



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:55 PM UTC

PDB ID : 6YK0 / pdb_00006yk0
Title : Crystal structure of mouse pyridoxal kinase in complex with ATP-gamma-S
Authors : Kasaragod, V.B.; Schindelin, H.
Deposited on : 2020-04-05
Resolution : 2.90 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

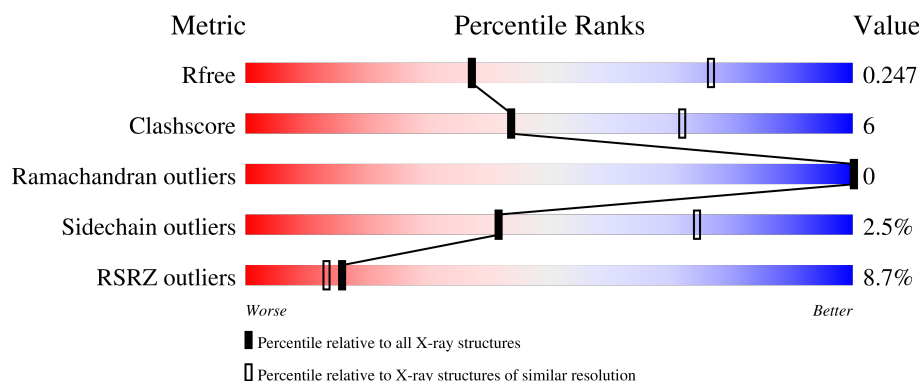
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

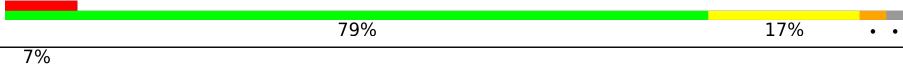
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	314	
1	B	314	
1	C	314	
1	D	314	

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
4	EDO	B	408	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19576 atoms, of which 9723 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.

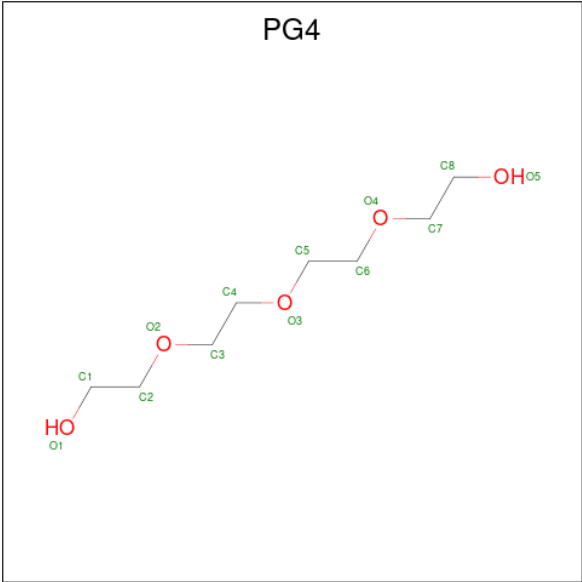
- Molecule 1 is a protein called Pyridoxal kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	H	N	O	S	0	0	0
			4759	1505	2366	414	456	18			
1	B	309	Total	C	H	N	O	S	1	0	0
			4775	1507	2378	419	453	18			
1	C	309	Total	C	H	N	O	S	1	0	0
			4787	1509	2384	422	454	18			
1	D	309	Total	C	H	N	O	S	2	0	0
			4793	1511	2388	420	456	18			

There are 8 discrepancies between the modelled and reference sequences:

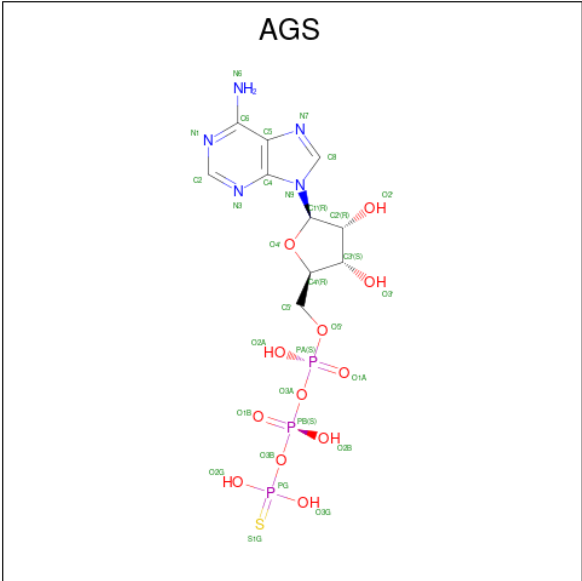
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8K183
A	0	PRO	-	expression tag	UNP Q8K183
B	-1	GLY	-	expression tag	UNP Q8K183
B	0	PRO	-	expression tag	UNP Q8K183
C	-1	GLY	-	expression tag	UNP Q8K183
C	0	PRO	-	expression tag	UNP Q8K183
D	-1	GLY	-	expression tag	UNP Q8K183
D	0	PRO	-	expression tag	UNP Q8K183

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			31	8	18	5		
2	A	1	Total	C	H	O	0	1
			19	5	11	3		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



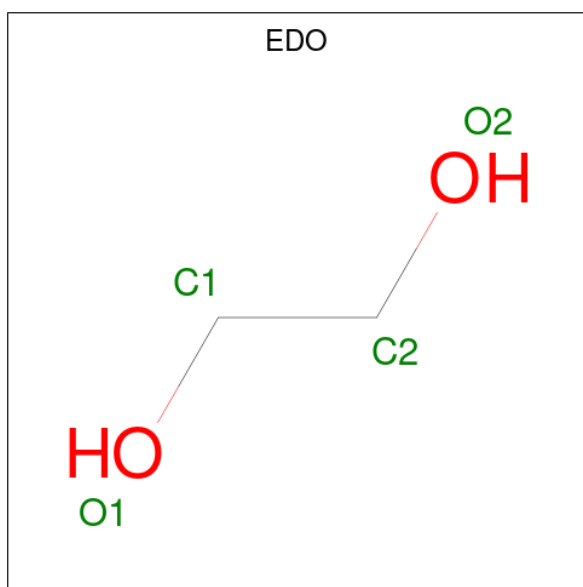
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



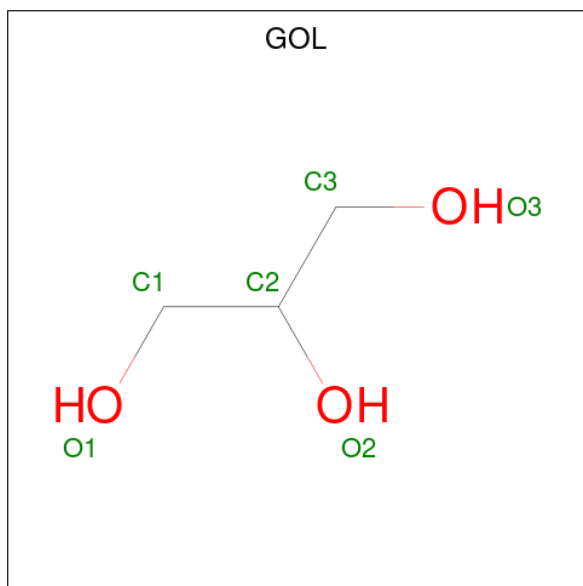
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

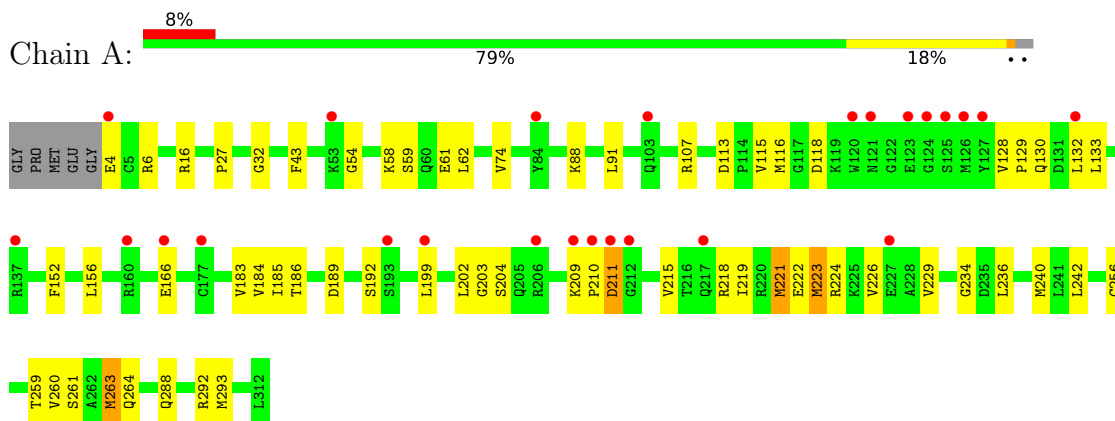
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	B	7	Total	O	0	0
			7	7		
6	C	6	Total	O	0	0
			6	6		
6	D	5	Total	O	0	0
			5	5		

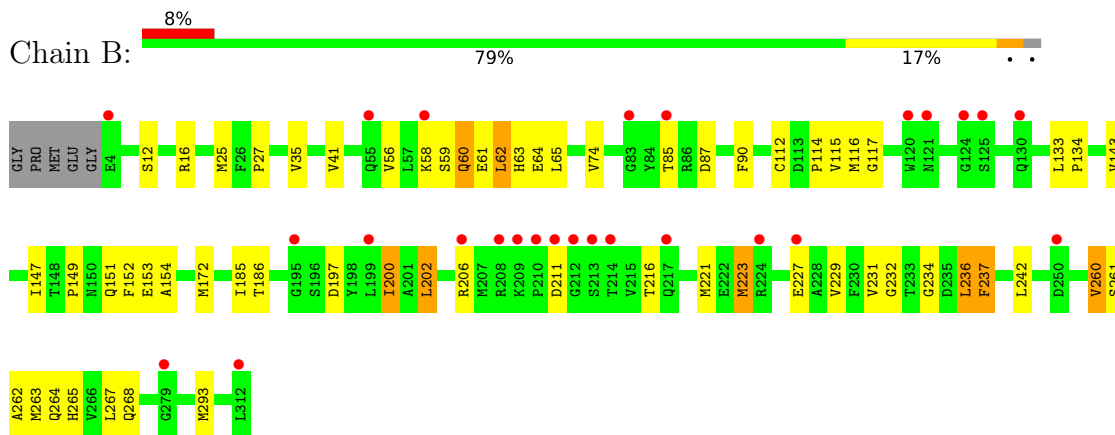
3 Residue-property plots [i](#)

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.

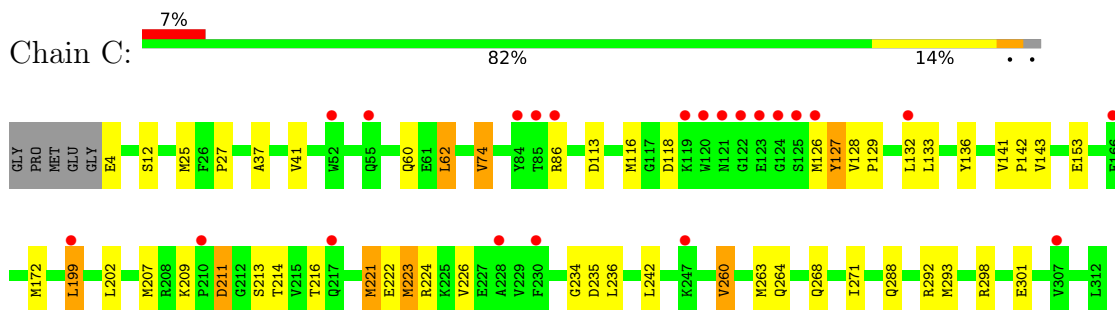
• Molecule 1: Pyridoxal kinase



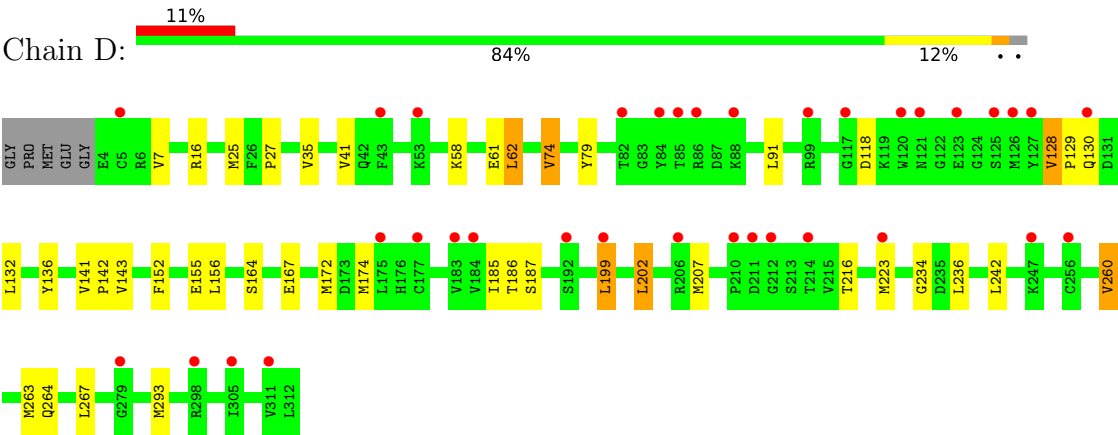
• Molecule 1: Pyridoxal kinase



• Molecule 1: Pyridoxal kinase



● Molecule 1: Pyridoxal kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	278.60Å 53.02Å 109.85Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	47.16 – 2.90 47.16 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.16-2.90) 99.5 (47.16-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.234 , 0.255 0.235 , 0.247	Depositor DCC
R_{free} test set	1760 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19576	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AGS, EDO, GOL, PG4

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	1.15	24/2436 (1.0%)	0.68	5/3299 (0.2%)
1	B	1.35	37/2440 (1.5%)	0.73	6/3303 (0.2%)
1	C	0.99	14/2446 (0.6%)	0.60	1/3311 (0.0%)
1	D	1.02	9/2448 (0.4%)	0.69	4/3313 (0.1%)
All	All	1.14	84/9770 (0.9%)	0.68	16/13226 (0.1%)

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	264	GLN	C-O	-8.77	1.14	1.24
1	A	264	GLN	C-O	-7.56	1.15	1.24
1	B	61	GLU	C-O	-7.49	1.15	1.24
1	A	184	VAL	C-O	-7.49	1.16	1.24
1	B	261	SER	C-O	-7.23	1.15	1.24
1	A	183	VAL	C-O	-6.93	1.17	1.24
1	B	236	LEU	C-O	-6.86	1.16	1.24
1	A	204	SER	C-O	-6.85	1.16	1.23
1	B	112	CYS	C-O	-6.69	1.16	1.24
1	B	264	GLN	C-O	-6.55	1.16	1.24
1	A	202	LEU	C-O	-6.53	1.15	1.23
1	B	147	ILE	C-O	-6.46	1.17	1.24
1	B	149	PRO	C-O	-6.41	1.15	1.23
1	B	268	GLN	C-O	-6.39	1.16	1.24
1	B	223	MET	C-O	-6.39	1.16	1.23
1	B	260	VAL	C-O	-6.38	1.16	1.24
1	B	63	HIS	C-O	-6.37	1.16	1.24
1	B	262	ALA	C-O	-6.24	1.16	1.24
1	A	259	THR	C-O	-6.23	1.17	1.24
1	B	65	LEU	C-O	-6.19	1.17	1.24
1	B	229	VAL	C-O	-6.18	1.17	1.24
1	A	263	MET	C-O	-6.10	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	C-O	-6.07	1.16	1.24
1	B	90	PHE	C-O	-6.07	1.16	1.24
1	A	62	LEU	C-O	-6.06	1.16	1.24
1	B	231	VAL	C-O	-6.00	1.18	1.24
1	C	221	MET	C-O	-5.97	1.16	1.23
1	D	155	GLU	C-O	-5.94	1.17	1.24
1	B	200	ILE	C-O	-5.94	1.17	1.24
1	B	64	GLU	C-O	-5.88	1.17	1.24
1	C	260	VAL	C-O	-5.87	1.16	1.24
1	D	58	LYS	C-O	-5.86	1.16	1.23
1	B	153	GLU	C-O	-5.85	1.17	1.24
1	B	152	PHE	C-O	-5.82	1.17	1.24
1	C	235	ASP	C-O	-5.82	1.17	1.24
1	A	229	VAL	C-O	-5.82	1.17	1.24
1	B	267	LEU	C-O	-5.80	1.17	1.24
1	B	151	GLN	C-O	-5.78	1.17	1.24
1	C	153	GLU	C-O	-5.78	1.17	1.24
1	C	263	MET	C-O	-5.77	1.17	1.24
1	B	237	PHE	C-O	-5.70	1.17	1.24
1	B	265	HIS	C-O	-5.67	1.17	1.24
1	B	58	LYS	C-O	-5.66	1.16	1.23
1	B	234	GLY	C-O	-5.65	1.17	1.23
1	D	61	GLU	C-O	-5.64	1.17	1.24
1	D	264	GLN	C-O	-5.63	1.17	1.24
1	B	221	MET	C-O	-5.62	1.17	1.23
1	B	117	GLY	C-O	-5.60	1.17	1.23
1	A	234	GLY	C-O	-5.56	1.16	1.23
1	B	114	PRO	CA-C	-5.54	1.47	1.53
1	D	234	GLY	C-O	-5.51	1.17	1.23
1	D	260	VAL	C-O	-5.50	1.17	1.24
1	B	154	ALA	C-O	-5.50	1.17	1.24
1	A	59	SER	C-O	-5.45	1.17	1.24
1	C	226	VAL	C-O	-5.44	1.18	1.24
1	D	62	LEU	C-O	-5.44	1.17	1.24
1	B	62	LEU	C-O	-5.42	1.17	1.24
1	B	149	PRO	CA-C	-5.40	1.47	1.53
1	A	113	ASP	C-O	-5.34	1.17	1.24
1	A	221	MET	C-O	-5.29	1.18	1.24
1	A	226	VAL	C-O	-5.29	1.18	1.24
1	C	222	GLU	C-O	-5.25	1.17	1.24
1	B	59	SER	C-O	-5.25	1.17	1.24
1	C	224	ARG	C-O	-5.23	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	MET	C-O	-5.23	1.17	1.24
1	A	261	SER	C-O	-5.21	1.18	1.24
1	A	189	ASP	C-O	-5.17	1.17	1.24
1	A	185	ILE	C-O	-5.17	1.17	1.23
1	C	199	LEU	C-O	-5.16	1.17	1.24
1	B	116	MET	C-O	-5.13	1.17	1.24
1	C	62	LEU	C-O	-5.13	1.18	1.24
1	A	203	GLY	C-O	-5.12	1.17	1.23
1	C	113	ASP	C-O	-5.12	1.17	1.24
1	A	218	ARG	C-O	-5.11	1.17	1.24
1	A	58	LYS	C-O	-5.11	1.17	1.23
1	A	224	ARG	C-O	-5.08	1.17	1.23
1	D	263	MET	C-O	-5.06	1.18	1.24
1	C	234	GLY	C-O	-5.05	1.17	1.23
1	B	232	GLY	C-O	-5.05	1.17	1.24
1	D	267	LEU	C-O	-5.04	1.18	1.24
1	B	115	VAL	C-O	-5.04	1.18	1.24
1	A	115	VAL	CA-CB	-5.03	1.48	1.53
1	B	60	GLN	C-O	-5.01	1.18	1.24
1	C	235	ASP	CA-C	-5.00	1.46	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	LEU	CA-C-N	9.39	130.38	121.46
1	D	202	LEU	C-N-CA	9.39	130.38	121.46
1	B	202	LEU	CA-C-N	9.21	130.21	121.46
1	B	202	LEU	C-N-CA	9.21	130.21	121.46
1	D	186	THR	N-CA-C	6.48	118.42	111.36
1	C	127	TYR	CB-CA-C	-6.28	100.11	110.72
1	B	186	THR	N-CA-C	6.26	118.11	111.28
1	A	115	VAL	CB-CA-C	-6.25	104.48	111.23
1	A	186	THR	N-CA-C	5.95	119.73	112.23
1	A	118	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	227	GLU	N-CA-C	5.28	117.54	109.62
1	D	118	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	224	ARG	N-CA-C	5.14	117.68	109.96
1	B	115	VAL	N-CA-C	5.04	116.01	108.54
1	B	263	MET	CB-CA-C	-5.04	102.42	110.79
1	A	226	VAL	N-CA-C	-5.04	101.11	108.17

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	2393	2366	2370	33	1
1	B	2397	2378	2382	30	0
1	C	2403	2384	2388	30	0
1	D	2405	2388	2392	25	1
2	A	21	29	18	1	0
3	A	31	13	12	4	0
3	B	31	13	12	2	0
3	C	31	13	12	0	0
3	D	31	13	12	3	0
4	A	12	18	18	0	0
4	B	28	42	42	4	0
4	C	24	36	36	1	0
4	D	4	6	6	0	0
5	A	6	8	8	0	0
5	B	6	8	8	0	0
5	C	6	8	8	0	0
6	A	6	0	0	0	0
6	B	7	0	0	0	0
6	C	6	0	0	0	0
6	D	5	0	0	0	0
All	All	9853	9723	9724	120	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (120) 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:192:SER:OG	1:A:222:GLU:OE1	1.87	0.92
1:A:88:LYS:HA	1:A:132:LEU:HD21	1.63	0.79
1:C:236:LEU:HD13	1:C:293:MET:HE1	1.66	0.77
1:A:74:VAL:HG11	1:B:16:ARG:CD	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:CD	1:B:74:VAL:HG11	2.16	0.76
1:A:288:GLN:O	1:A:292:ARG:NH2	2.21	0.73
1:A:209:LYS:HE3	1:A:215:VAL:HB	1.68	0.73
3:D:401:AGS:O2G	3:D:401:AGS:O1B	2.05	0.73
3:B:401:AGS:O2G	3:B:401:AGS:O2B	2.05	0.73
1:A:236:LEU:HD13	1:A:293:MET:HE1	1.71	0.72
1:D:236:LEU:HD13	1:D:293:MET:HE1	1.72	0.72
1:D:62:LEU:HD12	1:D:62:LEU:O	1.92	0.70
1:B:62:LEU:HD12	1:B:62:LEU:O	1.93	0.66
1:C:4:GLU:N	1:C:4:GLU:OE1	2.28	0.66
1:A:16:ARG:HD2	1:B:74:VAL:HG11	1.77	0.66
1:B:85:THR:HG23	4:B:408:EDO:O1	1.95	0.65
1:C:211:ASP:N	1:C:211:ASP:OD1	2.30	0.63
1:B:74:VAL:O	1:B:74:VAL:HG12	1.98	0.63
1:A:74:VAL:O	1:A:74:VAL:HG12	1.99	0.62
1:C:209:LYS:HE3	1:C:213:SER:HB3	1.81	0.62
1:C:288:GLN:O	1:C:292:ARG:NH2	2.32	0.62
1:C:62:LEU:O	1:C:62:LEU:HD12	1.99	0.62
1:D:27:PRO:HD3	1:D:293:MET:HE2	1.81	0.62
1:B:12:SER:HB2	1:B:41:VAL:HG22	1.81	0.62
1:C:116:MET:HE3	1:C:136:TYR:CD2	2.36	0.61
1:A:211:ASP:N	1:A:211:ASP:OD1	2.31	0.60
1:D:143:VAL:O	1:D:143:VAL:HG12	2.02	0.60
1:A:209:LYS:HE3	1:A:215:VAL:CB	2.32	0.59
1:C:128:VAL:CG1	1:C:132:LEU:HD22	2.33	0.58
1:A:74:VAL:HG11	1:B:16:ARG:HD3	1.86	0.57
1:A:74:VAL:HG11	1:B:16:ARG:HD2	1.87	0.57
1:B:27:PRO:HD3	1:B:293:MET:HE2	1.87	0.56
3:A:402:AGS:H8	3:A:402:AGS:H5'2	1.86	0.56
1:A:88:LYS:HA	1:A:132:LEU:CD2	2.33	0.55
1:C:25:MET:HE2	1:C:37:ALA:HB2	1.87	0.55
1:C:143:VAL:HG22	1:C:143:VAL:O	2.06	0.55
1:D:128:VAL:HG13	1:D:132:LEU:HD12	1.87	0.55
1:B:143:VAL:HG12	1:B:143:VAL:O	2.06	0.54
1:D:74:VAL:HG13	1:D:74:VAL:O	2.06	0.54
1:D:223:MET:HE3	1:D:260:VAL:HG13	1.88	0.54
1:D:242:LEU:C	1:D:242:LEU:HD23	2.33	0.53
1:D:25:MET:HG2	1:D:35:VAL:HG11	1.91	0.53
1:C:60:GLN:OE1	1:C:60:GLN:N	2.37	0.53
1:A:236:LEU:HG	1:A:240:MET:HE2	1.91	0.52
1:B:85:THR:HG23	4:B:408:EDO:C1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:MET:HE3	1:A:260:VAL:HG13	1.92	0.52
1:B:85:THR:HG22	1:B:87:ASP:H	1.76	0.51
1:C:27:PRO:HD3	1:C:293:MET:HE2	1.92	0.51
1:C:74:VAL:O	1:C:74:VAL:CG1	2.58	0.51
1:B:206:ARG:HG2	1:B:216:THR:OG1	2.11	0.50
1:C:12:SER:HB2	1:C:41:VAL:HG22	1.93	0.50
1:C:236:LEU:CD1	1:C:293:MET:HE1	2.39	0.49
1:C:116:MET:CE	1:C:136:TYR:CD2	2.95	0.49
1:D:187:SER:HA	1:D:199:LEU:HD11	1.95	0.49
1:A:74:VAL:CG1	1:B:16:ARG:HD2	2.43	0.49
1:A:152:PHE:CE2	1:A:156:LEU:HD11	2.48	0.49
1:C:223:MET:HE3	1:C:260:VAL:HG13	1.94	0.49
1:D:128:VAL:HG22	1:D:129:PRO:HD2	1.95	0.48
1:D:152:PHE:CE2	1:D:156:LEU:HD11	2.48	0.48
1:B:172:MET:HE1	1:B:202:LEU:HB2	1.96	0.47
1:C:133:LEU:HD12	1:C:133:LEU:O	2.14	0.47
1:A:27:PRO:HD3	1:A:293:MET:HE2	1.95	0.47
1:A:209:LYS:HB3	1:A:210:PRO:HD2	1.97	0.47
1:A:91:LEU:HD12	1:A:132:LEU:HD22	1.96	0.46
1:A:128:VAL:HG22	1:A:129:PRO:HD2	1.97	0.46
1:B:236:LEU:HD13	1:B:293:MET:HE1	1.97	0.46
1:C:128:VAL:HG13	1:C:129:PRO:HD2	1.97	0.46
1:B:60:GLN:OE1	1:B:60:GLN:N	2.36	0.46
1:A:242:LEU:C	1:A:242:LEU:HD23	2.41	0.46
1:C:128:VAL:HG11	1:C:132:LEU:HD22	1.98	0.46
1:A:43:PHE:HD2	2:A:401:PG4:HO1	1.61	0.46
3:A:402:AGS:H8	3:A:402:AGS:C5'	2.46	0.45
1:C:4:GLU:HG2	1:C:4:GLU:O	2.17	0.45
1:C:242:LEU:C	1:C:242:LEU:HD23	2.42	0.45
1:B:56:VAL:HG13	4:B:408:EDO:H22	1.99	0.45
1:B:56:VAL:HG13	4:B:408:EDO:C2	2.47	0.45
1:C:209:LYS:CE	1:C:213:SER:HB3	2.46	0.45
1:D:91:LEU:HD11	1:D:136:TYR:CE2	2.52	0.44
1:A:133:LEU:HD12	1:A:133:LEU:O	2.18	0.44
1:B:242:LEU:HD23	1:B:242:LEU:C	2.43	0.44
1:A:4:GLU:OE1	1:A:32:GLY:O	2.34	0.44
1:D:128:VAL:HG22	1:D:132:LEU:HD12	1.99	0.44
1:D:172:MET:HE1	1:D:202:LEU:CB	2.48	0.44
1:C:268:GLN:O	1:C:271:ILE:HG22	2.18	0.44
1:D:7:VAL:HG22	1:D:79:TYR:HB2	2.00	0.44
1:A:209:LYS:HE3	1:A:215:VAL:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:MET:HE1	1:B:202:LEU:CB	2.49	0.43
3:D:401:AGS:PG	3:D:401:AGS:O1A	2.77	0.43
1:A:43:PHE:CD1	1:A:54:GLY:HA3	2.52	0.43
1:D:128:VAL:CG1	1:D:132:LEU:HD12	2.48	0.43
1:A:130:GLN:N	1:A:130:GLN:OE1	2.52	0.43
3:A:402:AGS:C5'	3:A:402:AGS:C8	2.97	0.42
3:D:401:AGS:N3	3:D:401:AGS:O2'	2.52	0.42
1:D:223:MET:HE3	1:D:260:VAL:CG1	2.49	0.42
1:D:74:VAL:O	1:D:74:VAL:CG1	2.68	0.42
1:B:25:MET:HG2	1:B:35:VAL:HG11	2.02	0.42
1:B:74:VAL:O	1:B:74:VAL:CG1	2.67	0.42
1:A:221:MET:SD	1:A:256:CYS:HB3	2.60	0.41
1:D:62:LEU:HD12	1:D:62:LEU:C	2.41	0.41
1:B:260:VAL:O	1:B:260:VAL:HG12	2.18	0.41
3:B:401:AGS:PG	3:B:401:AGS:O2A	2.78	0.41
1:C:172:MET:HE1	1:C:202:LEU:CB	2.50	0.41
1:D:143:VAL:O	1:D:143:VAL:CG1	2.67	0.41
1:B:172:MET:HE2	1:B:185:ILE:HD12	2.03	0.41
1:D:141:VAL:N	1:D:142:PRO:CD	2.83	0.41
1:B:133:LEU:O	1:B:133:LEU:HD12	2.21	0.41
1:C:25:MET:HE2	1:C:37:ALA:CB	2.49	0.41
1:C:221:MET:HE3	1:C:221:MET:HB2	1.81	0.41
1:A:263:MET:HE2	3:A:402:AGS:H1'	2.02	0.41
1:A:221:MET:HE3	1:A:221:MET:HB2	1.87	0.40
1:B:133:LEU:HB3	1:B:134:PRO:HD3	2.04	0.40
1:D:164:SER:O	1:D:167:GLU:HB2	2.21	0.40
1:B:200:ILE:HD12	1:B:200:ILE:HG23	1.76	0.40
1:D:174:MET:HE2	1:D:174:MET:HB3	1.81	0.40
1:B:237:PHE:CD1	1:B:237:PHE:C	2.98	0.40
1:C:298:ARG:HD2	1:C:301:GLU:OE1	2.22	0.40
1:D:236:LEU:CD1	1:D:293:MET:HE1	2.47	0.40
1:C:86:ARG:NH1	4:C:407:EDO:O2	2.51	0.40
1:C:141:VAL:N	1:C:142:PRO:CD	2.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:OE2	1:D:130:GLN:HE22[1_554]	1.50	0.10

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	307/314 (98%)	301 (98%)	6 (2%)	0	100	100
1	B	307/314 (98%)	298 (97%)	9 (3%)	0	100	100
1	C	307/314 (98%)	297 (97%)	10 (3%)	0	100	100
1	D	307/314 (98%)	298 (97%)	9 (3%)	0	100	100
All	All	1228/1256 (98%)	1194 (97%)	34 (3%)	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	263/273 (96%)	258 (98%)	5 (2%)	50	79
1	B	263/273 (96%)	260 (99%)	3 (1%)	65	88
1	C	264/273 (97%)	254 (96%)	10 (4%)	29	64
1	D	265/273 (97%)	257 (97%)	8 (3%)	36	70
All	All	1055/1092 (97%)	1029 (98%)	26 (2%)	42	74

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ARG
1	A	199	LEU

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Mol	Chain	Res	Type
1	A	211	ASP
1	A	219	ILE
1	A	223	MET
1	B	197	ASP
1	B	211	ASP
1	B	223	MET
1	C	74	VAL
1	C	118	ASP
1	C	126	MET
1	C	127	TYR
1	C	199	LEU
1	C	207	MET
1	C	211	ASP
1	C	214	THR
1	C	216	THR
1	C	223	MET
1	D	16	ARG
1	D	41	VAL
1	D	74	VAL
1	D	128	VAL
1	D	185	ILE
1	D	199	LEU
1	D	207	MET
1	D	216	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	B	194	GLN
1	B	246	HIS
1	C	103	GLN
1	C	308	GLN
1	D	63	HIS
1	D	103	GLN
1	D	308	GLN

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](#)

27 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	$\# Z > 2$
4	EDO	B	409	-	3,3,3	0.36	0	2,2,2	1.32	0
4	EDO	C	405	-	3,3,3	0.44	0	2,2,2	0.40	0
4	EDO	C	402	-	3,3,3	0.44	0	2,2,2	0.36	0
4	EDO	C	406	-	3,3,3	0.44	0	2,2,2	0.40	0
3	AGS	D	401	-	32,33,33	3.13	14 (43%)	45,52,52	2.21	15 (33%)
4	EDO	C	404	-	3,3,3	0.45	0	2,2,2	0.32	0
4	EDO	A	403	-	3,3,3	0.45	0	2,2,2	0.40	0
5	GOL	B	403	-	5,5,5	0.70	0	5,5,5	1.09	0
4	EDO	B	408	-	3,3,3	0.43	0	2,2,2	0.48	0
4	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.30	0
4	EDO	A	407	-	3,3,3	0.47	0	2,2,2	0.28	0
3	AGS	C	401	-	32,33,33	3.15	19 (59%)	45,52,52	1.89	12 (26%)
4	EDO	B	406	-	3,3,3	0.46	0	2,2,2	0.38	0
2	PG4	A	401	-	12,12,12	0.56	0	11,11,11	0.42	0
3	AGS	B	401	-	32,33,33	2.91	17 (53%)	45,52,52	2.19	16 (35%)
4	EDO	A	406	-	3,3,3	0.45	0	2,2,2	0.34	0
5	GOL	A	405	-	5,5,5	0.63	0	5,5,5	0.89	0
4	EDO	C	407	-	3,3,3	0.45	0	2,2,2	0.44	0
4	EDO	B	402	-	3,3,3	0.43	0	2,2,2	0.29	0
5	GOL	C	403	-	5,5,5	0.79	0	5,5,5	1.17	1 (20%)
4	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	407	-	3,3,3	0.39	0	2,2,2	0.43	0
3	AGS	A	402	-	32,33,33	3.04	19 (59%)	45,52,52	2.09	15 (33%)
4	EDO	D	402	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	C	408	-	3,3,3	0.45	0	2,2,2	0.41	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
4	EDO	B	409	-	-	0/1/1/1	-
4	EDO	C	405	-	-	1/1/1/1	-
4	EDO	C	402	-	-	0/1/1/1	-
4	EDO	C	406	-	-	0/1/1/1	-
3	AGS	D	401	-	-	9/21/38/38	0/3/3/3
4	EDO	C	404	-	-	0/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-
5	GOL	B	403	-	-	3/4/4/4	-
4	EDO	B	408	-	-	0/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
3	AGS	C	401	-	-	3/21/38/38	0/3/3/3
4	EDO	B	406	-	-	1/1/1/1	-
2	PG4	A	401	-	-	5/10/10/10	-
3	AGS	B	401	-	-	8/21/38/38	0/3/3/3
4	EDO	A	406	-	-	0/1/1/1	-
5	GOL	A	405	-	-	2/4/4/4	-
4	EDO	C	407	-	-	0/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
5	GOL	C	403	-	-	2/4/4/4	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-
3	AGS	A	402	-	-	3/21/38/38	0/3/3/3
4	EDO	D	402	-	-	0/1/1/1	-
4	EDO	C	408	-	-	1/1/1/1	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	AGS	PA-O3A	-9.08	1.49	1.59
3	D	401	AGS	PB-O3A	-8.54	1.50	1.59
3	D	401	AGS	PA-O3A	-8.09	1.50	1.59
3	A	402	AGS	PB-O3A	-7.80	1.51	1.59
3	C	401	AGS	PB-O3A	-7.54	1.51	1.59
3	A	402	AGS	PA-O3A	-7.50	1.51	1.59
3	B	401	AGS	PA-O3A	-6.88	1.52	1.59
3	B	401	AGS	PB-O3B	-5.67	1.53	1.59
3	B	401	AGS	PB-O3A	-5.57	1.53	1.59
3	D	401	AGS	PB-O3B	-5.47	1.53	1.59
3	A	402	AGS	C5-N7	-5.26	1.29	1.39
3	C	401	AGS	C5-N7	-4.95	1.30	1.39
3	B	401	AGS	C5-N7	-4.75	1.30	1.39
3	B	401	AGS	PG-O3G	-4.73	1.39	1.54
3	C	401	AGS	C4-N9	-4.70	1.27	1.37
3	D	401	AGS	C5-N7	-4.44	1.31	1.39
3	D	401	AGS	C4-N9	-4.38	1.28	1.37
3	A	402	AGS	C4-N9	-4.31	1.28	1.37
3	B	401	AGS	C8-N9	-4.22	1.30	1.37
3	C	401	AGS	C8-N9	-4.18	1.30	1.37
3	D	401	AGS	PG-O3G	-4.15	1.41	1.54
3	B	401	AGS	C4-N9	-4.00	1.29	1.37
3	A	402	AGS	C8-N9	-3.98	1.30	1.37
3	C	401	AGS	PG-O3G	-3.95	1.41	1.54
3	D	401	AGS	C8-N9	-3.67	1.31	1.37
3	D	401	AGS	PG-S1G	3.65	1.98	1.90
3	A	402	AGS	PG-O3G	-3.63	1.43	1.54
3	A	402	AGS	PG-S1G	3.58	1.98	1.90
3	C	401	AGS	PA-O2A	-3.08	1.41	1.55
3	C	401	AGS	PB-O3B	-3.08	1.56	1.59
3	A	402	AGS	O4'-C4'	-3.02	1.38	1.45
3	B	401	AGS	PA-O2A	-2.91	1.41	1.55
3	A	402	AGS	PB-O3B	-2.88	1.56	1.59
3	A	402	AGS	PA-O1A	-2.77	1.41	1.50
3	D	401	AGS	O4'-C4'	-2.76	1.38	1.45
3	C	401	AGS	PG-S1G	2.72	1.96	1.90
3	C	401	AGS	C2'-C3'	-2.68	1.46	1.53
3	B	401	AGS	PG-S1G	2.60	1.96	1.90
3	C	401	AGS	PB-O2B	-2.60	1.43	1.55
3	D	401	AGS	PB-O2B	-2.57	1.43	1.55
3	A	402	AGS	C2'-C3'	-2.57	1.46	1.53
3	B	401	AGS	PB-O2B	-2.55	1.43	1.55
3	A	402	AGS	PB-O2B	-2.54	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	AGS	PA-O2A	-2.51	1.43	1.55
3	D	401	AGS	C2'-C1'	-2.51	1.45	1.53
3	C	401	AGS	O4'-C4'	-2.49	1.39	1.45
3	C	401	AGS	C6-N1	-2.47	1.28	1.35
3	D	401	AGS	PA-O1A	-2.45	1.42	1.50
3	A	402	AGS	O5'-C5'	-2.41	1.35	1.44
3	B	401	AGS	C2'-C3'	-2.41	1.46	1.53
3	B	401	AGS	O4'-C4'	-2.38	1.39	1.45
3	B	401	AGS	PB-O1B	-2.34	1.42	1.50
3	A	402	AGS	C2'-C1'	-2.22	1.46	1.53
3	C	401	AGS	PB-O1B	-2.20	1.43	1.50
3	A	402	AGS	PA-O5'	-2.17	1.50	1.59
3	B	401	AGS	PA-O5'	-2.14	1.51	1.59
3	B	401	AGS	C2-N1	-2.13	1.30	1.33
3	B	401	AGS	PA-O1A	-2.12	1.43	1.50
3	C	401	AGS	C3'-C4'	-2.10	1.47	1.53
3	C	401	AGS	C2-N3	-2.09	1.30	1.33
3	D	401	AGS	PB-O1B	-2.08	1.43	1.50
3	D	401	AGS	PA-O2A	-2.08	1.45	1.55
3	C	401	AGS	C2'-C1'	-2.06	1.47	1.53
3	C	401	AGS	C4-N3	-2.04	1.30	1.34
3	A	402	AGS	C3'-C4'	-2.03	1.47	1.53
3	C	401	AGS	PA-O1A	-2.02	1.43	1.50
3	B	401	AGS	C2-N3	-2.02	1.30	1.33
3	A	402	AGS	C2-N3	-2.01	1.30	1.33
3	A	402	AGS	PB-O1B	-2.01	1.43	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	AGS	C5-C4-N3	-6.13	118.28	126.72
3	A	402	AGS	C5-C4-N3	-5.54	119.09	126.72
3	C	401	AGS	C5-C4-N3	-5.16	119.61	126.72
3	D	401	AGS	C5-C4-N3	-5.07	119.74	126.72
3	D	401	AGS	PB-O3B-PG	-4.72	115.89	133.17
3	B	401	AGS	N3-C4-N9	4.44	134.71	127.17
3	A	402	AGS	N3-C4-N9	4.41	134.67	127.17
3	A	402	AGS	N3-C2-N1	-4.40	121.93	128.58
3	B	401	AGS	C2-N3-C4	4.34	122.43	111.83
3	B	401	AGS	N3-C2-N1	-4.29	122.09	128.58
3	D	401	AGS	N3-C4-N9	4.20	134.31	127.17
3	A	402	AGS	C2-N3-C4	4.01	121.63	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	AGS	N3-C2-N1	-3.92	122.66	128.58
3	C	401	AGS	N3-C4-N9	3.91	133.81	127.17
3	B	401	AGS	O2B-PB-O3A	3.80	117.54	107.27
3	D	401	AGS	N3-C2-N1	-3.78	122.85	128.58
3	B	401	AGS	PB-O3B-PG	-3.76	119.39	133.17
3	C	401	AGS	O2G-PG-O3B	3.69	116.95	104.64
3	D	401	AGS	O2B-PB-O3B	3.66	117.18	107.27
3	A	402	AGS	O3A-PB-O1B	-3.64	99.74	110.70
3	D	401	AGS	C2-N3-C4	3.53	120.45	111.83
3	D	401	AGS	O2'-C2'-C1'	-3.53	97.96	110.10
3	D	401	AGS	O2B-PB-O3A	-3.52	97.77	107.27
3	C	401	AGS	C2-N3-C4	3.51	120.40	111.83
3	D	401	AGS	O4'-C1'-N9	3.49	114.80	108.09
3	B	401	AGS	C4-C5-N7	-3.31	106.80	110.58
3	D	401	AGS	C4-N9-C8	3.31	109.21	105.74
3	B	401	AGS	O3G-PG-O3B	3.23	115.43	104.64
3	D	401	AGS	C2'-C1'-N9	-2.88	106.15	113.30
3	A	402	AGS	PB-O3B-PG	-2.87	122.66	133.17
3	C	401	AGS	C4-C5-N7	-2.82	107.36	110.58
3	A	402	AGS	O2'-C2'-C1'	-2.78	100.54	110.10
3	B	401	AGS	C3'-C2'-C1'	2.76	106.68	101.46
3	A	402	AGS	O2G-PG-O3B	2.64	113.46	104.64
3	C	401	AGS	C4-N9-C8	2.60	108.47	105.74
3	A	402	AGS	C2-N1-C6	2.60	123.00	118.73
3	B	401	AGS	O2'-C2'-C1'	-2.60	101.17	110.10
3	C	401	AGS	C2-N1-C6	2.54	122.90	118.73
3	A	402	AGS	C3'-C2'-C1'	2.53	106.24	101.46
3	A	402	AGS	C5'-C4'-C3'	-2.52	106.15	115.21
3	A	402	AGS	C4-C5-N7	-2.49	107.74	110.58
3	B	401	AGS	C6-C5-N7	2.45	136.81	132.09
3	D	401	AGS	C4-C5-N7	-2.42	107.81	110.58
3	C	401	AGS	C5'-C4'-C3'	-2.39	106.60	115.21
3	C	401	AGS	O3B-PB-O1B	2.38	117.86	110.70
3	D	401	AGS	O2'-C2'-C3'	2.23	118.97	111.82
3	D	401	AGS	N9-C8-N7	-2.20	110.81	113.94
3	C	401	AGS	O2A-PA-O1A	2.19	122.65	112.44
3	B	401	AGS	C4-N9-C8	2.17	108.02	105.74
3	C	401	AGS	O2'-C2'-C1'	-2.17	102.64	110.10
3	B	401	AGS	C5-N7-C8	2.13	106.80	103.45
3	B	401	AGS	O2G-PG-O3B	2.12	111.73	104.64
3	D	401	AGS	N6-C6-N1	2.09	123.03	118.38
3	A	402	AGS	N6-C6-N1	2.08	123.01	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	AGS	C2-N1-C6	2.07	122.12	118.73
5	C	403	GOL	C3-C2-C1	-2.06	104.25	111.80
3	A	402	AGS	PA-O5'-C5'	-2.05	109.59	121.35
3	A	402	AGS	C4-N9-C8	2.03	107.87	105.74
3	B	401	AGS	O3A-PB-O1B	-2.01	104.66	110.70

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	AGS	PB-O3B-PG-O2G
3	B	401	AGS	PB-O3B-PG-O3G
3	B	401	AGS	C5'-O5'-PA-O1A
3	B	401	AGS	C5'-O5'-PA-O2A
3	B	401	AGS	C5'-O5'-PA-O3A
3	C	401	AGS	O4'-C4'-C5'-O5'
3	C	401	AGS	C3'-C4'-C5'-O5'
3	D	401	AGS	PB-O3B-PG-O2G
3	D	401	AGS	PB-O3B-PG-O3G
3	D	401	AGS	C5'-O5'-PA-O1A
3	D	401	AGS	C5'-O5'-PA-O2A
3	D	401	AGS	C5'-O5'-PA-O3A
5	A	405	GOL	C1-C2-C3-O3
2	A	401	PG4	O1-C1-C2-O2
3	A	402	AGS	O4'-C4'-C5'-O5'
3	A	402	AGS	C3'-C4'-C5'-O5'
5	B	403	GOL	O1-C1-C2-C3
5	C	403	GOL	C1-C2-C3-O3
2	A	401	PG4	O4-C7-C8-O5
5	A	405	GOL	O2-C2-C3-O3
5	B	403	GOL	O1-C1-C2-O2
3	D	401	AGS	O4'-C4'-C5'-O5'
2	A	401	PG4	O3-C5-C6-O4
3	B	401	AGS	PB-O3A-PA-O1A
3	D	401	AGS	PB-O3A-PA-O1A
2	A	401	PG4	C3-C4-O3-C5
3	A	402	AGS	PG-O3B-PB-O1B
3	B	401	AGS	PB-O3A-PA-O2A
4	B	406	EDO	O1-C1-C2-O2
4	C	405	EDO	O1-C1-C2-O2
5	C	403	GOL	O2-C2-C3-O3
5	B	403	GOL	C1-C2-C3-O3

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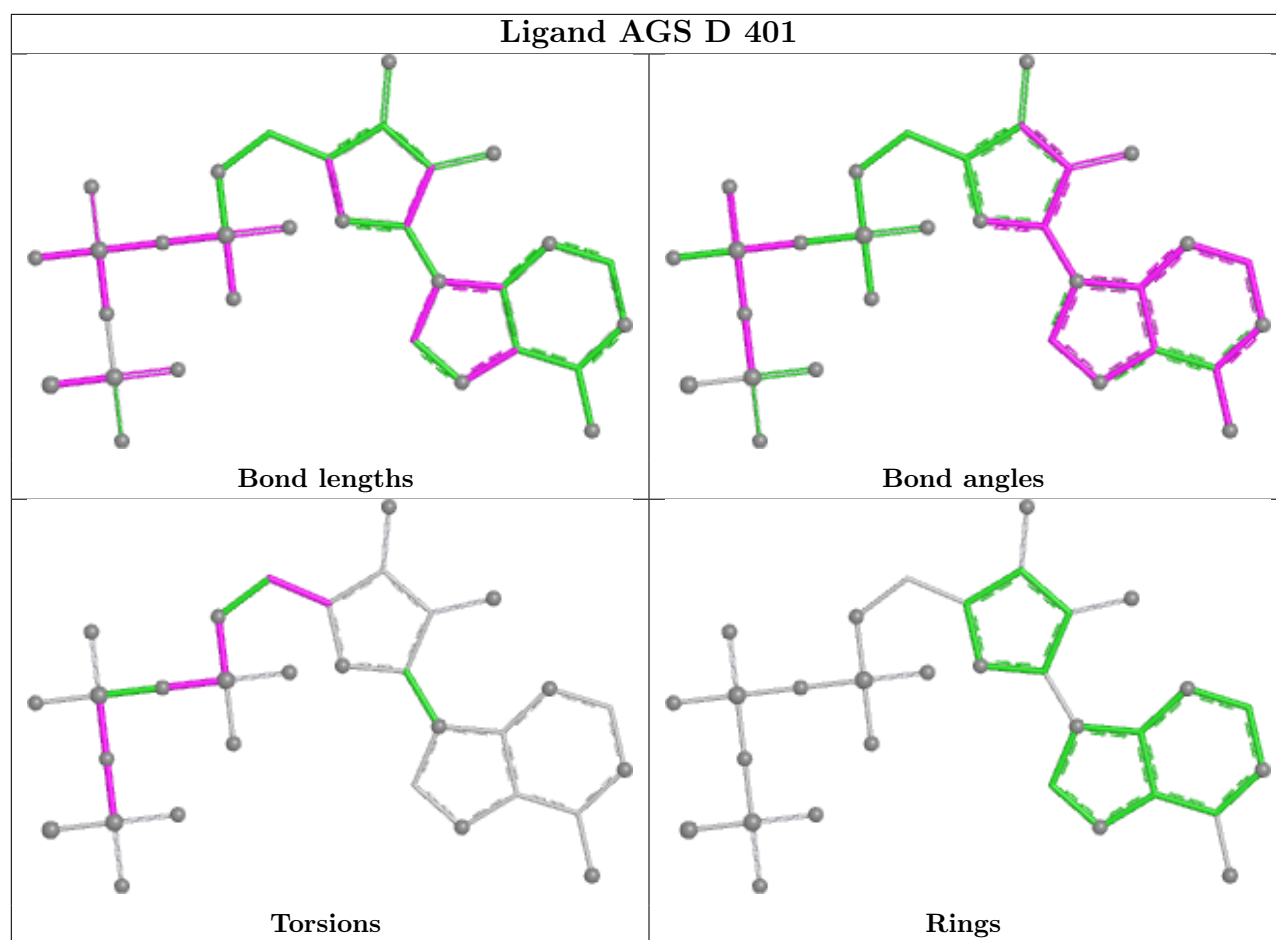
Mol	Chain	Res	Type	Atoms
3	B	401	AGS	PG-O3B-PB-O2B
3	C	401	AGS	PB-O3A-PA-O2A
4	C	408	EDO	O1-C1-C2-O2
3	D	401	AGS	PG-O3B-PB-O2B
3	D	401	AGS	C3'-C4'-C5'-O5'
2	A	401	PG4	C5-C6-O4-C7
4	A	403	EDO	O1-C1-C2-O2

There are no ring outliers.

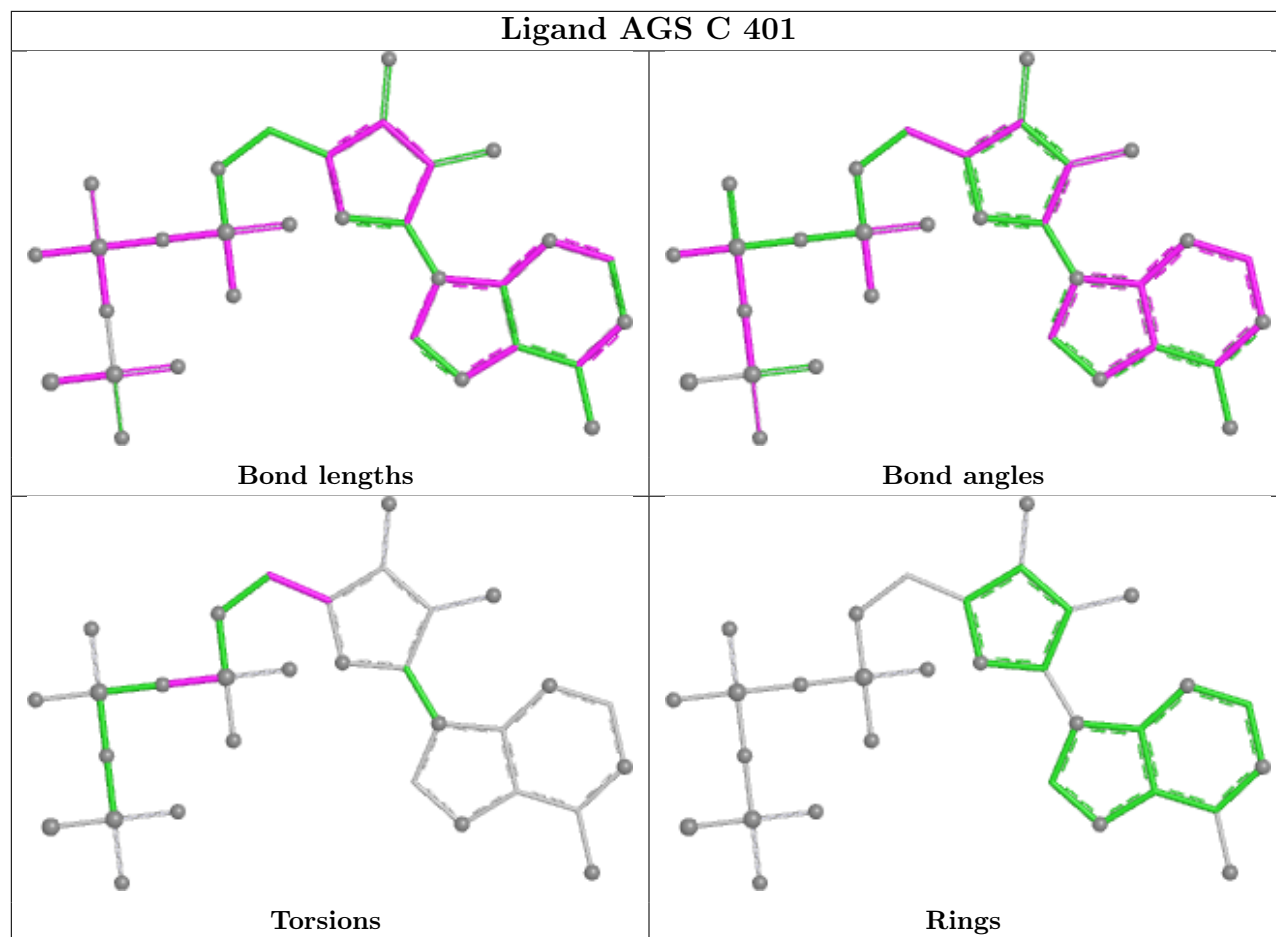
6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	AGS	3	0
4	B	408	EDO	4	0
2	A	401	PG4	1	0
3	B	401	AGS	2	0
4	C	407	EDO	1	0
3	A	402	AGS	4	0

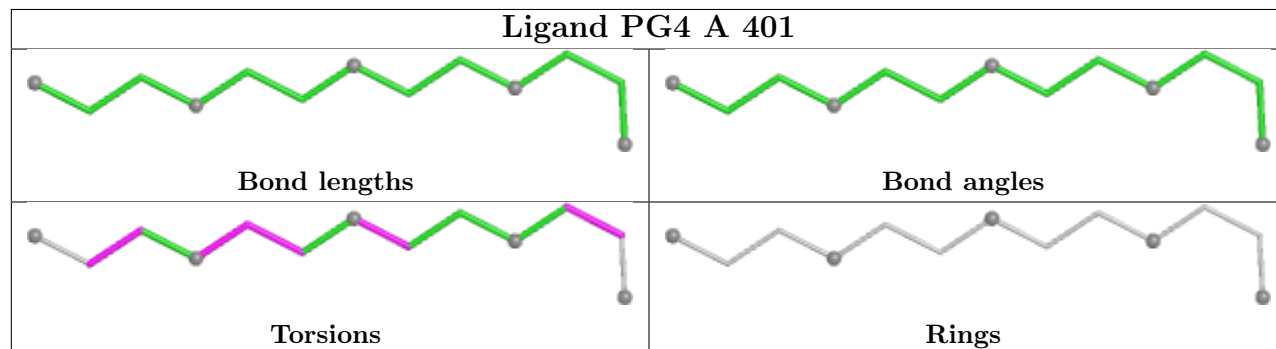
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



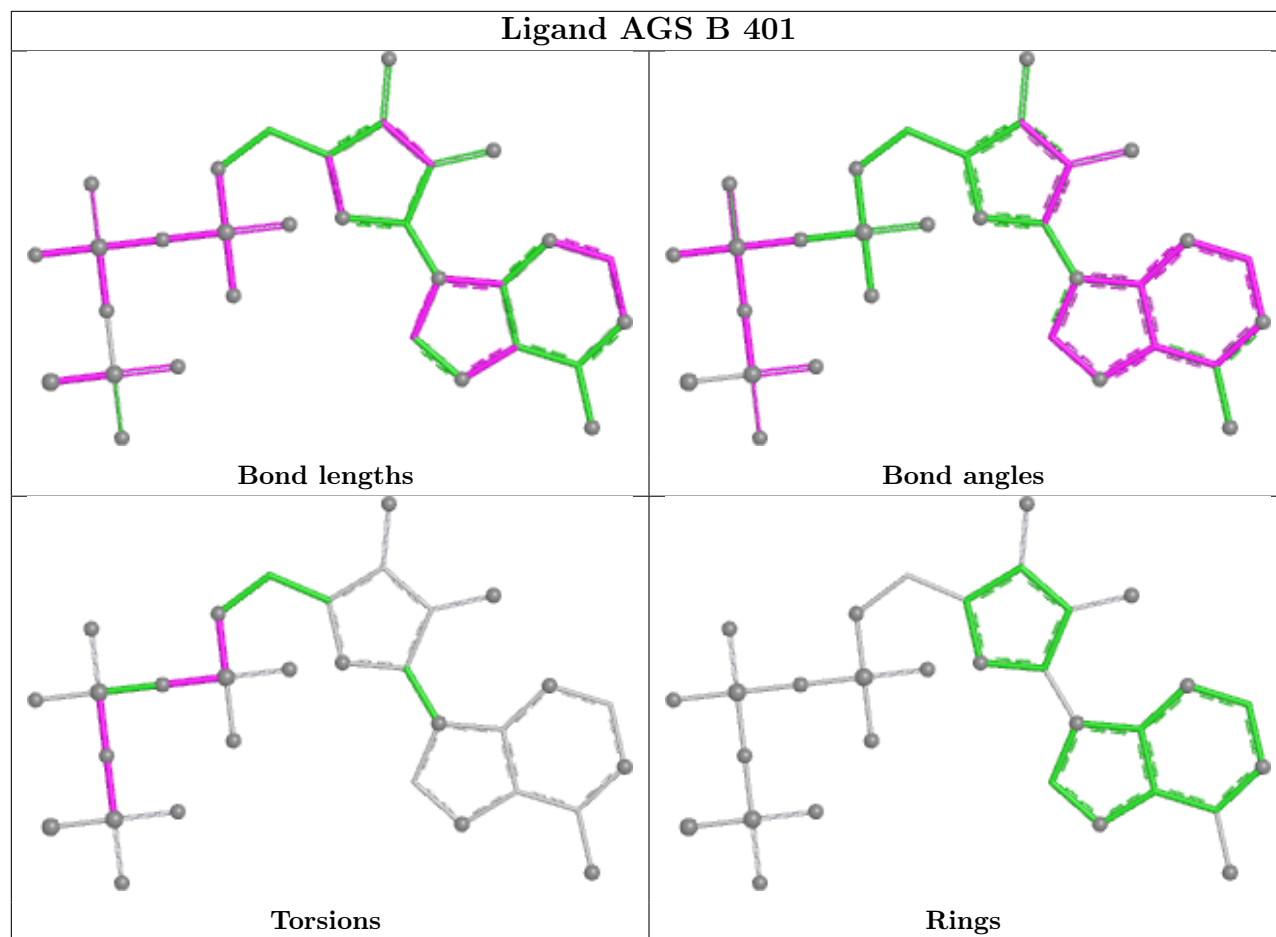
Ligand AGS C 401

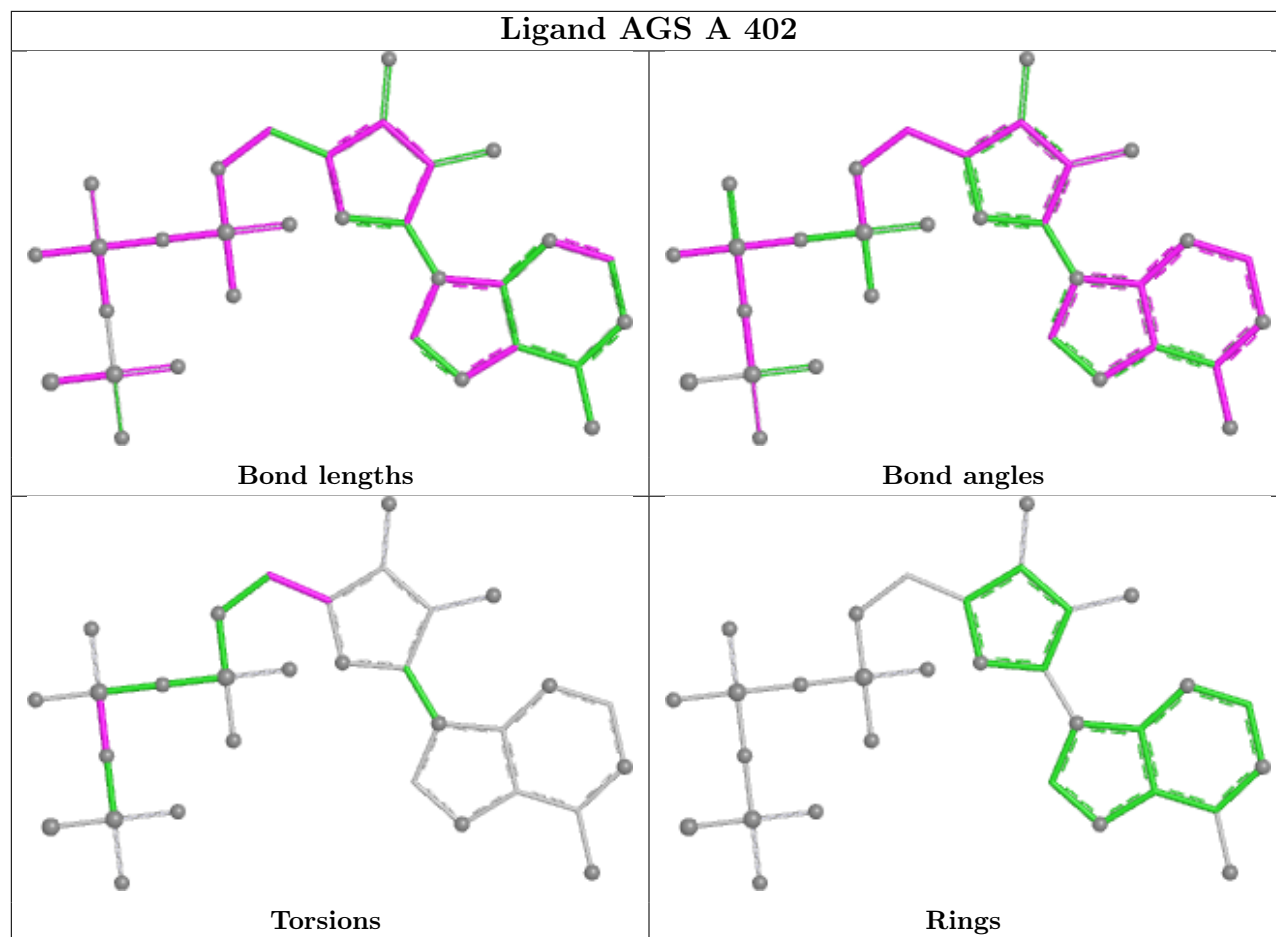


Ligand PG4 A 401



Ligand AGS B 401





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, 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	309/314 (98%)	0.78	25 (8%) 18 15	75, 100, 119, 134	0
1	B	309/314 (98%)	0.84	26 (8%) 17 14	75, 99, 119, 146	0
1	C	309/314 (98%)	0.81	22 (7%) 22 17	75, 104, 121, 133	0
1	D	309/314 (98%)	1.05	35 (11%) 10 9	75, 112, 142, 154	0
All	All	1236/1256 (98%)	0.87	108 (8%) 16 13	75, 103, 128, 154	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120	TRP	4.5
1	A	121	ASN	4.5
1	D	199	LEU	4.5
1	D	120	TRP	4.3
1	B	199	LEU	3.9
1	A	120	TRP	3.8
1	B	208	ARG	3.8
1	B	213	SER	3.7
1	B	210	PRO	3.7
1	A	123	GLU	3.6
1	C	85	THR	3.6
1	B	55	GLN	3.6
1	D	127	TYR	3.6
1	B	121	ASN	3.5
1	B	217	GLN	3.4
1	A	127	TYR	3.4
1	D	84	TYR	3.4
1	D	211	ASP	3.3
1	D	121	ASN	3.3
1	D	85	THR	3.3
1	C	125	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	166	GLU	3.2
1	B	211	ASP	3.2
1	C	228	ALA	3.1
1	D	126	MET	3.1
1	D	212	GLY	3.1
1	A	137	ARG	3.0
1	D	130	GLN	3.0
1	A	211	ASP	2.9
1	D	123	GLU	2.9
1	D	125	SER	2.9
1	A	160	ARG	2.9
1	B	120	TRP	2.9
1	D	210	PRO	2.9
1	B	212	GLY	2.8
1	C	307	VAL	2.8
1	C	123	GLU	2.8
1	D	279	GLY	2.8
1	A	4	GLU	2.7
1	B	209	LYS	2.7
1	C	199	LEU	2.7
1	A	126	MET	2.7
1	A	53	LYS	2.7
1	B	206	ARG	2.7
1	B	130	GLN	2.7
1	C	55	GLN	2.6
1	A	193	SER	2.6
1	A	124	GLY	2.6
1	B	4	GLU	2.6
1	C	119	LYS	2.6
1	B	312	LEU	2.6
1	D	177	CYS	2.6
1	A	210	PRO	2.5
1	B	83	GLY	2.5
1	B	125	SER	2.5
1	C	84	TYR	2.5
1	C	210	PRO	2.5
1	C	217	GLN	2.5
1	B	85	THR	2.5
1	B	58	LYS	2.5
1	D	53	LYS	2.5
1	A	132	LEU	2.4
1	B	250	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	311	VAL	2.4
1	C	124	GLY	2.4
1	D	223	MET	2.4
1	B	214	THR	2.4
1	D	184	VAL	2.4
1	C	247	LYS	2.3
1	A	177	CYS	2.3
1	D	43	PHE	2.3
1	A	84	TYR	2.3
1	C	86	ARG	2.3
1	D	99	ARG	2.3
1	A	212	GLY	2.3
1	B	124	GLY	2.3
1	C	230	PHE	2.2
1	A	103	GLN	2.2
1	B	195	GLY	2.2
1	D	5	CYS	2.2
1	A	206	ARG	2.2
1	D	88	LYS	2.2
1	A	199	LEU	2.2
1	D	86	ARG	2.1
1	B	279	GLY	2.1
1	A	125	SER	2.1
1	D	192	SER	2.1
1	B	224	ARG	2.1
1	C	121	ASN	2.1
1	A	227	GLU	2.1
1	D	256	CYS	2.1
1	C	132	LEU	2.1
1	D	175	LEU	2.1
1	D	82	THR	2.1
1	D	298	ARG	2.1
1	A	166	GLU	2.1
1	D	117	GLY	2.1
1	C	52	TRP	2.1
1	A	209	LYS	2.0
1	C	122	GLY	2.0
1	D	305	ILE	2.0
1	B	227	GLU	2.0
1	A	217	GLN	2.0
1	D	206	ARG	2.0
1	D	214	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	247	LYS	2.0
1	C	126	MET	2.0
1	D	183	VAL	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.

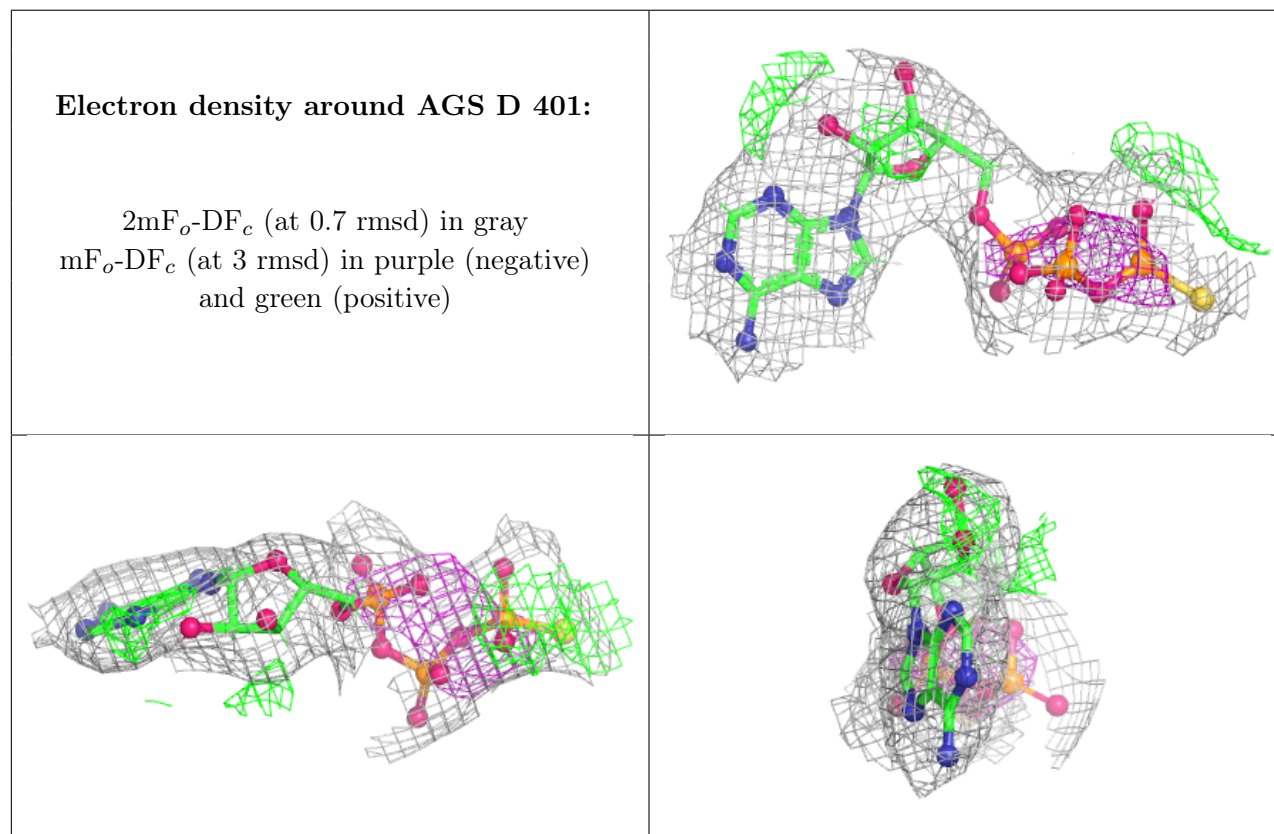
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	C	407	4/4	0.42	0.22	102,123,124,125	0
4	EDO	B	409	4/4	0.66	0.34	92,111,112,113	0
4	EDO	C	406	4/4	0.72	0.28	86,103,104,105	0
4	EDO	B	408	4/4	0.75	0.28	88,106,107,109	0
4	EDO	A	406	4/4	0.75	0.20	104,125,126,126	0
4	EDO	B	405	4/4	0.76	0.22	95,114,114,115	0
2	PG4	A	404[A]	8/13	0.77	0.24	90,108,110,115	1
2	PG4	A	404[B]	8/13	0.77	0.24	90,108,110,115	1
5	GOL	A	405	6/6	0.78	0.22	90,108,110,110	0
4	EDO	C	402	4/4	0.79	0.15	91,109,109,110	0
4	EDO	B	406	4/4	0.81	0.15	88,106,107,109	0
4	EDO	C	404	4/4	0.82	0.29	96,115,117,117	0
4	EDO	A	407	4/4	0.82	0.29	80,97,100,102	0
4	EDO	A	403	4/4	0.82	0.24	89,107,109,109	0
3	AGS	D	401	31/31	0.82	0.16	105,110,132,134	0
3	AGS	B	401	31/31	0.83	0.15	90,92,110,112	0
5	GOL	C	403	6/6	0.83	0.17	97,117,119,120	0
4	EDO	B	407	4/4	0.84	0.14	83,100,100,103	0
3	AGS	A	402	31/31	0.85	0.16	92,98,112,117	0
2	PG4	A	401	13/13	0.85	0.22	88,106,116,118	0

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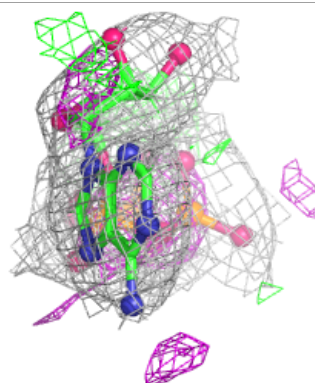
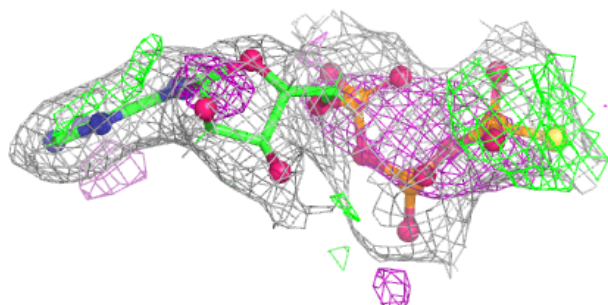
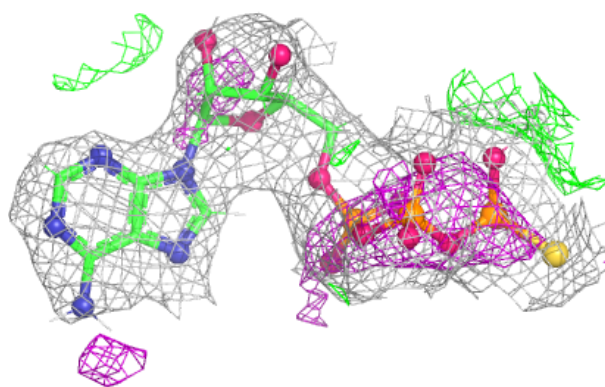
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	403	6/6	0.85	0.17	84,101,104,104	0
3	AGS	C	401	31/31	0.85	0.14	94,98,113,124	0
4	EDO	B	402	4/4	0.90	0.14	90,108,110,111	0
4	EDO	B	404	4/4	0.90	0.17	84,101,103,104	0
4	EDO	C	405	4/4	0.92	0.15	86,103,106,109	0
4	EDO	C	408	4/4	0.92	0.16	90,108,109,111	0
4	EDO	D	402	4/4	0.92	0.18	90,108,108,109	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.

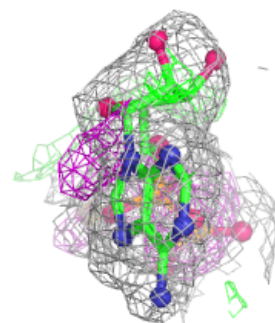
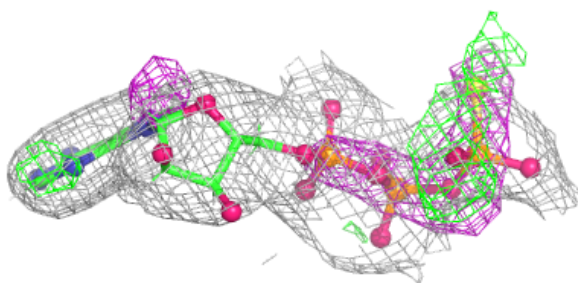
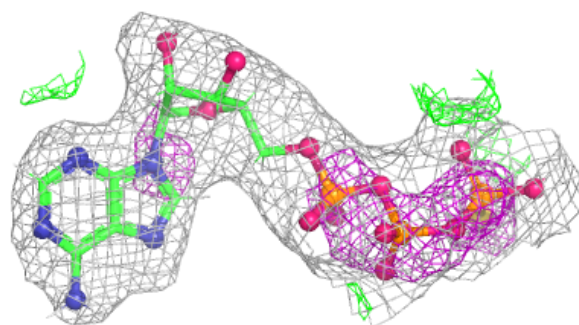


Electron density around AGS B 401:

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

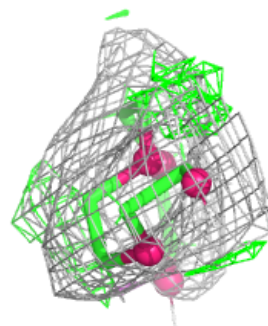
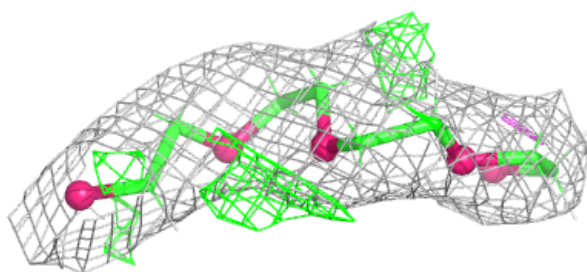
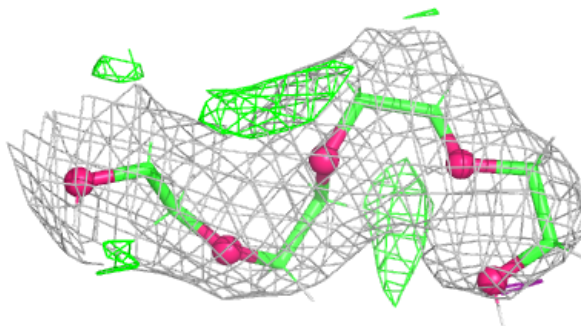
**Electron density around AGS A 402:**

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

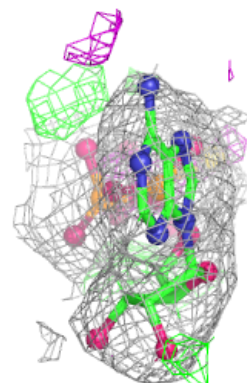
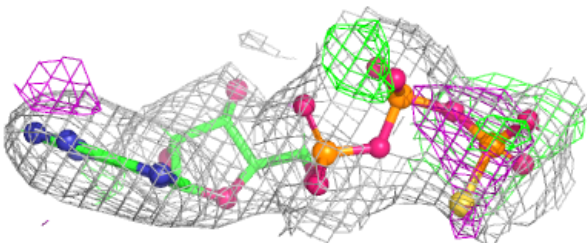
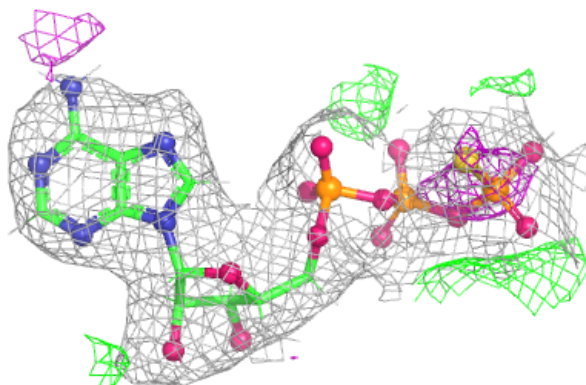


Electron density around PG4 A 401:

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

**Electron density around AGS C 401:**

$2mF_o-DF_c$ (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.