wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2025 – 06:14 PM EST

PDB ID	:	1NF7
Title	:	Ternary complex of the human type II Inosine Monophosphate Dedhydrogenase with Ribavirin Monophosphate and C2-Mycophenolic Adenine Dinucleotide
Authors	:	Risal, D.; Strickler, M.D.; Goldstein, B.M.
Deposited on	:	2002-12-13
Resolution	:	2.65 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:

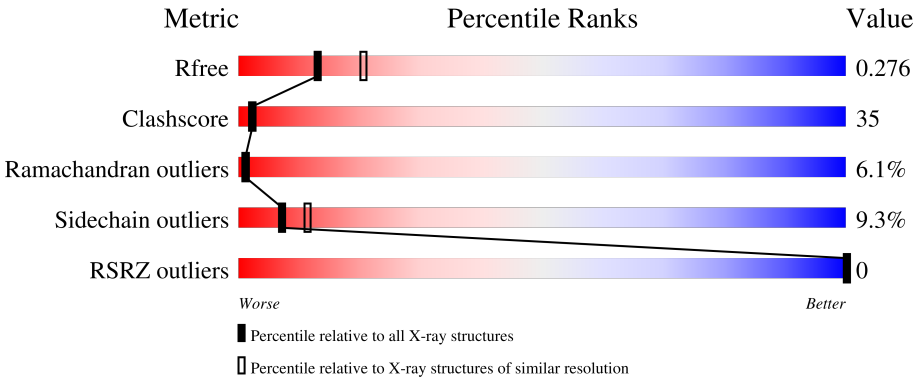
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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	514	42% 39% 7% 12%
1	B	514	41% 39% 8% 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7114 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.

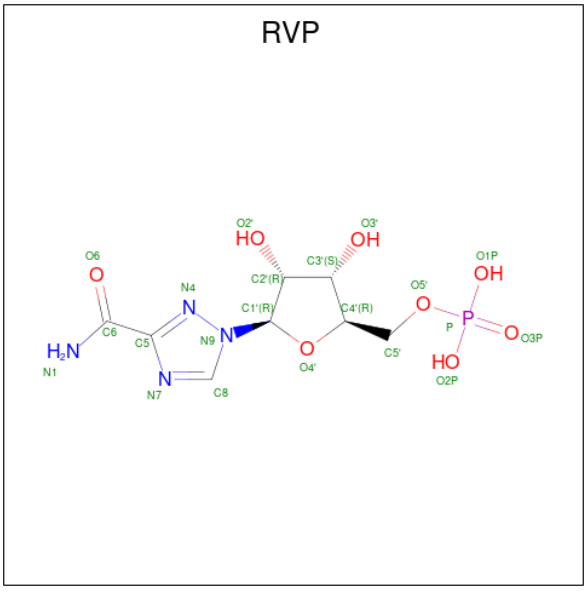
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3440	2176	587	658	19			
1	B	454	Total	C	N	O	S	0	0	0
			3440	2176	587	658	19			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

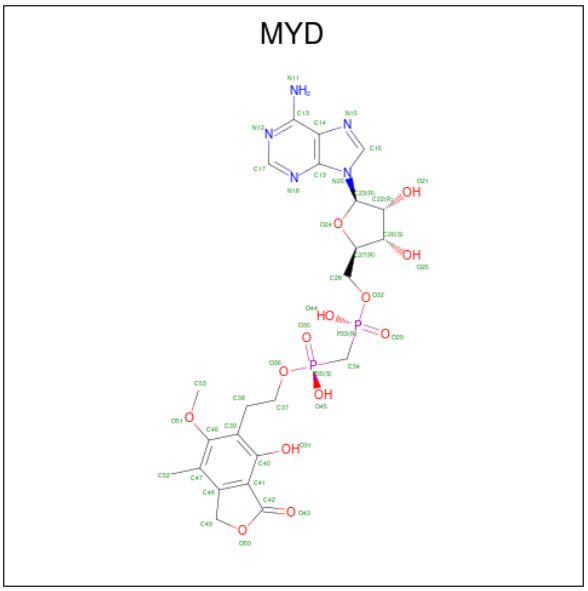
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is RIBAVIRIN MONOPHOSPHATE (three-letter code: RVP) (formula: $C_8H_{13}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	8	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			21	8	4	8	1		

- Molecule 4 is {[5-(6-AMINO-PURIN-7-YL)-3,4-DIHYDROXY-TETRAHYDRO-FURAN-2-YLMETHOXY]-HYDROXY-PHOSPHORYLMETHYL}-PHOSPHONIC ACID MONO-[2-(4-HYDROXY-6-METHOXY-7-METHYL-3-OXO-1,3-DIHYDRO-ISOBENZOFURAN-5-YL)-ETHYL] ESTER (three-letter code: MYD) (formula: $C_{23}H_{29}N_5O_{13}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			43	23	5	13	2		
4	B	1	Total	C	N	O	P	0	0
			43	23	5	13	2		

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total	C	0	0
			11	11		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		

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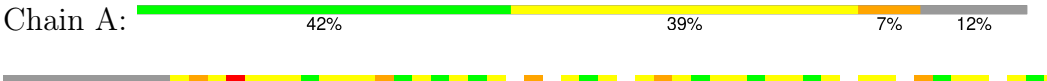
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	47	47	47	0	0

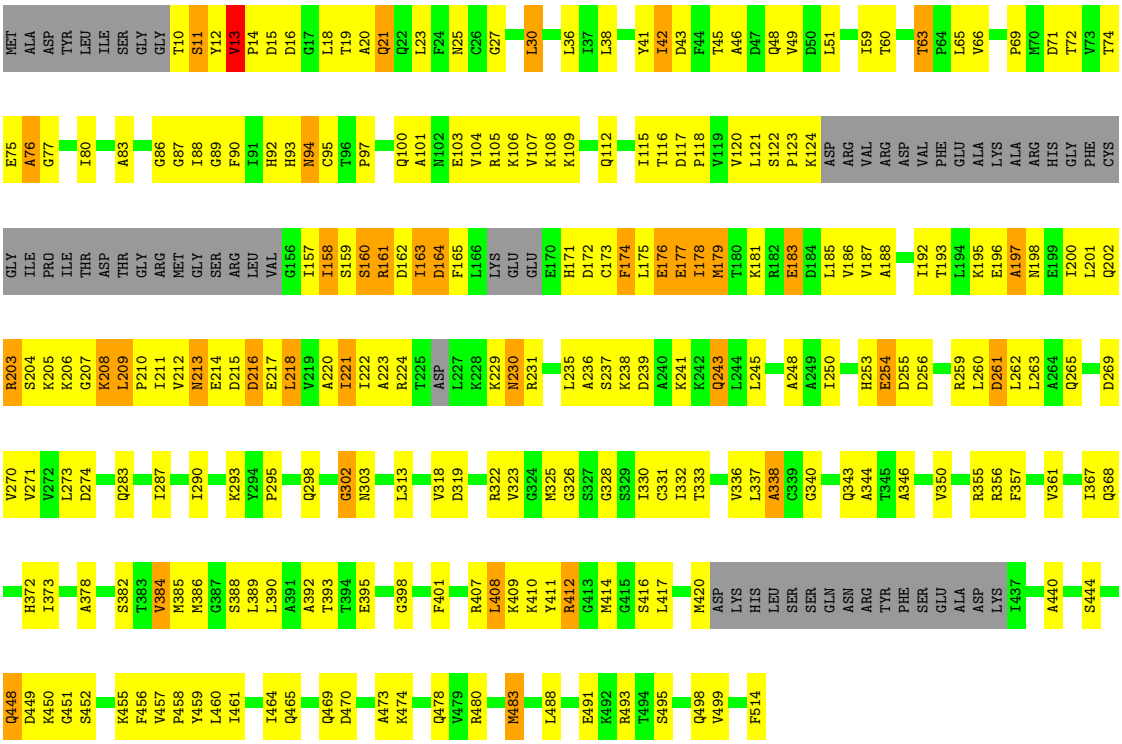
3 Residue-property plots (i)

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: Inosine-5'-monophosphate dehydrogenase 2

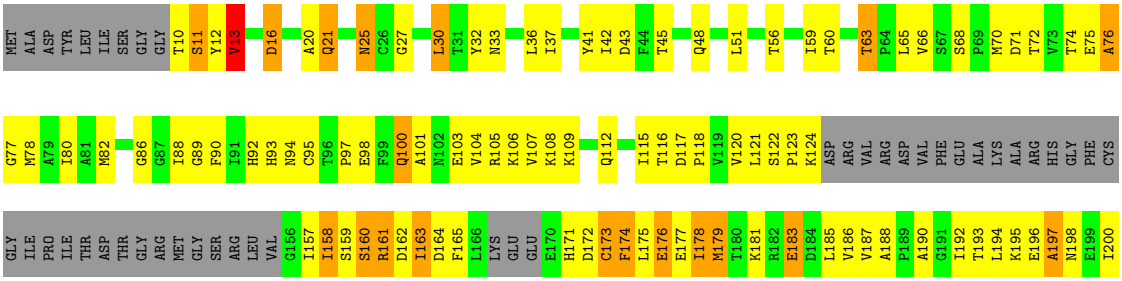
Chain A:

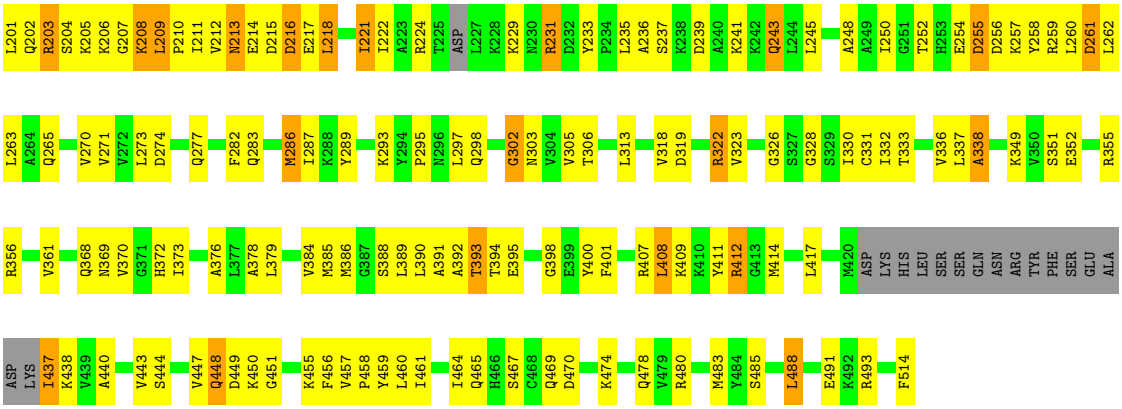




• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain B:




L201 Q202 R203 S204 K205 K206 G207 K208 L209 P210 I211 V212 N213 E214 D215 D216 E217 L218 I221 I222 A223 R224 T225 ASP L227 K228 K229 N230 R231 D232 Y233 P234 L235 A236 S237 K238 D239 A240 K241 K242 Q243 L244 L245 A248 A249 I250 G251 T252 H253 E254 D255 D256 K257 Y258 R259 L260 D261 L262
L263 A264 Q265 V270 V271 V272 L273 D274 Q277 F282 Q283 M286 I287 K288 Y289 K293 Y294 P295 N296 L297 Q298 G302 N303 V304 V305 T306 L313 V318 D319 R322 V323 G326 S327 G328 S329 I330 C331 I332 T333 V336 L337 A338 K349 V350 S351 E352 R355
R356 V361 Q368 N369 V370 G371 H372 I373 A376 L377 A378 L379 V384 M385 M386 G387 S388 L389 L390 A391 A392 T393 T394 E395 G398 E399 Y400 F401 R407 L408 K409 K410 Y411 R412 G413 M414 L417 M420 ASP LYS HIS LEU SER SER GLN ASN ARG TYR PHE SER GLU ALA
ASP LYS I437 K438 V439 A440 V443 S444 V447 Q448 D449 K450 G451 K455 F456 V457 P458 Y459 L460 I461 I464 Q465 H466 S467 C468 Q469 D470 K474 Q478 V479 R480 M483 Y484 S485 L488 E491 K492 R493 F514

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	146.58Å 146.58Å 128.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.24 – 2.65 41.24 – 2.65	Depositor EDS
% Data completeness (in resolution range)	64.7 (41.24-2.65) 75.9 (41.24-2.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	0.59 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.277 0.258 , 0.276	Depositor DCC
R_{free} test set	2984 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.560	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.429 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7114	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: K, MYD, RVP, UNL

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	0.58	0/3489	0.63	0/4705
1	B	0.58	1/3489 (0.0%)	0.64	1/4705 (0.0%)
All	All	0.58	1/6978 (0.0%)	0.63	1/9410 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	437	ILE	CG1-CD1	5.48	1.88	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	437	ILE	CB-CG1-CD1	-8.72	89.47	113.90

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	3440	0	3498	243	0
1	B	3440	0	3498	247	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	0	11	1	0
3	B	21	0	11	1	0
4	A	43	0	25	4	0
4	B	43	0	25	5	0
5	B	11	0	0	1	0
6	A	46	0	0	2	0
6	B	47	0	0	6	0
All	All	7114	0	7068	496	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 35.

The worst 5 of 496 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ILE:CG1	1:B:437:ILE:CD1	1.88	1.52
1:B:179:MET:HE1	1:B:181:LYS:HE2	1.38	1.05
1:A:157:ILE:HD12	1:A:157:ILE:H	1.27	0.99
1:B:437:ILE:CD1	1:B:437:ILE:CB	2.41	0.98
1:B:270:VAL:HG12	1:B:298:GLN:HB2	1.45	0.97

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	444/514 (86%)	348 (78%)	69 (16%)	27 (6%)	1 1
1	B	444/514 (86%)	349 (79%)	68 (15%)	27 (6%)	1 1
All	All	888/1028 (86%)	697 (78%)	137 (15%)	54 (6%)	1 1

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ALA
1	A	116	THR
1	A	160	SER
1	A	197	ALA
1	A	216	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/420 (88%)	334 (90%)	36 (10%)	6	10
1	B	370/420 (88%)	337 (91%)	33 (9%)	8	12
All	All	740/840 (88%)	671 (91%)	69 (9%)	7	11

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	255	ASP
1	B	277	GLN
1	B	412	ARG
1	A	243	GLN
1	A	231	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	372	HIS
1	B	441	GLN
1	A	466	HIS
1	A	441	GLN
1	B	466	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)

Of 17 ligands modelled in this entry, 2 are monoatomic and 11 are unknown - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MYD	B	702	-	39,47,47	2.17	10 (25%)	49,72,72	2.35	21 (42%)
4	MYD	A	701	-	39,47,47	2.24	10 (25%)	49,72,72	2.39	21 (42%)
3	RVP	B	601	-	18,22,22	2.28	4 (22%)	22,33,33	1.58	4 (18%)
3	RVP	A	600	-	18,22,22	2.22	4 (22%)	22,33,33	1.51	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MYD	B	702	-	-	2/21/50/50	0/5/5/5
4	MYD	A	701	-	-	2/21/50/50	0/5/5/5
3	RVP	B	601	-	-	0/6/30/30	0/2/2/2
3	RVP	A	600	-	-	0/6/30/30	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	RVP	O4'-C1'	6.69	1.49	1.40
3	A	600	RVP	O4'-C1'	6.13	1.48	1.40
4	A	701	MYD	O50-C42	5.76	1.43	1.36
4	A	701	MYD	C49-C48	5.60	1.56	1.50
4	A	701	MYD	O24-C23	5.34	1.47	1.40

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	702	MYD	N18-C17-N12	-6.64	119.66	128.67
4	A	701	MYD	N18-C17-N12	-6.45	119.92	128.67
4	A	701	MYD	C22-C26-C27	-4.84	93.26	102.61
4	A	701	MYD	C27-O24-C23	-4.83	105.50	109.92
4	A	701	MYD	O50-C49-C48	-4.74	100.81	104.57

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	MYD	C39-C46-O51-C53
4	B	702	MYD	C39-C46-O51-C53
4	A	701	MYD	P33-C34-P35-O30
4	B	702	MYD	P33-C34-P35-O30

There are no ring outliers.

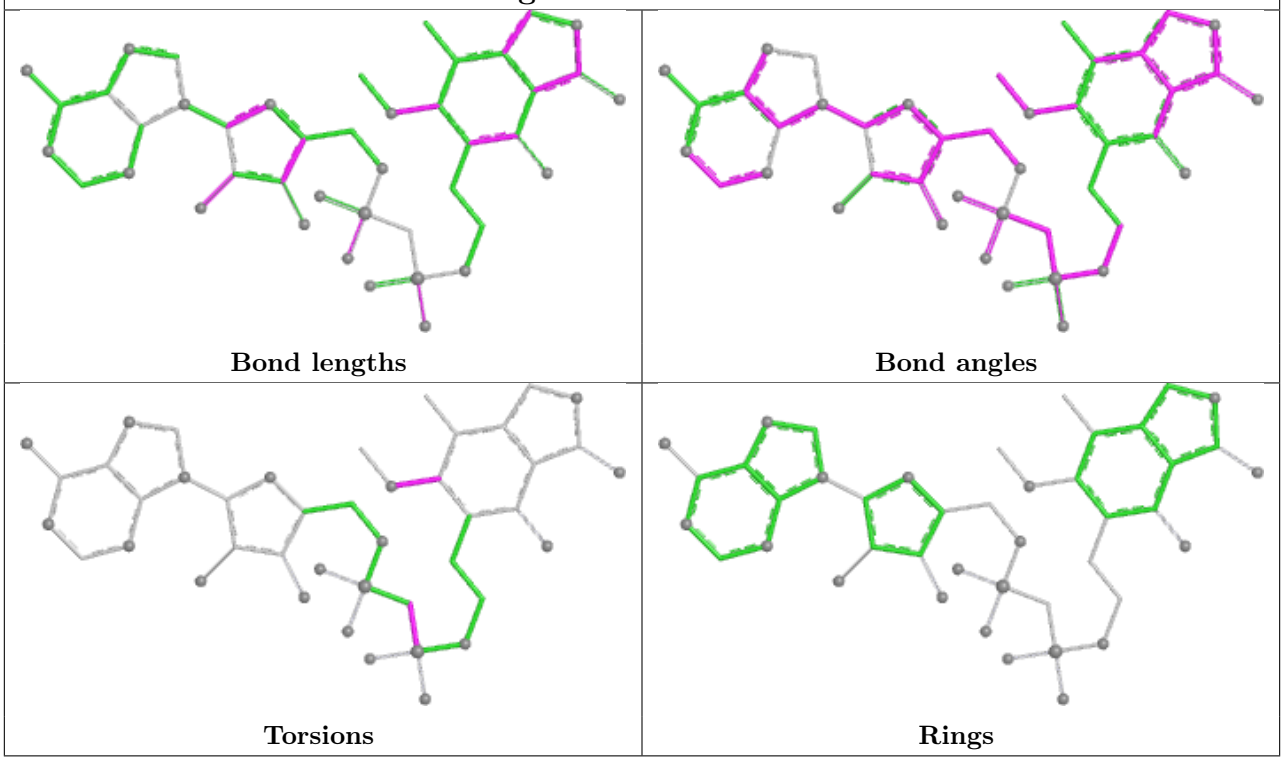
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	702	MYD	5	0
4	A	701	MYD	4	0
3	B	601	RVP	1	0
3	A	600	RVP	1	0

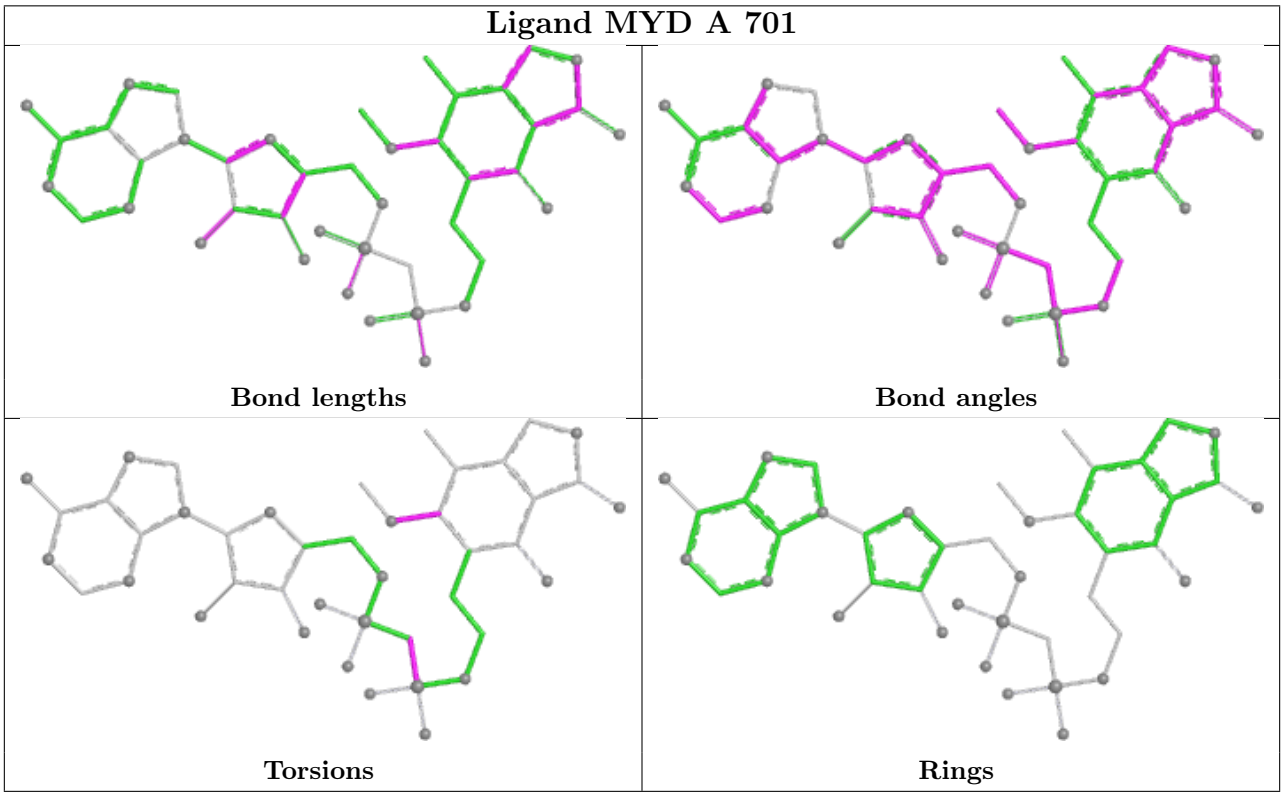
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

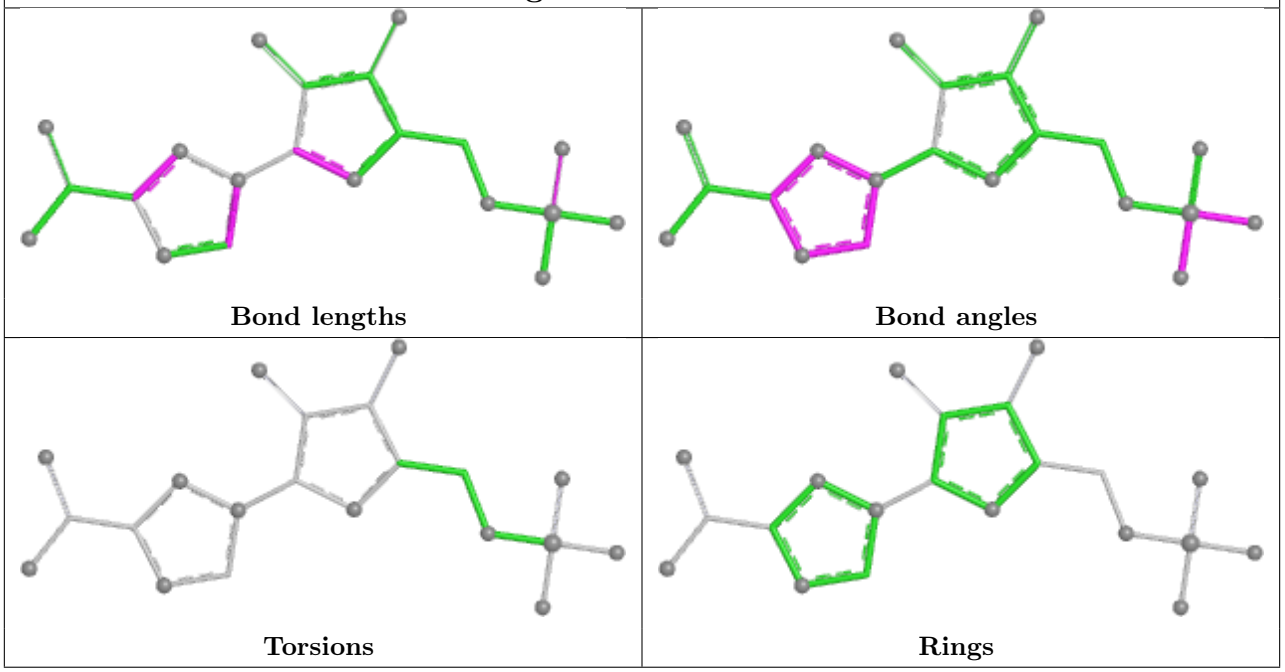
Ligand MYD B 702



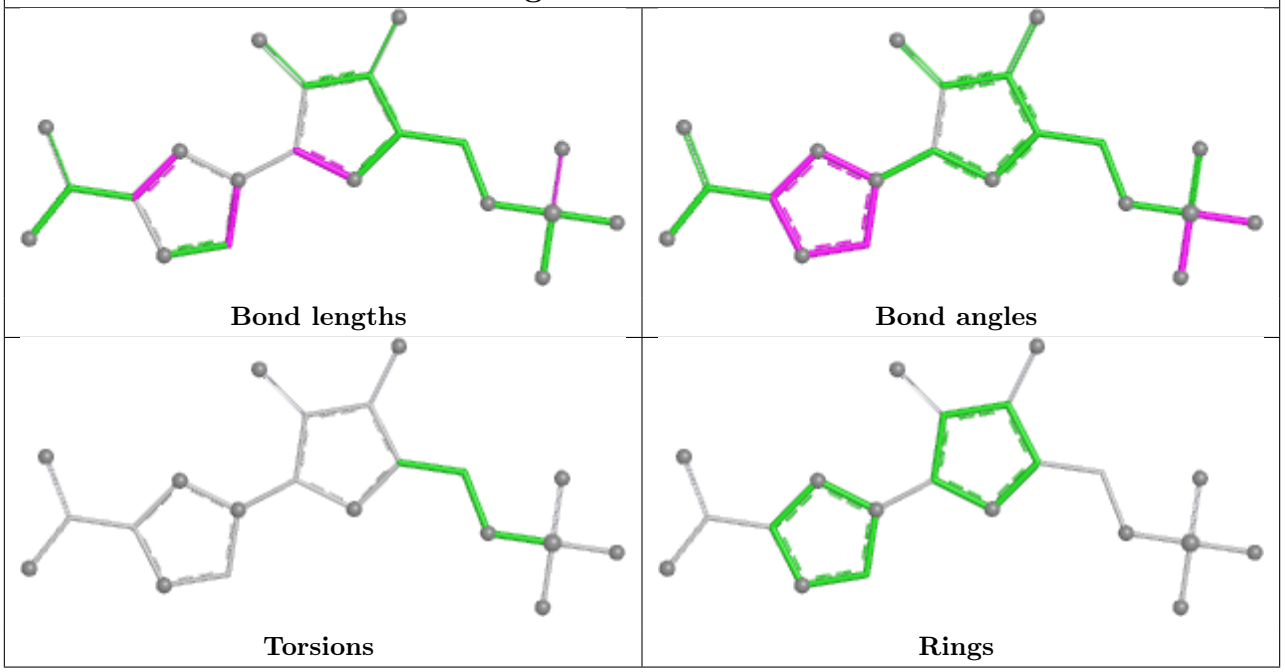
Ligand MYD A 701



Ligand RVP B 601



Ligand RVP A 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	454/514 (88%)	-1.32	0	100	100	12, 41, 116, 140	0
1	B	454/514 (88%)	-1.34	0	100	100	10, 41, 110, 143	0
All	All	908/1028 (88%)	-1.33	0	100	100	10, 41, 114, 143	0

There are no RSRZ outliers to report.

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, 95^{th} 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
5	UNL	B	806	1/-	0.93	0.10	20,20,20,20	0
5	UNL	B	803	1/-	0.97	0.05	20,20,20,20	0
5	UNL	B	801	1/-	0.98	0.06	20,20,20,20	0
5	UNL	B	804	1/-	0.98	0.05	20,20,20,20	0
5	UNL	B	802	1/-	0.98	0.06	20,20,20,20	0
5	UNL	B	807	1/-	0.98	0.12	20,20,20,20	0
5	UNL	B	809	1/-	0.98	0.04	20,20,20,20	0

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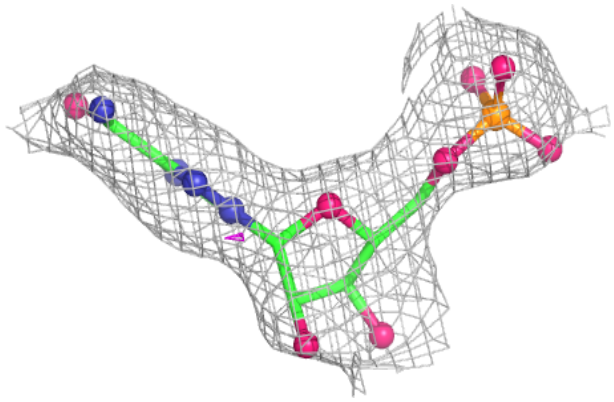
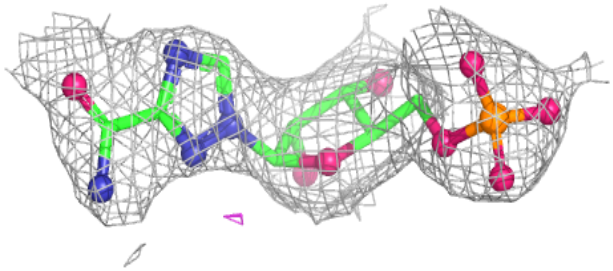
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	K	B	901	1/1	0.99	0.16	106,106,106,106	0
3	RVP	A	600	21/21	0.99	0.03	53,53,53,53	0
3	RVP	B	601	21/21	0.99	0.05	56,56,56,56	0
5	UNL	B	805	1/-	0.99	0.09	20,20,20,20	0
4	MYD	A	701	43/43	0.99	0.04	58,58,58,58	0
4	MYD	B	702	43/43	0.99	0.05	60,60,60,60	0
5	UNL	B	808	1/-	0.99	0.05	20,20,20,20	0
2	K	A	902	1/1	0.99	0.12	100,100,100,100	0
5	UNL	B	810	1/-	0.99	0.11	20,20,20,20	0
5	UNL	B	811	1/-	1.00	0.10	20,20,20,20	0

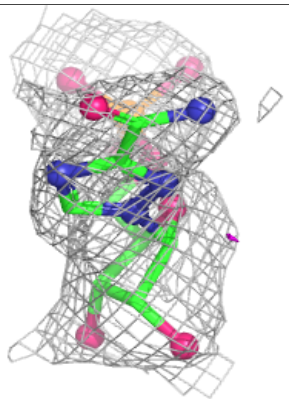
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RVP A 600:

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

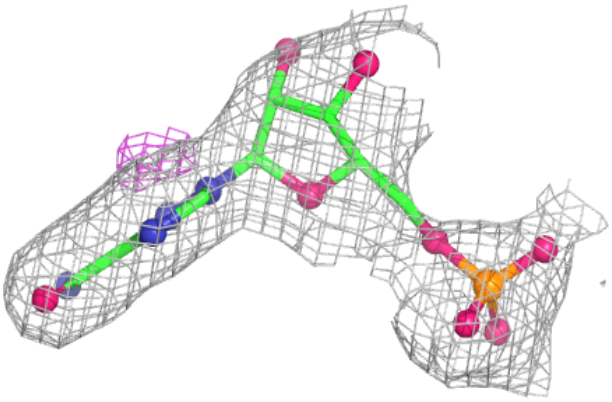


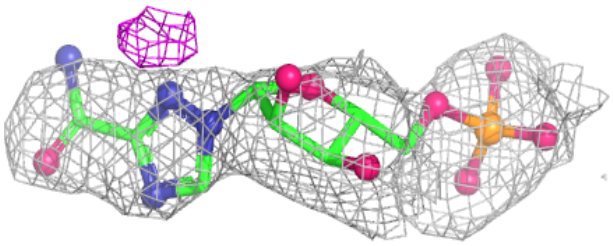


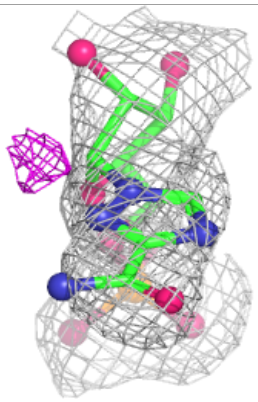


Electron density around RVP B 601:

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

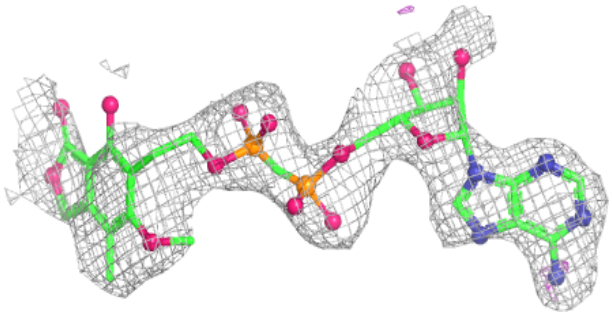


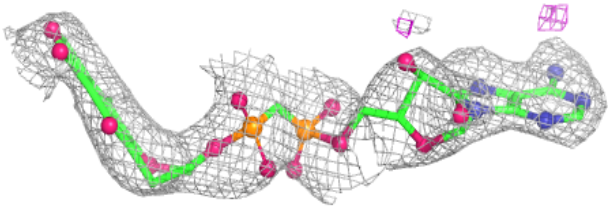


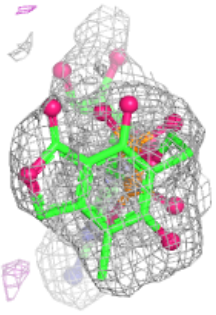


Electron density around MYD A 701:

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

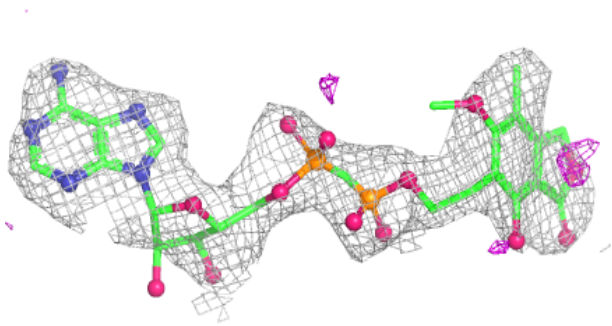


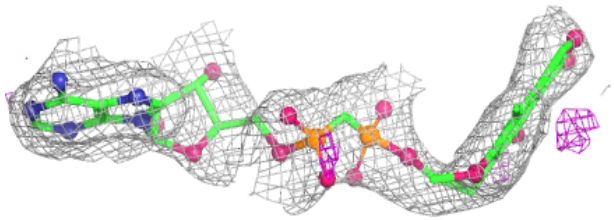


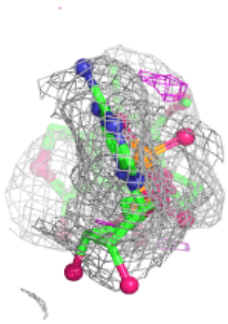


Electron density around MYD B 702:

$2mF_o$-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.