W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 12, 2024 – 04:46 AM EST

PDB ID	:	3GMD
Title	:	Structure-based design of 7-Azaindole-pyrrolidines as inhibitors of 11beta-Hydroxysteroid-Dehydrogenase type I
Authors	:	Valeur, E.; Lepifre, F.; Roche, D.; Christmann-Franck, S.; Hillertz, P.; Musil, D.
Deposited on	:	2009-03-13
Resolution	:	2.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

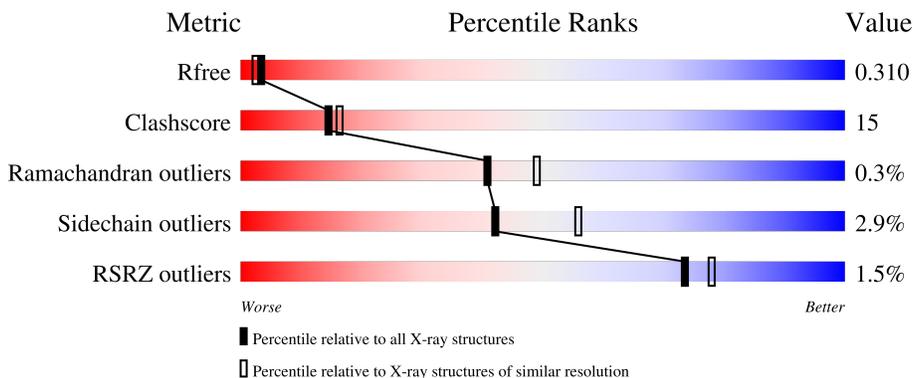|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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:
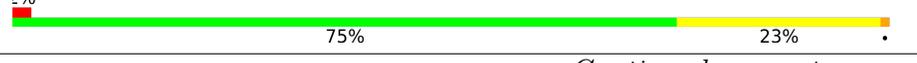*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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.
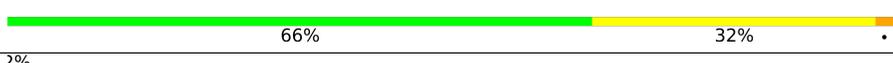
Metric	Percentile Ranks	Value
Rfree		0.310
Clashscore		15
Ramachandran outliers		0.3%
Sidechain outliers		2.9%
RSRZ outliers		1.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	264	2% — 65% — 34% — •
1	B	264	3% — 57% — 41% — •
1	C	264	% — 75% — 23% — •
1	D	264	2% — 75% — 23% — •

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Mol	Chain	Length	Quality of chain
1	E	264	% 67% 32%
1	F	264	2% 69% 30%
1	G	264	66% 32%
1	H	264	2% 70% 28%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 17364 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	27	0	0
			2025	1297	337	374	17			
1	B	264	Total	C	N	O	S	10	0	0
			2025	1297	337	374	17			
1	C	264	Total	C	N	O	S	17	0	0
			2025	1297	337	374	17			
1	D	264	Total	C	N	O	S	29	0	0
			2025	1297	337	374	17			
1	E	264	Total	C	N	O	S	23	0	0
			2025	1297	337	374	17			
1	F	264	Total	C	N	O	S	15	0	0
			2025	1297	337	374	17			
1	G	264	Total	C	N	O	S	30	0	0
			2025	1297	337	374	17			
1	H	264	Total	C	N	O	S	25	0	0
			2025	1297	337	374	17			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	VAL	MET	engineered mutation	UNP P50172
A	177	TYR	GLN	engineered mutation	UNP P50172
A	180	VAL	ILE	engineered mutation	UNP P50172
A	226	ALA	GLU	engineered mutation	UNP P50172
A	227	VAL	ILE	engineered mutation	UNP P50172
A	231	VAL	ILE	engineered mutation	UNP P50172
B	175	VAL	MET	engineered mutation	UNP P50172
B	177	TYR	GLN	engineered mutation	UNP P50172
B	180	VAL	ILE	engineered mutation	UNP P50172
B	226	ALA	GLU	engineered mutation	UNP P50172
B	227	VAL	ILE	engineered mutation	UNP P50172
B	231	VAL	ILE	engineered mutation	UNP P50172
C	175	VAL	MET	engineered mutation	UNP P50172

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Chain	Residue	Modelled	Actual	Comment	Reference
C	177	TYR	GLN	engineered mutation	UNP P50172
C	180	VAL	ILE	engineered mutation	UNP P50172
C	226	ALA	GLU	engineered mutation	UNP P50172
C	227	VAL	ILE	engineered mutation	UNP P50172
C	231	VAL	ILE	engineered mutation	UNP P50172
D	175	VAL	MET	engineered mutation	UNP P50172
D	177	TYR	GLN	engineered mutation	UNP P50172
D	180	VAL	ILE	engineered mutation	UNP P50172
D	226	ALA	GLU	engineered mutation	UNP P50172
D	227	VAL	ILE	engineered mutation	UNP P50172
D	231	VAL	ILE	engineered mutation	UNP P50172
E	175	VAL	MET	engineered mutation	UNP P50172
E	177	TYR	GLN	engineered mutation	UNP P50172
E	180	VAL	ILE	engineered mutation	UNP P50172
E	226	ALA	GLU	engineered mutation	UNP P50172
E	227	VAL	ILE	engineered mutation	UNP P50172
E	231	VAL	ILE	engineered mutation	UNP P50172
F	175	VAL	MET	engineered mutation	UNP P50172
F	177	TYR	GLN	engineered mutation	UNP P50172
F	180	VAL	ILE	engineered mutation	UNP P50172
F	226	ALA	GLU	engineered mutation	UNP P50172
F	227	VAL	ILE	engineered mutation	UNP P50172
F	231	VAL	ILE	engineered mutation	UNP P50172
G	175	VAL	MET	engineered mutation	UNP P50172
G	177	TYR	GLN	engineered mutation	UNP P50172
G	180	VAL	ILE	engineered mutation	UNP P50172
G	226	ALA	GLU	engineered mutation	UNP P50172
G	227	VAL	ILE	engineered mutation	UNP P50172
G	231	VAL	ILE	engineered mutation	UNP P50172
H	175	VAL	MET	engineered mutation	UNP P50172
H	177	TYR	GLN	engineered mutation	UNP P50172
H	180	VAL	ILE	engineered mutation	UNP P50172
H	226	ALA	GLU	engineered mutation	UNP P50172
H	227	VAL	ILE	engineered mutation	UNP P50172
H	231	VAL	ILE	engineered mutation	UNP P50172

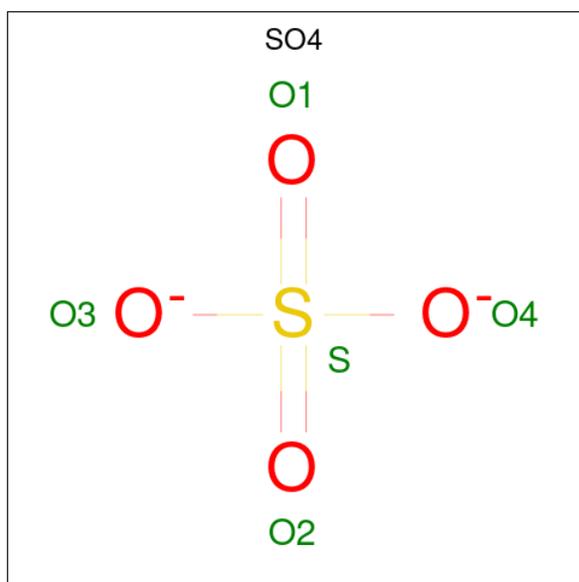- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

NDP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-methyl-3-{(3S)-1-[(1-pyridin-2-ylcyclopropyl)carbonyl]pyrrolidin-3-yl}-1H-pyrrolo[2,3-b]pyridine (three-letter code: 2M3) (formula: $C_{21}H_{22}N_4O$).

W O R L D W I D E
PDB
PROTEIN DATA BANK

2M3
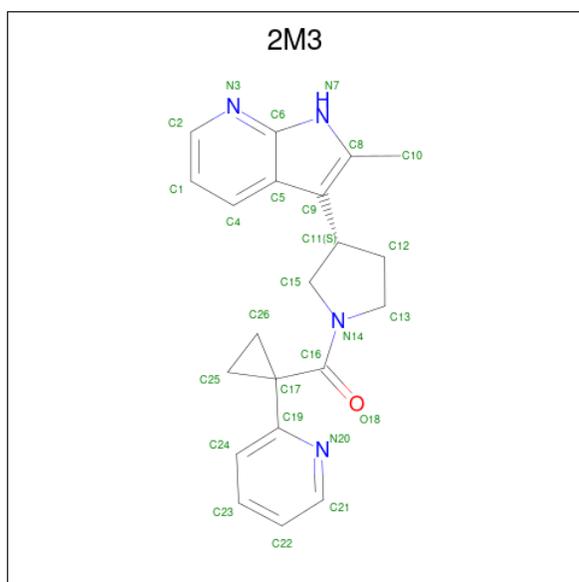
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			26	21	4	1		
3	B	1	Total	C	N	O	0	0
			26	21	4	1		
3	C	1	Total	C	N	O	0	0
			26	21	4	1		
3	D	1	Total	C	N	O	0	0
			26	21	4	1		
3	E	1	Total	C	N	O	0	0
			26	21	4	1		
3	F	1	Total	C	N	O	0	0
			26	21	4	1		
3	G	1	Total	C	N	O	0	0
			26	21	4	1		
3	H	1	Total	C	N	O	0	0
			26	21	4	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O3   O⁻ — S — O⁻ O4

S

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	H	1	Total 5	O 4	S 1	0	0
4	H	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total 72	O 72	0	0
5	B	56	Total 56	O 56	0	0
5	C	86	Total 86	O 86	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	70	Total 70	O 70	0	0
5	E	71	Total 71	O 71	0	0
5	F	61	Total 61	O 61	0	0
5	G	64	Total 64	O 64	0	0
5	H	47	Total 47	O 47	0	0

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: Corticosteroid 11-beta-dehydrogenase isozyme 1
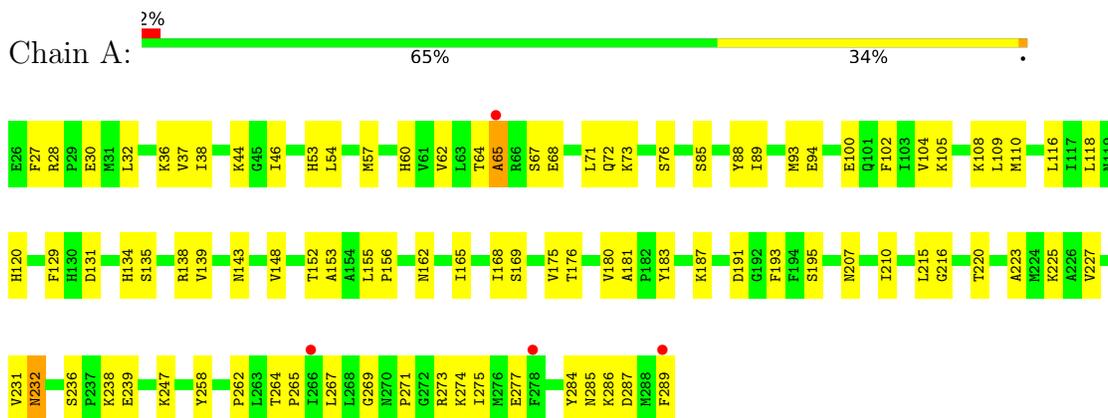
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain D:

- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain E:

- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain F:

- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain G:

Y257 Y258 P262 L263 T264 P265 I266 L267 L268 G269 N270 P271 G272 R273 Y283 Y284 N285 M288 F289

• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain H:

2%

70%   28%   ·

E26 F27 R28 M31 L32 V39 A42 I46 M50 S55 K56 M57 R66 S67 E68 L71 V75 S76 R77 L81 G82 A83 Y88 I89 A90 E94 T122 L126 S127 L128 D131 V136 R137 R138 V139 M140 E141 V142 N143 F144 L155 P156 M157

L158 I168 S169 S170 L171 A172 V175 T176 Y177 A181 P182 Y183 S184 L190 F193 F194 S195 T196 I197 E200 T204 L212 C213 V214 L215 G216 E221 V231 Q234 A242 L243 E244 I245 R252 Y258 D259 K260 S261 P262 L263 T264 P265 I266 L267 N270

P271 G272 R273 M276 E277 Y283 Y284 N285 K286 D287 M288 F289
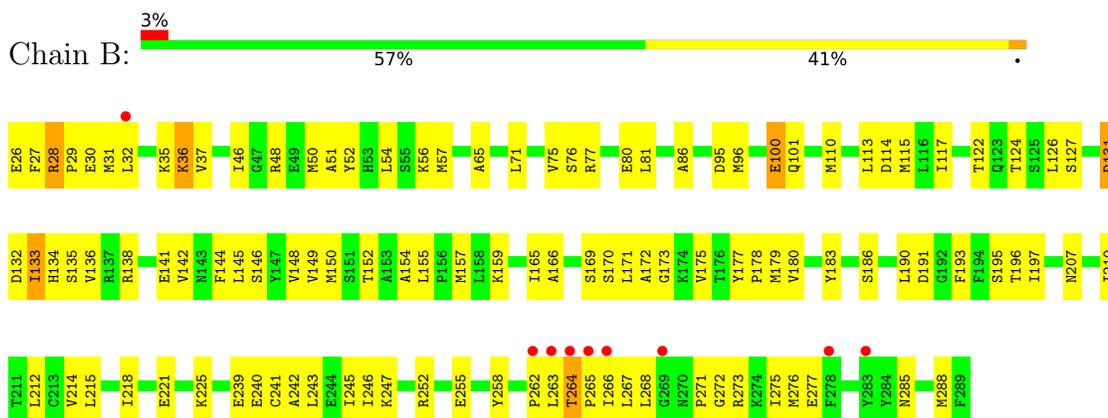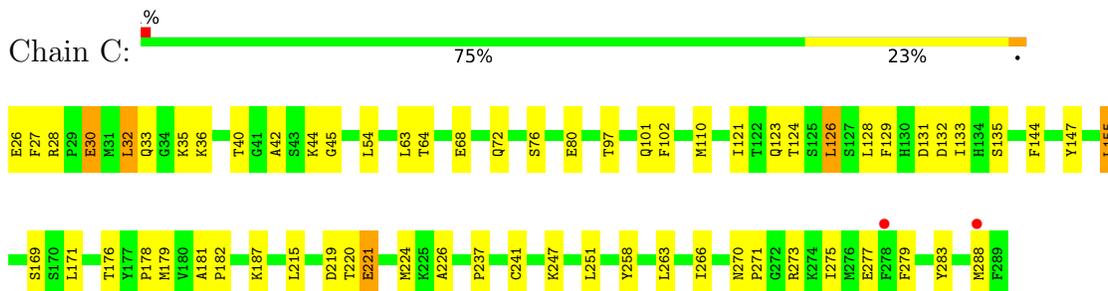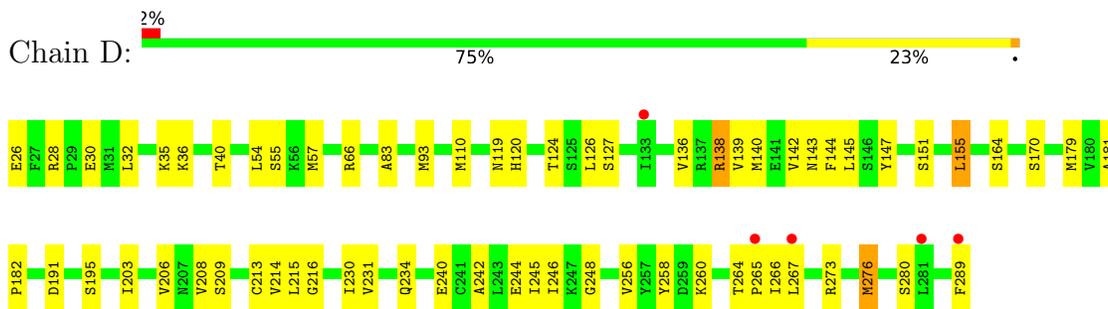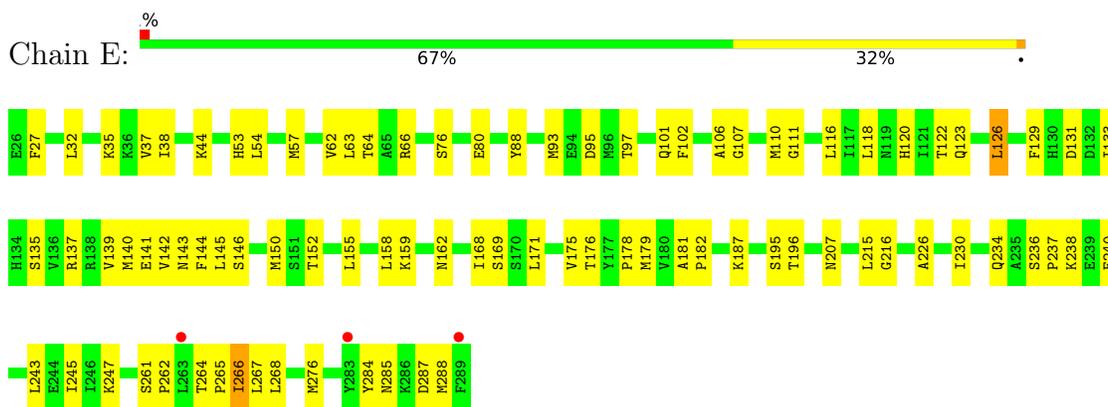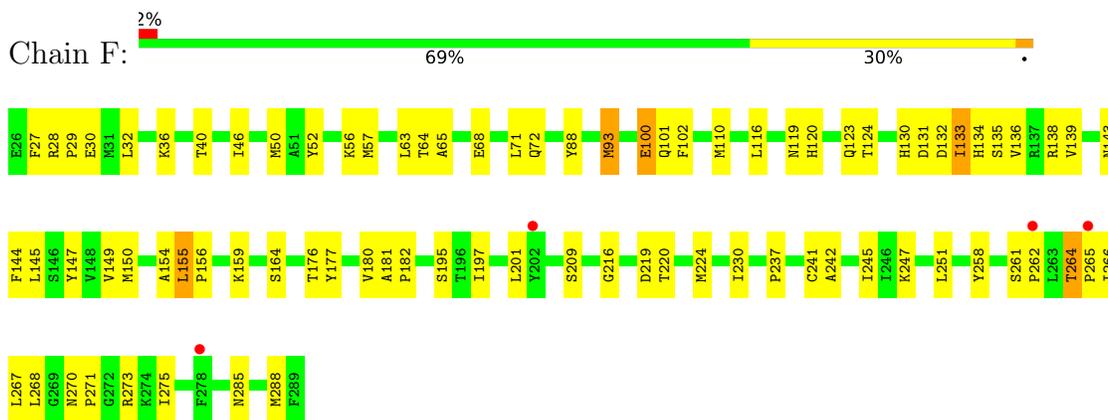
4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.34Å 70.49Å 132.96Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	70.00 – 2.28 48.35 – 2.28	Depositor EDS
% Data completeness (in resolution range)	95.4 (70.00-2.28) 95.9 (48.35-2.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.29Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.252 , 0.306 0.261 , 0.310	Depositor DCC
R_{free} test set	1260 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	1.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.160 for h,-k,-l 0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17364	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2618e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 2M3, SO4

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	0.33	0/2059	0.50	0/2775
1	B	0.32	0/2059	0.51	0/2775
1	C	0.37	0/2059	0.53	0/2775
1	D	0.36	0/2059	0.53	0/2775
1	E	0.39	0/2059	0.55	0/2775
1	F	0.35	0/2059	0.54	0/2775
1	G	0.33	0/2059	0.52	0/2775
1	H	0.33	0/2059	0.52	0/2775
All	All	0.35	0/16472	0.52	0/22200

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2025	0	2092	70	0
1	B	2025	0	2092	109	0
1	C	2025	0	2092	48	0
1	D	2025	0	2092	58	0
1	E	2025	0	2092	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2025	0	2092	64	0
1	G	2025	0	2092	79	0
1	H	2025	0	2092	66	0
2	A	48	0	26	2	0
2	B	48	0	26	2	0
2	C	48	0	26	0	0
2	D	48	0	26	3	0
2	E	48	0	26	4	0
2	F	48	0	26	3	0
2	G	48	0	26	4	0
2	H	48	0	26	2	0
3	A	26	0	22	0	0
3	B	26	0	22	5	0
3	C	26	0	22	5	0
3	D	26	0	22	3	0
3	E	26	0	22	3	0
3	F	26	0	22	4	0
3	G	26	0	22	2	0
3	H	26	0	22	1	0
4	B	5	0	0	1	0
4	C	10	0	0	1	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	10	0	0	0	0
5	A	72	0	0	2	0
5	B	56	0	0	2	0
5	C	86	0	0	2	0
5	D	70	0	0	2	0
5	E	71	0	0	5	0
5	F	61	0	0	0	0
5	G	64	0	0	2	0
5	H	47	0	0	0	0
All	All	17364	0	17120	516	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 15.

The worst 5 of 516 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:133:ILE:HD11	1:F:145:LEU:HG	1.43	1.01
1:A:273:ARG:HG3	1:B:175:VAL:HG12	1.46	0.98
1:C:133:ILE:HD11	1:D:145:LEU:HG	1.52	0.91
1:B:36:LYS:HG3	1:B:110:MET:HB3	1.54	0.90
1:D:138:ARG:HH11	1:D:138:ARG:HG3	1.39	0.87

There are no symmetry-related clashes.

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	262/264 (99%)	245 (94%)	16 (6%)	1 (0%)	34	40
1	B	262/264 (99%)	247 (94%)	13 (5%)	2 (1%)	19	22
1	C	262/264 (99%)	248 (95%)	14 (5%)	0	100	100
1	D	262/264 (99%)	251 (96%)	11 (4%)	0	100	100
1	E	262/264 (99%)	255 (97%)	7 (3%)	0	100	100
1	F	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	34	40
1	G	262/264 (99%)	246 (94%)	14 (5%)	2 (1%)	19	22
1	H	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	34	40
All	All	2096/2112 (99%)	1990 (95%)	99 (5%)	7 (0%)	41	49

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ALA
1	G	179	MET
1	G	219	ASP
1	H	131	ASP
1	B	131	ASP

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	222/222 (100%)	216 (97%)	6 (3%)	44	59
1	B	222/222 (100%)	218 (98%)	4 (2%)	59	72
1	C	222/222 (100%)	213 (96%)	9 (4%)	30	41
1	D	222/222 (100%)	215 (97%)	7 (3%)	39	52
1	E	222/222 (100%)	218 (98%)	4 (2%)	59	72
1	F	222/222 (100%)	215 (97%)	7 (3%)	39	52
1	G	222/222 (100%)	215 (97%)	7 (3%)	39	52
1	H	222/222 (100%)	214 (96%)	8 (4%)	35	47
All	All	1776/1776 (100%)	1724 (97%)	52 (3%)	42	56

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	215	LEU
1	F	155	LEU
1	H	270	ASN
1	E	266	ILE
1	F	100	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	207	ASN
1	H	285	ASN
1	F	162	ASN
1	H	162	ASN
1	F	134	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

25 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	NDP	B	300	-	45,52,52	1.59	9 (20%)	53,80,80	1.31	4 (7%)
3	2M3	B	1	-	26,30,30	2.27	5 (19%)	32,45,45	2.22	14 (43%)
4	SO4	H	3	-	4,4,4	0.29	0	6,6,6	0.16	0
3	2M3	A	2	-	26,30,30	2.28	5 (19%)	32,45,45	2.18	12 (37%)
2	NDP	F	300	-	45,52,52	1.63	9 (20%)	53,80,80	1.25	4 (7%)
3	2M3	F	290	-	26,30,30	2.15	7 (26%)	32,45,45	2.23	12 (37%)
2	NDP	G	300	-	45,52,52	1.61	7 (15%)	53,80,80	1.26	4 (7%)
3	2M3	G	8	-	26,30,30	2.25	5 (19%)	32,45,45	2.31	15 (46%)
2	NDP	D	300	-	45,52,52	1.46	7 (15%)	53,80,80	1.32	6 (11%)
2	NDP	C	300	-	45,52,52	1.63	10 (22%)	53,80,80	1.24	4 (7%)
4	SO4	G	9	-	4,4,4	0.28	0	6,6,6	0.10	0
3	2M3	C	4	-	26,30,30	2.26	6 (23%)	32,45,45	2.19	12 (37%)
4	SO4	E	4	-	4,4,4	0.27	0	6,6,6	0.10	0
4	SO4	H	6	-	4,4,4	0.27	0	6,6,6	0.09	0
3	2M3	D	3	-	26,30,30	2.22	5 (19%)	32,45,45	2.19	13 (40%)
4	SO4	C	8	-	4,4,4	0.28	0	6,6,6	0.15	0
4	SO4	C	7	-	4,4,4	0.27	0	6,6,6	0.09	0
4	SO4	F	5	-	4,4,4	0.27	0	6,6,6	0.11	0
2	NDP	E	300	-	45,52,52	1.61	7 (15%)	53,80,80	1.24	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NDP	A	300	-	45,52,52	1.61	8 (17%)	53,80,80	1.17	5 (9%)
4	SO4	D	1	-	4,4,4	0.24	0	6,6,6	0.06	0
2	NDP	H	300	-	45,52,52	1.64	8 (17%)	53,80,80	1.24	3 (5%)
4	SO4	B	2	-	4,4,4	0.26	0	6,6,6	0.11	0
3	2M3	E	7	-	26,30,30	2.28	5 (19%)	32,45,45	2.21	14 (43%)
3	2M3	H	290	-	26,30,30	2.35	6 (23%)	32,45,45	2.27	13 (40%)

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	NDP	B	300	-	-	11/30/77/77	0/5/5/5
3	2M3	C	4	-	-	2/14/33/33	0/5/5/5
2	NDP	E	300	-	-	5/30/77/77	0/5/5/5
3	2M3	F	290	-	-	0/14/33/33	0/5/5/5
2	NDP	A	300	-	-	9/30/77/77	0/5/5/5
2	NDP	G	300	-	-	6/30/77/77	0/5/5/5
3	2M3	B	1	-	-	0/14/33/33	0/5/5/5
3	2M3	D	3	-	-	1/14/33/33	0/5/5/5
3	2M3	G	8	-	-	2/14/33/33	0/5/5/5
2	NDP	H	300	-	-	8/30/77/77	0/5/5/5
3	2M3	H	290	-	-	0/14/33/33	0/5/5/5
3	2M3	A	2	-	-	0/14/33/33	0/5/5/5
2	NDP	F	300	-	-	10/30/77/77	0/5/5/5
2	NDP	D	300	-	-	6/30/77/77	0/5/5/5
2	NDP	C	300	-	-	8/30/77/77	0/5/5/5
3	2M3	E	7	-	-	2/14/33/33	0/5/5/5

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	290	2M3	C9-C5	6.21	1.47	1.40
3	B	1	2M3	C9-C5	6.09	1.47	1.40
3	A	2	2M3	C9-C5	6.03	1.47	1.40
3	E	7	2M3	C9-C5	5.95	1.47	1.40
3	E	7	2M3	C1-C2	5.92	1.55	1.37

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	300	NDP	N3A-C2A-N1A	-4.86	121.08	128.68
2	E	300	NDP	N3A-C2A-N1A	-4.86	121.08	128.68
3	D	3	2M3	C21-N20-C19	4.83	124.09	117.49
2	D	300	NDP	N3A-C2A-N1A	-4.80	121.18	128.68
3	H	290	2M3	C26-C17-C25	-4.79	56.30	58.33

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	NDP	C2B-O2B-P2B-O2X
2	A	300	NDP	C5D-O5D-PN-O1N
2	A	300	NDP	C5D-O5D-PN-O2N
2	B	300	NDP	C5B-O5B-PA-O3
2	B	300	NDP	O4B-C4B-C5B-O5B

There are no ring outliers.

17 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	300	NDP	2	0
3	B	1	2M3	5	0
2	F	300	NDP	3	0
3	F	290	2M3	4	0
2	G	300	NDP	4	0
3	G	8	2M3	2	0
2	D	300	NDP	3	0
3	C	4	2M3	5	0
4	E	4	SO4	1	0
3	D	3	2M3	3	0
4	C	8	SO4	1	0
2	E	300	NDP	4	0
2	A	300	NDP	2	0
2	H	300	NDP	2	0
4	B	2	SO4	1	0
3	E	7	2M3	3	0
3	H	290	2M3	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 NDP B 300

Bond lengths

Bond angles

Torsions

Rings

Ligand 2M3 B 1

Bond lengths

Bond angles

Torsions

Rings

Ligand 2M3 A 2

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP F 300

Bond lengths

Bond angles

Torsions

Rings

Ligand 2M3 F 290

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP G 300

Bond lengths

Bond angles

Torsions

Rings

Ligand 2M3 G 8

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP D 300

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP C 300

Bond lengths

Bond angles

Torsions

Rings

Ligand 2M3 C 4

Bond lengths

Bond angles

Torsions

Rings

Ligand 2M3 D 3

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP E 300

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 300

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP H 300

Bond lengths

Bond angles

Torsions

Rings

Ligand 2M3 E 7

Bond lengths

Bond angles

Torsions

Rings

Ligand 2M3 H 290

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	264/264 (100%)	0.13	4 (1%)	73	78	17, 30, 49, 71	6 (2%)
1	B	264/264 (100%)	0.31	9 (3%)	45	50	19, 30, 53, 58	9 (3%)
1	C	264/264 (100%)	-0.22	2 (0%)	86	89	5, 18, 40, 56	5 (1%)
1	D	264/264 (100%)	-0.20	5 (1%)	66	72	5, 18, 45, 58	7 (2%)
1	E	264/264 (100%)	-0.14	3 (1%)	80	84	8, 20, 43, 72	5 (1%)
1	F	263/264 (99%)	-0.15	4 (1%)	73	78	7, 20, 44, 57	2 (0%)
1	G	264/264 (100%)	0.03	0	100	100	14, 27, 48, 58	8 (3%)
1	H	264/264 (100%)	0.12	5 (1%)	66	72	15, 28, 53, 69	6 (2%)
All	All	2111/2112 (99%)	-0.02	32 (1%)	73	78	5, 25, 48, 72	48 (2%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	LEU	7.0
1	B	264	THR	4.7
1	H	262	PRO	4.0
1	A	289	PHE	3.7
1	B	266	ILE	3.4

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
3	2M3	B	1	26/26	0.84	0.25	44,51,54,55	0
3	2M3	H	290	26/26	0.88	0.21	39,42,44,44	0
3	2M3	F	290	26/26	0.89	0.20	32,42,43,44	0
3	2M3	A	2	26/26	0.90	0.19	29,31,35,36	0
3	2M3	D	3	26/26	0.92	0.15	27,31,34,36	0
3	2M3	E	7	26/26	0.92	0.17	19,24,28,29	0
4	SO4	H	3	5/5	0.92	0.13	57,57,58,59	0
4	SO4	G	9	5/5	0.93	0.14	48,49,51,51	0
3	2M3	G	8	26/26	0.93	0.17	26,29,30,31	0
4	SO4	E	4	5/5	0.95	0.14	46,47,47,48	0
3	2M3	C	4	26/26	0.95	0.19	14,22,23,24	0
2	NDP	G	300	48/48	0.95	0.12	19,28,30,31	0
2	NDP	H	300	48/48	0.96	0.11	16,29,33,36	0
2	NDP	B	300	48/48	0.96	0.11	24,28,31,34	0
2	NDP	A	300	48/48	0.96	0.12	17,27,33,34	0
4	SO4	H	6	5/5	0.96	0.19	60,60,61,61	0
2	NDP	F	300	48/48	0.97	0.11	9,14,18,20	0
4	SO4	B	2	5/5	0.97	0.12	48,48,49,50	0
2	NDP	D	300	48/48	0.97	0.11	5,13,19,21	0
4	SO4	D	1	5/5	0.98	0.13	34,36,36,36	0
2	NDP	C	300	48/48	0.98	0.10	11,14,20,20	0
4	SO4	F	5	5/5	0.98	0.11	27,30,31,32	0
2	NDP	E	300	48/48	0.98	0.10	11,15,19,19	0
4	SO4	C	7	5/5	0.98	0.10	48,49,49,50	0
4	SO4	C	8	5/5	0.98	0.13	35,37,37,37	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.
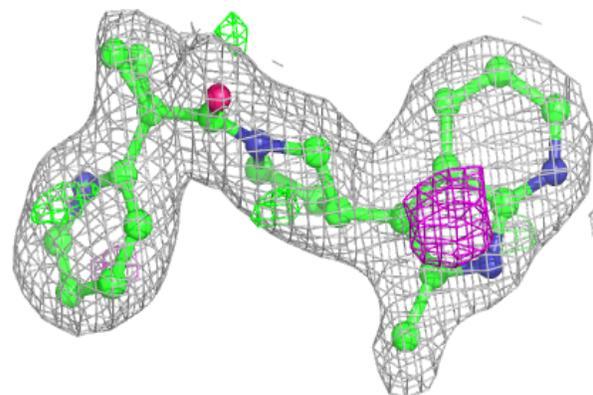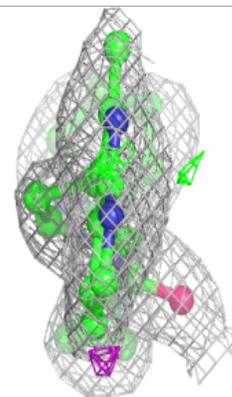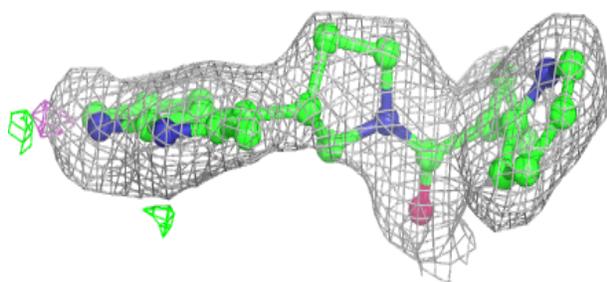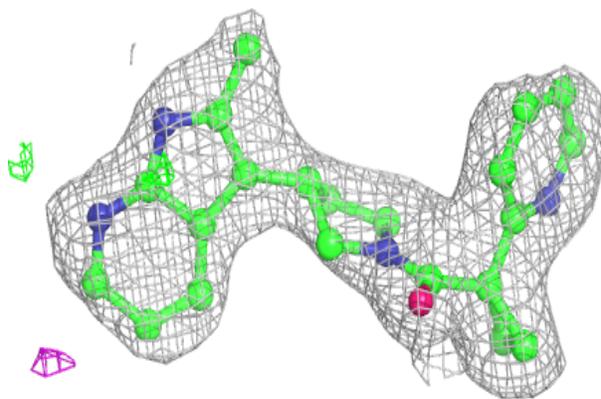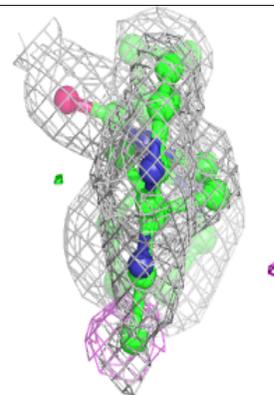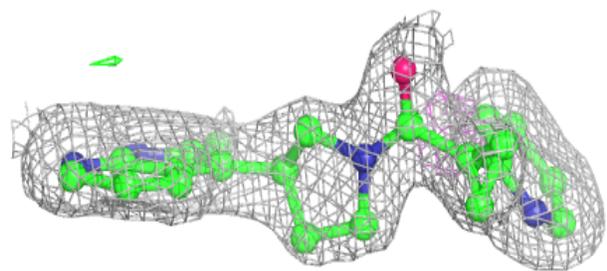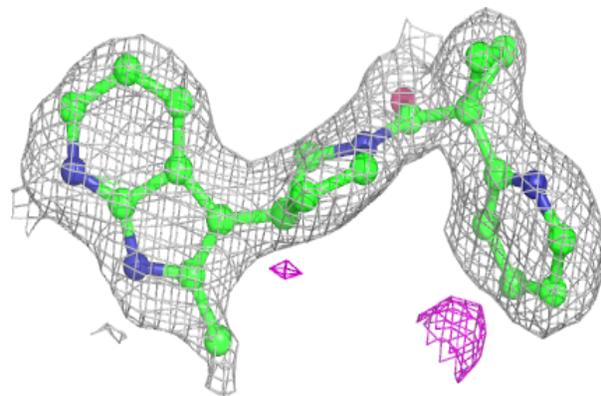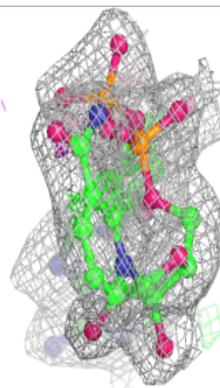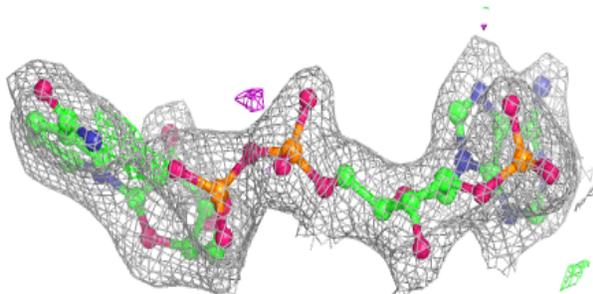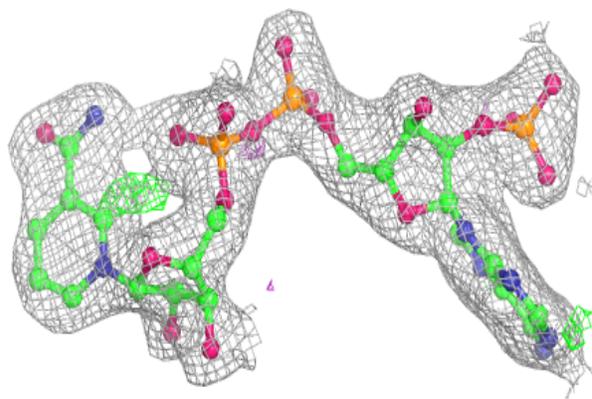
Electron density around 2M3 B 1:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
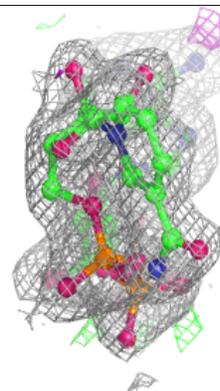mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
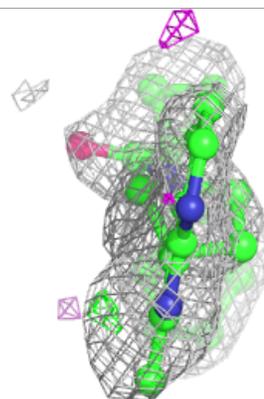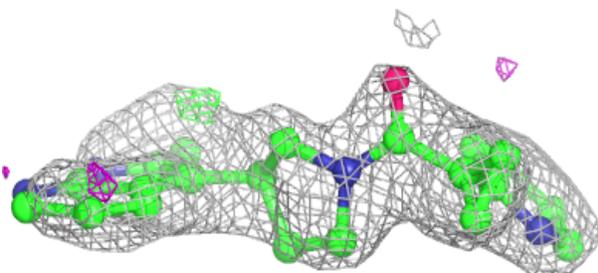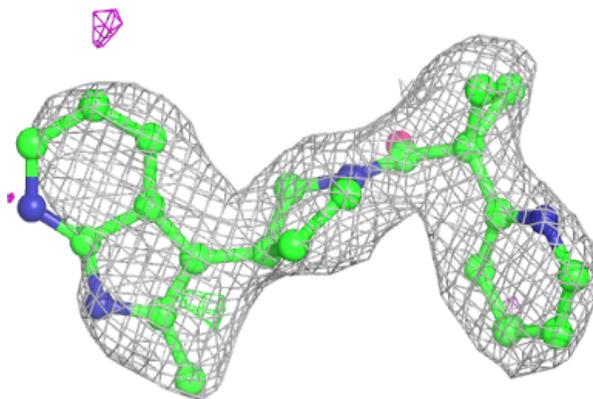
Electron density around 2M3 H 290:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
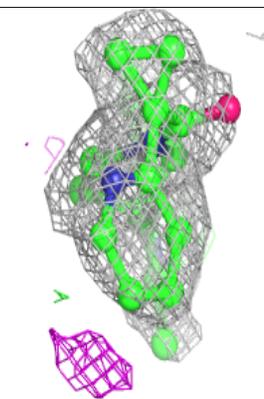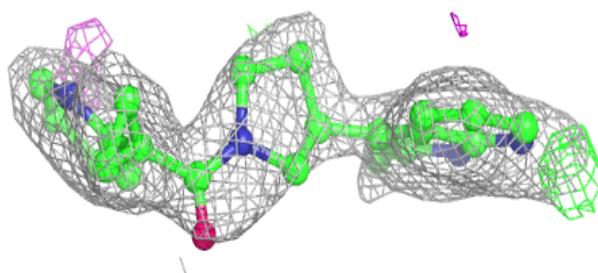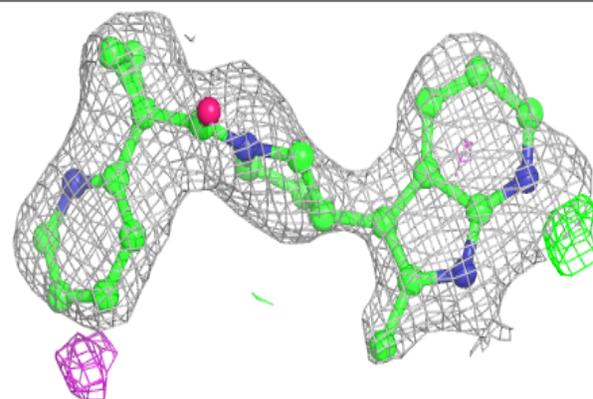
Electron density around 2M3 F 290:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
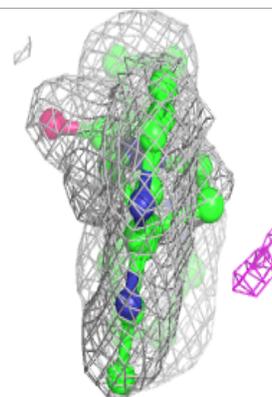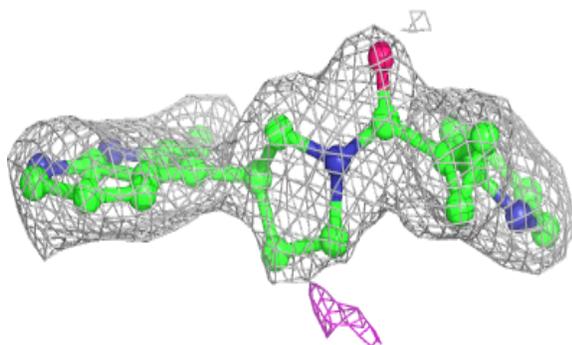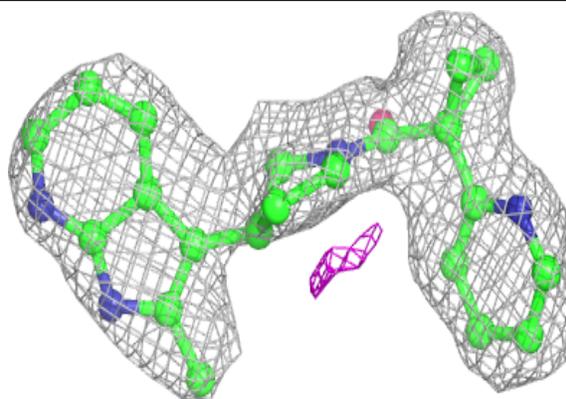
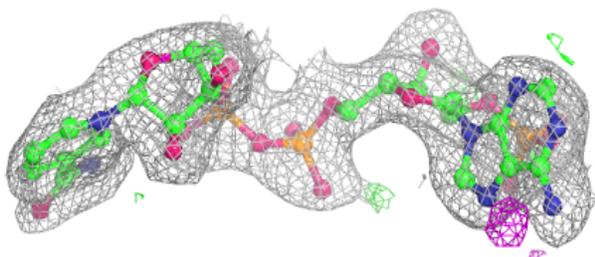**Electron density around 2M3 A 2:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
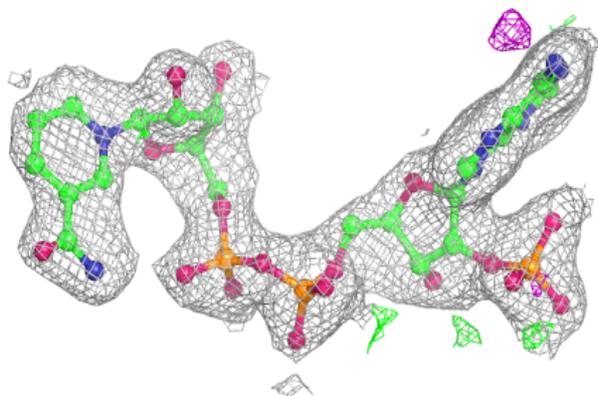and green (positive)
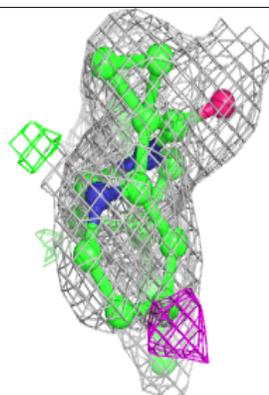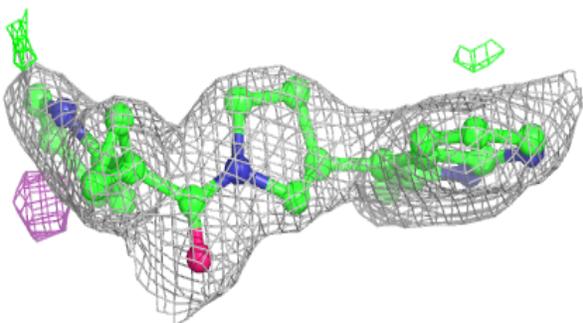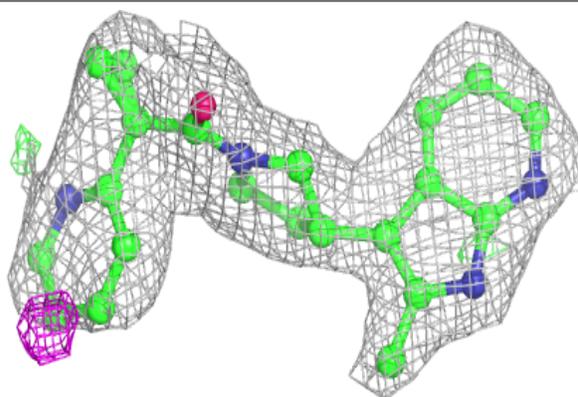
Electron density around 2M3 D 3:

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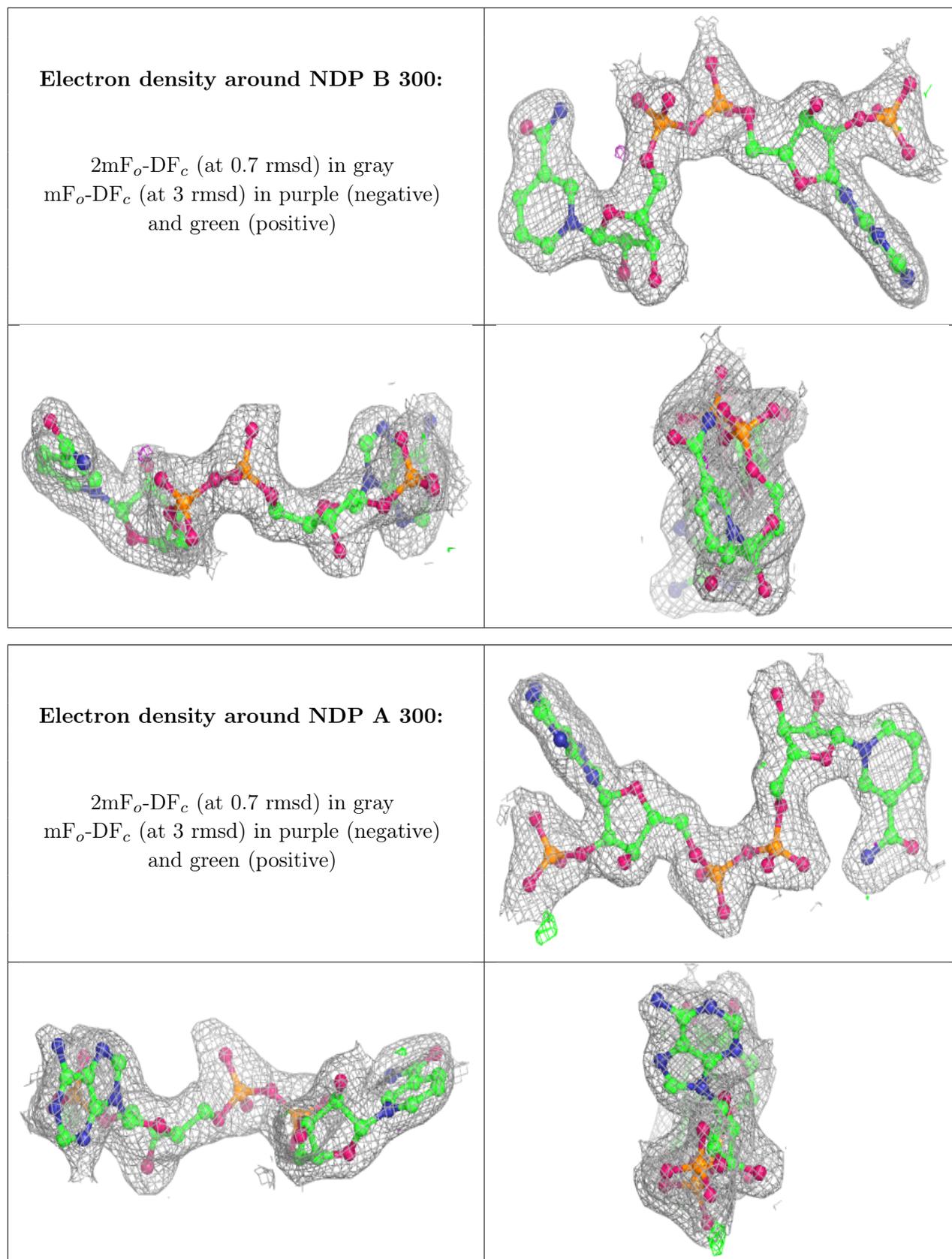mF_o-DF_c (at 3 rmsd) in purple (negative)
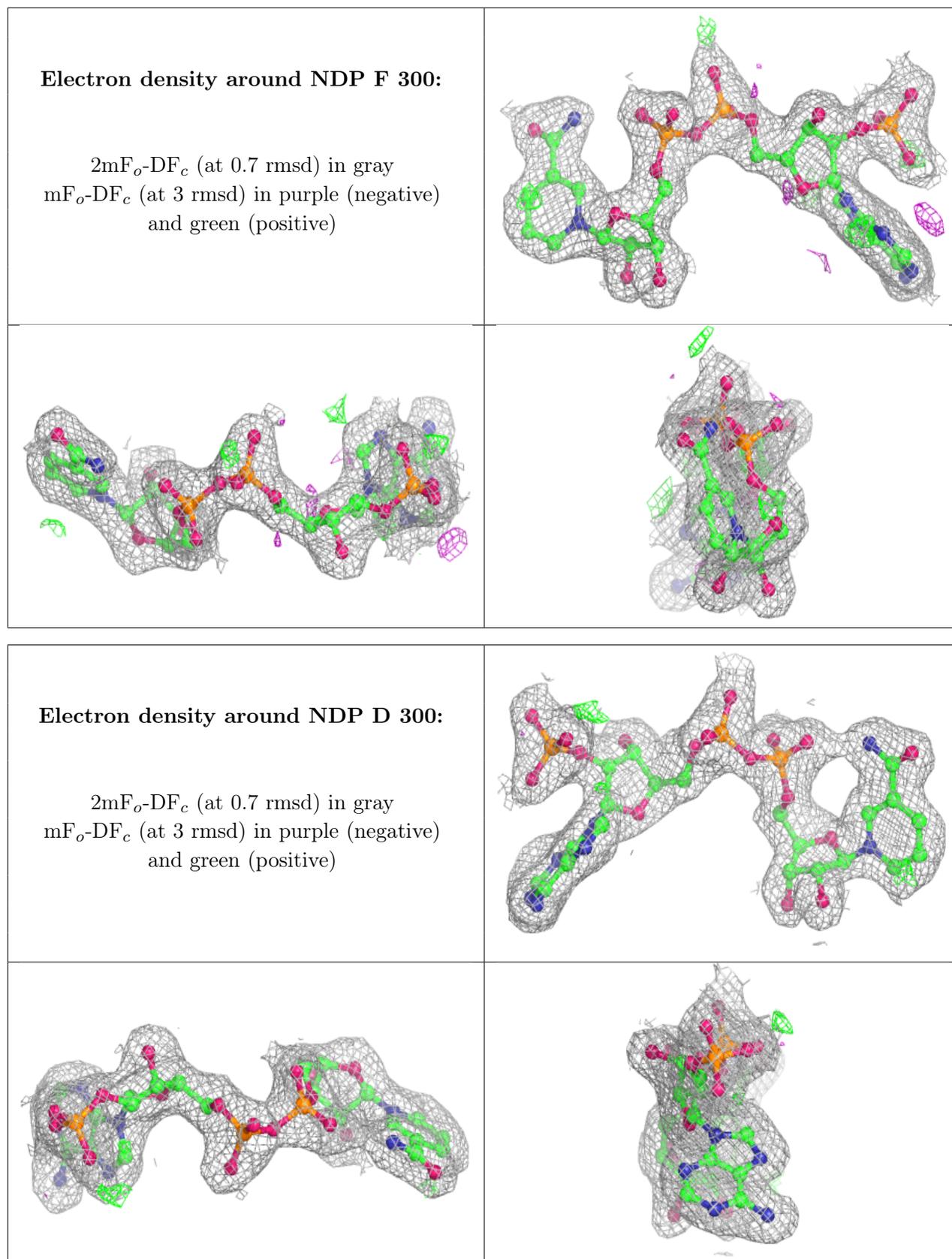and green (positive)
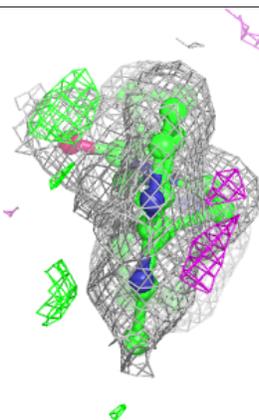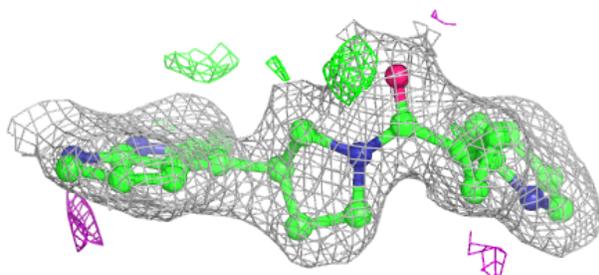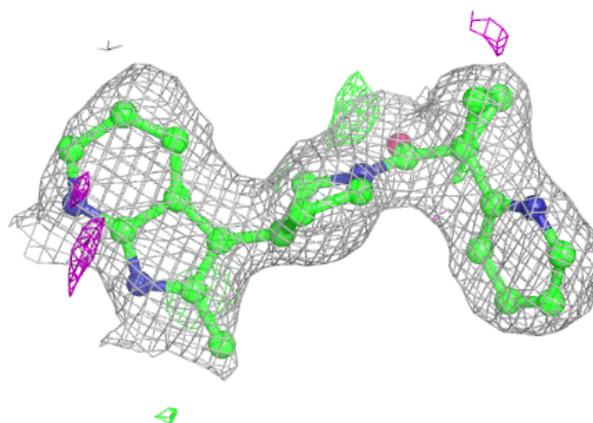
Electron density around 2M3 E 7:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
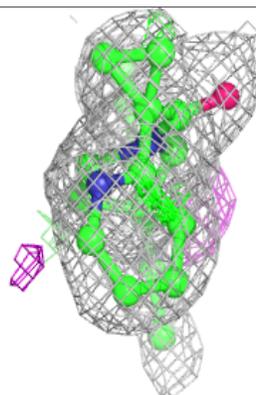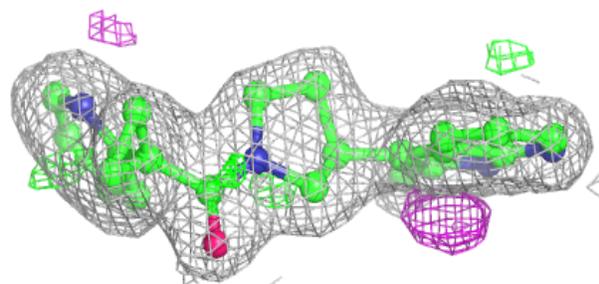
Electron density around 2M3 G 8:

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

Electron density around 2M3 C 4:

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

Electron density around NDP G 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 NDP H 300:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
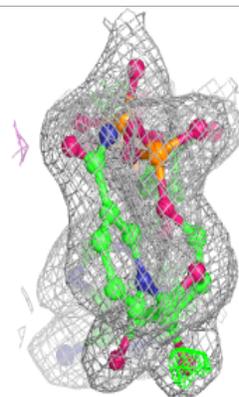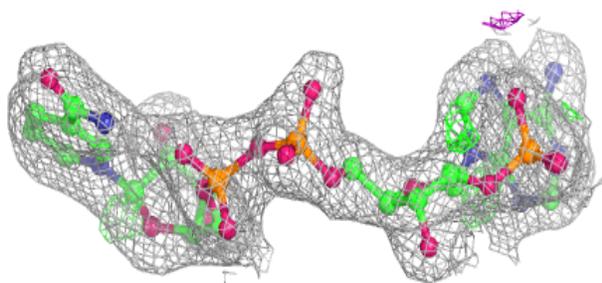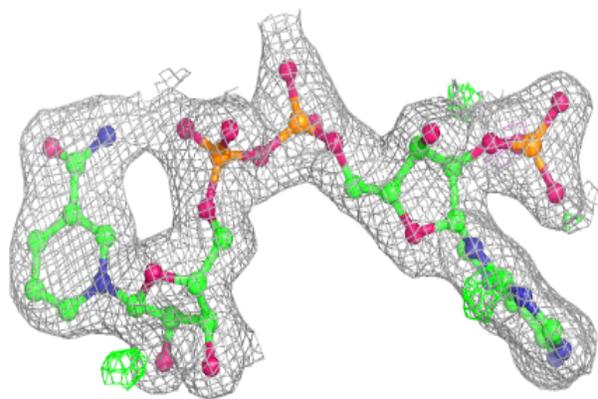mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NDP B 300:

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

Electron density around NDP A 300:

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

Electron density around NDP F 300:

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

Electron density around NDP D 300:

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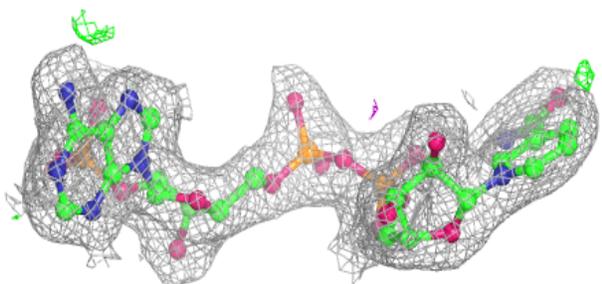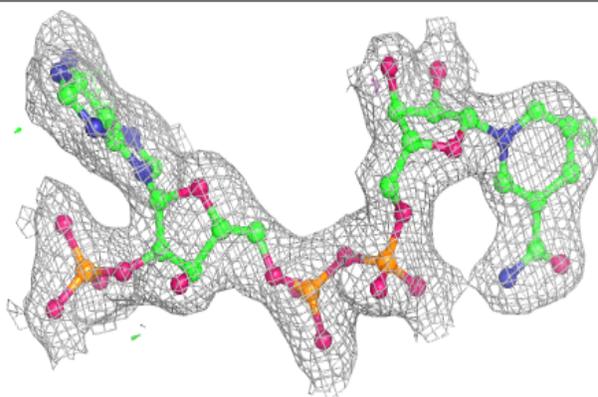$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NDP C 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 NDP E 300:

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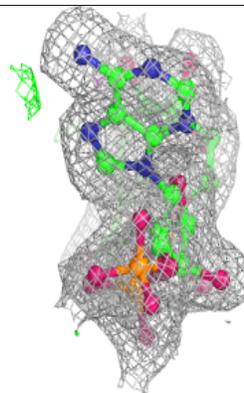
6.5 Other polymers (i)

There are no such residues in this entry.