



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:27 AM UTC

PDB ID : 6YK1 / pdb_00006yk1
Title : Crystal structure of mouse pyridoxal kinase in complex with ATP-gamma-S and artesunate
Authors : Kasaragod, V.B.; Schindelin, H.
Deposited on : 2020-04-05
Resolution : 2.40 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

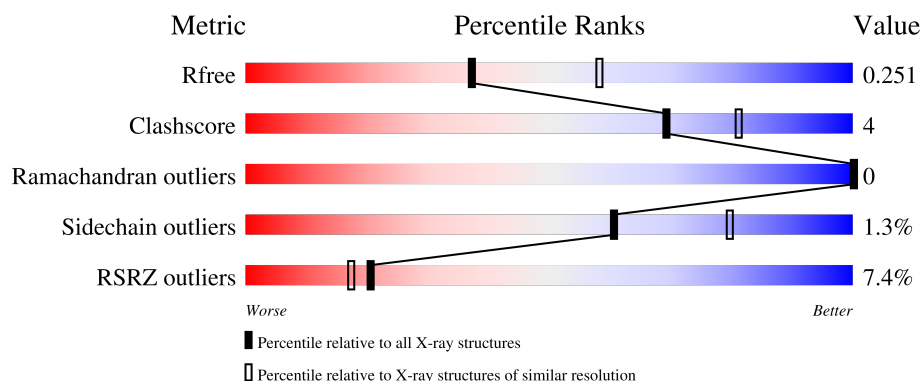
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	 6% 83% 13% ..
1	B	314	 8% 83% 13% .
1	C	314	 4% 88% 9% .
1	D	314	 10% 86% 11% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19493 atoms, of which 9601 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	305	Total	C	H	N	O	S	0	1	0
			4710	1492	2341	412	446	19			
1	B	304	Total	C	H	N	O	S	0	1	0
			4736	1497	2357	414	449	19			
1	C	304	Total	C	H	N	O	S	0	0	0
			4705	1490	2339	409	449	18			
1	D	305	Total	C	H	N	O	S	0	0	0
			4597	1470	2262	399	448	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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



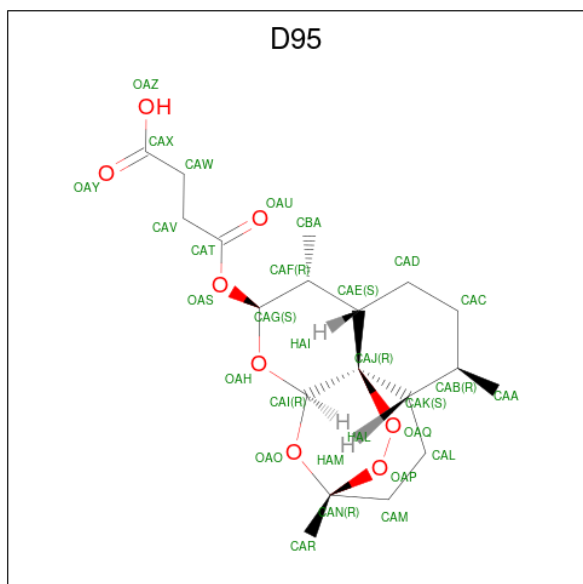
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			13	3	7	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



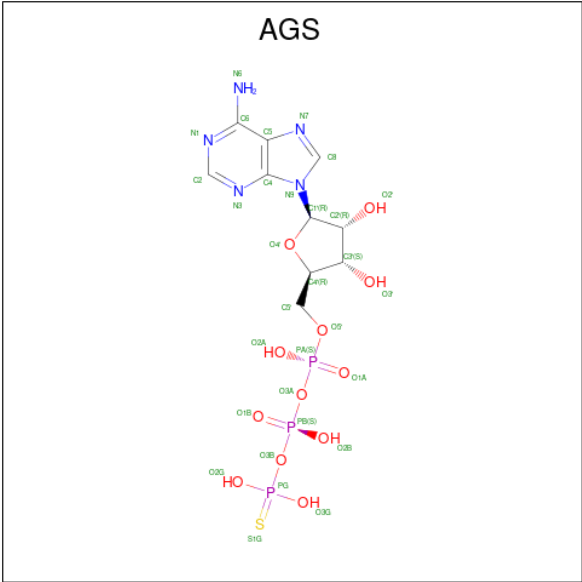
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 4 is Artesunate (CCD ID: D95) (formula: $C_{19}H_{28}O_8$) (labeled as "Ligand of Interest" by depositor).



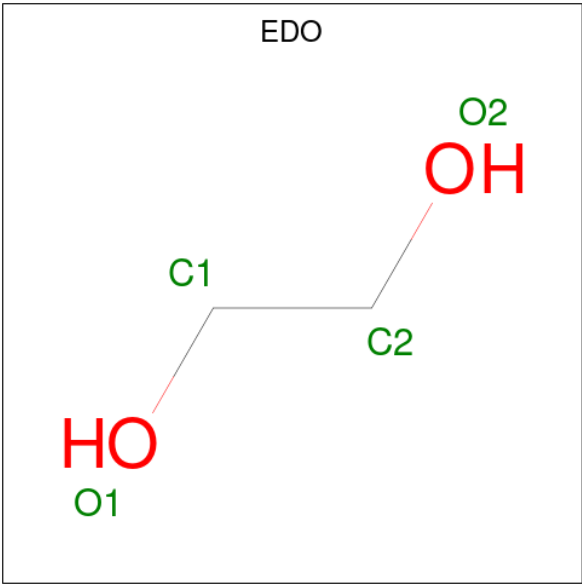
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			55	19	28	8		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
5	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
5	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
5	D	1	Total	C	H	N	O	P	S	0	0
			45	10	14	5	12	3	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

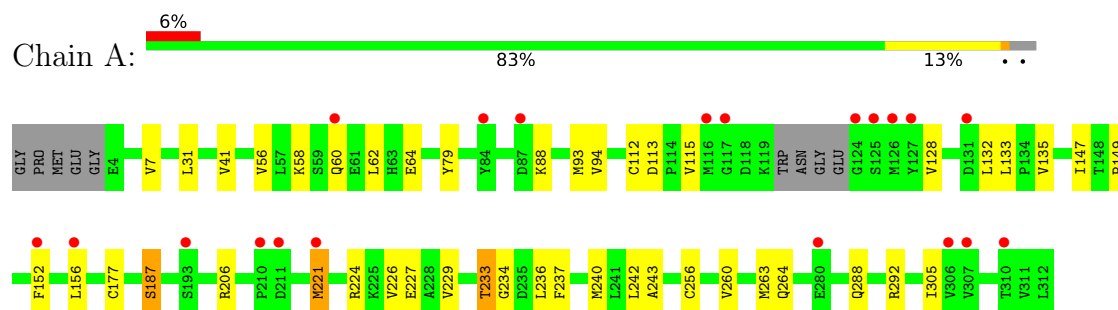
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	B	60	Total	O	0	0
			60	60		
7	C	26	Total	O	0	0
			26	26		
7	D	12	Total	O	0	0
			12	12		

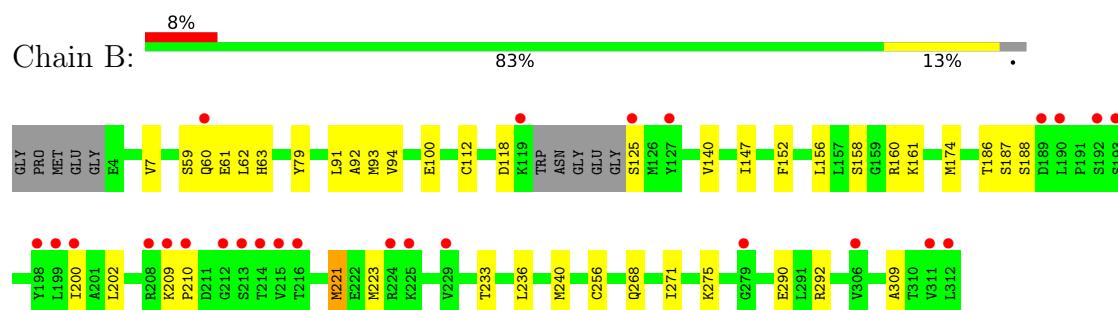
3 Residue-property plots [i](#)

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.

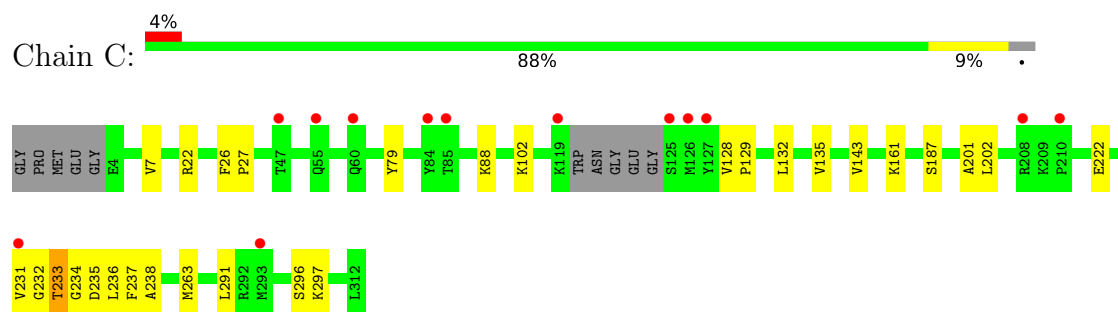
• Molecule 1: Pyridoxal kinase



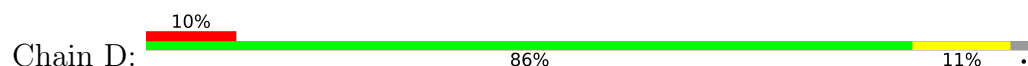
• Molecule 1: Pyridoxal kinase

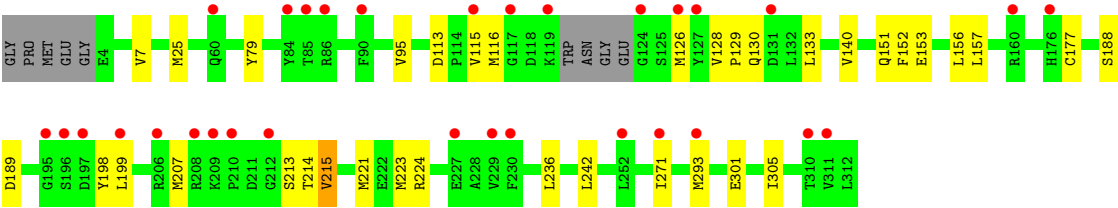


• Molecule 1: Pyridoxal kinase



• 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	279.38Å 53.04Å 110.15Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	47.20 – 2.40 47.20 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.20-2.40) 99.6 (47.20-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.209 , 0.254 0.217 , 0.251	Depositor DCC
R_{free} test set	3237 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19493	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: GOL, AGS, D95, PG4, EDO

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	1.03	18/2414 (0.7%)	0.56	3/3268 (0.1%)
1	B	0.86	16/2424 (0.7%)	0.55	4/3280 (0.1%)
1	C	0.84	13/2408 (0.5%)	0.49	2/3260 (0.1%)
1	D	0.61	0/2377	0.46	0/3227
All	All	0.85	47/9623 (0.5%)	0.52	9/13035 (0.1%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221[A]	MET	CA-C	9.83	1.64	1.52
1	A	221[B]	MET	CA-C	9.83	1.64	1.52
1	B	221[A]	MET	N-CA	8.24	1.56	1.46
1	B	221[B]	MET	N-CA	8.24	1.56	1.46
1	B	221[A]	MET	CA-C	7.60	1.61	1.52
1	B	221[B]	MET	CA-C	7.60	1.61	1.52
1	B	61	GLU	C-O	-7.45	1.15	1.24
1	B	63	HIS	C-O	-7.14	1.15	1.24
1	B	93	MET	C-O	-7.14	1.15	1.24
1	A	115	VAL	C-O	-6.93	1.17	1.23
1	B	59	SER	C-O	-6.64	1.16	1.24
1	B	62	LEU	C-O	-6.61	1.16	1.24
1	C	187	SER	C-O	-6.61	1.15	1.23
1	A	237	PHE	C-O	-6.50	1.16	1.24
1	B	94	VAL	C-O	-6.45	1.16	1.24
1	B	188	SER	C-O	-6.13	1.16	1.23
1	C	234	GLY	C-O	-6.10	1.16	1.23
1	C	235	ASP	C-O	-6.07	1.16	1.24
1	C	291	LEU	C-O	-5.99	1.16	1.23
1	C	231	VAL	C-O	-5.93	1.18	1.24
1	A	113	ASP	C-O	-5.84	1.17	1.24
1	B	187	SER	C-O	-5.82	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	ILE	C-O	-5.82	1.17	1.24
1	A	260	VAL	C-O	-5.79	1.16	1.24
1	C	201	ALA	C-O	-5.78	1.17	1.24
1	A	94	VAL	C-O	-5.77	1.17	1.24
1	A	64	GLU	C-O	-5.74	1.17	1.24
1	A	233	THR	C-O	-5.74	1.17	1.24
1	C	236	LEU	C-O	-5.72	1.17	1.24
1	A	234	GLY	C-O	-5.70	1.17	1.23
1	B	92	ALA	C-O	-5.68	1.17	1.24
1	A	264	GLN	C-O	-5.66	1.17	1.24
1	C	237	PHE	C-O	-5.65	1.17	1.24
1	B	186	THR	C-O	-5.57	1.17	1.24
1	C	232	GLY	C-O	-5.52	1.16	1.24
1	A	226	VAL	C-O	-5.52	1.18	1.24
1	A	224	ARG	C-O	-5.46	1.17	1.23
1	C	233	THR	C-O	-5.45	1.17	1.24
1	C	238	ALA	C-O	-5.37	1.17	1.24
1	C	263	MET	C-O	-5.36	1.17	1.24
1	A	93	MET	C-O	-5.32	1.17	1.24
1	A	62	LEU	C-O	-5.32	1.17	1.24
1	A	187	SER	C-O	-5.32	1.17	1.23
1	A	229	VAL	C-O	-5.09	1.18	1.24
1	C	222	GLU	C-O	-5.09	1.17	1.24
1	B	202	LEU	C-O	-5.04	1.17	1.23
1	A	149	PRO	C-O	-5.04	1.17	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	LEU	CA-C-N	8.44	129.48	121.46
1	C	202	LEU	C-N-CA	8.44	129.48	121.46
1	B	221[A]	MET	CA-C-O	6.96	128.66	120.66
1	B	221[B]	MET	CA-C-O	6.96	128.66	120.66
1	A	221[A]	MET	CA-C-O	6.68	128.62	120.60
1	A	221[B]	MET	CA-C-O	6.68	128.62	120.60
1	A	227	GLU	N-CA-C	5.49	118.12	109.39
1	B	200	ILE	N-CA-C	5.14	115.37	108.17
1	B	202	LEU	O-C-N	-5.04	116.59	123.10

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	2369	2341	2357	17	1
1	B	2379	2357	2373	17	0
1	C	2366	2339	2353	9	0
1	D	2335	2262	2277	23	1
2	A	6	8	8	1	0
2	B	12	16	16	0	0
2	C	18	23	24	0	0
3	A	13	18	18	0	0
4	A	27	28	0	0	0
5	A	31	13	12	1	0
5	B	31	13	12	1	0
5	C	31	13	12	1	0
5	D	31	14	12	1	0
6	A	44	66	65	0	0
6	B	20	30	30	1	0
6	C	28	42	42	0	0
6	D	12	18	18	0	0
7	A	41	0	0	0	0
7	B	60	0	0	1	0
7	C	26	0	0	1	0
7	D	12	0	0	0	0
All	All	9892	9601	9629	68	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 4.

All (68) 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)
5:C:505:AGS:O2B	5:C:505:AGS:S1G	2.29	0.90
1:D:7:VAL:HG22	1:D:79:TYR:HB2	1.67	0.76
1:D:128:VAL:HG22	1:D:129:PRO:HD2	1.67	0.74
5:A:504:AGS:O2G	5:A:504:AGS:O2B	2.05	0.72
2:A:501:GOL:O3	2:A:501:GOL:O1	2.06	0.71
1:D:236:LEU:HD22	1:D:293:MET:HE1	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:LYS:HG3	1:C:135:VAL:HG21	1.80	0.63
1:D:95:VAL:CG2	1:D:140:VAL:HG22	2.28	0.63
1:B:7:VAL:HG22	1:B:79:TYR:HB2	1.81	0.63
1:A:7:VAL:HG22	1:A:79:TYR:HB2	1.83	0.59
1:D:198:TYR:N	1:D:198:TYR:CD2	2.72	0.58
1:B:160:ARG:HD3	1:B:174:MET:HE1	1.87	0.57
1:A:58:LYS:HA	1:A:58:LYS:HE3	1.88	0.55
5:B:403:AGS:S1G	5:B:403:AGS:O1B	2.65	0.55
1:B:158:SER:HB2	1:B:174:MET:HE2	1.91	0.53
1:B:118:ASP:O	1:B:125:SER:N	2.41	0.53
1:B:100:GLU:OE1	6:B:408:EDO:O1	2.25	0.52
1:B:236:LEU:HG	1:B:240:MET:HE2	1.90	0.52
1:B:91:LEU:HD22	1:B:140:VAL:HG21	1.92	0.52
1:C:128:VAL:HG13	1:C:129:PRO:HD2	1.93	0.52
1:A:236:LEU:HG	1:A:240:MET:HE2	1.93	0.51
1:A:133:LEU:HD12	1:A:133:LEU:O	2.11	0.50
1:B:209:LYS:HB3	1:B:210:PRO:HD2	1.93	0.50
1:D:151:GLN:NE2	1:D:189:ASP:OD1	2.44	0.50
1:A:305:ILE:H	1:A:305:ILE:HD12	1.76	0.49
1:A:242:LEU:C	1:A:242:LEU:HD23	2.38	0.49
1:D:207:MET:HB2	1:D:215:VAL:HG13	1.95	0.49
1:D:305:ILE:HD12	1:D:305:ILE:H	1.77	0.49
1:D:133:LEU:HD12	1:D:133:LEU:O	2.12	0.49
1:A:58:LYS:HA	1:A:58:LYS:CE	2.43	0.48
1:C:7:VAL:HG22	1:C:79:TYR:HB2	1.96	0.47
1:A:128:VAL:CG2	1:A:132:LEU:HD12	2.45	0.46
1:A:128:VAL:HG21	1:A:132:LEU:HD12	1.97	0.46
1:D:116:MET:HE1	1:D:157:LEU:HD21	1.98	0.46
1:B:221[A]:MET:HE1	1:B:256:CYS:HB3	1.98	0.46
1:A:152:PHE:CE2	1:A:156:LEU:HD11	2.51	0.46
1:C:297:LYS:NZ	1:D:301:GLU:OE2	2.38	0.46
1:A:221[B]:MET:SD	1:A:256:CYS:HB3	2.56	0.45
1:D:126:MET:HE1	1:D:130:GLN:HA	1.97	0.45
1:D:128:VAL:HG22	1:D:129:PRO:CD	2.43	0.45
1:D:113:ASP:OD1	5:D:402:AGS:S1G	2.75	0.45
1:C:102:LYS:NZ	1:C:143:VAL:O	2.48	0.45
1:D:221:MET:HE2	1:D:221:MET:HB3	1.84	0.45
1:A:288:GLN:O	1:A:292:ARG:NH2	2.50	0.44
1:A:305:ILE:HD12	1:A:305:ILE:N	2.32	0.44
1:B:271:ILE:O	1:B:275:LYS:HG2	2.18	0.44
1:B:290:GLU:O	1:B:292:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLN:OE1	1:D:188:SER:HB2	2.18	0.43
1:B:161:LYS:NZ	7:B:503:HOH:O	2.51	0.43
1:A:31:LEU:HD13	1:A:243:ALA:CB	2.49	0.43
1:B:112:CYS:O	1:B:147:ILE:HA	2.18	0.43
1:B:268:GLN:O	1:B:271:ILE:HG22	2.19	0.43
1:C:161:LYS:NZ	7:C:602:HOH:O	2.51	0.43
1:B:152:PHE:CE2	1:B:156:LEU:HD11	2.54	0.43
1:D:115:VAL:HA	1:D:153:GLU:OE2	2.19	0.42
1:D:271:ILE:HD12	1:D:271:ILE:HA	1.92	0.42
1:B:221[A]:MET:HE2	1:B:309:ALA:HB2	2.00	0.42
1:C:26:PHE:HB3	1:C:27:PRO:HD3	2.01	0.42
1:B:221[B]:MET:HB3	1:B:221[B]:MET:HE2	1.86	0.41
1:D:213:SER:OG	1:D:214:THR:N	2.50	0.41
1:A:88:LYS:HG3	1:A:135:VAL:HG21	2.03	0.41
1:D:223:MET:HE2	1:D:223:MET:HB2	1.86	0.41
1:C:296:SER:O	1:C:297:LYS:C	2.64	0.40
1:A:41:VAL:HG12	1:A:56:VAL:HA	2.03	0.40
1:A:112:CYS:O	1:A:147:ILE:HA	2.22	0.40
1:D:152:PHE:CE2	1:D:156:LEU:HD11	2.56	0.40
1:C:22:ARG:CZ	1:D:25:MET:HE1	2.51	0.40
1:D:242:LEU:C	1:D:242:LEU:HD23	2.47	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:177:CYS:HG	1:D:177:CYS:SG[2_556]	0.90	0.70

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	302/314 (96%)	293 (97%)	9 (3%)	0	100	100
1	B	301/314 (96%)	294 (98%)	7 (2%)	0	100	100
1	C	300/314 (96%)	290 (97%)	10 (3%)	0	100	100
1	D	301/314 (96%)	289 (96%)	12 (4%)	0	100	100
All	All	1204/1256 (96%)	1166 (97%)	38 (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	261/273 (96%)	256 (98%)	5 (2%)	50	71
1	B	264/273 (97%)	261 (99%)	3 (1%)	65	82
1	C	262/273 (96%)	260 (99%)	2 (1%)	73	86
1	D	254/273 (93%)	251 (99%)	3 (1%)	63	81
All	All	1041/1092 (95%)	1028 (99%)	13 (1%)	61	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	187	SER
1	A	206	ARG
1	A	233	THR
1	A	263	MET
1	B	60	GLN
1	B	223	MET
1	B	233	THR
1	C	132	LEU
1	C	233	THR
1	D	199	LEU
1	D	215	VAL
1	D	224	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	163	HIS
1	A	246	HIS
1	A	248	HIS
1	B	11	GLN
1	B	60	GLN
1	B	194	GLN
1	C	51	HIS
1	C	60	GLN
1	C	248	HIS
1	C	265	HIS
1	D	104	GLN
1	D	194	GLN
1	D	288	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](#)

38 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
6	EDO	A	515	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	D	403	-	3,3,3	0.42	0	2,2,2	0.36	0
6	EDO	C	509	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	A	507	-	3,3,3	0.80	0	2,2,2	0.95	0
5	AGS	C	505	-	32,33,33	2.81	11 (34%)	45,52,52	1.94	13 (28%)
2	GOL	C	502	-	5,5,5	0.90	0	5,5,5	1.03	0
6	EDO	A	514	-	3,3,3	0.43	0	2,2,2	0.37	0
5	AGS	A	504	-	32,33,33	2.51	11 (34%)	45,52,52	2.06	12 (26%)
3	PG4	A	502	-	12,12,12	0.53	0	11,11,11	0.28	0
6	EDO	B	408	-	3,3,3	0.41	0	2,2,2	0.59	0
6	EDO	A	505	-	3,3,3	0.43	0	2,2,2	0.36	0
6	EDO	B	406	-	3,3,3	0.44	0	2,2,2	0.31	0
6	EDO	C	511	-	3,3,3	0.43	0	2,2,2	0.32	0
2	GOL	C	503	-	5,5,5	0.89	0	5,5,5	1.09	0
6	EDO	B	404	-	3,3,3	0.42	0	2,2,2	0.38	0
6	EDO	D	401	-	3,3,3	0.43	0	2,2,2	0.33	0
6	EDO	A	508	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	A	506	-	3,3,3	0.40	0	2,2,2	0.37	0
6	EDO	D	404	-	3,3,3	0.43	0	2,2,2	0.35	0
2	GOL	C	504	-	5,5,5	0.89	0	5,5,5	1.02	0
6	EDO	C	510	-	3,3,3	0.42	0	2,2,2	0.30	0
2	GOL	B	401	-	5,5,5	0.88	0	5,5,5	0.99	0
6	EDO	A	513	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	A	512	-	3,3,3	0.44	0	2,2,2	0.34	0
6	EDO	B	405	-	3,3,3	0.43	0	2,2,2	0.36	0
2	GOL	A	501	-	5,5,5	0.89	0	5,5,5	0.93	0
5	AGS	D	402	-	32,33,33	2.47	10 (31%)	45,52,52	2.14	13 (28%)
6	EDO	B	407	-	3,3,3	0.40	0	2,2,2	0.37	0
6	EDO	A	511	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	C	506	-	3,3,3	0.42	0	2,2,2	0.36	0
5	AGS	B	403	-	32,33,33	2.37	12 (37%)	45,52,52	2.03	14 (31%)
2	GOL	B	402	-	5,5,5	0.91	0	5,5,5	1.06	0
6	EDO	A	509	-	3,3,3	0.43	0	2,2,2	0.35	0
6	EDO	C	501	-	3,3,3	0.42	0	2,2,2	0.36	0
6	EDO	C	507	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	C	508	-	3,3,3	0.43	0	2,2,2	0.39	0
6	EDO	A	510	-	3,3,3	0.43	0	2,2,2	0.37	0
4	D95	A	503	-	30,30,30	0.33	0	46,47,47	1.24	5 (10%)

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
6	EDO	A	515	-	-	0/1/1/1	-
6	EDO	D	403	-	-	0/1/1/1	-
6	EDO	C	509	-	-	0/1/1/1	-
6	EDO	A	507	-	-	0/1/1/1	-
5	AGS	C	505	-	-	5/21/38/38	0/3/3/3
2	GOL	C	502	-	-	2/4/4/4	-
6	EDO	A	514	-	-	0/1/1/1	-
5	AGS	A	504	-	-	2/21/38/38	0/3/3/3
3	PG4	A	502	-	-	3/10/10/10	-
6	EDO	B	408	-	-	0/1/1/1	-
6	EDO	A	505	-	-	0/1/1/1	-
6	EDO	B	406	-	-	1/1/1/1	-
6	EDO	C	511	-	-	0/1/1/1	-
2	GOL	C	503	-	-	2/4/4/4	-
6	EDO	B	404	-	-	1/1/1/1	-
6	EDO	D	401	-	-	0/1/1/1	-
6	EDO	A	508	-	-	0/1/1/1	-
6	EDO	A	506	-	-	0/1/1/1	-
6	EDO	D	404	-	-	0/1/1/1	-
2	GOL	C	504	-	-	0/4/4/4	-
6	EDO	C	510	-	-	1/1/1/1	-
2	GOL	B	401	-	-	0/4/4/4	-
6	EDO	A	513	-	-	0/1/1/1	-
6	EDO	A	512	-	-	1/1/1/1	-
6	EDO	B	405	-	-	0/1/1/1	-
2	GOL	A	501	-	-	0/4/4/4	-
5	AGS	D	402	-	-	5/21/38/38	0/3/3/3
6	EDO	B	407	-	-	0/1/1/1	-
6	EDO	A	511	-	-	0/1/1/1	-
6	EDO	C	506	-	-	0/1/1/1	-
5	AGS	B	403	-	-	4/21/38/38	0/3/3/3
2	GOL	B	402	-	-	2/4/4/4	-
6	EDO	A	509	-	-	0/1/1/1	-
6	EDO	C	501	-	-	0/1/1/1	-
6	EDO	C	507	-	-	0/1/1/1	-
6	EDO	C	508	-	-	0/1/1/1	-
6	EDO	A	510	-	-	0/1/1/1	-
4	D95	A	503	-	-	5/9/66/66	0/5/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	505	AGS	PA-O3A	-7.76	1.51	1.59
5	C	505	AGS	PB-O3A	-6.11	1.52	1.59
5	D	402	AGS	PG-S1G	5.75	2.03	1.90
5	A	504	AGS	PG-S1G	5.18	2.01	1.90
5	A	504	AGS	PB-O3B	-5.14	1.53	1.59
5	D	402	AGS	PB-O3B	-5.08	1.54	1.59
5	B	403	AGS	PG-S1G	5.05	2.01	1.90
5	D	402	AGS	PB-O3A	-4.77	1.54	1.59
5	A	504	AGS	PA-O3A	-4.77	1.54	1.59
5	D	402	AGS	PA-O3A	-4.74	1.54	1.59
5	C	505	AGS	C5-N7	-4.59	1.30	1.39
5	A	504	AGS	PB-O3A	-4.54	1.54	1.59
5	C	505	AGS	PG-S1G	4.46	2.00	1.90
5	B	403	AGS	C5-N7	-4.45	1.31	1.39
5	A	504	AGS	C5-N7	-4.33	1.31	1.39
5	B	403	AGS	PA-O3A	-4.20	1.55	1.59
5	B	403	AGS	C4-N9	-4.14	1.29	1.37
5	D	402	AGS	C5-N7	-3.98	1.31	1.39
5	C	505	AGS	C4-N9	-3.95	1.29	1.37
5	B	403	AGS	PG-O3G	-3.94	1.42	1.54
5	B	403	AGS	C8-N9	-3.88	1.31	1.37
5	C	505	AGS	C8-N9	-3.87	1.31	1.37
5	C	505	AGS	PG-O3G	-3.82	1.42	1.54
5	C	505	AGS	PB-O3B	-3.75	1.55	1.59
5	A	504	AGS	C4-N9	-3.64	1.30	1.37
5	A	504	AGS	C8-N9	-3.60	1.31	1.37
5	D	402	AGS	C4-N9	-3.51	1.30	1.37
5	A	504	AGS	PG-O3G	-3.42	1.43	1.54
5	B	403	AGS	PB-O3A	-3.38	1.55	1.59
5	D	402	AGS	PG-O3G	-3.16	1.44	1.54
5	D	402	AGS	C8-N9	-2.92	1.32	1.37
5	D	402	AGS	O4'-C4'	-2.89	1.38	1.45
5	D	402	AGS	C5-C4	2.78	1.44	1.39
5	B	403	AGS	PB-O3B	-2.63	1.56	1.59
5	A	504	AGS	C5-C4	2.47	1.43	1.39
5	C	505	AGS	C5-C4	2.37	1.43	1.39
5	B	403	AGS	PA-O2A	-2.37	1.44	1.55
5	B	403	AGS	O4'-C4'	-2.34	1.39	1.45
5	A	504	AGS	O4'-C4'	-2.32	1.39	1.45
5	A	504	AGS	PA-O2A	-2.27	1.44	1.55
5	C	505	AGS	PA-O2A	-2.24	1.45	1.55
5	B	403	AGS	PA-O1A	-2.08	1.43	1.50
5	C	505	AGS	PA-O1A	-2.06	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	AGS	PB-O2B	-2.00	1.46	1.55

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	AGS	PB-O3B-PG	-6.43	109.64	133.17
5	D	402	AGS	PB-O3B-PG	-6.25	110.28	133.17
5	D	402	AGS	C5-C4-N3	-5.94	118.54	126.72
4	A	503	D95	CAI-OAH-CAG	5.63	127.84	115.07
5	A	504	AGS	C5-C4-N3	-5.39	119.30	126.72
5	C	505	AGS	PB-O3B-PG	-5.32	113.70	133.17
5	C	505	AGS	C5-C4-N3	-5.12	119.67	126.72
5	B	403	AGS	C5-C4-N3	-4.88	120.00	126.72
5	D	402	AGS	N3-C4-N9	4.71	135.19	127.17
5	A	504	AGS	N3-C4-N9	4.54	134.89	127.17
5	B	403	AGS	N3-C4-N9	4.37	134.60	127.17
5	B	403	AGS	C4-N9-C8	4.18	110.13	105.74
5	C	505	AGS	N3-C4-N9	4.17	134.25	127.17
5	B	403	AGS	N3-C2-N1	-3.90	122.68	128.58
5	D	402	AGS	C2-N3-C4	3.88	121.32	111.83
5	D	402	AGS	N3-C2-N1	-3.82	122.79	128.58
5	B	403	AGS	C2-N3-C4	3.64	120.71	111.83
5	B	403	AGS	PB-O3B-PG	-3.62	119.92	133.17
5	A	504	AGS	N3-C2-N1	-3.48	123.31	128.58
5	A	504	AGS	C2-N3-C4	3.46	120.29	111.83
5	C	505	AGS	O2G-PG-O3B	3.39	115.95	104.64
5	C	505	AGS	C4-C5-N7	-3.37	106.73	110.58
5	C	505	AGS	C2-N3-C4	3.36	120.04	111.83
5	C	505	AGS	N3-C2-N1	-3.13	123.84	128.58
5	B	403	AGS	N9-C8-N7	-3.05	109.60	113.94
5	D	402	AGS	C4-C5-N7	-3.04	107.11	110.58
5	B	403	AGS	C4-C5-N7	-3.04	107.11	110.58
4	A	503	D95	OAP-OAQ-CAJ	3.01	114.26	111.72
5	A	504	AGS	C4-C5-N7	-2.97	107.19	110.58
4	A	503	D95	OAQ-OAP-CAN	2.96	111.56	108.46
5	A	504	AGS	C4-N9-C8	2.81	108.69	105.74
5	D	402	AGS	O2B-PB-O3A	2.75	114.69	107.27
5	A	504	AGS	O2B-PB-O1B	2.74	125.21	112.44
5	B	403	AGS	O2G-PG-O3B	2.73	113.76	104.64
5	D	402	AGS	C4-N9-C8	2.72	108.59	105.74
5	B	403	AGS	C5-N7-C8	2.71	107.70	103.45
5	C	505	AGS	C4-N9-C8	2.59	108.46	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	AGS	O2B-PB-O3B	-2.58	100.31	107.27
5	A	504	AGS	C2-N1-C6	2.57	122.96	118.73
5	D	402	AGS	C2'-C3'-C4'	2.56	107.55	102.61
5	C	505	AGS	C5-N7-C8	2.43	107.27	103.45
5	C	505	AGS	C2-N1-C6	2.34	122.57	118.73
5	B	403	AGS	C6-C5-N7	2.30	136.53	132.09
5	D	402	AGS	C5-N7-C8	2.27	107.02	103.45
5	D	402	AGS	O3A-PA-O1A	-2.27	103.87	110.70
5	A	504	AGS	C5-N7-C8	2.25	106.99	103.45
5	A	504	AGS	O3G-PG-O3B	2.25	112.16	104.64
5	D	402	AGS	C2-N1-C6	2.23	122.39	118.73
5	B	403	AGS	C2-N1-C6	2.20	122.34	118.73
4	A	503	D95	OAH-CAI-CAJ	2.19	114.96	112.62
5	C	505	AGS	O3B-PB-O1B	2.17	117.23	110.70
5	C	505	AGS	C6-C5-N7	2.15	136.24	132.09
4	A	503	D95	CAM-CAL-CAK	2.13	119.27	114.60
5	D	402	AGS	N9-C8-N7	-2.07	111.00	113.94
5	C	505	AGS	O3A-PB-O1B	-2.06	104.49	110.70
5	B	403	AGS	C2'-C1'-N9	2.06	118.43	113.30
5	B	403	AGS	O2B-PB-O3A	2.05	112.82	107.27

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	GOL	O1-C1-C2-C3
4	A	503	D95	OAU-CAT-OAS-CAG
5	A	504	AGS	O4'-C4'-C5'-O5'
5	C	505	AGS	O4'-C4'-C5'-O5'
5	D	402	AGS	C5'-O5'-PA-O2A
5	D	402	AGS	C5'-O5'-PA-O3A
5	A	504	AGS	C3'-C4'-C5'-O5'
5	C	505	AGS	C3'-C4'-C5'-O5'
5	B	403	AGS	O4'-C4'-C5'-O5'
5	B	403	AGS	C3'-C4'-C5'-O5'
5	D	402	AGS	O4'-C4'-C5'-O5'
5	D	402	AGS	C3'-C4'-C5'-O5'
2	C	503	GOL	O1-C1-C2-C3
3	A	502	PG4	O3-C5-C6-O4
2	C	502	GOL	O1-C1-C2-C3
4	A	503	D95	CAV-CAT-OAS-CAG
2	C	502	GOL	O2-C2-C3-O3

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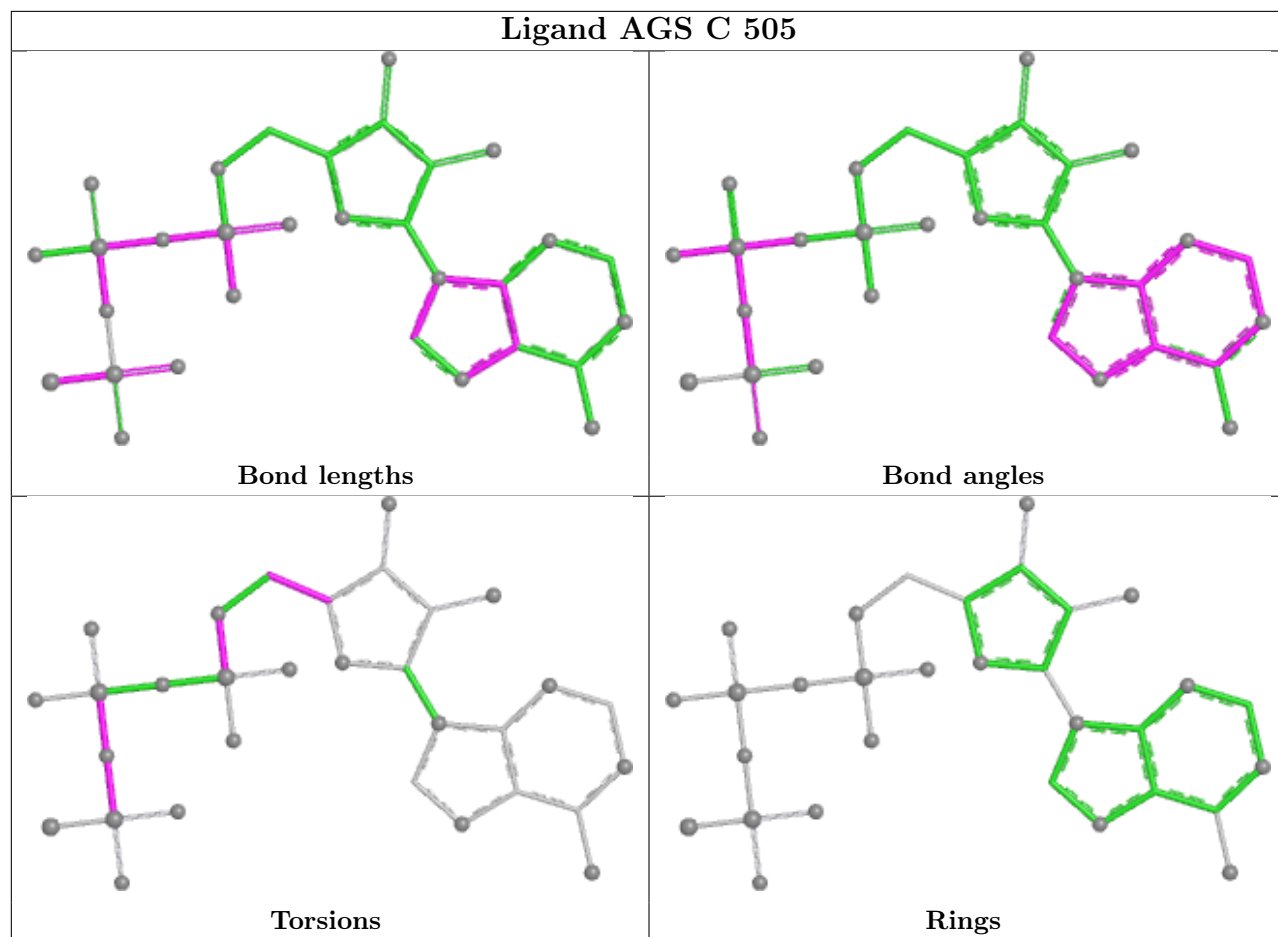
Mol	Chain	Res	Type	Atoms
2	C	503	GOL	O1-C1-C2-O2
2	B	402	GOL	O1-C1-C2-O2
5	B	403	AGS	PB-O3A-PA-O2A
4	A	503	D95	CAT-CAV-CAW-CAX
3	A	502	PG4	O4-C7-C8-O5
5	C	505	AGS	C5'-O5'-PA-O1A
5	D	402	AGS	C5'-O5'-PA-O1A
3	A	502	PG4	O2-C3-C4-O3
6	C	510	EDO	O1-C1-C2-O2
4	A	503	D95	CAV-CAW-CAX-OAY
6	B	404	EDO	O1-C1-C2-O2
5	C	505	AGS	PG-O3B-PB-O2B
5	C	505	AGS	PB-O3B-PG-O3G
4	A	503	D95	CAV-CAW-CAX-OAZ
6	A	512	EDO	O1-C1-C2-O2
6	B	406	EDO	O1-C1-C2-O2
5	B	403	AGS	PB-O3A-PA-O1A

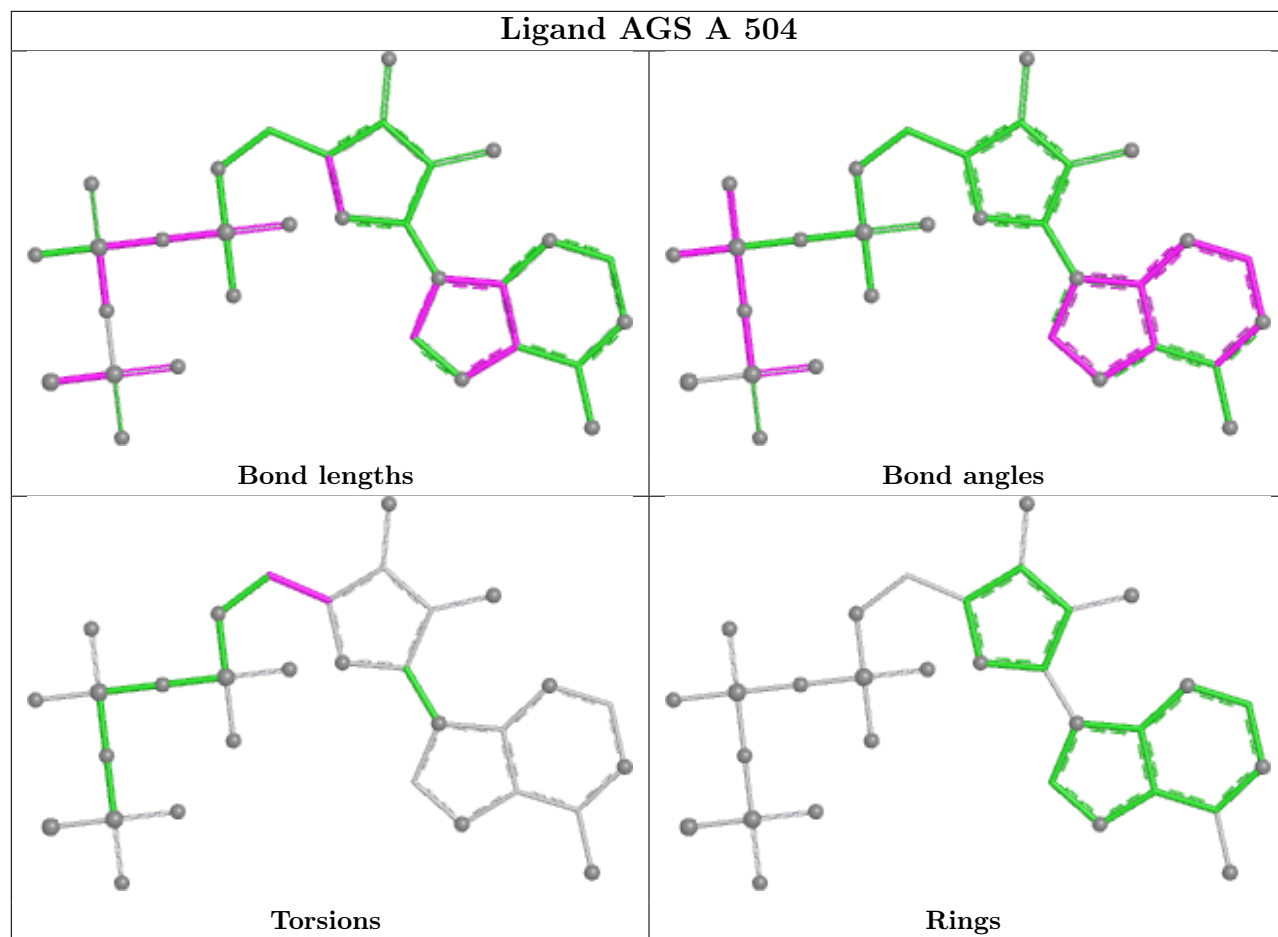
There are no ring outliers.

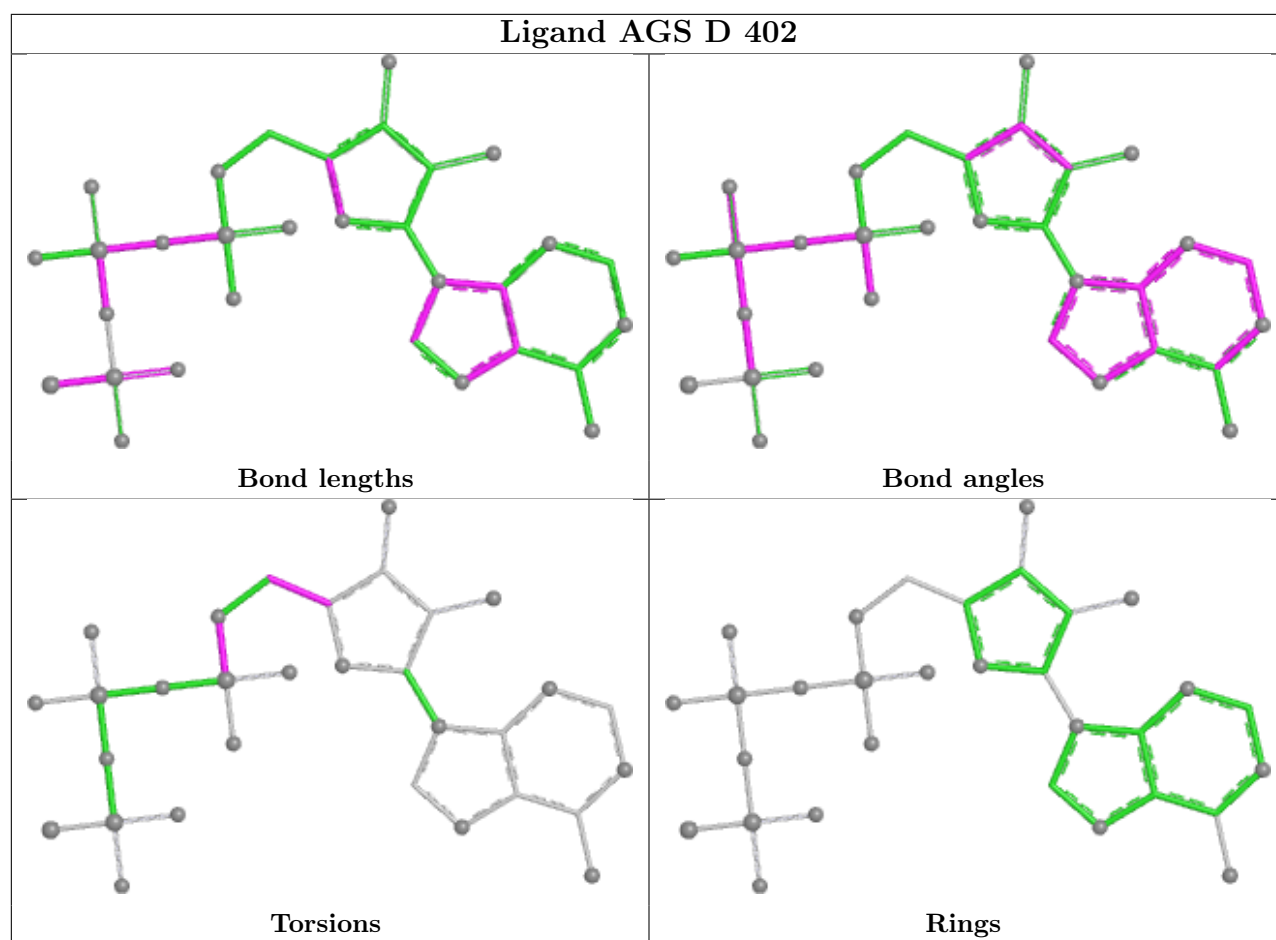
6 monomers are involved in 6 short contacts:

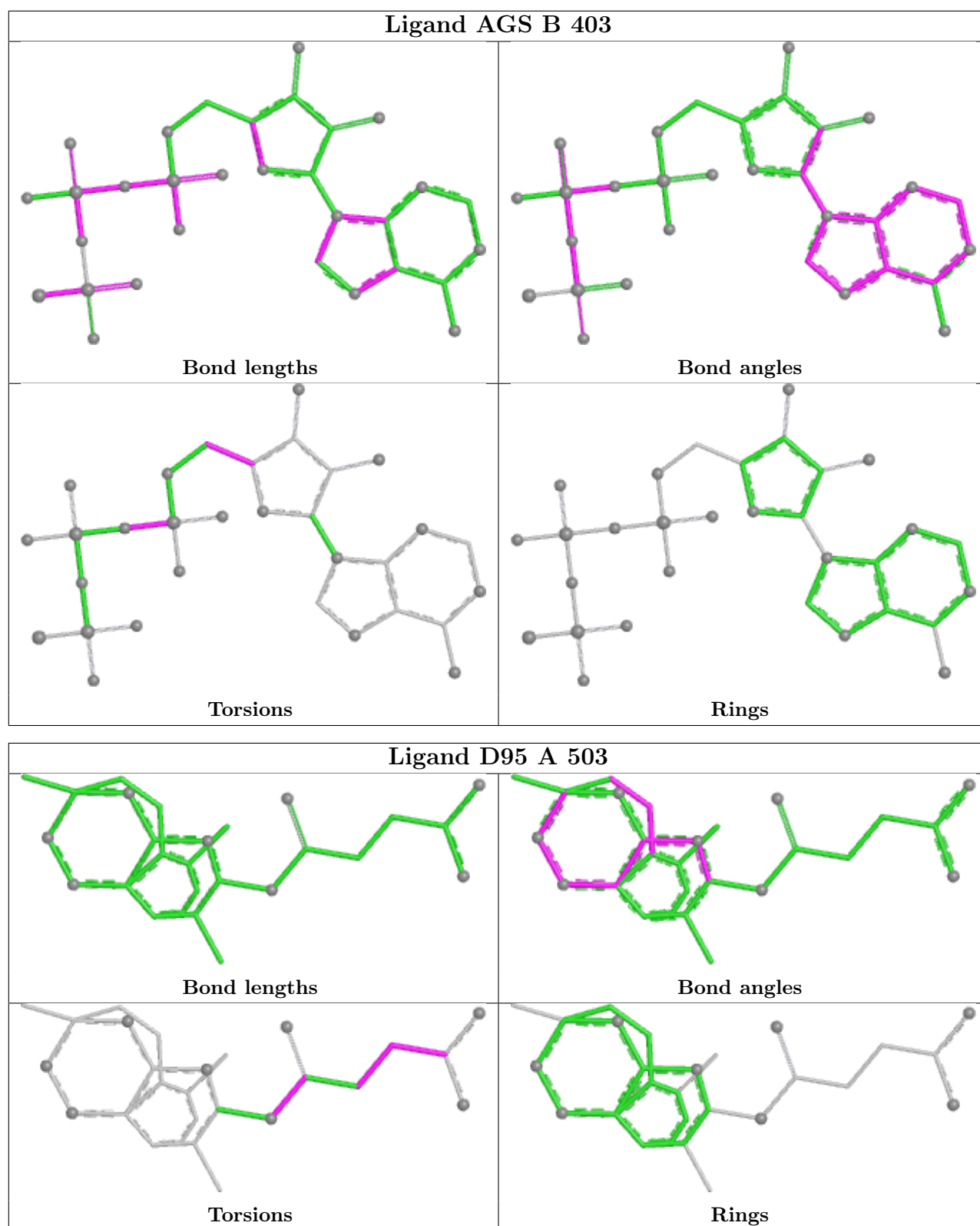
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	505	AGS	1	0
5	A	504	AGS	1	0
6	B	408	EDO	1	0
2	A	501	GOL	1	0
5	D	402	AGS	1	0
5	B	403	AGS	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	305/314 (97%)	0.36	20 (6%)	24 20	42, 66, 102, 145	1 (0%)
1	B	304/314 (96%)	0.47	26 (8%)	16 13	43, 63, 106, 303	1 (0%)
1	C	304/314 (96%)	0.37	13 (4%)	40 36	48, 69, 108, 148	0
1	D	305/314 (97%)	0.88	31 (10%)	12 9	52, 84, 132, 150	0
All	All	1218/1256 (96%)	0.52	90 (7%)	20 17	42, 69, 115, 303	2 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	GLY	5.7
1	B	214	THR	5.3
1	D	60	GLN	4.4
1	D	127	TYR	4.2
1	B	213	SER	4.2
1	A	126	MET	4.2
1	B	210	PRO	3.9
1	C	125	SER	3.9
1	B	119	LYS	3.8
1	B	312	LEU	3.6
1	D	119	LYS	3.5
1	D	208	ARG	3.4
1	D	86	ARG	3.3
1	D	227	GLU	3.3
1	A	117	GLY	3.2
1	B	209	LYS	3.1
1	D	199	LEU	3.1
1	A	152	PHE	3.0
1	C	231	VAL	2.9
1	C	126	MET	2.9
1	D	126	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	60	GLN	2.9
1	D	210	PRO	2.9
1	D	206	ARG	2.8
1	A	211	ASP	2.8
1	C	208	ARG	2.8
1	D	209	LYS	2.8
1	A	193	SER	2.8
1	A	131	ASP	2.8
1	B	198	TYR	2.8
1	D	196	SER	2.8
1	B	229	VAL	2.7
1	B	60	GLN	2.7
1	C	210	PRO	2.7
1	A	306	VAL	2.6
1	C	85	THR	2.6
1	D	90	PHE	2.6
1	B	199	LEU	2.6
1	B	190	LEU	2.6
1	D	85	THR	2.6
1	A	116	MET	2.5
1	B	200	ILE	2.5
1	A	307	VAL	2.5
1	D	229	VAL	2.5
1	D	293	MET	2.5
1	A	125	SER	2.5
1	D	197	ASP	2.4
1	B	215	VAL	2.4
1	D	310	THR	2.4
1	A	124	GLY	2.4
1	D	131	ASP	2.4
1	D	311	VAL	2.4
1	D	124	GLY	2.4
1	D	212	GLY	2.4
1	A	60	GLN	2.4
1	B	189	ASP	2.4
1	B	192	SER	2.3
1	A	156	LEU	2.3
1	B	216	THR	2.3
1	C	127	TYR	2.3
1	B	208	ARG	2.3
1	B	193	SER	2.3
1	A	127	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	84	TYR	2.3
1	B	125	SER	2.2
1	B	311	VAL	2.2
1	D	115	VAL	2.2
1	B	127	TYR	2.2
1	A	221[A]	MET	2.2
1	D	252	LEU	2.2
1	B	224	ARG	2.2
1	B	225	LYS	2.2
1	C	55	GLN	2.2
1	C	47	THR	2.2
1	C	293	MET	2.1
1	B	279	GLY	2.1
1	D	160	ARG	2.1
1	C	119	LYS	2.1
1	D	176	HIS	2.1
1	B	306	VAL	2.1
1	D	230	PHE	2.1
1	D	117	GLY	2.1
1	D	195	GLY	2.1
1	A	84	TYR	2.1
1	A	87	ASP	2.1
1	A	280	GLU	2.0
1	A	310	THR	2.0
1	D	271	ILE	2.0
1	A	210	PRO	2.0
1	C	84	TYR	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](#)

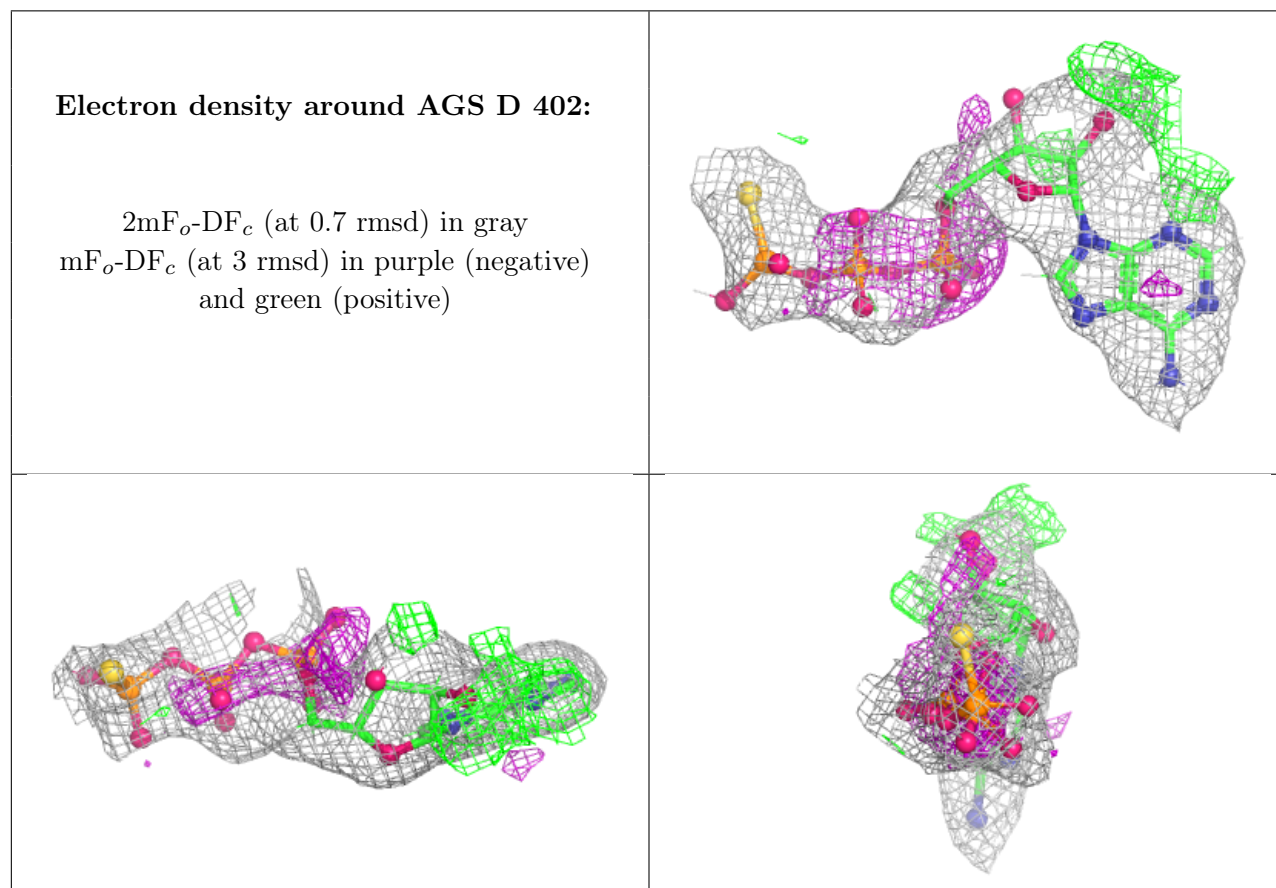
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
2	GOL	C	502	6/6	0.40	0.18	105,127,141,148	0
6	EDO	A	505	4/4	0.53	0.19	88,106,114,114	0
3	PG4	A	502	13/13	0.61	0.19	95,114,125,126	0
2	GOL	A	501	6/6	0.61	0.23	115,138,147,155	0
5	AGS	D	402	31/31	0.62	0.17	83,109,136,163	0
2	GOL	C	504	6/6	0.63	0.20	66,88,94,106	0
6	EDO	C	501	4/4	0.65	0.14	87,105,112,124	0
6	EDO	A	509	4/4	0.66	0.16	96,116,124,124	0
2	GOL	B	401	6/6	0.70	0.14	83,100,113,115	0
6	EDO	A	506	4/4	0.71	0.26	55,67,82,99	0
6	EDO	B	404	4/4	0.75	0.24	65,79,83,86	0
6	EDO	C	506	4/4	0.75	0.15	77,93,101,101	0
6	EDO	C	507	4/4	0.77	0.19	70,84,91,95	0
6	EDO	A	512	4/4	0.78	0.22	74,89,100,105	0
6	EDO	B	406	4/4	0.79	0.22	76,92,96,101	0
5	AGS	A	504	31/31	0.79	0.14	64,81,106,114	0
6	EDO	D	403	4/4	0.79	0.23	68,82,86,88	0
5	AGS	C	505	31/31	0.81	0.13	61,80,111,123	0
6	EDO	A	511	4/4	0.81	0.17	64,77,79,92	0
5	AGS	B	403	31/31	0.81	0.14	65,80,93,97	0
6	EDO	A	507	4/4	0.82	0.24	48,58,64,66	0
2	GOL	C	503	6/6	0.82	0.22	78,95,116,116	0
6	EDO	A	515	4/4	0.82	0.19	60,73,78,91	0
6	EDO	D	404	4/4	0.83	0.20	74,89,93,96	0
4	D95	A	503	27/27	0.84	0.23	65,96,114,115	0
6	EDO	B	408	4/4	0.85	0.19	71,86,90,93	0
6	EDO	A	513	4/4	0.85	0.14	65,81,97,100	0
6	EDO	C	509	4/4	0.86	0.18	76,91,95,95	0
6	EDO	A	514	4/4	0.86	0.17	68,82,90,99	0
6	EDO	C	508	4/4	0.86	0.21	63,76,87,91	0
2	GOL	B	402	6/6	0.87	0.11	62,74,88,90	0
6	EDO	C	511	4/4	0.87	0.19	82,99,103,113	0
6	EDO	A	508	4/4	0.88	0.27	69,83,90,94	0
6	EDO	A	510	4/4	0.89	0.17	71,85,98,102	0
6	EDO	C	510	4/4	0.90	0.17	63,76,83,88	0
6	EDO	D	401	4/4	0.91	0.17	43,60,78,94	0
6	EDO	B	407	4/4	0.92	0.13	43,52,60,65	0
6	EDO	B	405	4/4	0.93	0.14	62,75,84,87	0

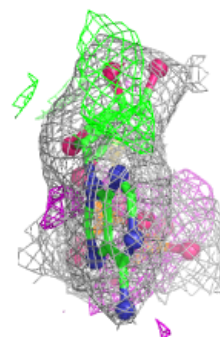
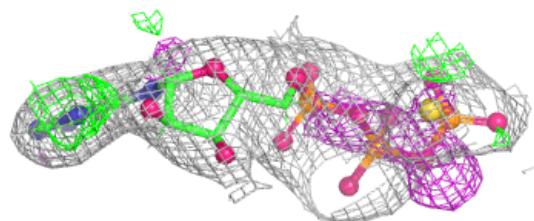
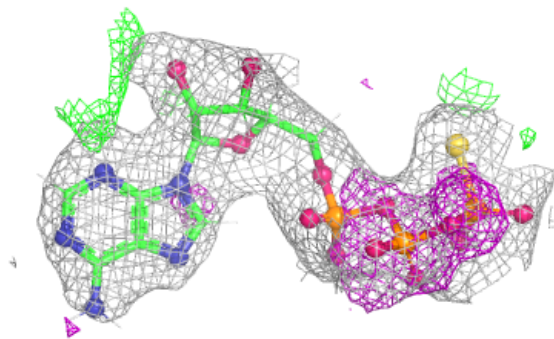
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

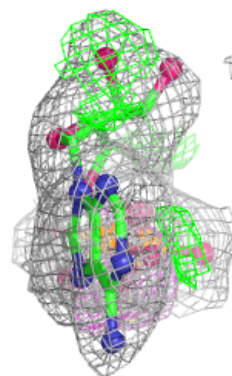
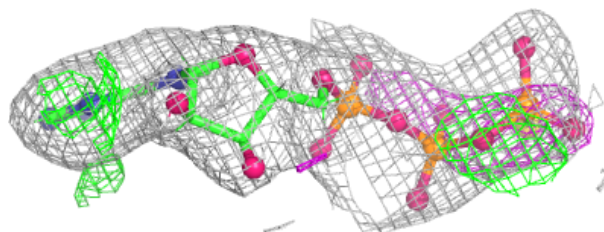
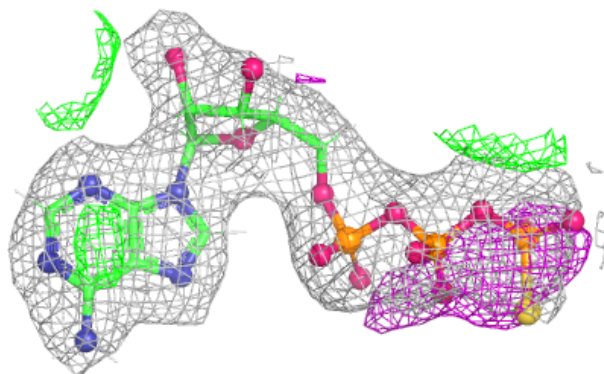


Electron density around AGS A 504:

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

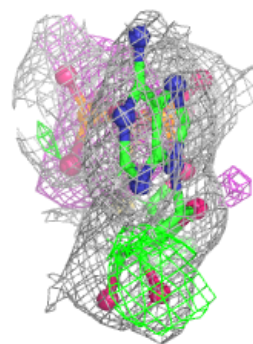
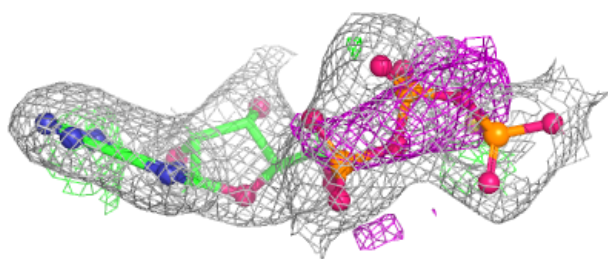
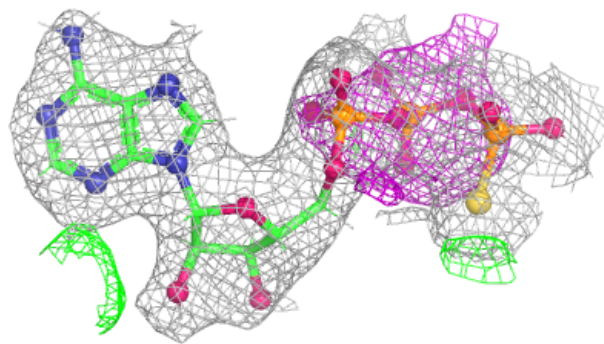
**Electron density around AGS C 505:**

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

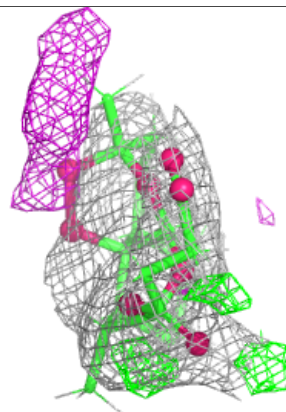
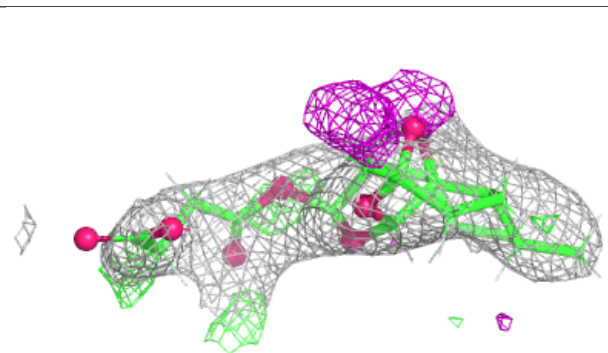
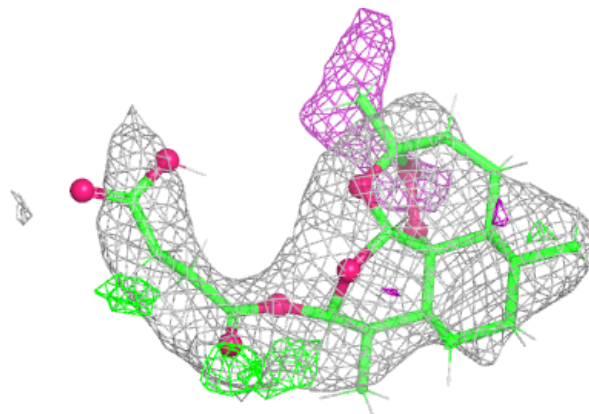


Electron density around AGS B 403:

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

**Electron density around D95 A 503:**

$2mF_o-DF_c$ (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.