



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2025 – 03:08 pm GMT

PDB ID : 8S1Y
Title : ThaOS V79A
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Deposited on : 2024-02-16
Resolution : 1.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

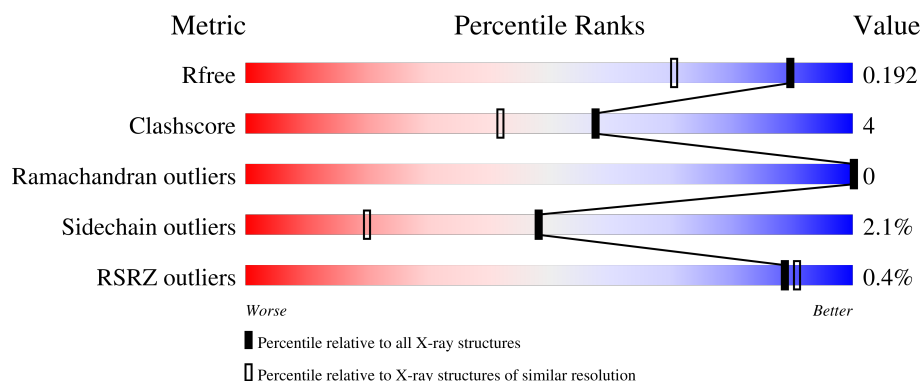
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.50 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	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13231 atoms, of which 6419 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 8-amino-7-oxononanoate synthase/2-amino-3-ketobutyrate coenzyme A ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	398	Total	C	H	N	O	S	84	2	0
			6241	1970	3155	546	567	3			
1	B	395	Total	C	H	N	O	S	84	3	0
			6225	1965	3150	544	564	2			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP Q5SHZ8
A	-23	SER	-	expression tag	UNP Q5SHZ8
A	-22	TYR	-	expression tag	UNP Q5SHZ8
A	-21	TYR	-	expression tag	UNP Q5SHZ8
A	-20	HIS	-	expression tag	UNP Q5SHZ8
A	-19	HIS	-	expression tag	UNP Q5SHZ8
A	-18	HIS	-	expression tag	UNP Q5SHZ8
A	-17	HIS	-	expression tag	UNP Q5SHZ8
A	-16	HIS	-	expression tag	UNP Q5SHZ8
A	-15	HIS	-	expression tag	UNP Q5SHZ8
A	-14	ASP	-	expression tag	UNP Q5SHZ8
A	-13	TYR	-	expression tag	UNP Q5SHZ8
A	-12	ASP	-	expression tag	UNP Q5SHZ8
A	-11	ILE	-	expression tag	UNP Q5SHZ8
A	-10	PRO	-	expression tag	UNP Q5SHZ8
A	-9	THR	-	expression tag	UNP Q5SHZ8
A	-8	THR	-	expression tag	UNP Q5SHZ8
A	-7	GLU	-	expression tag	UNP Q5SHZ8
A	-6	ASN	-	expression tag	UNP Q5SHZ8
A	-5	LEU	-	expression tag	UNP Q5SHZ8
A	-4	TYR	-	expression tag	UNP Q5SHZ8
A	-3	PHE	-	expression tag	UNP Q5SHZ8
A	-2	GLN	-	expression tag	UNP Q5SHZ8
A	-1	GLY	-	expression tag	UNP Q5SHZ8

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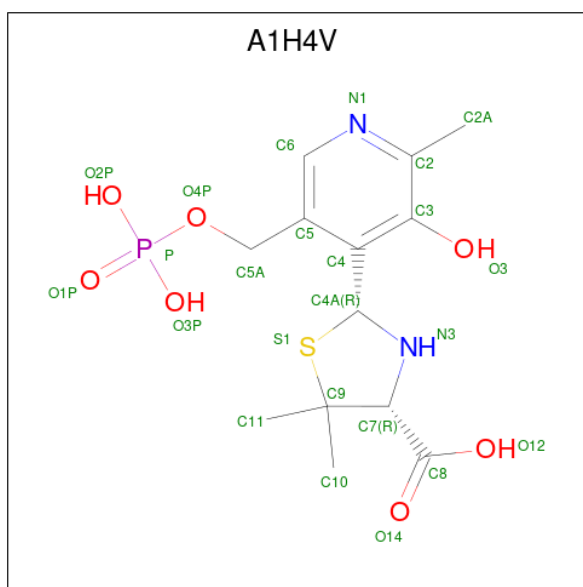
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP Q5SHZ8
A	1	MET	-	expression tag	UNP Q5SHZ8
A	2	GLY	-	expression tag	UNP Q5SHZ8
A	79	ALA	VAL	engineered mutation	UNP Q5SHZ8
B	-24	MET	-	initiating methionine	UNP Q5SHZ8
B	-23	SER	-	expression tag	UNP Q5SHZ8
B	-22	TYR	-	expression tag	UNP Q5SHZ8
B	-21	TYR	-	expression tag	UNP Q5SHZ8
B	-20	HIS	-	expression tag	UNP Q5SHZ8
B	-19	HIS	-	expression tag	UNP Q5SHZ8
B	-18	HIS	-	expression tag	UNP Q5SHZ8
B	-17	HIS	-	expression tag	UNP Q5SHZ8
B	-16	HIS	-	expression tag	UNP Q5SHZ8
B	-15	HIS	-	expression tag	UNP Q5SHZ8
B	-14	ASP	-	expression tag	UNP Q5SHZ8
B	-13	TYR	-	expression tag	UNP Q5SHZ8
B	-12	ASP	-	expression tag	UNP Q5SHZ8
B	-11	ILE	-	expression tag	UNP Q5SHZ8
B	-10	PRO	-	expression tag	UNP Q5SHZ8
B	-9	THR	-	expression tag	UNP Q5SHZ8
B	-8	THR	-	expression tag	UNP Q5SHZ8
B	-7	GLU	-	expression tag	UNP Q5SHZ8
B	-6	ASN	-	expression tag	UNP Q5SHZ8
B	-5	LEU	-	expression tag	UNP Q5SHZ8
B	-4	TYR	-	expression tag	UNP Q5SHZ8
B	-3	PHE	-	expression tag	UNP Q5SHZ8
B	-2	GLN	-	expression tag	UNP Q5SHZ8
B	-1	GLY	-	expression tag	UNP Q5SHZ8
B	0	ALA	-	expression tag	UNP Q5SHZ8
B	1	MET	-	expression tag	UNP Q5SHZ8
B	2	GLY	-	expression tag	UNP Q5SHZ8
B	79	ALA	VAL	engineered mutation	UNP Q5SHZ8

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	1	0
			22	6	14	2		
2	A	1	Total	C	H	O	1	0
			22	6	14	2		
2	B	1	Total	C	H	O	1	0
			22	6	14	2		
2	B	1	Total	C	H	O	1	0
			22	6	14	2		
2	B	1	Total	C	H	O	1	0
			22	6	14	2		

- Molecule 3 is (2 {R},4 {R})-5,5-dimethyl-2-[2-methyl-3-oxidanyl-5-(phosphonooxymethyl)pyridin-4-yl]-1,3-thiazolidine-4-carboxylic acid (three-letter code: A1H4V) (formula: C₁₃H₁₉N₂O₇PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			39	13	15	2	7	1	1		
3	B	1	Total	C	H	N	O	P	S	0	0
			39	13	15	2	7	1	1		

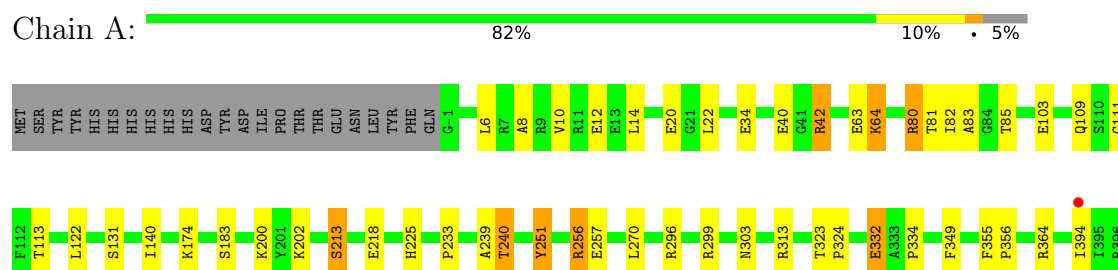
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	273	Total	O	0	0
			273	273		
4	B	282	Total	O	0	0
			282	282		

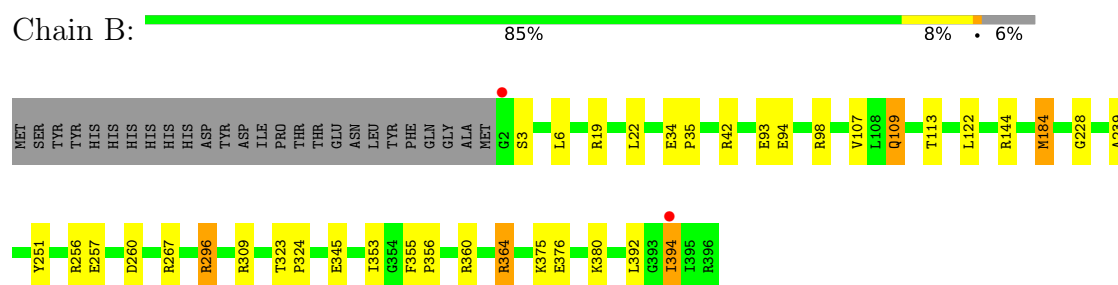
3 Residue-property plots

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: 8-amino-7-oxononanoate synthase/2-amino-3-ketobutyrate coenzyme A ligase



- Molecule 1: 8-amino-7-oxononanoate synthase/2-amino-3-ketobutyrate coenzyme A ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.43Å 63.94Å 65.97Å 64.80° 70.29° 68.18°	Depositor
Resolution (Å)	43.76 – 1.50 43.76 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (43.76-1.50) 96.1 (43.76-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.159 , 0.192 0.159 , 0.192	Depositor DCC
R_{free} test set	5892 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13231	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1H4V, MPD

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	0.80	5/3152 (0.2%)	1.05	8/4260 (0.2%)
1	B	0.78	1/3144 (0.0%)	1.06	5/4249 (0.1%)
All	All	0.79	6/6296 (0.1%)	1.05	13/8509 (0.2%)

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	3
1	B	0	5
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	GLU	CD-OE1	7.98	1.34	1.25
1	A	103	GLU	CD-OE1	7.11	1.33	1.25
1	A	34	GLU	CD-OE2	-6.00	1.19	1.25
1	A	63	GLU	CD-OE1	-5.79	1.19	1.25
1	B	376	GLU	CD-OE1	-5.27	1.19	1.25
1	A	183	SER	CB-OG	5.15	1.49	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	364	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	299	ARG	NE-CZ-NH2	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	SER	CB-CA-C	5.34	120.25	110.10
1	A	251	TYR	CB-CG-CD1	5.30	124.18	121.00
1	A	240	THR	CA-CB-CG2	-5.22	105.09	112.40
1	B	184	MET	CG-SD-CE	-5.19	91.90	100.20
1	B	360	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	364	ARG	CD-NE-CZ	5.15	130.82	123.60
1	A	80	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	349	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	A	200	LYS	CB-CA-C	5.06	120.52	110.40
1	B	296	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	ARG	Sidechain
1	A	296	ARG	Sidechain
1	A	42	ARG	Sidechain
1	B	144	ARG	Sidechain
1	B	256	ARG	Sidechain
1	B	267	ARG	Sidechain
1	B	296	ARG	Sidechain
1	B	309	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	3086	3155	3148	33	0
1	B	3075	3150	3141	22	0
2	A	16	28	28	10	0
2	B	32	56	56	1	0
3	A	24	15	0	1	0
3	B	24	15	0	1	0
4	A	273	0	0	11	0
4	B	282	0	0	9	0
All	All	6812	6419	6373	56	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 4.

All (56) 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:19:ARG:HD3	4:B:588:HOH:O	1.67	0.94
1:A:131[A]:SER:OG	4:A:501:HOH:O	1.91	0.88
2:A:401:MPD:HM3	2:A:401:MPD:O4	1.85	0.76
1:A:239:ALA:HB3	1:A:251:TYR:CZ	2.21	0.76
1:A:10:VAL:HG11	1:B:257:GLU:HB3	1.67	0.75
1:A:40:GLU:OE2	4:A:502:HOH:O	2.06	0.72
1:B:345:GLU:OE1	4:B:501:HOH:O	2.08	0.71
1:A:213:SER:HB3	4:A:618:HOH:O	1.90	0.71
1:A:85:THR:HG21	2:A:401:MPD:HM2	1.74	0.70
1:A:64:LYS:HE2	4:A:525:HOH:O	1.90	0.70
1:A:42:ARG:CZ	4:A:573:HOH:O	2.41	0.69
1:B:380:LYS:HD2	4:B:712:HOH:O	1.94	0.67
1:A:80:ARG:HH21	2:A:401:MPD:CM	2.08	0.66
2:A:402:MPD:O4	2:A:402:MPD:HM1	1.99	0.62
1:A:257:GLU:HG3	4:B:647:HOH:O	1.99	0.61
1:B:107:VAL:HG21	4:B:759:HOH:O	2.00	0.60
1:A:80:ARG:HH21	2:A:401:MPD:HM1	1.67	0.59
1:A:109[B]:GLN:HG3	1:A:113:THR:OG1	2.04	0.57
1:B:94:GLU:OE1	4:B:502:HOH:O	2.18	0.56
1:A:83:ALA:HB1	4:A:580:HOH:O	2.07	0.54
1:A:82:ILE:O	1:A:83:ALA:HB3	2.06	0.53
1:A:80:ARG:NH2	2:A:401:MPD:HM1	2.23	0.53
1:A:111:GLY:HA3	1:A:240:THR:HG22	1.92	0.52
1:A:233:PRO:O	1:B:6:LEU:HD23	2.10	0.52
2:A:401:MPD:O4	2:A:401:MPD:CM	2.56	0.51
3:A:403:A1H4V:O3	3:A:403:A1H4V:N3	2.43	0.50
1:B:375:LYS:HB2	2:B:403:MPD:H13	1.92	0.49
1:A:225:HIS:HD2	4:A:651:HOH:O	1.96	0.49
1:B:392:LEU:HB2	1:B:394:ILE:HD13	1.95	0.49
1:A:10:VAL:CG1	1:B:257:GLU:HB3	2.40	0.49
1:A:14:LEU:HD11	1:B:260:ASP:HB3	1.96	0.48
1:B:239:ALA:HB3	1:B:251:TYR:CZ	2.49	0.48
1:B:228:GLY:HA2	4:B:530:HOH:O	2.13	0.48
1:B:93:GLU:OE2	1:B:107:VAL:HG22	2.13	0.48
1:B:355:PHE:CG	1:B:356:PRO:HA	2.49	0.48
1:B:34:GLU:HB3	1:B:35:PRO:HD2	1.96	0.47
1:A:80:ARG:HH21	2:A:401:MPD:HM2	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:HG21	1:A:270:LEU:HD23	1.97	0.47
1:A:332:GLU:HB3	1:A:334:PRO:HD2	1.97	0.46
1:A:323:THR:HB	1:A:324:PRO:CD	2.46	0.45
1:A:303:ASN:OD1	2:A:402:MPD:H12	2.17	0.45
1:A:8:ALA:O	1:A:12:GLU:HG3	2.18	0.44
2:A:402:MPD:O4	2:A:402:MPD:CM	2.66	0.43
1:A:20:GLU:HA	1:A:20:GLU:OE1	2.19	0.43
1:B:184:MET:SD	1:B:353:ILE:HD13	2.59	0.42
1:A:355:PHE:CG	1:A:356:PRO:HA	2.54	0.42
1:B:323:THR:HB	1:B:324:PRO:CD	2.50	0.42
1:A:218:GLU:HG3	4:A:738:HOH:O	2.19	0.42
1:A:140:ILE:HD13	4:A:501:HOH:O	2.20	0.42
1:B:109[B]:GLN:HG3	1:B:113:THR:OG1	2.21	0.41
1:B:98:ARG:NH1	4:B:505:HOH:O	2.39	0.41
1:A:313:ARG:NH1	4:A:514:HOH:O	2.54	0.41
1:A:332:GLU:OE1	4:A:503:HOH:O	2.22	0.41
1:B:42:ARG:CZ	4:B:600:HOH:O	2.68	0.41
3:B:405:A1H4V:O3	3:B:405:A1H4V:N3	2.54	0.41
1:A:174:LYS:HE3	1:B:3:SER:OG	2.21	0.40

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	398/421 (94%)	390 (98%)	8 (2%)	0	100	100
1	B	396/421 (94%)	386 (98%)	10 (2%)	0	100	100
All	All	794/842 (94%)	776 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	317/338 (94%)	309 (98%)	8 (2%)	42	15
1	B	317/338 (94%)	311 (98%)	6 (2%)	52	24
All	All	634/676 (94%)	620 (98%)	14 (2%)	48	18

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	22	LEU
1	A	64	LYS
1	A	122	LEU
1	A	202	LYS
1	A	256	ARG
1	A	364	ARG
1	A	394	ILE
1	B	22	LEU
1	B	109[A]	GLN
1	B	109[B]	GLN
1	B	122	LEU
1	B	364	ARG
1	B	394	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	225	HIS

5.3.3 RNA ⓘ

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](#)

8 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	MPD	A	401	-	7,7,7	0.53	0	9,10,10	0.81	0
2	MPD	B	401	-	7,7,7	0.48	0	9,10,10	0.71	0
2	MPD	B	403	-	7,7,7	0.20	0	9,10,10	0.79	0
2	MPD	B	402	-	7,7,7	0.66	0	9,10,10	0.96	0
3	A1H4V	B	405	-	21,25,25	0.90	0	28,39,39	1.41	4 (14%)
3	A1H4V	A	403	-	21,25,25	1.19	2 (9%)	28,39,39	2.17	9 (32%)
2	MPD	B	404	-	7,7,7	0.17	0	9,10,10	0.42	0
2	MPD	A	402	-	7,7,7	0.45	0	9,10,10	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	A	401	-	-	0/5/5/5	-
2	MPD	B	401	-	-	0/5/5/5	-
2	MPD	B	403	-	-	0/5/5/5	-
2	MPD	B	402	-	-	0/5/5/5	-
3	A1H4V	B	405	-	-	1/13/29/29	0/2/2/2
3	A1H4V	A	403	-	-	2/13/29/29	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	B	404	-	-	2/5/5/5	-
2	MPD	A	402	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	A1H4V	O3-C3	-3.59	1.28	1.37
3	A	403	A1H4V	O12-C8	-2.66	1.21	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	A1H4V	C7-C9-S1	-6.16	91.59	103.81
3	A	403	A1H4V	C11-C9-S1	5.79	118.91	109.21
3	B	405	A1H4V	C4-C4A-S1	4.25	123.49	113.29
3	B	405	A1H4V	C3-C4-C4A	3.39	124.09	118.08
3	A	403	A1H4V	C8-C7-N3	-3.23	105.65	110.70
3	A	403	A1H4V	C10-C9-C7	-2.81	103.03	112.33
3	A	403	A1H4V	C4-C4A-S1	2.75	119.90	113.29
3	B	405	A1H4V	C7-C9-S1	-2.63	98.59	103.81
3	B	405	A1H4V	C11-C9-S1	2.58	113.53	109.21
3	A	403	A1H4V	O3P-P-O2P	2.55	117.40	107.64
3	A	403	A1H4V	C3-C4-C4A	2.41	122.36	118.08
3	A	403	A1H4V	O4P-P-O1P	-2.13	100.51	106.47
3	A	403	A1H4V	C11-C9-C7	2.12	119.38	112.33

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	MPD	O2-C2-C3-C4
2	A	402	MPD	CM-C2-C3-C4
2	B	404	MPD	C2-C3-C4-O4
3	A	403	A1H4V	C4-C5-C5A-O4P
2	B	404	MPD	C2-C3-C4-C5
3	B	405	A1H4V	C3-C4-C4A-S1
3	A	403	A1H4V	C6-C5-C5A-O4P

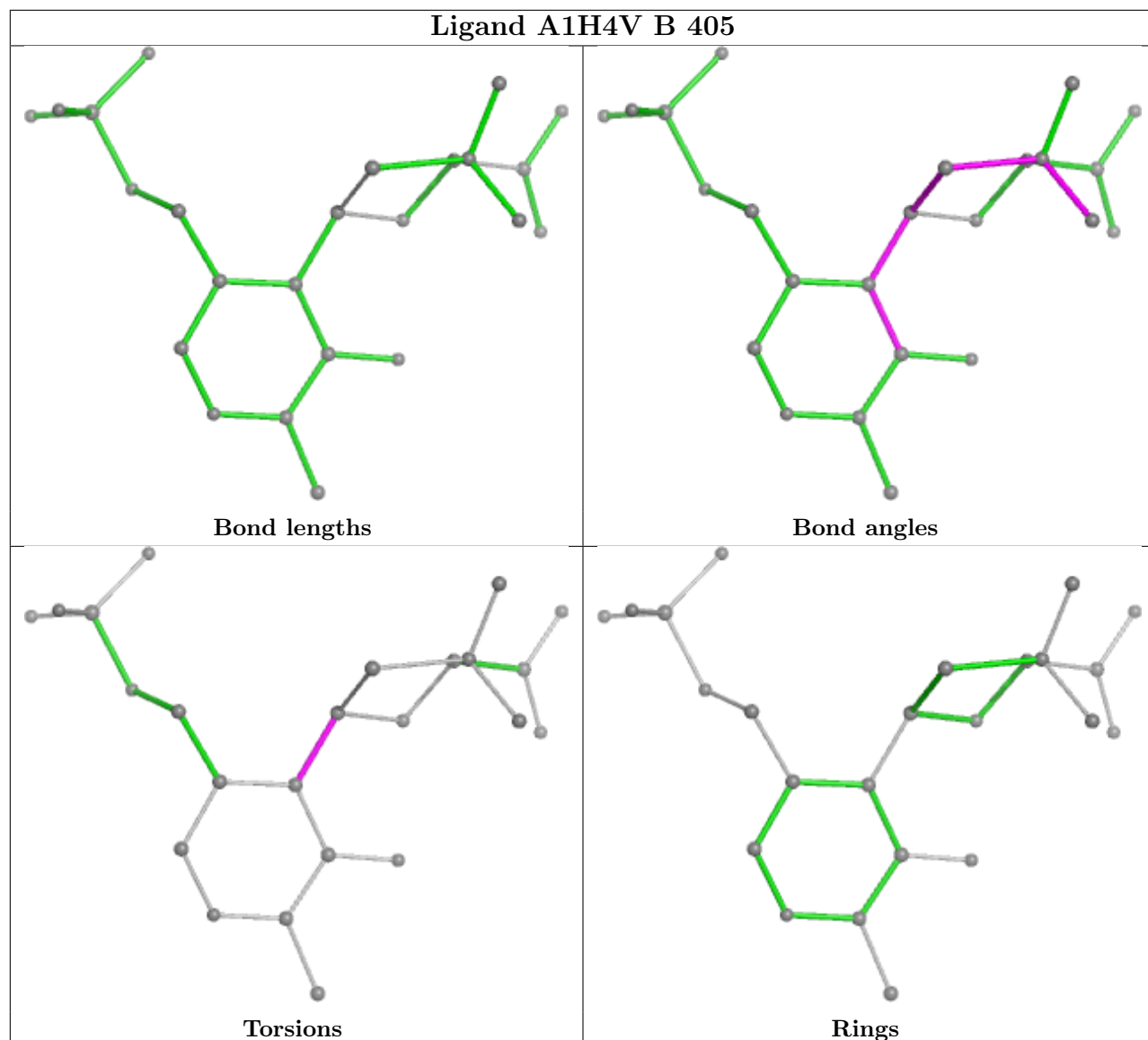
There are no ring outliers.

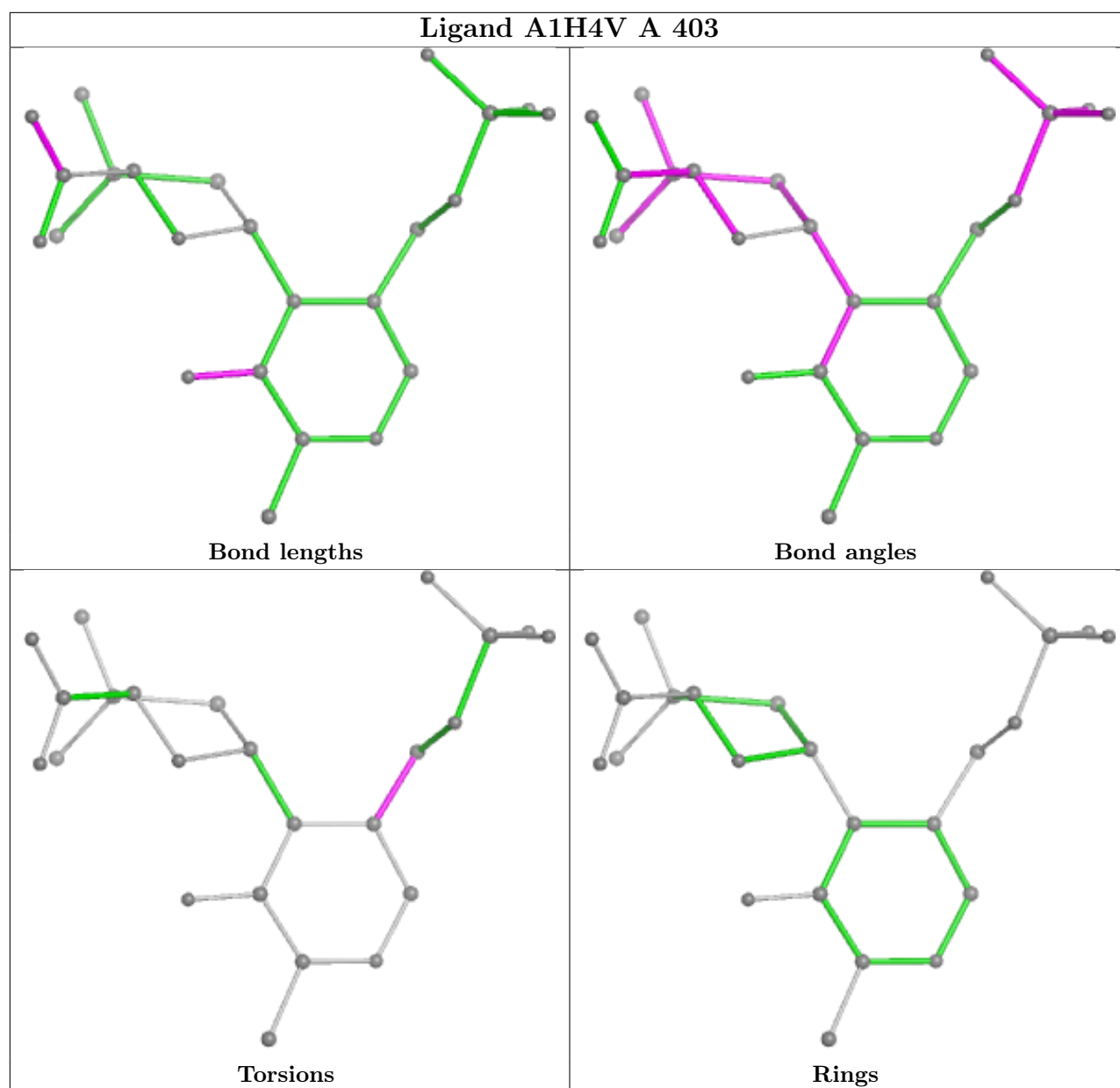
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	MPD	7	0
2	B	403	MPD	1	0
3	B	405	A1H4V	1	0
3	A	403	A1H4V	1	0
2	A	402	MPD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1H4V B 405





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	398/421 (94%)	-0.42	1 (0%) 90 92	7, 24, 44, 77	2 (0%)
1	B	395/421 (93%)	-0.51	2 (0%) 87 89	7, 23, 42, 68	3 (0%)
All	All	793/842 (94%)	-0.47	3 (0%) 89 91	7, 23, 43, 77	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	394	ILE	3.0
1	B	2	GLY	2.5
1	A	394	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MPD	A	402	8/8	0.89	0.13	44,49,61,74	1
2	MPD	B	403	8/8	0.90	0.11	49,56,63,79	1

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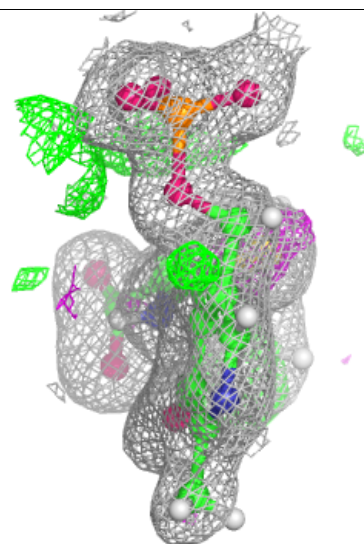
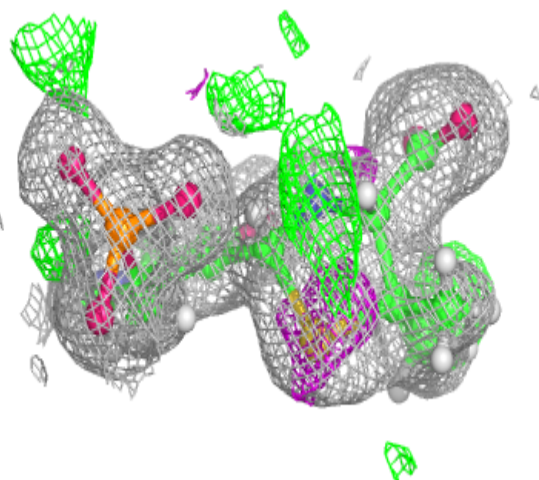
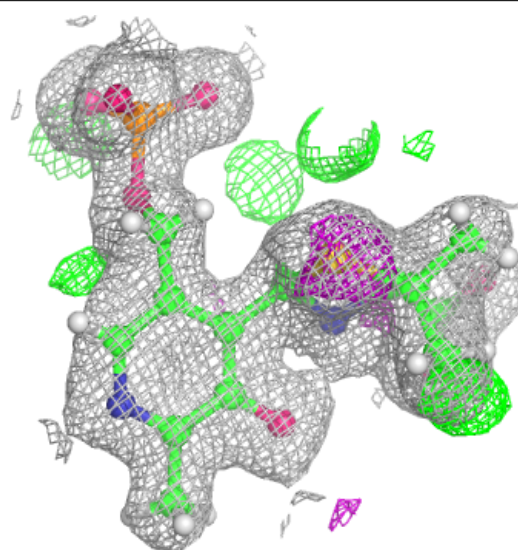
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MPD	B	402	8/8	0.93	0.09	29,33,51,54	1
2	MPD	B	404	8/8	0.93	0.09	45,52,58,70	1
2	MPD	A	401	8/8	0.94	0.08	22,32,41,44	1
2	MPD	B	401	8/8	0.95	0.06	23,24,25,34	1
3	A1H4V	A	403	24/24	0.97	0.06	16,24,36,37	0
3	A1H4V	B	405	24/24	0.97	0.06	16,21,29,30	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.

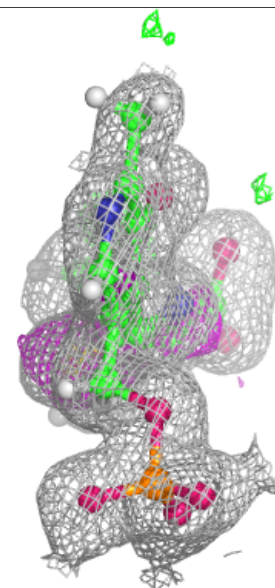
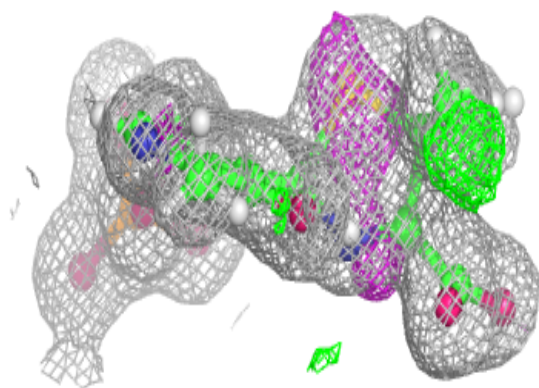
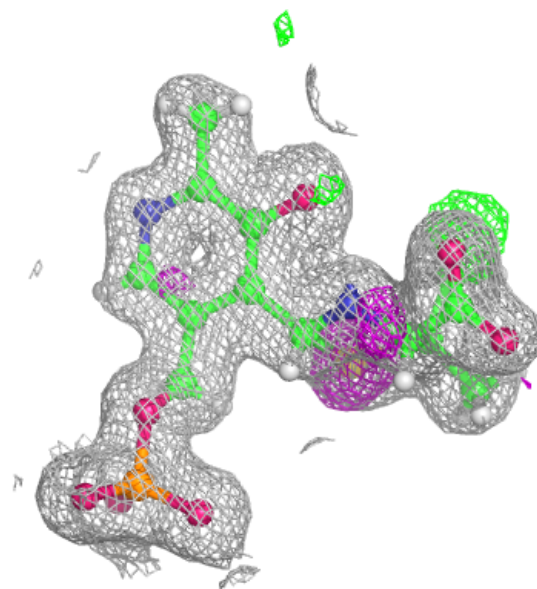
Electron density around A1H4V A 403:

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 A1H4V B 405:

$2mF_o-DF_c$ (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.