Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 01:27 PM EST

PDB ID : 1EJB
Title : LUMAZINE SYNTHASE FROM SACCHAROMYCES CEREVISIAE
Authors : Meining, W.; Mortl, S.; Fischer, M.; Cushman, M.; Bacher, A.; Ladenstein, R.
Deposited on : 2000-03-02
Resolution : 1.85 Å(reported)

The following versions of software and data (see references (i)) 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 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.
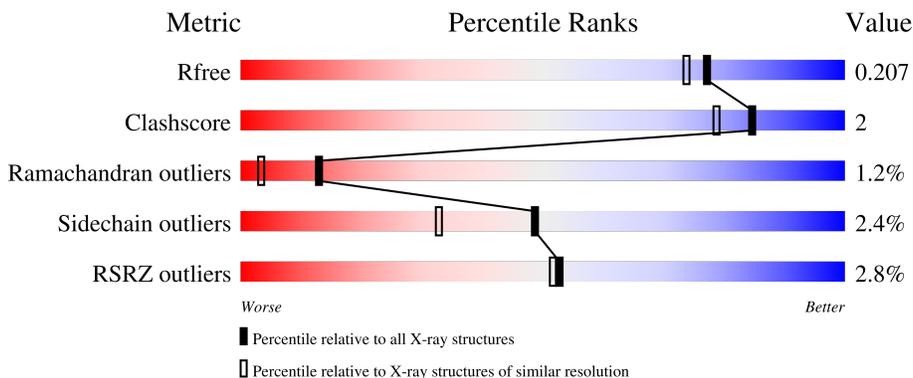
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	3% / 87% / 12% / •
1	B	168	3% / 86% / 11% / •
1	C	168	4% / 85% / 14% / ••
1	D	168	2% / 86% / 13% / •
1	E	168	2% / 88% / 11% / ••

2 Entry composition (i)

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 (three-letter code: INJ) (formula: $C_{14}H_{26}N_3O_9P$).
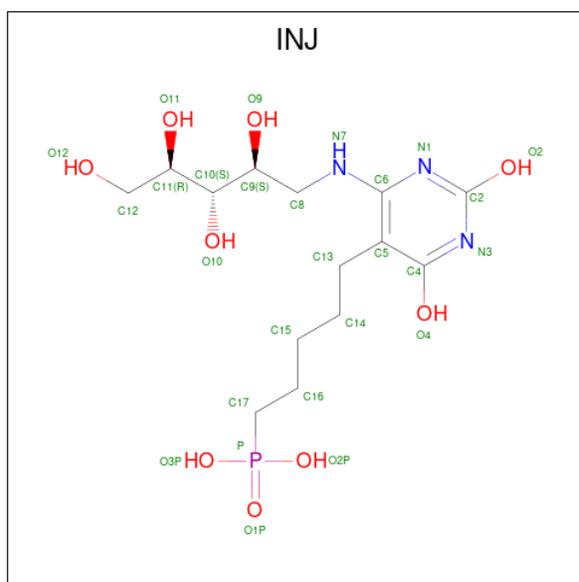
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	14	3	9	1		
2	B	1	Total	C	N	O	P	0	0
			27	14	3	9	1		
2	C	1	Total	C	N	O	P	0	0
			27	14	3	9	1		
2	D	1	Total	C	N	O	P	0	0
			27	14	3	9	1		
2	E	1	Total	C	N	O	P	0	0
			27	14	3	9	1		

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

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

• Molecule 1: LUMAZINE SYNTHASE
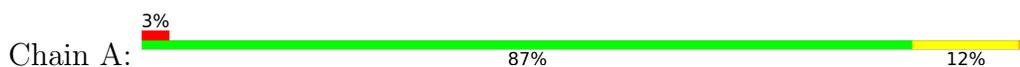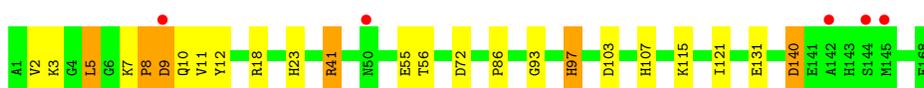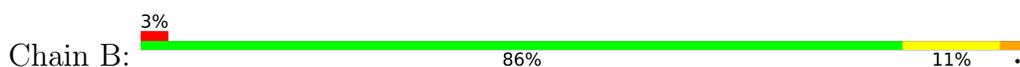
Chain A:

• Molecule 1: LUMAZINE SYNTHASE

Chain B:

• Molecule 1: LUMAZINE SYNTHASE

Chain C:

• Molecule 1: LUMAZINE SYNTHASE

Chain D:
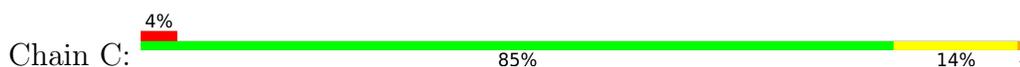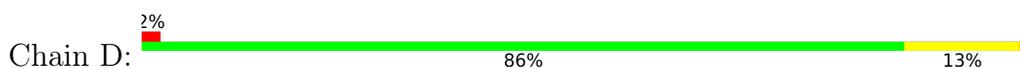
• Molecule 1: LUMAZINE SYNTHASE

Chain E:
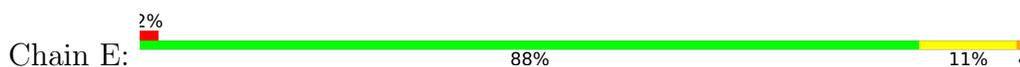
4 Data and refinement statistics ⓘ

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 24.90 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.85) 99.8 (24.90-1.85)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 50.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.88	9/1319 (0.7%)	1.31	17/1781 (1.0%)
1	B	1.29	6/1319 (0.5%)	2.23	11/1781 (0.6%)
1	C	1.32	7/1319 (0.5%)	1.43	23/1781 (1.3%)
1	D	2.60	16/1319 (1.2%)	1.42	18/1781 (1.0%)
1	E	1.60	6/1319 (0.5%)	1.96	18/1781 (1.0%)
All	All	1.64	44/6595 (0.7%)	1.71	87/8905 (1.0%)

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 (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	GLU	CD-OE1	-53.11	0.67	1.25
1	D	114	GLU	CD-OE2	41.42	1.71	1.25
1	B	41	ARG	CZ-NH2	-35.05	0.87	1.33
1	E	73	ARG	CZ-NH1	30.85	1.73	1.33
1	C	48	GLU	CD-OE2	30.49	1.59	1.25
1	E	48	GLU	CD-OE2	28.30	1.56	1.25
1	D	10	GLN	CD-OE1	-27.43	0.63	1.24
1	D	114	GLU	CG-CD	26.69	1.92	1.51
1	E	48	GLU	CD-OE1	-25.34	0.97	1.25
1	D	10	GLN	CG-CD	24.66	2.07	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	141	GLU	CD-OE1	-21.23	1.02	1.25
1	D	141	GLU	CD-OE2	20.94	1.48	1.25
1	D	73	ARG	CZ-NH1	15.39	1.53	1.33
1	C	50	ASN	CG-OD1	-15.13	0.90	1.24
1	C	49	GLU	CG-CD	15.12	1.74	1.51
1	C	131	GLU	CD-OE1	12.23	1.39	1.25
1	D	73	ARG	CZ-NH2	-11.71	1.17	1.33
1	D	10	GLN	CD-NE2	11.30	1.61	1.32
1	E	73	ARG	NE-CZ	-10.72	1.19	1.33
1	D	141	GLU	CG-CD	10.61	1.67	1.51
1	B	115	LYS	CG-CD	-9.79	1.19	1.52
1	B	131	GLU	CG-CD	9.69	1.66	1.51
1	C	131	GLU	CG-CD	-9.40	1.37	1.51
1	E	73	ARG	CZ-NH2	-9.06	1.21	1.33
1	E	26	TRP	CD2-CE3	8.98	1.53	1.40
1	A	73	ARG	CZ-NH1	8.63	1.44	1.33
1	B	131	GLU	CD-OE2	-8.57	1.16	1.25
1	C	115	LYS	CG-CD	-8.44	1.23	1.52
1	A	1	ALA	CA-CB	-8.33	1.34	1.52
1	D	50	ASN	CG-OD1	-7.79	1.06	1.24
1	B	10	GLN	CB-CG	7.51	1.72	1.52
1	A	1	ALA	C-N	-7.50	1.16	1.34
1	D	36	LYS	CD-CE	7.50	1.70	1.51
1	C	50	ASN	CB-CG	7.39	1.68	1.51
1	A	115	LYS	CG-CD	-7.32	1.27	1.52
1	A	2	VAL	CB-CG1	7.21	1.68	1.52
1	D	40	GLU	CD-OE1	-6.31	1.18	1.25
1	A	73	ARG	NE-CZ	-6.18	1.25	1.33
1	A	40	GLU	CG-CD	-5.53	1.43	1.51
1	D	73	ARG	CD-NE	-5.50	1.37	1.46
1	A	130	GLU	CG-CD	-5.36	1.44	1.51
1	A	7	LYS	CD-CE	-5.23	1.38	1.51
1	D	40	GLU	CD-OE2	-5.16	1.20	1.25
1	B	8	PRO	N-CA	-5.08	1.38	1.47

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	41	ARG	NE-CZ-NH2	70.12	155.36	120.30
1	E	73	ARG	NE-CZ-NH1	-41.28	99.66	120.30
1	E	73	ARG	NE-CZ-NH2	40.40	140.50	120.30
1	B	41	ARG	NH1-CZ-NH2	-36.17	79.61	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	114	GLU	CG-CD-OE2	-16.99	84.32	118.30
1	D	10	GLN	OE1-CD-NE2	16.36	159.54	121.90
1	C	49	GLU	CG-CD-OE1	-14.95	88.39	118.30
1	E	73	ARG	CD-NE-CZ	14.86	144.41	123.60
1	E	26	TRP	NE1-CE2-CZ2	13.54	145.30	130.40
1	D	10	GLN	CG-CD-NE2	-13.33	84.71	116.70
1	E	115	LYS	CD-CE-NZ	13.08	141.78	111.70
1	B	115	LYS	CB-CG-CD	12.91	145.16	111.60
1	A	1	ALA	N-CA-CB	12.89	128.15	110.10
1	A	41	ARG	NE-CZ-NH1	12.57	126.59	120.30
1	E	26	TRP	CG-CD2-CE3	-12.53	122.62	133.90
1	E	26	TRP	CD2-CE2-CZ2	-12.44	107.38	122.30
1	C	48	GLU	CG-CD-OE2	-11.90	94.50	118.30
1	C	48	GLU	OE1-CD-OE2	11.63	137.26	123.30
1	A	73	ARG	CD-NE-CZ	11.19	139.26	123.60
1	D	114	GLU	OE1-CD-OE2	10.91	136.39	123.30
1	D	73	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	E	73	ARG	NH1-CZ-NH2	-10.74	107.59	119.40
1	C	2	VAL	CA-C-N	-10.60	93.88	117.20
1	D	114	GLU	CG-CD-OE1	10.33	138.96	118.30
1	C	7	LYS	CA-CB-CG	10.22	135.88	113.40
1	A	18	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	E	48	GLU	CG-CD-OE1	9.29	136.88	118.30
1	C	115	LYS	CB-CG-CD	9.22	135.57	111.60
1	E	26	TRP	CH2-CZ2-CE2	8.96	126.36	117.40
1	C	5	LEU	CB-CG-CD2	8.94	126.20	111.00
1	E	26	TRP	CE2-CD2-CE3	8.66	129.09	118.70
1	C	2	VAL	C-N-CA	8.63	143.28	121.70
1	D	141	GLU	CG-CD-OE2	-8.48	101.34	118.30
1	A	1	ALA	N-CA-C	-8.47	88.13	111.00
1	E	48	GLU	CG-CD-OE2	-8.27	101.76	118.30
1	C	5	LEU	CB-CA-C	8.24	125.86	110.20
1	B	131	GLU	OE1-CD-OE2	8.16	133.09	123.30
1	E	18	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	C	1	ALA	C-N-CA	-8.06	101.55	121.70
1	C	25	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	E	115	LYS	CB-CG-CD	7.49	131.06	111.60
1	A	41	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	1	ALA	CB-CA-C	-7.32	99.12	110.10
1	C	2	VAL	O-C-N	7.22	134.25	122.70
1	D	114	GLU	CB-CG-CD	-7.07	95.11	114.20
1	D	10	GLN	CB-CA-C	6.77	123.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ASP	CB-CG-OD1	6.77	124.39	118.30
1	C	18	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	D	18	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	E	69	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	E	11	VAL	CG1-CB-CG2	-6.57	100.39	110.90
1	C	2	VAL	N-CA-C	6.56	128.70	111.00
1	C	28	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	C	41	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	140	ASP	CB-CA-C	-6.20	98.00	110.40
1	B	11	VAL	CG1-CB-CG2	-6.11	101.12	110.90
1	E	136	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	2	VAL	CA-CB-CG2	6.01	119.92	110.90
1	A	41	ARG	CD-NE-CZ	6.01	132.01	123.60
1	D	50	ASN	CB-CG-ND2	-5.95	102.42	116.70
1	A	73	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	B	18	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	D	70	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	A	25	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	8	PRO	O-C-N	5.77	131.94	122.70
1	E	140	ASP	CB-CG-OD1	5.76	123.49	118.30
1	C	13	ASP	CB-CG-OD2	5.76	123.49	118.30
1	D	41	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	5	LEU	CB-CG-CD1	5.71	120.70	111.00
1	B	9	ASP	CA-CB-CG	-5.68	100.91	113.40
1	B	55	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	C	2	VAL	CA-C-O	5.60	131.87	120.10
1	A	40	GLU	CB-CG-CD	5.50	129.05	114.20
1	D	141	GLU	CG-CD-OE1	5.50	129.29	118.30
1	C	131	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	D	18	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	69	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	40	GLU	CG-CD-OE2	5.42	129.14	118.30
1	D	16	LYS	CB-CG-CD	5.40	125.64	111.60
1	A	115	LYS	CB-CG-CD	5.33	125.45	111.60
1	A	5	LEU	CB-CG-CD1	5.31	120.03	111.00
1	D	124	LEU	CA-CB-CG	5.29	127.47	115.30
1	D	100	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	40	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	C	18	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	32	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	50	ASN	CB-CG-OD1	5.11	131.81	121.60

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
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	1309	7	0
1	B	1294	0	1310	7	0
1	C	1294	0	1309	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	1	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	6658	29	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 (29) 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	0.77
1:C:49:GLU:CD	1:C:49:GLU:CB	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:96:MET:HE2	3:C:525:HOH:O	2.00	0.60
1:A:103:ASP:OD2	1:B:107:HIS:HE1	1.87	0.58
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:103:ASP:OD2	1:D:107:HIS:HE1	1.91	0.54
1:B:9:ASP:OD1	1:B:12:TYR:OH	2.28	0.52
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: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%)	8	2
1	C	166/168 (99%)	161 (97%)	3 (2%)	2 (1%)	13	3
1	D	166/168 (99%)	164 (99%)	2 (1%)	0	100	100
1	E	166/168 (99%)	155 (93%)	6 (4%)	5 (3%)	4	0
All	All	830/840 (99%)	797 (96%)	23 (3%)	10 (1%)	13	3

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%)	135 (99%)	1 (1%)	84	79
1	B	136/136 (100%)	130 (96%)	6 (4%)	28	12
1	C	136/136 (100%)	134 (98%)	2 (2%)	65	53
1	D	136/136 (100%)	133 (98%)	3 (2%)	52	36
1	E	136/136 (100%)	132 (97%)	4 (3%)	42	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	680/680 (100%)	664 (98%)	16 (2%)	49 33

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	B	3	LYS
1	B	5	LEU
1	B	7	LYS
1	B	41	ARG
1	B	97	HIS
1	B	140	ASP
1	C	2	VAL
1	C	97	HIS
1	D	49	GLU
1	D	97	HIS
1	D	115	LYS
1	E	5	LEU
1	E	7	LYS
1	E	16	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	A	148	HIS
1	B	107	HIS
1	C	107	HIS
1	C	148	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	C	400	-	24,27,27	3.55	8 (33%)	27,37,37	2.37	11 (40%)
2	INJ	E	800	-	24,27,27	3.46	12 (50%)	27,37,37	2.49	11 (40%)
2	INJ	B	300	-	24,27,27	3.62	10 (41%)	27,37,37	2.45	14 (51%)
2	INJ	D	600	-	24,27,27	3.46	12 (50%)	27,37,37	2.41	11 (40%)
2	INJ	A	200	-	24,27,27	3.52	9 (37%)	27,37,37	2.67	15 (55%)

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	C	400	-	-	6/24/24/24	0/1/1/1
2	INJ	E	800	-	-	5/24/24/24	0/1/1/1
2	INJ	B	300	-	-	6/24/24/24	0/1/1/1
2	INJ	D	600	-	-	6/24/24/24	0/1/1/1
2	INJ	A	200	-	-	6/24/24/24	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	INJ	C5-C4	9.99	1.50	1.39
2	A	200	INJ	C5-C4	9.64	1.50	1.39
2	E	800	INJ	C5-C4	9.29	1.50	1.39
2	B	300	INJ	C5-C4	9.07	1.49	1.39
2	D	600	INJ	C5-C4	8.95	1.49	1.39
2	B	300	INJ	C11-C10	7.46	1.67	1.53
2	C	400	INJ	C13-C5	-7.41	1.41	1.52
2	D	600	INJ	C13-C5	-7.15	1.41	1.52
2	E	800	INJ	C13-C5	-6.98	1.41	1.52
2	A	200	INJ	C8-C9	6.96	1.61	1.52
2	A	200	INJ	C13-C5	-6.84	1.42	1.52
2	B	300	INJ	C13-C5	-6.57	1.42	1.52
2	C	400	INJ	C8-C9	6.49	1.61	1.52
2	D	600	INJ	C11-C10	6.31	1.65	1.53
2	E	800	INJ	C11-C10	6.23	1.65	1.53
2	C	400	INJ	C11-C10	6.16	1.65	1.53
2	B	300	INJ	C8-C9	5.99	1.60	1.52
2	A	200	INJ	C11-C10	5.94	1.64	1.53
2	E	800	INJ	C8-C9	5.85	1.60	1.52
2	D	600	INJ	C8-C9	5.61	1.60	1.52
2	B	300	INJ	P-C17	5.54	1.84	1.78
2	A	200	INJ	C6-N1	4.61	1.43	1.34
2	B	300	INJ	C6-N1	4.36	1.42	1.34
2	C	400	INJ	C6-N1	4.21	1.42	1.34
2	E	800	INJ	C6-N1	4.21	1.42	1.34
2	D	600	INJ	C6-N1	3.92	1.41	1.34
2	A	200	INJ	C8-N7	3.77	1.53	1.45
2	D	600	INJ	C8-N7	3.74	1.53	1.45
2	A	200	INJ	C6-N7	3.62	1.40	1.34
2	E	800	INJ	P-C17	3.48	1.82	1.78
2	C	400	INJ	P-O1P	-3.42	1.43	1.50
2	E	800	INJ	C8-N7	3.38	1.52	1.45
2	C	400	INJ	C8-N7	3.25	1.52	1.45
2	D	600	INJ	C6-N7	3.24	1.39	1.34
2	C	400	INJ	C6-N7	3.22	1.39	1.34
2	B	300	INJ	C6-N7	3.11	1.39	1.34
2	E	800	INJ	C6-N7	3.09	1.39	1.34
2	B	300	INJ	C8-N7	2.97	1.51	1.45
2	D	600	INJ	C5-C6	2.80	1.47	1.42
2	B	300	INJ	C12-C11	2.79	1.59	1.52
2	D	600	INJ	P-O1P	-2.74	1.44	1.50
2	B	300	INJ	P-O1P	-2.66	1.44	1.50
2	D	600	INJ	C12-C11	2.64	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	INJ	P-C17	2.54	1.81	1.78
2	E	800	INJ	C12-C11	2.36	1.58	1.52
2	E	800	INJ	C9-C10	2.34	1.57	1.53
2	E	800	INJ	P-O1P	-2.30	1.45	1.50
2	A	200	INJ	P-O1P	-2.21	1.45	1.50
2	A	200	INJ	C5-C6	2.18	1.46	1.42
2	E	800	INJ	C5-C6	2.18	1.46	1.42
2	D	600	INJ	P-O2P	-2.17	1.49	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	200	INJ	C8-N7-C6	-5.71	113.09	123.25
2	E	800	INJ	C8-N7-C6	-5.39	113.65	123.25
2	D	600	INJ	C8-N7-C6	-5.22	113.97	123.25
2	A	200	INJ	C2-N3-C4	5.01	126.15	115.49
2	D	600	INJ	C2-N3-C4	4.83	125.78	115.49
2	E	800	INJ	C2-N3-C4	4.82	125.75	115.49
2	B	300	INJ	C2-N3-C4	4.69	125.47	115.49
2	C	400	INJ	C8-N7-C6	-4.53	115.19	123.25
2	A	200	INJ	O3P-P-O1P	-4.49	100.50	112.39
2	A	200	INJ	O11-C11-C10	-4.46	98.25	109.10
2	B	300	INJ	C8-N7-C6	-4.45	115.33	123.25
2	D	600	INJ	O3P-P-O1P	-4.39	100.78	112.39
2	E	800	INJ	O11-C11-C10	-4.27	98.71	109.10
2	C	400	INJ	C2-N3-C4	4.21	124.44	115.49
2	B	300	INJ	O10-C10-C11	-4.12	98.86	108.81
2	B	300	INJ	O11-C11-C10	-4.08	99.17	109.10
2	B	300	INJ	O3P-P-O1P	-4.05	101.67	112.39
2	C	400	INJ	C2-N1-C6	3.94	122.83	113.80
2	E	800	INJ	O3P-P-O1P	-3.92	102.02	112.39
2	C	400	INJ	O3P-P-O1P	-3.82	102.30	112.39
2	C	400	INJ	O11-C11-C10	-3.76	99.97	109.10
2	D	600	INJ	O10-C10-C11	-3.70	99.87	108.81
2	E	800	INJ	C2-N1-C6	3.52	121.86	113.80
2	C	400	INJ	O1P-P-C17	3.47	117.82	111.40
2	E	800	INJ	O10-C10-C11	-3.46	100.45	108.81
2	B	300	INJ	C15-C14-C13	-3.35	100.73	113.76
2	C	400	INJ	C15-C14-C13	-3.32	100.86	113.76
2	E	800	INJ	P-C17-C16	3.30	119.11	114.98
2	D	600	INJ	C2-N1-C6	3.26	121.25	113.80
2	A	200	INJ	C15-C14-C13	-3.26	101.10	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	200	INJ	C2-N1-C6	3.24	121.22	113.80
2	D	600	INJ	O12-C12-C11	-3.10	104.32	111.07
2	A	200	INJ	O10-C10-C11	-3.09	101.34	108.81
2	C	400	INJ	O10-C10-C11	-2.94	101.71	108.81
2	C	400	INJ	C14-C13-C5	2.93	121.46	113.82
2	A	200	INJ	C14-C13-C5	2.90	121.39	113.82
2	B	300	INJ	C2-N1-C6	2.90	120.44	113.80
2	A	200	INJ	C12-C11-C10	2.82	118.53	112.41
2	D	600	INJ	O11-C11-C10	-2.80	102.29	109.10
2	B	300	INJ	O12-C12-C11	-2.74	105.09	111.07
2	E	800	INJ	C14-C13-C5	2.73	120.93	113.82
2	A	200	INJ	O12-C12-C11	-2.71	105.16	111.07
2	E	800	INJ	C15-C14-C13	-2.66	103.42	113.76
2	B	300	INJ	C14-C13-C5	2.65	120.72	113.82
2	A	200	INJ	P-C17-C16	2.59	118.23	114.98
2	D	600	INJ	C15-C14-C13	-2.56	103.79	113.76
2	E	800	INJ	C12-C11-C10	2.51	117.86	112.41
2	E	800	INJ	O3P-P-O2P	2.50	115.39	108.08
2	B	300	INJ	O11-C11-C12	-2.46	103.39	109.14
2	B	300	INJ	O3P-P-O2P	2.40	115.08	108.08
2	A	200	INJ	O1P-P-C17	2.38	115.80	111.40
2	B	300	INJ	O2P-P-O1P	2.30	118.46	112.39
2	B	300	INJ	C8-C9-C10	2.28	118.14	110.93
2	D	600	INJ	O10-C10-C9	-2.27	103.33	108.81
2	B	300	INJ	O10-C10-C9	-2.27	103.34	108.81
2	A	200	INJ	O9-C9-C8	-2.20	105.25	109.69
2	C	400	INJ	C8-C9-C10	2.20	117.90	110.93
2	A	200	INJ	O11-C11-C12	-2.15	104.11	109.14
2	D	600	INJ	C8-C9-C10	2.12	117.64	110.93
2	D	600	INJ	C14-C13-C5	2.09	119.26	113.82
2	A	200	INJ	O10-C10-C9	-2.03	103.91	108.81
2	C	400	INJ	C12-C11-C10	2.01	116.78	112.41

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	200	INJ	N7-C8-C9-O9
2	D	600	INJ	C15-C16-C17-P
2	E	800	INJ	C15-C16-C17-P
2	A	200	INJ	C15-C16-C17-P
2	B	300	INJ	C15-C16-C17-P

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

Ligand INJ C 400	
Bond lengths	Bond angles
Torsions	Rings

Ligand INJ E 800	
Bond lengths	Bond angles
Torsions	Rings

Ligand INJ B 300

Bond lengths

Bond angles

Torsions

Rings

Ligand INJ D 600

Bond lengths

Bond angles

Torsions

Rings

Ligand INJ A 200

Bond lengths

Bond angles

Torsions

Rings
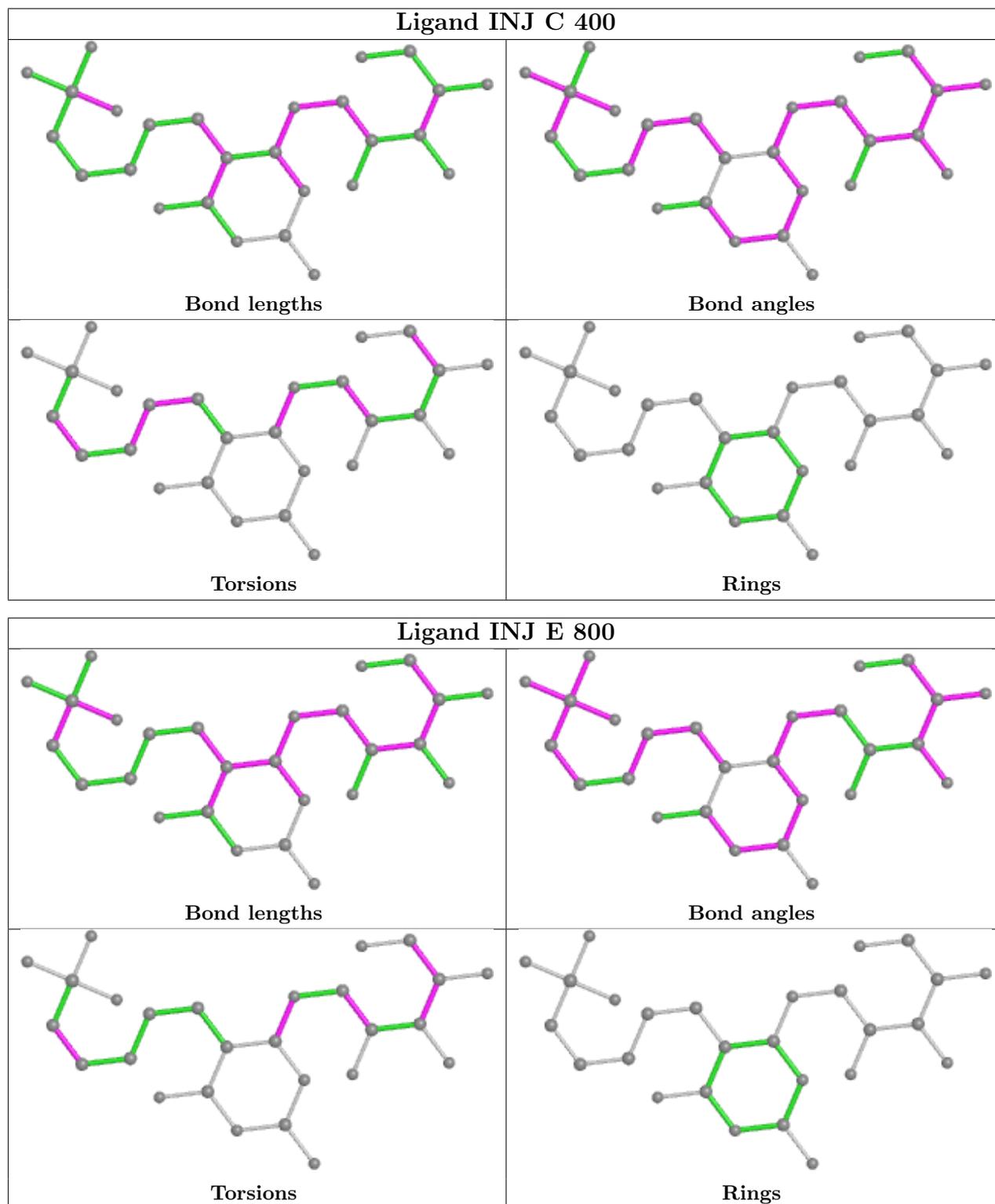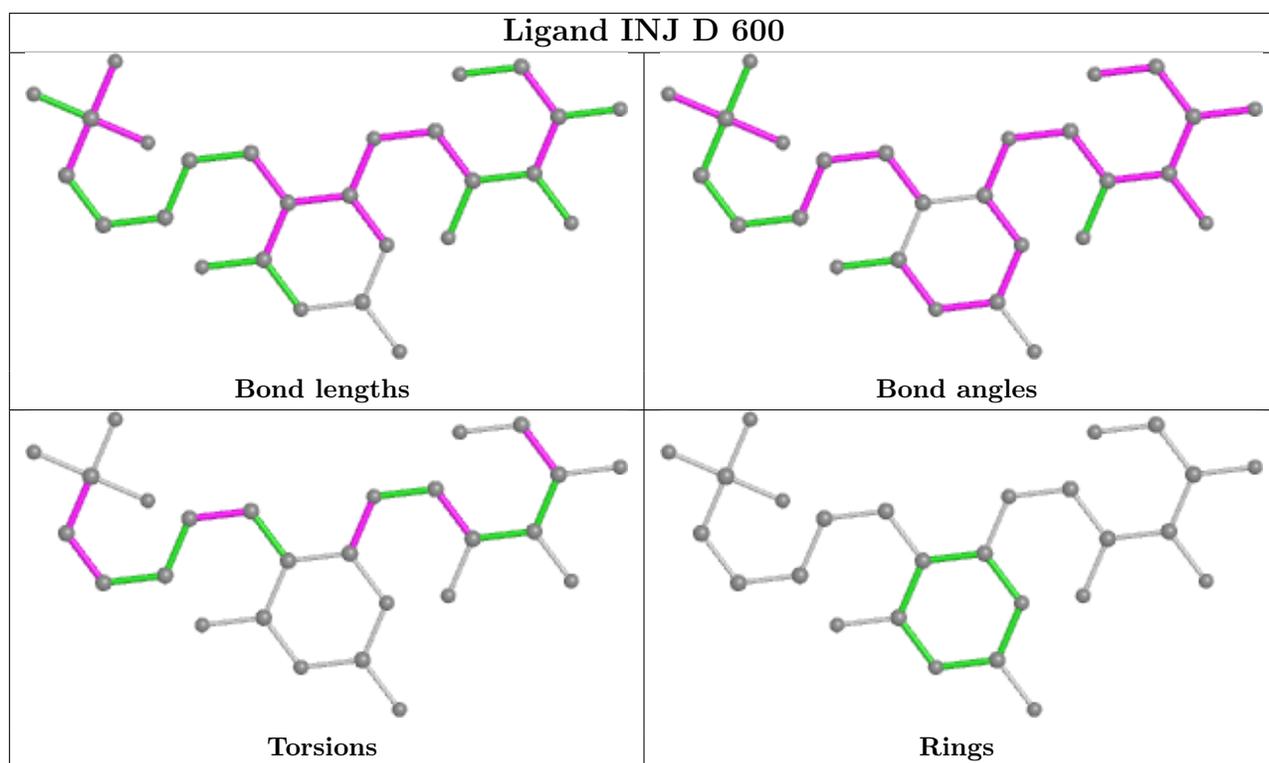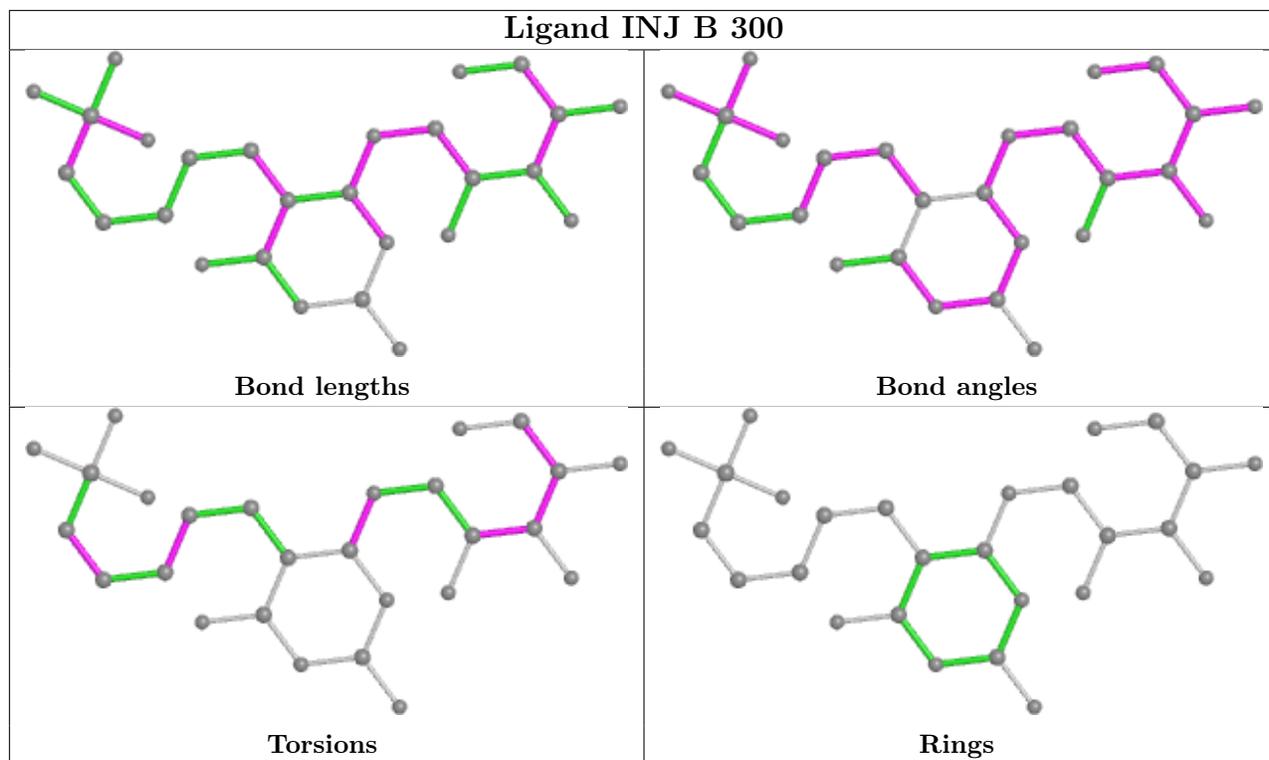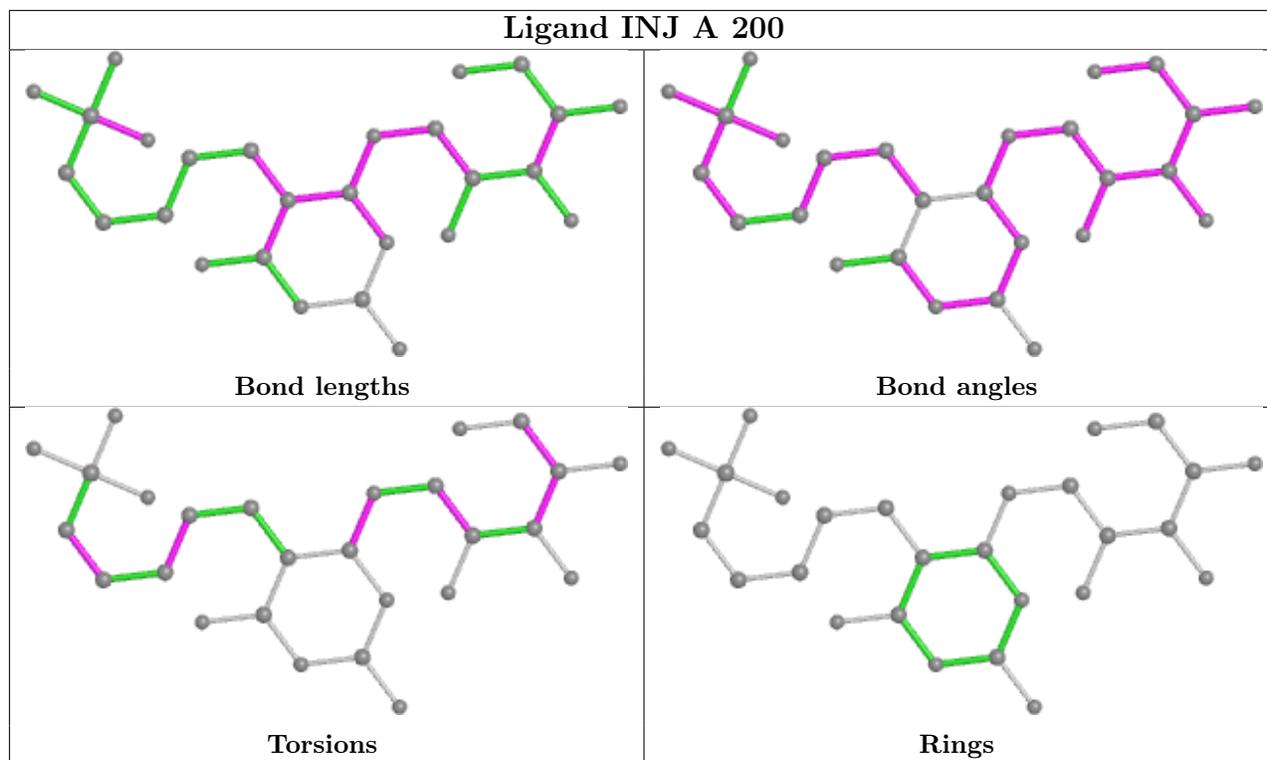
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	168/168 (100%)	-0.12	5 (2%)	50	48	13, 20, 34, 55	14 (8%)
1	B	160/168 (95%)	-0.05	5 (3%)	49	47	13, 19, 35, 46	11 (6%)
1	C	166/168 (98%)	-0.06	7 (4%)	36	34	13, 19, 35, 49	14 (8%)
1	D	168/168 (100%)	-0.17	3 (1%)	68	68	13, 19, 32, 37	14 (8%)
1	E	159/168 (94%)	-0.27	3 (1%)	66	66	13, 19, 27, 39	9 (5%)
All	All	821/840 (97%)	-0.13	23 (2%)	53	52	13, 19, 32, 55	62 (7%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	ALA	6.3
1	C	4	GLY	5.2
1	C	3	LYS	4.0
1	B	9	ASP	3.7
1	A	143	HIS	3.5
1	D	6	GLY	3.4
1	C	5	LEU	3.4
1	E	11	VAL	3.4
1	A	142	ALA	3.1
1	B	142	ALA	2.9
1	D	1	ALA	2.9
1	B	145	MET	2.7
1	A	141	GLU	2.6
1	D	49	GLU	2.5
1	C	143	HIS	2.5
1	A	2	VAL	2.4
1	B	144	SER	2.3
1	E	121	ILE	2.2
1	E	50	ASN	2.2
1	A	144	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	50	ASN	2.1
1	C	141	GLU	2.1
1	C	140	ASP	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	INJ	A	200	27/27	0.94	0.11	17,22,28,28	0
2	INJ	E	800	27/27	0.94	0.10	17,21,28,28	0
2	INJ	D	600	27/27	0.95	0.10	17,22,28,28	0
2	INJ	C	400	27/27	0.95	0.09	17,22,28,28	0
2	INJ	B	300	27/27	0.96	0.09	17,21,27,28	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)
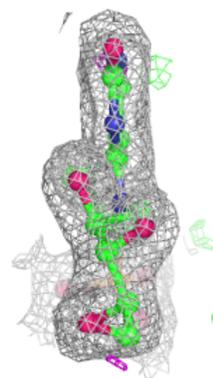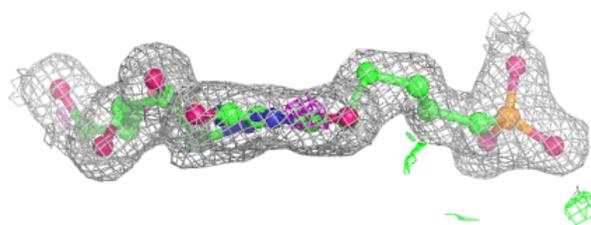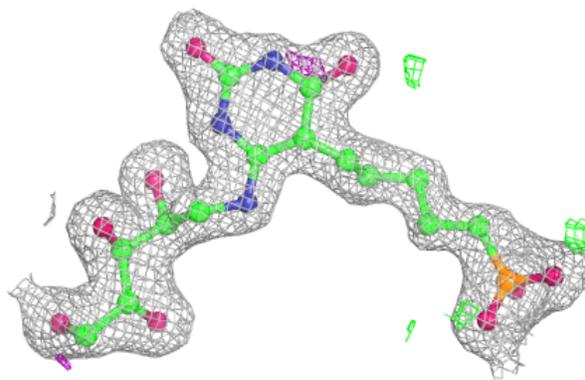
Electron density around INJ E 800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
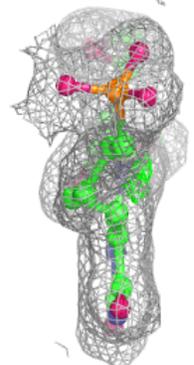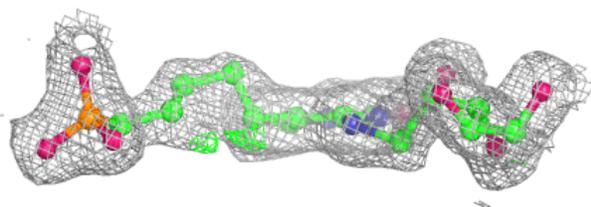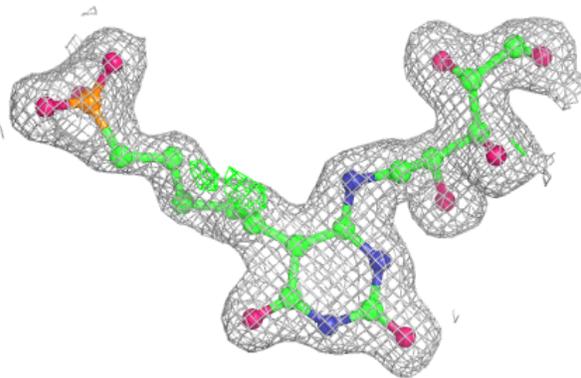
**Electron density around INJ D 600:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
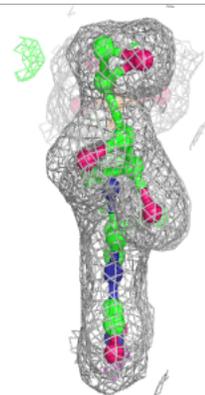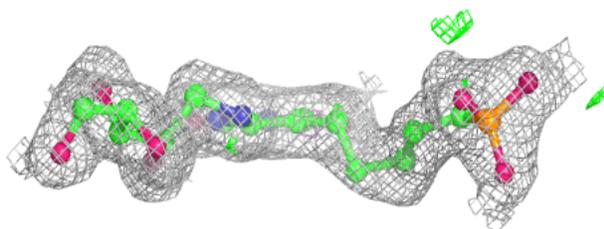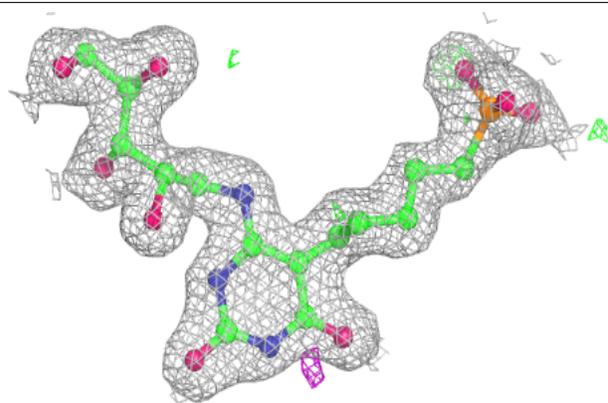
Electron density around INJ C 400:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)

6.5 Other polymers ⓘ

There are no such residues in this entry.