



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 3ST8 / pdb_00003st8
Title : Crystal structure of GlmU from Mycobacterium tuberculosis in complex with COENZYME A, GLUCOSAMINE 1-PHOSPHATE and URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE
Authors : Jagtap, P.A.; Prakash, B.
Deposited on : 2011-07-09
Resolution : 1.98 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

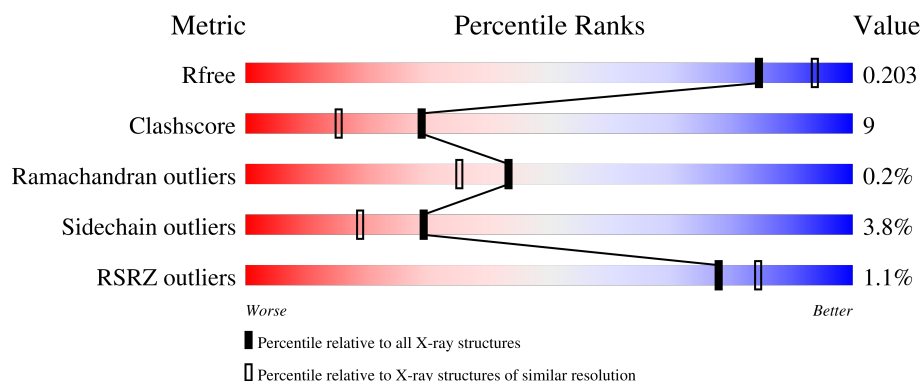
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	501	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4115 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 Bifunctional protein glmU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3479	2150	636	686	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P96382
A	-4	HIS	-	expression tag	UNP P96382
A	-3	HIS	-	expression tag	UNP P96382
A	-2	HIS	-	expression tag	UNP P96382
A	-1	HIS	-	expression tag	UNP P96382
A	0	HIS	-	expression tag	UNP P96382

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

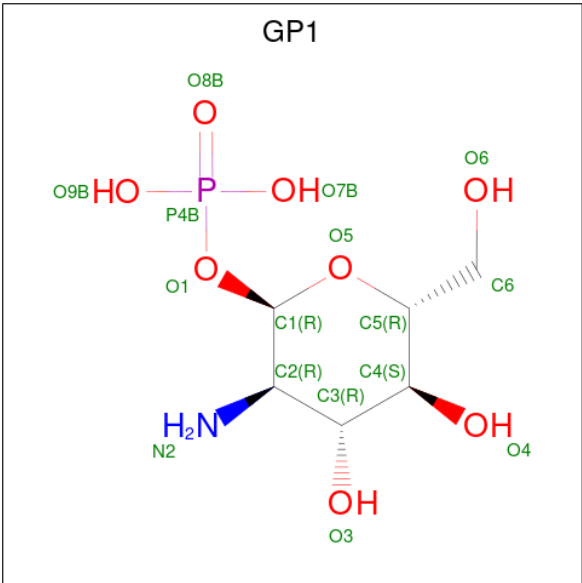
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mg	0	0
			4	4		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



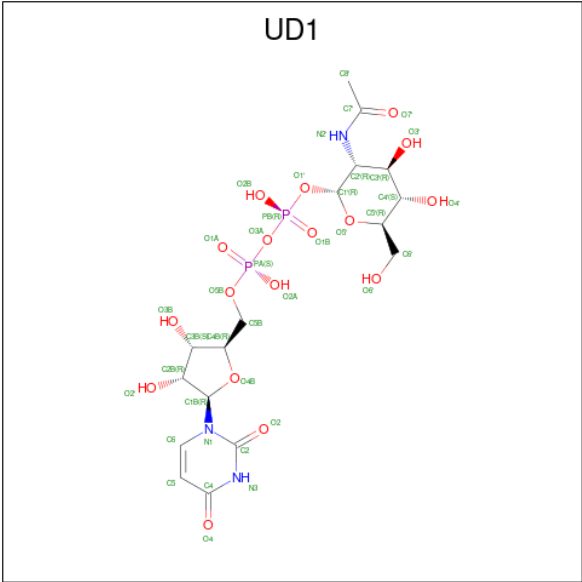
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	16	3		

- Molecule 4 is 2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose (CCD ID: GP1) (formula: C₆H₁₄NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (CCD ID: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

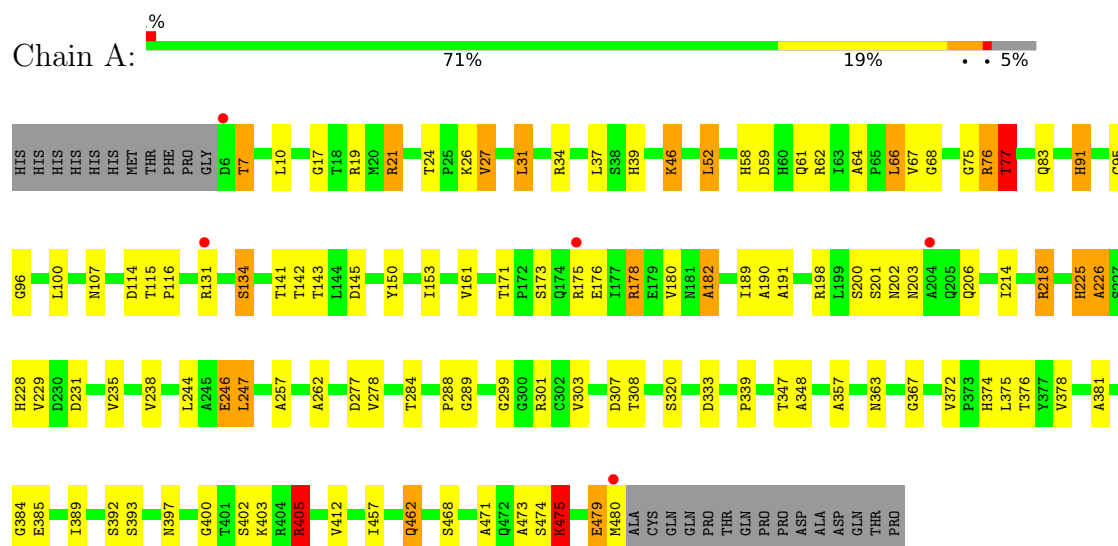
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	529	Total	O	0	0
			529	529		

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: Bifunctional protein glmU



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	110.31Å 110.31Å 360.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.71 – 1.98 19.71 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.71-1.98) 99.7 (19.71-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.202 0.169 , 0.203	Depositor DCC
R_{free} test set	1017 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4115	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.62% 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: GP1, COA, UD1, MG

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	1.87	52/3533 (1.5%)	1.51	28/4826 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	ALA	CA-CB	8.80	1.67	1.53
1	A	153	ILE	CA-C	7.82	1.62	1.52
1	A	468	SER	CA-CB	7.33	1.63	1.53
1	A	226	ALA	CA-CB	-7.26	1.42	1.53
1	A	173	SER	CA-C	7.17	1.61	1.52
1	A	284	THR	CB-OG1	-7.09	1.32	1.43
1	A	142	THR	CA-CB	6.96	1.64	1.53
1	A	238	VAL	CA-CB	-6.60	1.45	1.53
1	A	178	ARG	CA-C	6.59	1.61	1.52
1	A	225	HIS	CA-C	6.39	1.60	1.52
1	A	347	THR	CA-CB	6.36	1.62	1.53
1	A	246	GLU	CG-CD	6.36	1.68	1.52
1	A	257	ALA	CA-CB	6.34	1.63	1.53
1	A	64	ALA	CA-CB	6.30	1.62	1.53
1	A	17	GLY	N-CA	6.22	1.54	1.45
1	A	27	VAL	CB-CG1	-6.12	1.32	1.52
1	A	24	THR	CA-C	-6.10	1.44	1.52
1	A	299	GLY	C-O	6.06	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	ALA	CA-CB	6.03	1.62	1.53
1	A	402	SER	N-CA	5.96	1.53	1.45
1	A	182	ALA	CA-CB	-5.95	1.42	1.53
1	A	288	PRO	CA-CB	5.95	1.61	1.53
1	A	363	ASN	CA-C	5.92	1.60	1.53
1	A	412	VAL	CA-C	5.84	1.59	1.53
1	A	24	THR	CA-CB	5.77	1.61	1.53
1	A	68	GLY	N-CA	5.75	1.53	1.45
1	A	378	VAL	CA-CB	-5.75	1.46	1.53
1	A	218	ARG	CA-C	5.67	1.60	1.52
1	A	95	CYS	N-CA	5.61	1.53	1.46
1	A	381	ALA	CA-C	-5.54	1.46	1.52
1	A	278	VAL	CA-CB	5.51	1.59	1.54
1	A	473	ALA	CA-CB	5.51	1.61	1.53
1	A	475	LYS	N-CA	5.50	1.52	1.46
1	A	203	ASN	CA-C	-5.47	1.46	1.52
1	A	141	THR	C-O	-5.47	1.16	1.23
1	A	389	ILE	CA-CB	5.45	1.60	1.54
1	A	384	GLY	N-CA	5.45	1.51	1.45
1	A	115	THR	CA-CB	5.41	1.58	1.53
1	A	231	ASP	N-CA	5.40	1.53	1.46
1	A	191	ALA	CA-CB	5.38	1.61	1.53
1	A	262	ALA	CA-CB	5.33	1.62	1.53
1	A	284	THR	N-CA	5.26	1.52	1.46
1	A	301	ARG	NE-CZ	5.25	1.38	1.33
1	A	214	ILE	CA-C	5.21	1.59	1.52
1	A	67	VAL	CA-C	5.15	1.59	1.52
1	A	66	LEU	CB-CG	5.14	1.63	1.53
1	A	229	VAL	N-CA	5.13	1.52	1.46
1	A	385	GLU	CA-CB	5.12	1.61	1.53
1	A	457	ILE	CB-CG2	5.10	1.69	1.52
1	A	384	GLY	C-O	5.09	1.28	1.23
1	A	91	HIS	N-CA	5.02	1.52	1.46
1	A	190	ALA	CA-CB	5.02	1.61	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASN	N-CA-C	-7.11	97.34	108.14
1	A	201	SER	CA-C-N	-7.07	113.02	122.42
1	A	201	SER	C-N-CA	-7.07	113.02	122.42
1	A	76	ARG	NE-CZ-NH1	-6.93	114.57	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	GLY	N-CA-C	-6.60	106.05	114.37
1	A	145	ASP	N-CA-C	-6.54	104.23	111.82
1	A	59	ASP	CB-CA-C	-6.53	99.52	110.81
1	A	202	ASN	N-CA-CB	6.11	119.93	110.21
1	A	189	ILE	N-CA-C	6.03	116.77	110.62
1	A	100	LEU	CA-C-N	-5.97	113.82	119.85
1	A	100	LEU	C-N-CA	-5.97	113.82	119.85
1	A	474	SER	N-CA-CB	5.75	119.16	110.30
1	A	61	GLN	CA-CB-CG	-5.72	102.66	114.10
1	A	145	ASP	CA-C-N	-5.71	114.50	122.66
1	A	145	ASP	C-N-CA	-5.71	114.50	122.66
1	A	77	THR	CA-C-O	-5.61	114.47	120.92
1	A	66	LEU	CA-CB-CG	-5.60	96.69	116.30
1	A	367	GLY	N-CA-C	5.50	120.92	112.51
1	A	76	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	405	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	A	244	LEU	CB-CA-C	-5.36	102.43	110.90
1	A	21	ARG	CG-CD-NE	-5.30	100.34	112.00
1	A	405	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	A	320	SER	N-CA-CB	-5.20	101.94	110.68
1	A	277	ASP	CB-CA-C	-5.16	101.47	110.09
1	A	333	ASP	CB-CA-C	-5.04	101.35	109.72
1	A	77	THR	CA-CB-OG1	-5.01	102.08	109.60
1	A	462	GLN	CB-CA-C	-5.01	101.05	110.67

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	VAL	Mainchain

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	3479	0	3483	60	0
2	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	32	1	0
4	A	16	0	0	0	0
5	A	39	0	25	1	0
6	A	529	0	0	26	2
All	All	4115	0	3540	62	2

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 9.

All (62) 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:A:246:GLU:HG3	6:A:896:HOH:O	1.31	1.25
1:A:376:THR:HB	6:A:589:HOH:O	1.00	1.15
1:A:198:ARG:CZ	6:A:1023:HOH:O	1.97	1.09
1:A:76:ARG:NE	6:A:792:HOH:O	1.84	1.03
1:A:198:ARG:NH2	6:A:1023:HOH:O	1.88	1.03
1:A:76:ARG:NH1	1:A:77:THR:O	1.93	1.01
1:A:198:ARG:NE	6:A:1023:HOH:O	1.90	1.00
1:A:83:GLN:HE21	1:A:91:HIS:HD2	1.16	0.92
1:A:66:LEU:HB3	6:A:643:HOH:O	1.69	0.91
1:A:76:ARG:CZ	6:A:792:HOH:O	2.15	0.91
1:A:374:HIS:O	1:A:376:THR:HG23	1.69	0.90
1:A:27:VAL:CG1	1:A:37:LEU:HB2	2.03	0.89
1:A:376:THR:HG22	1:A:393:SER:H	1.37	0.87
1:A:475:LYS:HG2	6:A:850:HOH:O	1.74	0.86
1:A:76:ARG:NH2	6:A:792:HOH:O	2.09	0.86
1:A:62:ARG:HD2	6:A:883:HOH:O	1.77	0.84
1:A:19:ARG:CZ	6:A:797:HOH:O	2.27	0.81
3:A:498:COA:O2A	3:A:498:COA:O5A	2.00	0.79
1:A:83:GLN:HE21	1:A:91:HIS:CD2	2.01	0.78
1:A:376:THR:CB	6:A:589:HOH:O	1.75	0.76
1:A:228:HIS:HE1	6:A:681:HOH:O	1.69	0.76
1:A:62:ARG:CD	6:A:883:HOH:O	2.34	0.74
1:A:107:ASN:OD1	6:A:841:HOH:O	2.06	0.72
1:A:39:HIS:HD2	6:A:551:HOH:O	1.72	0.71
1:A:161:VAL:HG21	1:A:226:ALA:HB2	1.72	0.69
1:A:161:VAL:HG21	1:A:226:ALA:CB	2.25	0.67
1:A:27:VAL:HG12	1:A:37:LEU:HB2	1.76	0.66
1:A:175:ARG:HD2	6:A:1016:HOH:O	1.96	0.65
1:A:143:THR:HG22	1:A:228:HIS:CE1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:O	1:A:39:HIS:HE1	1.85	0.60
1:A:375:LEU:O	1:A:392:SER:HA	2.06	0.55
1:A:116:PRO:HG2	1:A:247:LEU:HD23	1.89	0.55
1:A:107:ASN:HD21	1:A:131:ARG:HE	1.56	0.54
1:A:46:LYS:NZ	6:A:904:HOH:O	2.42	0.53
1:A:134:SER:HB3	6:A:902:HOH:O	2.09	0.52
1:A:27:VAL:HG13	1:A:37:LEU:HB2	1.87	0.51
1:A:150:TYR:HB3	1:A:180:VAL:HB	1.92	0.51
1:A:225:HIS:HE1	6:A:521:HOH:O	1.94	0.50
1:A:228:HIS:CE1	6:A:681:HOH:O	2.53	0.49
1:A:479:GLU:O	1:A:480:MET:O	2.31	0.49
1:A:107:ASN:ND2	1:A:131:ARG:HH21	2.10	0.48
5:A:502:UD1:H6	5:A:502:UD1:O5B	2.13	0.47
1:A:34:ARG:HB2	1:A:39:HIS:CE1	2.50	0.47
1:A:52:LEU:HB3	1:A:76:ARG:NH1	2.30	0.47
1:A:218:ARG:HD2	6:A:909:HOH:O	2.14	0.46
1:A:7:THR:HB	1:A:107:ASN:HB2	1.97	0.46
1:A:182:ALA:HB1	1:A:235:VAL:HB	1.97	0.46
1:A:289:GLY:O	1:A:307:ASP:HA	2.16	0.45
1:A:339:PRO:O	1:A:357:ALA:HA	2.16	0.45
1:A:171:THR:O	1:A:175:ARG:HG3	2.17	0.44
1:A:75:GLY:HA2	6:A:616:HOH:O	2.17	0.43
1:A:26:LYS:HE3	1:A:114:ASP:HB3	2.00	0.43
1:A:376:THR:HG22	1:A:393:SER:N	2.19	0.43
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.83	0.42
1:A:10:LEU:HD13	1:A:96:GLY:HA3	2.01	0.42
1:A:462:GLN:HE22	1:A:475:LYS:HE3	1.84	0.42
1:A:161:VAL:HG21	1:A:226:ALA:HB3	2.01	0.42
1:A:21:ARG:NE	6:A:889:HOH:O	2.53	0.41
1:A:178:ARG:NH2	6:A:834:HOH:O	2.54	0.41
1:A:372:VAL:HG12	1:A:376:THR:OG1	2.20	0.41
1:A:405:ARG:HH11	1:A:405:ARG:HD3	1.75	0.40
1:A:397:ASN:O	1:A:403:LYS:HA	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:777:HOH:O	6:A:833:HOH:O[3_555]	2.15	0.05
6:A:658:HOH:O	6:A:942:HOH:O[4_555]	2.19	0.01

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	473/501 (94%)	463 (98%)	9 (2%)	1 (0%)	43	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	479	GLU

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	371/394 (94%)	357 (96%)	14 (4%)	29	19

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

Mol	Chain	Res	Type
1	A	7	THR
1	A	31	LEU
1	A	46	LYS
1	A	52	LEU
1	A	58	HIS
1	A	77	THR
1	A	134	SER
1	A	176	GLU
1	A	200	SER
1	A	206	GLN

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Mol	Chain	Res	Type
1	A	247	LEU
1	A	308	THR
1	A	405	ARG
1	A	475	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	50	GLN
1	A	91	HIS
1	A	107	ASN
1	A	228	HIS
1	A	388	ASN
1	A	462	GLN

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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
3	COA	A	498	-	47,50,50	1.68	9 (19%)	69,75,75	2.34	25 (36%)
5	UD1	A	502	2	40,41,41	0.98	2 (5%)	59,62,62	1.36	6 (10%)
4	GP1	A	499	-	15,16,16	2.17	7 (46%)	24,24,24	1.59	5 (20%)

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
3	COA	A	498	-	-	5/48/64/64	0/3/3/3
5	UD1	A	502	2	-	4/26/63/63	0/3/3/3
4	GP1	A	499	-	-	0/6/27/27	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	498	COA	P3B-O3B	5.27	1.68	1.59
4	A	499	GP1	P4B-O1	4.17	1.66	1.59
3	A	498	COA	C8A-N7A	3.91	1.39	1.31
3	A	498	COA	P1A-O3A	3.53	1.63	1.59
3	A	498	COA	OAP-CAP	3.51	1.48	1.42
4	A	499	GP1	C3-C2	2.98	1.57	1.53
3	A	498	COA	O4B-C4B	2.86	1.51	1.45
4	A	499	GP1	C4-C5	2.83	1.59	1.53
4	A	499	GP1	P4B-O8B	2.82	1.59	1.50
5	A	502	UD1	C4-N3	-2.54	1.34	1.38
3	A	498	COA	O4B-C1B	2.46	1.47	1.42
3	A	498	COA	CCP-CBP	2.30	1.56	1.52
3	A	498	COA	O5P-C5P	2.27	1.27	1.23
4	A	499	GP1	O5-C1	2.25	1.47	1.41
4	A	499	GP1	O5-C5	2.20	1.49	1.44
4	A	499	GP1	C2-N2	2.15	1.50	1.47
5	A	502	UD1	C2-N3	-2.11	1.34	1.38
3	A	498	COA	O6A-CCP	-2.05	1.37	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	498	COA	O2A-P1A-O3A	5.99	123.46	107.27
3	A	498	COA	O4B-C1B-N9A	-4.99	98.50	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	UD1	C4-N3-C2	-4.81	120.64	126.61
3	A	498	COA	C5A-C4A-N3A	-4.77	120.15	126.72
3	A	498	COA	CDP-CBP-CCP	4.70	115.97	108.22
3	A	498	COA	O8A-P3B-O7A	4.39	127.94	110.83
3	A	498	COA	C7P-C6P-C5P	-4.38	105.10	112.39
3	A	498	COA	N9A-C8A-N7A	-4.24	107.92	113.94
5	A	502	UD1	N3-C2-N1	4.14	120.28	114.89
4	A	499	GP1	C3-C4-C5	3.90	117.30	110.23
5	A	502	UD1	C5-C4-N3	3.87	120.22	114.80
3	A	498	COA	O5B-P1A-O1A	3.83	124.12	108.94
3	A	498	COA	O5B-C5B-C4B	-3.68	96.45	108.99
3	A	498	COA	N3A-C2A-N1A	-3.48	123.32	128.58
3	A	498	COA	O3B-P3B-O7A	-3.33	97.48	109.33
3	A	498	COA	O2B-C2B-C1B	-3.28	98.81	110.10
4	A	499	GP1	C1-C2-N2	-3.22	104.40	110.20
3	A	498	COA	O2A-P1A-O5B	-3.20	93.05	107.57
3	A	498	COA	O6A-CCP-CBP	-3.20	105.41	110.55
3	A	498	COA	C4A-N9A-C8A	3.08	108.97	105.74
4	A	499	GP1	C3-C2-N2	3.03	117.26	111.05
5	A	502	UD1	O4-C4-C5	-3.02	119.96	125.16
3	A	498	COA	C4A-C5A-N7A	-2.74	107.45	110.58
3	A	498	COA	O4B-C4B-C5B	2.72	118.06	109.33
4	A	499	GP1	O5-C5-C6	2.72	113.19	106.44
3	A	498	COA	C2A-N3A-C4A	2.64	118.28	111.83
3	A	498	COA	N3A-C4A-N9A	2.58	131.55	127.17
3	A	498	COA	O3B-C3B-C4B	-2.54	101.09	110.03
5	A	502	UD1	C3B-C2B-C1B	2.51	106.21	101.46
3	A	498	COA	C3P-N4P-C5P	2.44	127.36	122.82
3	A	498	COA	C5A-N7A-C8A	2.42	107.25	103.45
5	A	502	UD1	O2-C2-N1	-2.27	119.84	122.80
3	A	498	COA	O4B-C1B-C2B	-2.23	101.83	106.62
3	A	498	COA	C5A-C4A-N9A	2.23	108.25	105.81
3	A	498	COA	O3A-P1A-O1A	-2.19	104.12	110.70
4	A	499	GP1	P4B-O1-C1	-2.16	117.74	123.54

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	UD1	C1'-O1'-PB-O3A
3	A	498	COA	P2A-O3A-P1A-O2A
3	A	498	COA	C5B-O5B-P1A-O1A

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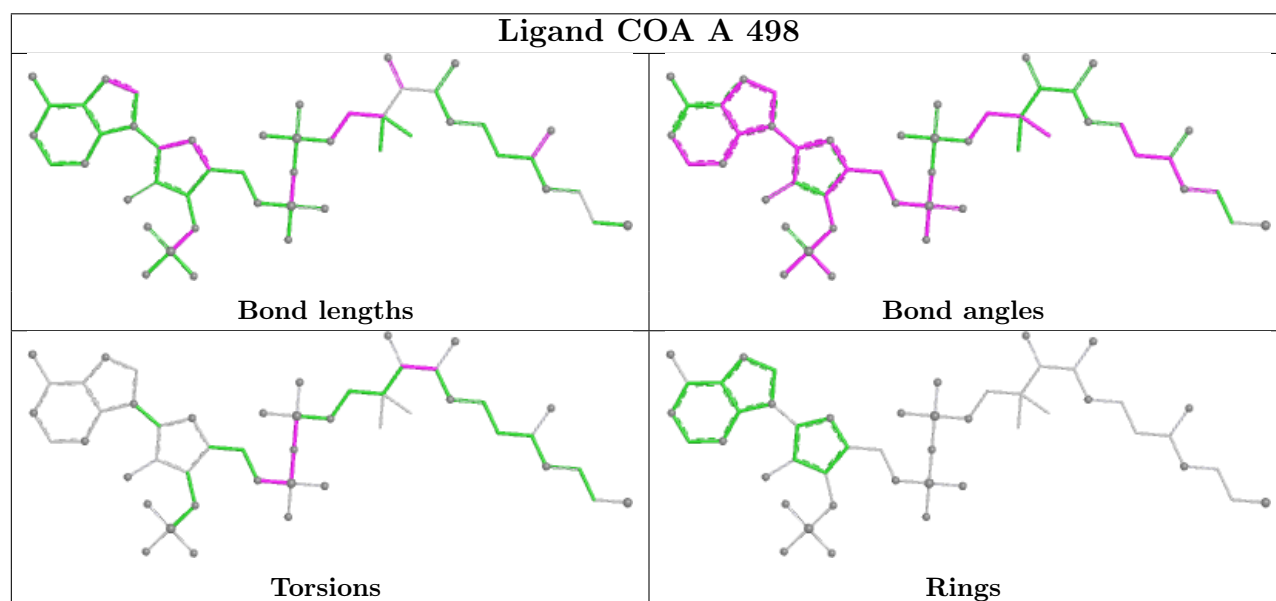
Mol	Chain	Res	Type	Atoms
5	A	502	UD1	O4B-C4B-C5B-O5B
3	A	498	COA	P1A-O3A-P2A-O4A
3	A	498	COA	P1A-O3A-P2A-O5A
5	A	502	UD1	C3B-C4B-C5B-O5B
5	A	502	UD1	C1'-O1'-PB-O1B
3	A	498	COA	N8P-C9P-CAP-OAP

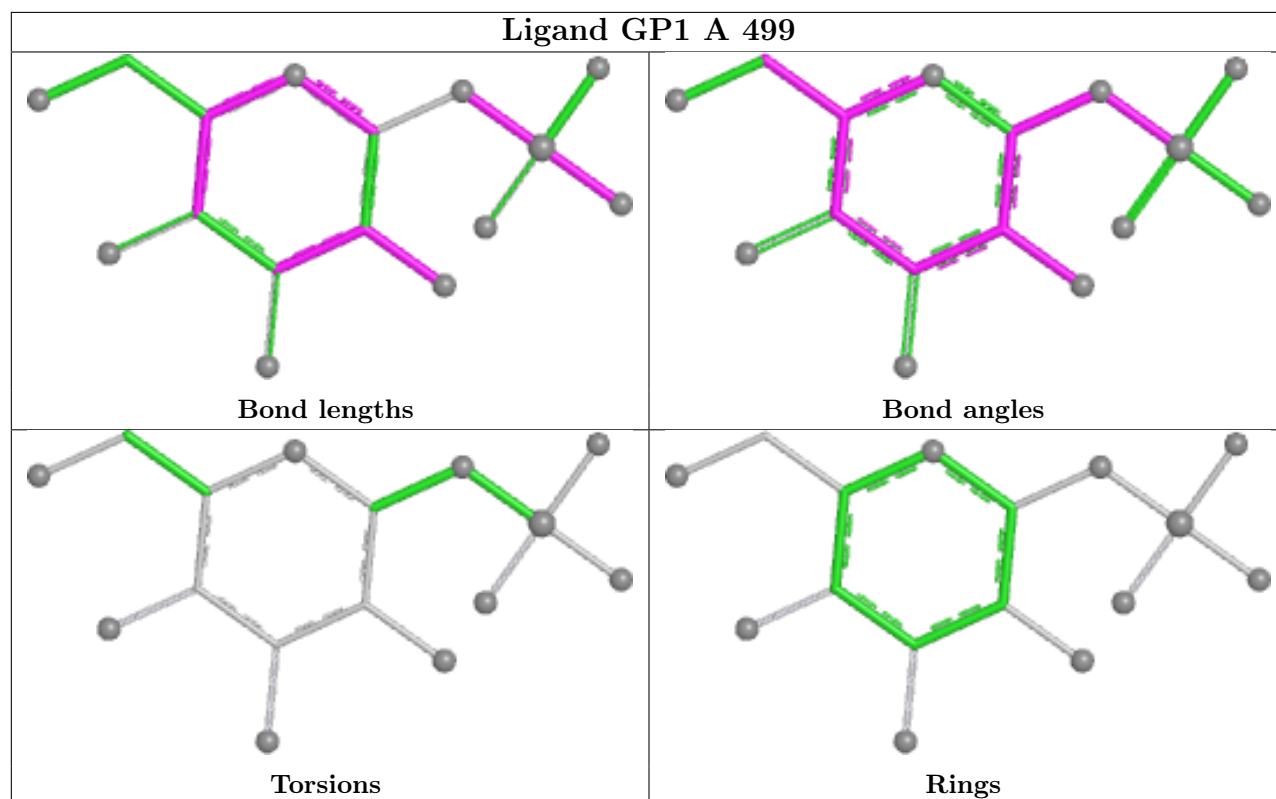
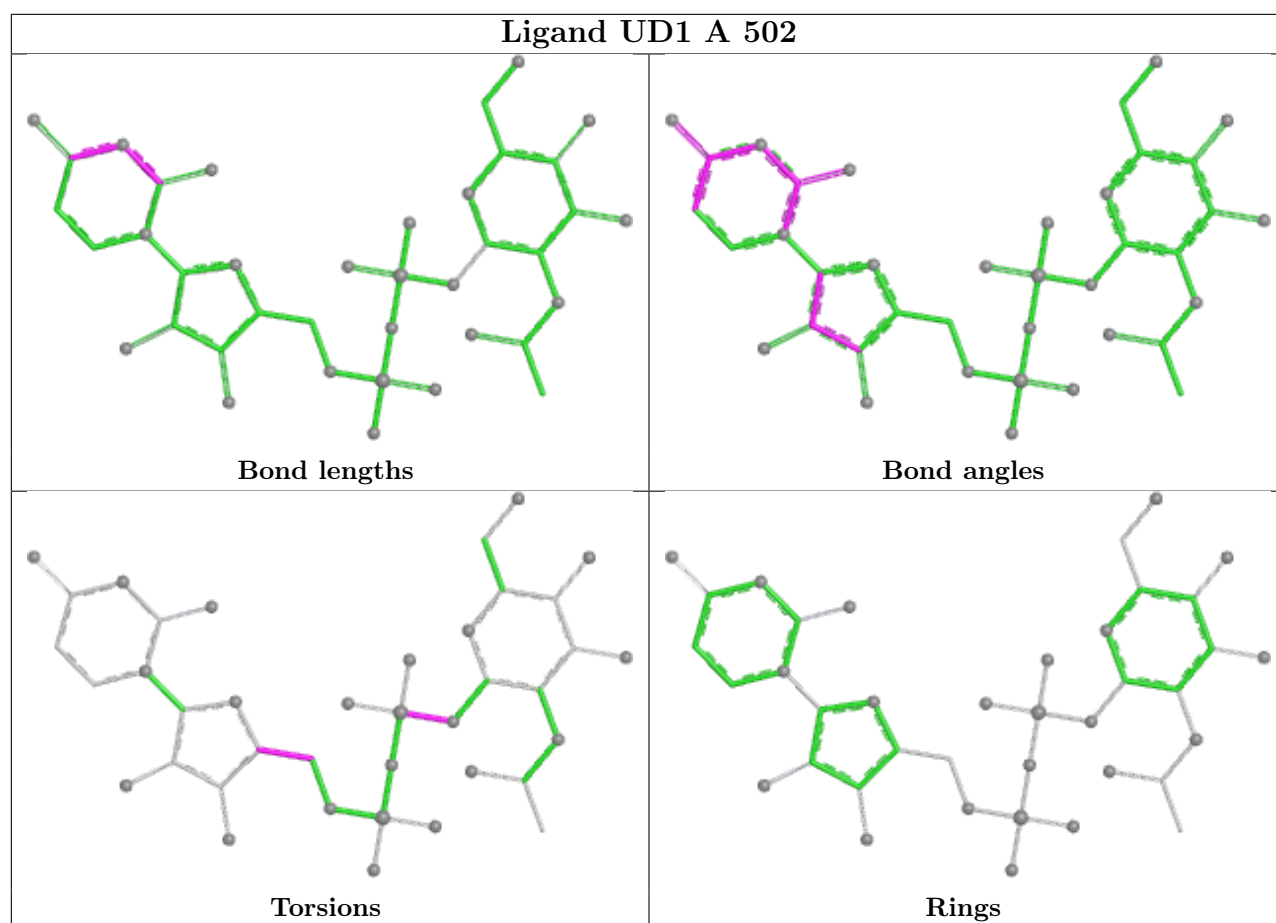
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	498	COA	1	0
5	A	502	UD1	1	0

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





5.7 Other polymers [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	475/501 (94%)	-0.47	5 (1%) 78 84	11, 21, 40, 85	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	480	MET	4.6
1	A	204	ALA	2.5
1	A	6	ASP	2.1
1	A	131	ARG	2.0
1	A	175	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	UD1	A	502	39/39	0.88	0.11	16,22,27,28	0
3	COA	A	498	48/48	0.96	0.06	15,22,46,53	0

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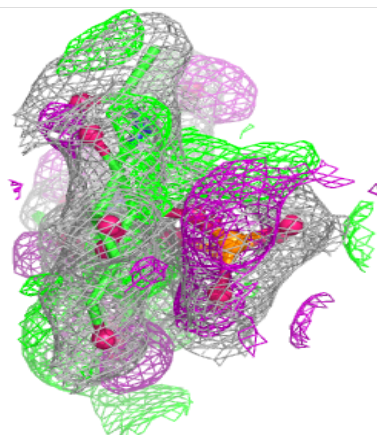
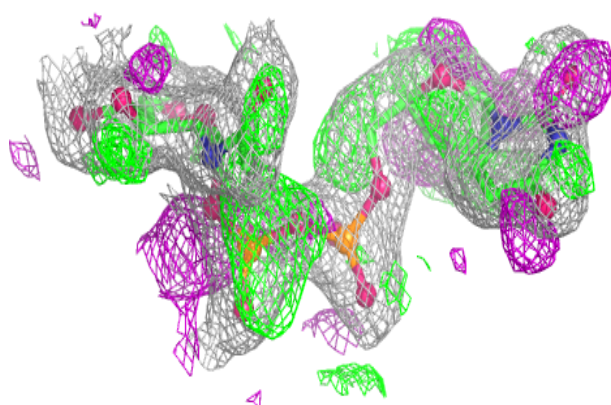
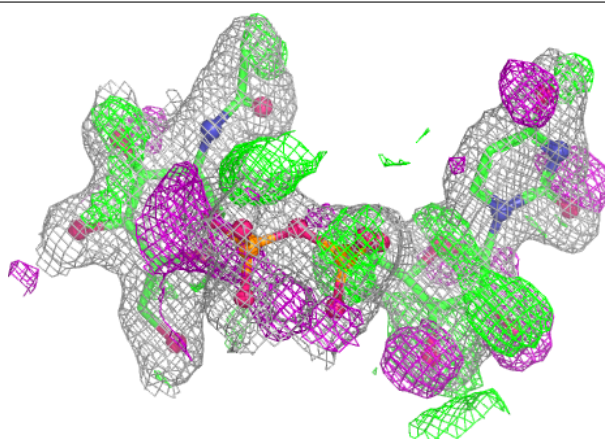
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	501	1/1	0.97	0.04	19,19,19,19	1
4	GP1	A	499	16/16	0.98	0.05	19,22,24,25	0
2	MG	A	496	1/1	0.98	0.09	25,25,25,25	0
2	MG	A	500	1/1	0.99	0.05	21,21,21,21	1
2	MG	A	497	1/1	1.00	0.06	16,16,16,16	1

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.

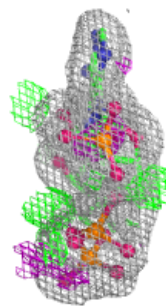
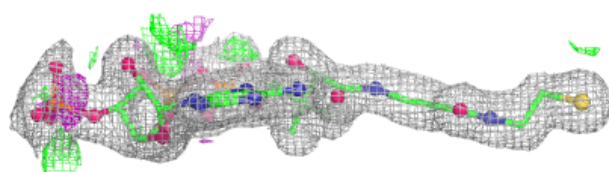
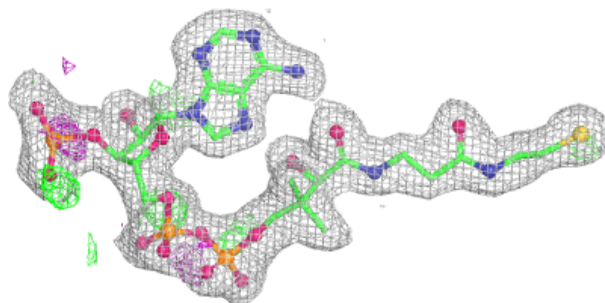
Electron density around UD1 A 502:

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



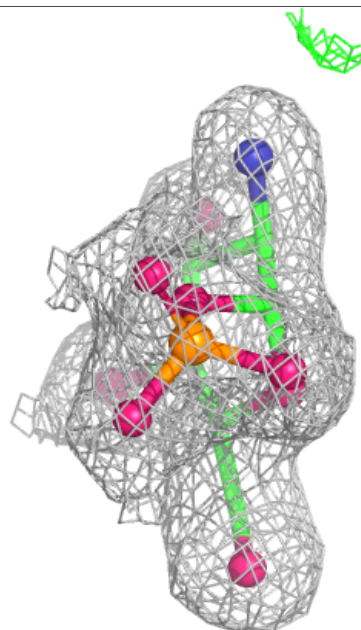
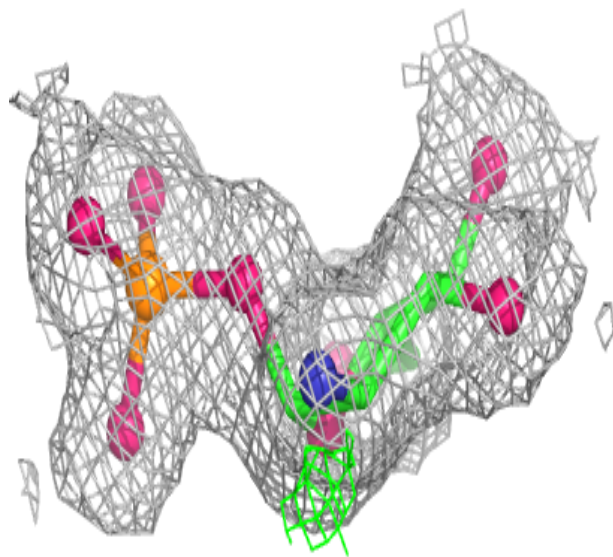
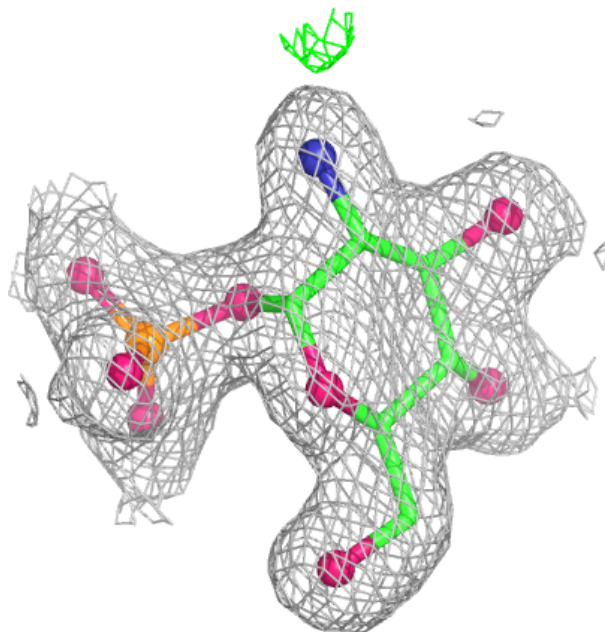
Electron density around COA A 498:

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



Electron density around GP1 A 499:

$2mF_o-DF_c$ (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.