



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:21 AM UTC

PDB ID : 7KDY / pdb_00007kdy
Title : Crystal structure of Streptomyces tokunonesis TokK with hydroxycobalamin, 5'-deoxyadenosine, methionine, and (2R)-pantetheinylated carbapenam
Authors : Knox, H.L.; Booker, S.J.; Boal, A.K.
Deposited on : 2020-10-09
Resolution : 1.94 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

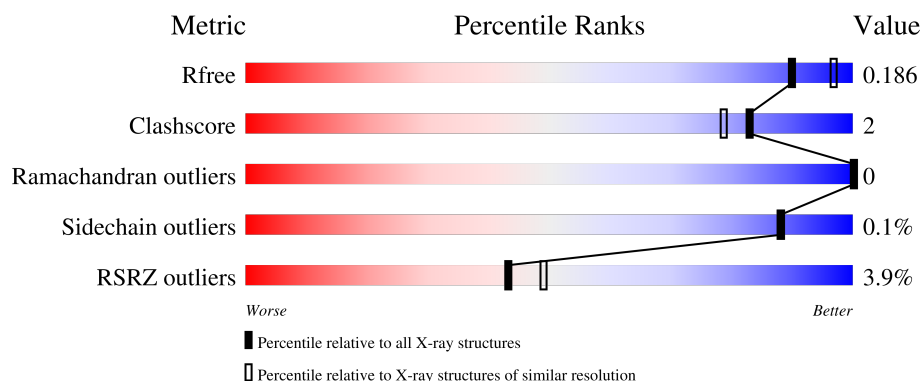
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	681	6% 90% 7% .
1	B	681	2% 93% . .

2 Entry composition [i](#)

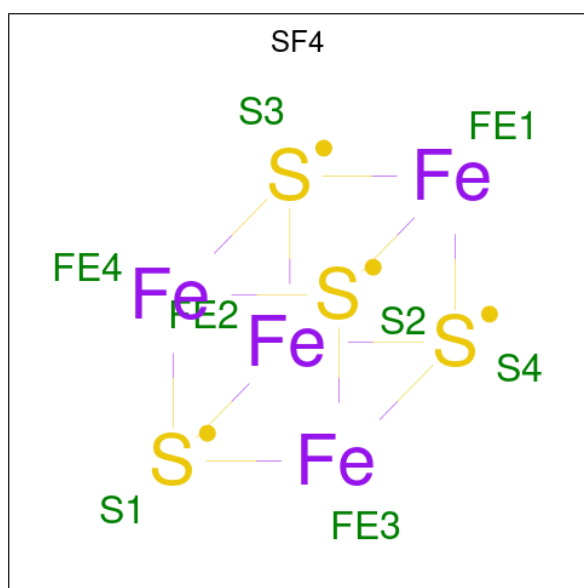
There are 9 unique types of molecules in this entry. The entry contains 12159 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Methyltransferase TokK.

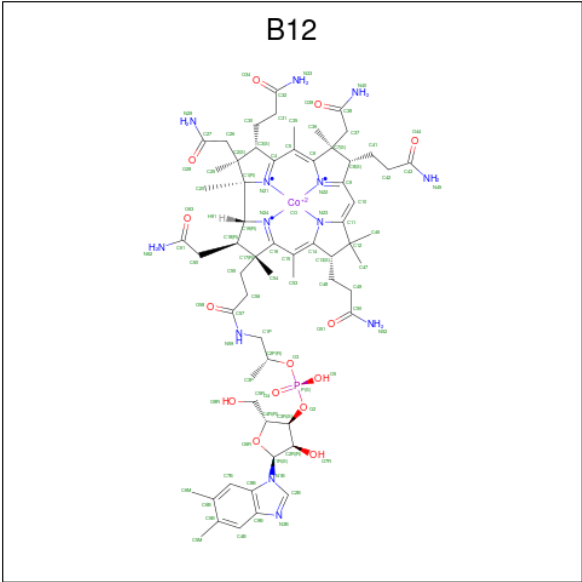
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	4	0
			5328	3387	937	976	28			
1	B	664	Total	C	N	O	S	0	3	0
			5341	3395	937	981	28			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



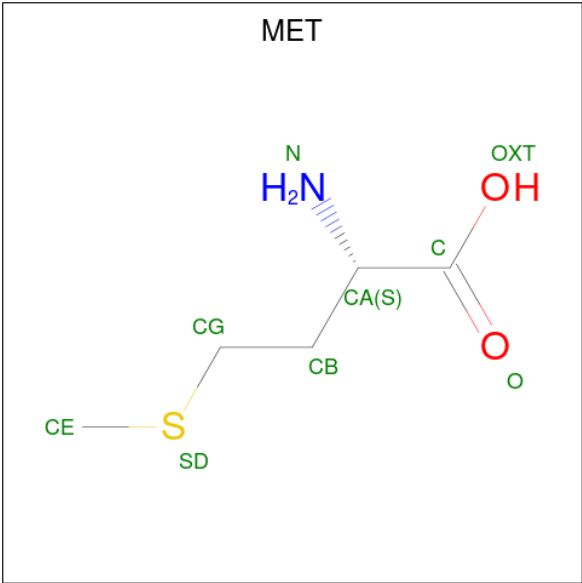
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $\text{C}_{62}\text{H}_{89}\text{CoN}_{13}\text{O}_{14}\text{P}$) (labeled as "Ligand of Interest" by depositor).



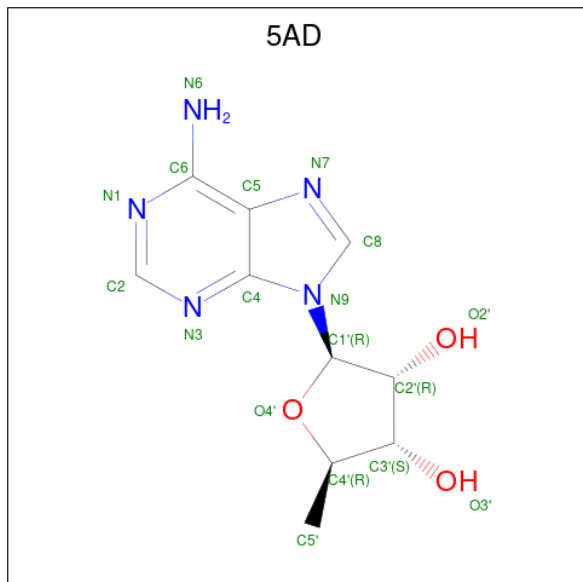
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
3	B	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 4 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



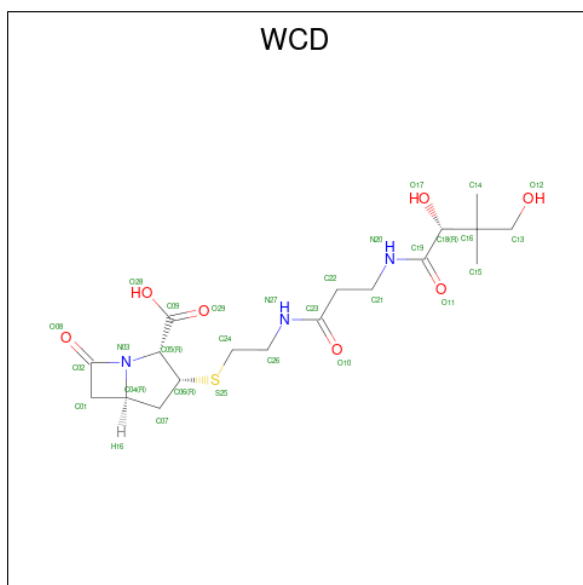
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 5 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	10	5	3		
5	B	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is (2R,3R,5R)-3-{{2-({N-[(2R)-2,4-dihydroxy-3,3-dimethylbutanoyl]-beta-alanyl} amino)ethyl}sulfanyl}-7-oxo-1-azabicyclo[3.2.0]heptane-2-carboxylic acid (CCD ID: WCD) (formula: $C_{18}H_{29}N_3O_7S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			29	18	3	7	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

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

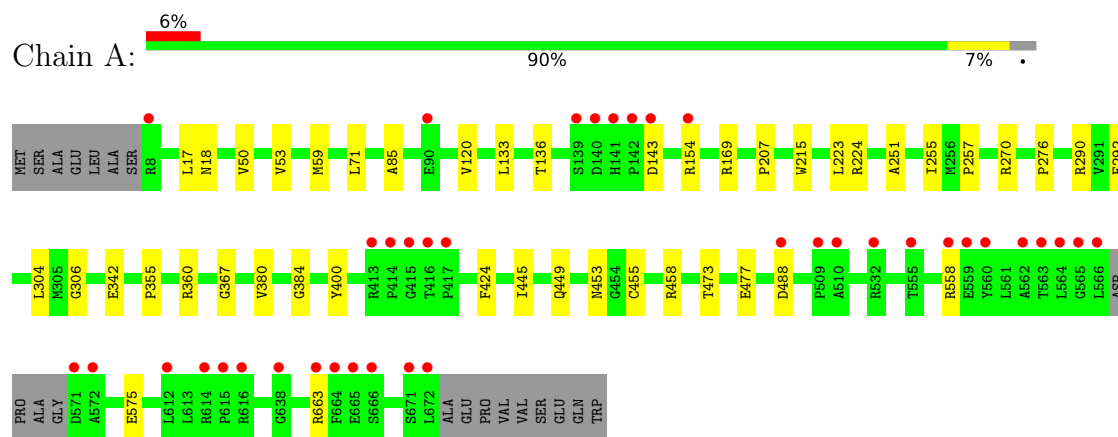
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	513	Total	O	0	0
			513	513		
9	B	680	Total	O	0	0
			680	680		

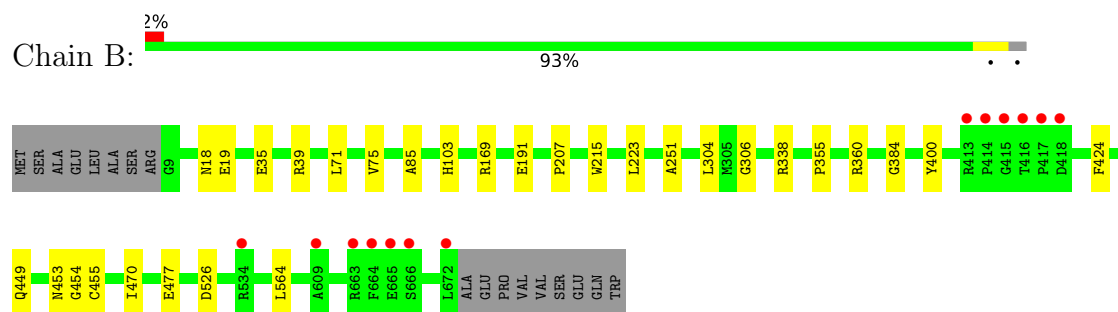
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Methyltransferase TokK



• Molecule 1: Methyltransferase TokK



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.50Å 132.82Å 155.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.19 – 1.94 44.19 – 1.94	Depositor EDS
% Data completeness (in resolution range)	77.9 (44.19-1.94) 96.5 (44.19-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.157 , 0.188 0.157 , 0.186	Depositor DCC
R_{free} test set	2000 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12159	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: K, B12, SF4, 5AD, GOL, WCD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.15	0/5478	0.40	0/7434
1	B	0.17	0/5490	0.41	0/7454
All	All	0.16	0/10968	0.40	0/14888

There are no bond length outliers.

There are no bond angle outliers.

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	5328	0	5178	25	0
1	B	5341	0	5181	20	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	91	0	88	5	0
3	B	91	0	88	6	0
4	A	9	0	8	0	0
4	B	9	0	8	0	0
5	A	18	0	13	0	0
5	B	18	0	13	0	0
6	A	29	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
9	A	513	0	0	2	1
9	B	680	0	0	5	1
All	All	12159	0	10593	52	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 2.

All (52) 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)
3:B:702:B12:H351	3:B:702:B12:H371	1.69	0.73
3:A:702:B12:H351	3:A:702:B12:H371	1.70	0.72
3:A:702:B12:H203	3:A:702:B12:H301	1.74	0.68
3:B:702:B12:H552	3:B:702:B12:H531	1.76	0.66
1:A:18:ASN:HD22	3:A:702:B12:H521	1.41	0.66
1:B:360:ARG:NH1	1:B:477:GLU:OE2	2.28	0.65
3:A:702:B12:H531	3:A:702:B12:H552	1.78	0.64
3:B:702:B12:H301	3:B:702:B12:H203	1.80	0.63
1:B:169[A]:ARG:NH1	9:B:804:HOH:O	2.33	0.61
1:B:18:ASN:ND2	1:B:19:GLU:H	2.02	0.57
1:B:207:PRO:HD3	1:B:223:LEU:HD21	1.86	0.57
1:B:75:VAL:H	3:B:702:B12:H332	1.52	0.57
1:A:255:ILE:HD11	1:B:191:GLU:HG2	1.88	0.56
1:A:558:ARG:NH1	1:A:575:GLU:OE1	2.33	0.56
1:B:338:ARG:NH1	9:B:803:HOH:O	2.28	0.54
1:B:470:ILE:HD13	1:B:564:LEU:HD13	1.92	0.52
1:A:207:PRO:HD3	1:A:223:LEU:HD21	1.92	0.51
1:A:663:ARG:NH1	9:A:804:HOH:O	2.44	0.51
1:B:526:ASP:OD2	9:B:801:HOH:O	2.19	0.50
1:A:215:TRP:CD1	1:A:251:ALA:HB2	2.47	0.49
1:B:304:LEU:HG	1:B:306:GLY:H	1.76	0.49
1:A:488:ASP:OD2	9:A:801:HOH:O	2.20	0.49
3:B:702:B12:H401	3:B:702:B12:C6	2.26	0.49
1:B:384:GLY:HA3	1:B:424:PHE:CZ	2.48	0.48
1:A:17:LEU:HD13	1:A:53:VAL:HG22	1.96	0.47
1:A:71:LEU:HD11	1:A:85:ALA:HB2	1.95	0.47
1:A:355:PRO:HB3	1:A:400:TYR:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:NH2	9:B:819:HOH:O	2.48	0.47
1:A:120:VAL:HG11	1:A:133:LEU:HD11	1.96	0.47
1:A:455[A]:CYS:SG	1:A:458:ARG:NH2	2.88	0.46
1:B:454:GLY:O	1:B:455[A]:CYS:HB2	2.16	0.46
1:A:292:PHE:HZ	1:A:342:GLU:HG3	1.81	0.46
1:B:18:ASN:HD22	1:B:19:GLU:H	1.62	0.45
1:B:71:LEU:HD11	1:B:85:ALA:HB2	1.98	0.45
1:B:355:PRO:HB3	1:B:400:TYR:CG	2.51	0.45
1:B:449:GLN:O	1:B:453:ASN:HB2	2.16	0.45
1:A:367:GLY:HA3	1:A:473:THR:OG1	2.16	0.45
3:A:702:B12:C6	3:A:702:B12:H401	2.30	0.45
1:B:35:GLU:OE1	9:B:802:HOH:O	2.21	0.45
1:B:18:ASN:OD1	3:B:702:B12:N52	2.50	0.44
1:A:154:ARG:HD3	1:A:154:ARG:HA	1.86	0.44
1:A:50:VAL:HG11	1:A:59:MET:HE3	2.00	0.44
1:A:136:THR:HG23	1:A:143:ASP:H	1.82	0.44
1:A:360:ARG:NH2	1:A:477:GLU:OE2	2.50	0.44
1:A:380:VAL:HB	1:A:445:ILE:HD13	2.01	0.43
1:A:169:ARG:HA	1:A:224:ARG:HG2	2.00	0.42
1:B:215:TRP:CD1	1:B:251:ALA:HB2	2.53	0.42
1:A:270:ARG:HD3	1:A:276:PRO:O	2.19	0.42
1:A:384:GLY:HA3	1:A:424:PHE:CZ	2.55	0.42
1:A:257:PRO:HA	1:A:290:ARG:NE	2.34	0.42
1:A:304:LEU:HG	1:A:306:GLY:H	1.85	0.41
1:A:449:GLN:O	1:A:453:ASN:HB2	2.21	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)
9:A:865:HOH:O	9:B:1035:HOH:O[3_544]	2.18	0.02

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	661/681 (97%)	644 (97%)	17 (3%)	0	100	100
1	B	665/681 (98%)	647 (97%)	18 (3%)	0	100	100
All	All	1326/1362 (97%)	1291 (97%)	35 (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	558/569 (98%)	558 (100%)	0	100	100
1	B	558/569 (98%)	557 (100%)	1 (0%)	87	87
All	All	1116/1138 (98%)	1115 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	103	HIS

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	36	GLN
1	A	141	HIS
1	A	540	ASN
1	A	625	GLN
1	B	36	GLN
1	B	141	HIS
1	B	264	HIS
1	B	343	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z > 2$
2	SF4	B	701	1,4	0,12,12	-	-	-		
5	5AD	A	704	-	20,20,20	0.10	0	28,30,30	0.32	0
3	B12	A	702	9	94,101,101	0.86	4 (4%)	149,166,166	1.10	9 (6%)
3	B12	B	702	9	94,101,101	0.91	4 (4%)	149,166,166	1.13	10 (6%)
4	MET	B	703	2	7,8,8	0.89	1 (14%)	5,9,9	1.31	1 (20%)
6	WCD	A	705	-	25,30,30	0.86	1 (4%)	30,43,43	2.36	8 (26%)
4	MET	A	703	2	7,8,8	0.91	1 (14%)	5,9,9	1.26	1 (20%)
2	SF4	A	701	1,4	0,12,12	-	-	-		
5	5AD	B	704	-	20,20,20	0.12	0	28,30,30	0.27	0
7	GOL	B	705	-	5,5,5	1.12	0	5,5,5	0.77	0
7	GOL	A	706	-	5,5,5	0.83	0	5,5,5	1.02	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	701	1,4	-	-	0/6/5/5
5	5AD	A	704	-	-	0/4/20/20	0/3/3/3
3	B12	A	702	9	-	15/56/223/223	0/3/11/11
3	B12	B	702	9	-	15/56/223/223	0/3/11/11
4	MET	B	703	2	-	2/8/8/8	-
6	WCD	A	705	-	-	1/30/54/54	0/2/2/2
4	MET	A	703	2	-	1/8/8/8	-
5	5AD	B	704	-	-	0/4/20/20	0/3/3/3
7	GOL	B	705	-	-	2/4/4/4	-
2	SF4	A	701	1,4	-	-	0/6/5/5
7	GOL	A	706	-	-	0/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	B12	C14-N23	5.80	1.42	1.35
3	A	702	B12	C14-N23	5.36	1.42	1.35
3	B	702	B12	C16-C15	3.93	1.55	1.44
3	A	702	B12	C16-C15	3.64	1.54	1.44
3	B	702	B12	O3-C2P	-2.99	1.37	1.45
3	A	702	B12	O3-C2P	-2.68	1.38	1.45
3	B	702	B12	C9-N22	2.28	1.36	1.30
4	A	703	MET	OXT-C	-2.26	1.23	1.30
6	A	705	WCD	C05-N03	-2.14	1.44	1.47
3	A	702	B12	C9-N22	2.13	1.35	1.30
4	B	703	MET	OXT-C	-2.13	1.23	1.30

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	705	WCD	C01-C02-N03	-7.92	86.13	92.52
3	B	702	B12	C1-C19-N24	-5.12	100.55	106.25
6	A	705	WCD	O29-C09-C05	-4.94	116.30	123.45
3	A	702	B12	C1-C19-N24	-4.60	101.13	106.25
6	A	705	WCD	C04-N03-C02	4.24	100.51	94.19
6	A	705	WCD	C05-N03-C02	3.89	137.15	125.72
3	A	702	B12	C9-N22-C6	3.81	109.86	105.28
3	B	702	B12	C19-N24-C16	3.69	111.32	107.29
6	A	705	WCD	O28-C09-C05	3.67	118.00	111.92
6	A	705	WCD	O08-C02-N03	3.63	136.17	130.31
3	B	702	B12	C9-N22-C6	3.56	109.56	105.28
3	A	702	B12	C19-N24-C16	3.49	111.10	107.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	B12	C35-C5-C4	-3.11	110.50	116.79
3	A	702	B12	C15-C16-N24	-3.10	118.01	122.42
3	B	702	B12	C20-C1-C19	-3.05	106.41	109.35
3	A	702	B12	C35-C5-C4	-2.99	110.74	116.79
4	B	703	MET	OXT-C-O	-2.91	117.48	124.08
3	B	702	B12	C15-C16-N24	-2.85	118.36	122.42
4	A	703	MET	OXT-C-O	-2.81	117.71	124.08
3	B	702	B12	C35-C5-C6	2.57	126.55	122.41
3	A	702	B12	C35-C5-C6	2.41	126.30	122.41
3	B	702	B12	C37-C7-C6	2.37	114.45	107.11
3	A	702	B12	C30-C3-C4	-2.36	104.13	109.66
3	A	702	B12	C20-C1-C19	-2.35	107.09	109.35
3	A	702	B12	C37-C7-C6	2.29	114.21	107.11
3	B	702	B12	C19-C1-N21	2.27	104.48	102.14
6	A	705	WCD	C22-C21-N20	-2.25	107.22	112.00
3	B	702	B12	C13-C14-C15	2.24	127.72	124.32
6	A	705	WCD	C09-C05-N03	2.09	116.72	113.28

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	B12	C7-C37-C38-O39
3	A	702	B12	C3R-O2-P-O5
3	B	702	B12	C7-C37-C38-O39
3	B	702	B12	C3R-O2-P-O5
7	B	705	GOL	O1-C1-C2-C3
3	A	702	B12	C7-C37-C38-N40
3	B	702	B12	C7-C37-C38-N40
3	B	702	B12	C2R-C1R-N1B-C8B
7	B	705	GOL	O1-C1-C2-O2
3	B	702	B12	C30-C31-C32-N33
3	B	702	B12	C30-C31-C32-O34
4	A	703	MET	C-CA-CB-CG
4	B	703	MET	C-CA-CB-CG
3	A	702	B12	C2R-C1R-N1B-C8B
3	A	702	B12	C38-C37-C7-C36
3	B	702	B12	C38-C37-C7-C36
3	A	702	B12	C41-C42-C43-O44
3	B	702	B12	O6R-C1R-N1B-C8B
6	A	705	WCD	C26-C24-S25-C06
3	A	702	B12	C2R-C1R-N1B-C2B

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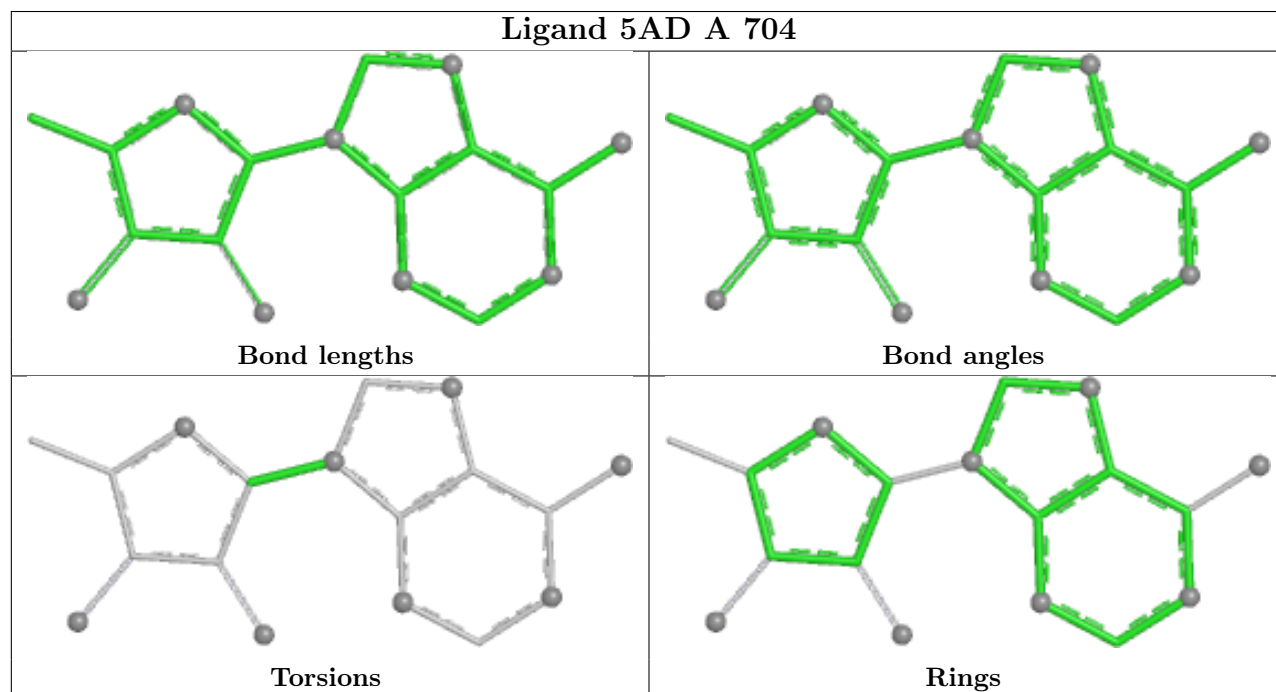
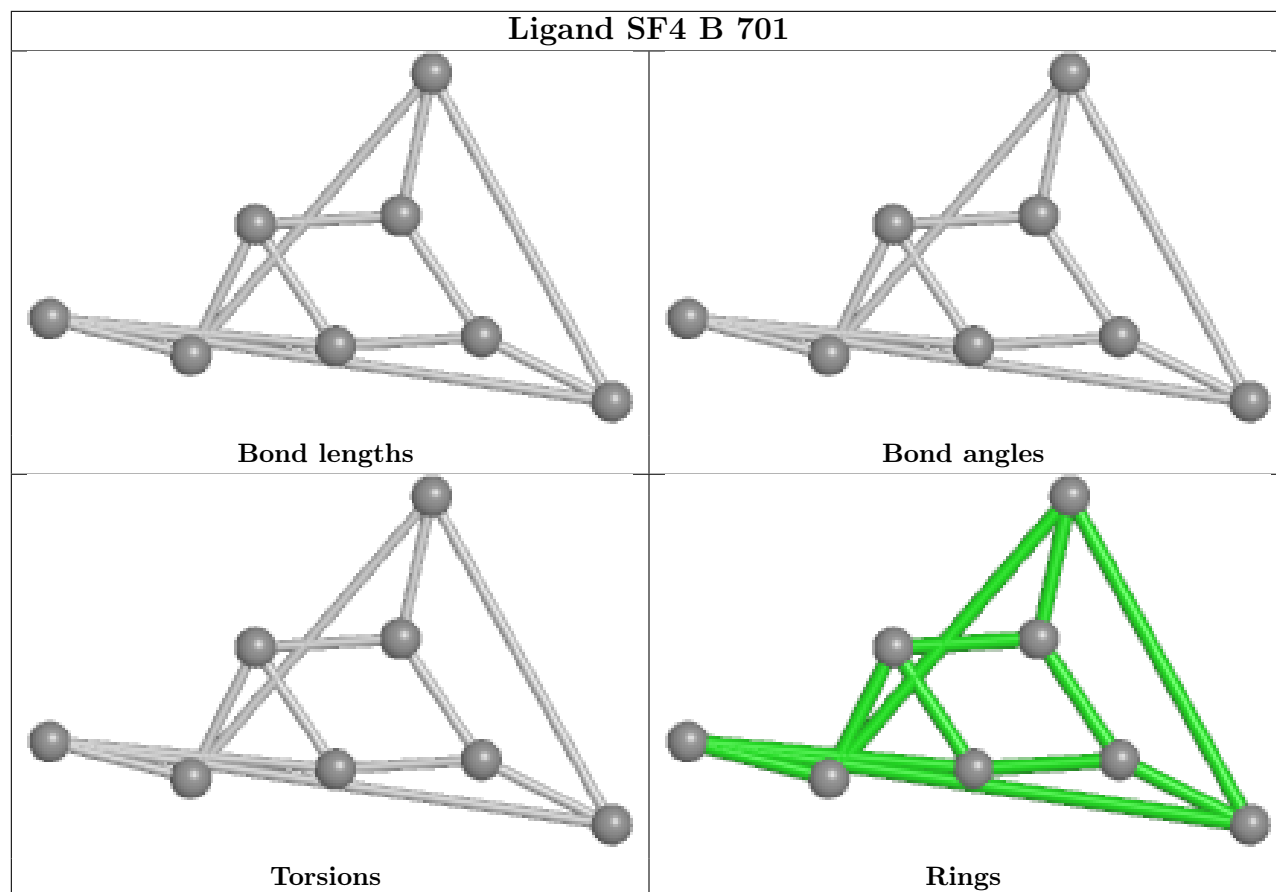
Mol	Chain	Res	Type	Atoms
3	B	702	B12	C2R-C1R-N1B-C2B
3	A	702	B12	C3R-O2-P-O4
3	B	702	B12	C3R-O2-P-O4
3	A	702	B12	C41-C42-C43-N45
3	A	702	B12	O6R-C1R-N1B-C8B
3	A	702	B12	C48-C49-C50-O51
3	B	702	B12	C55-C56-C57-O58
3	A	702	B12	C48-C49-C50-N52
3	B	702	B12	C55-C56-C57-N59
3	A	702	B12	C55-C56-C57-O58
3	B	702	B12	O6R-C1R-N1B-C2B
3	A	702	B12	C55-C56-C57-N59
3	B	702	B12	C48-C49-C50-O51
3	A	702	B12	O6R-C1R-N1B-C2B
3	B	702	B12	C48-C49-C50-N52
4	B	703	MET	OXT-C-CA-N

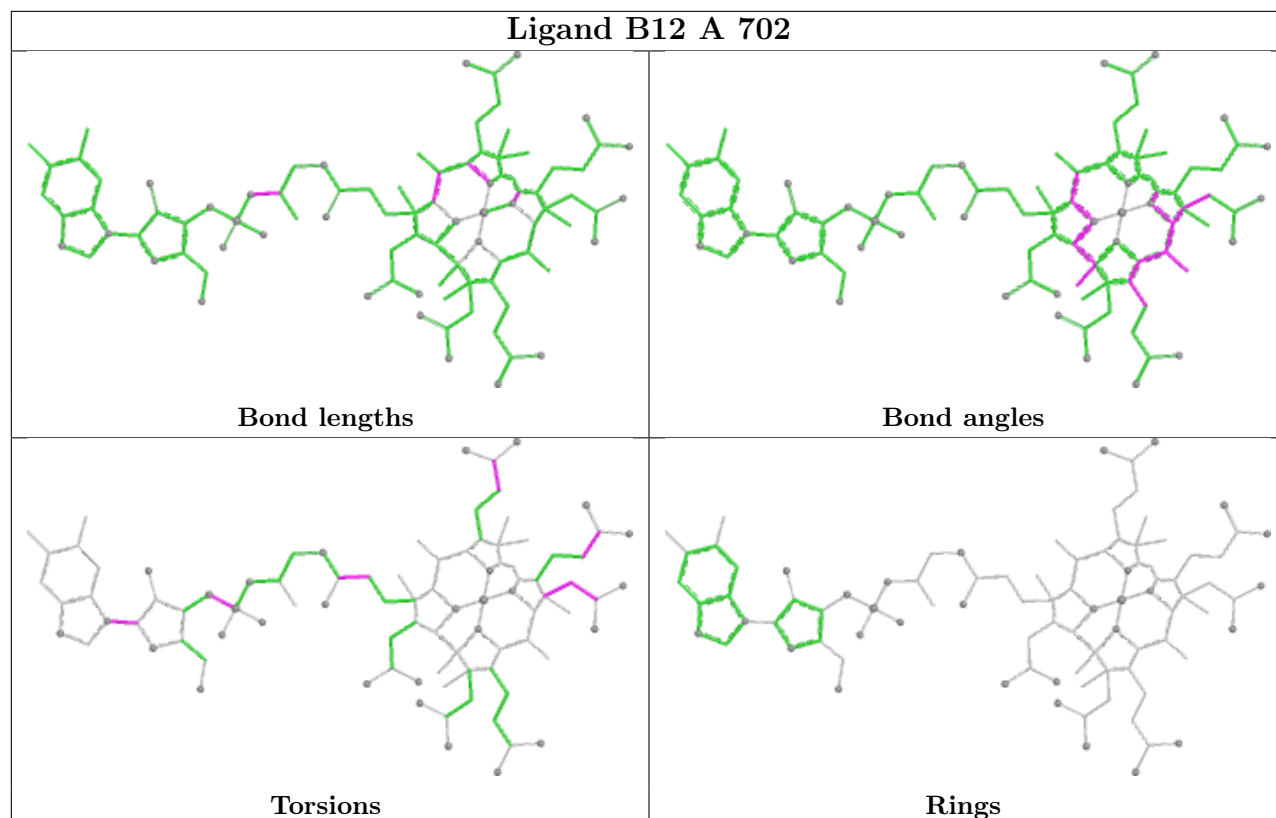
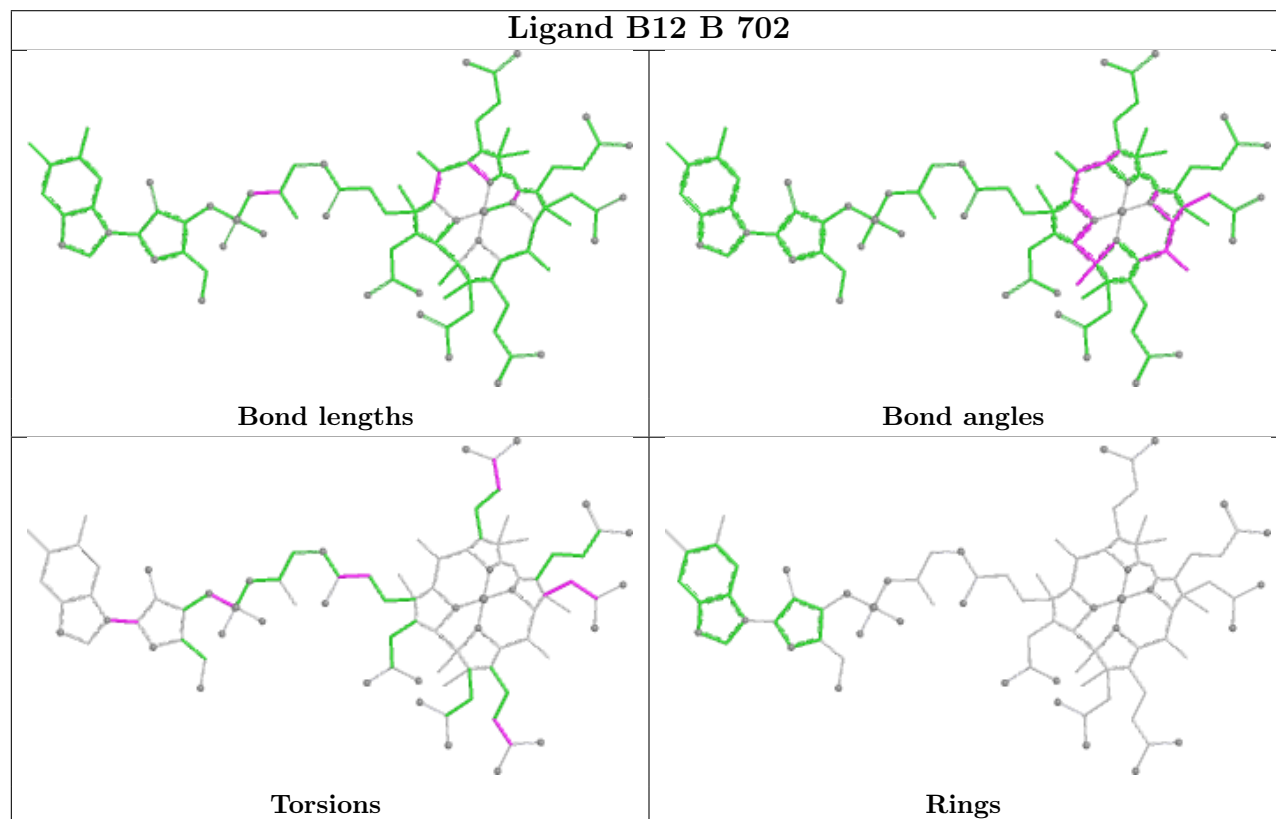
There are no ring outliers.

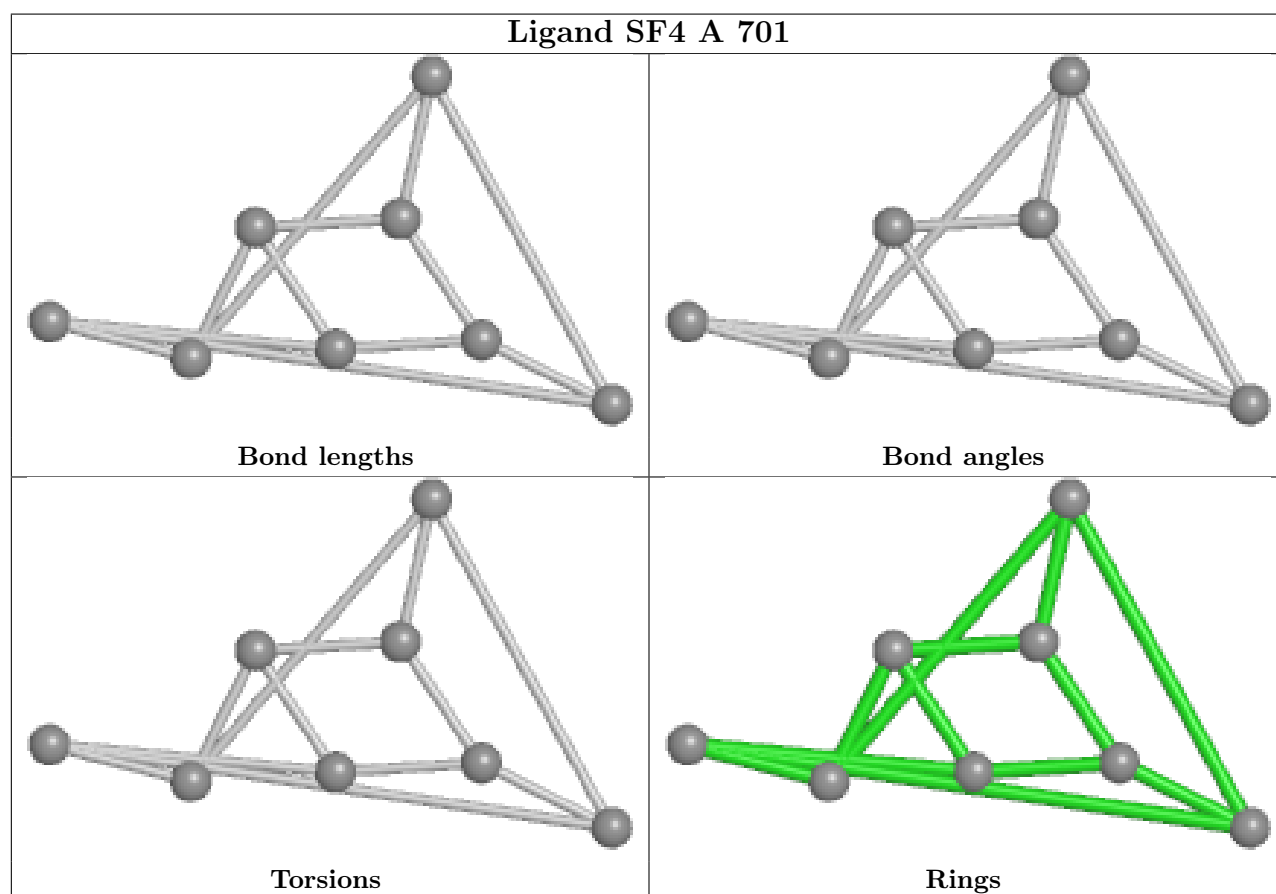
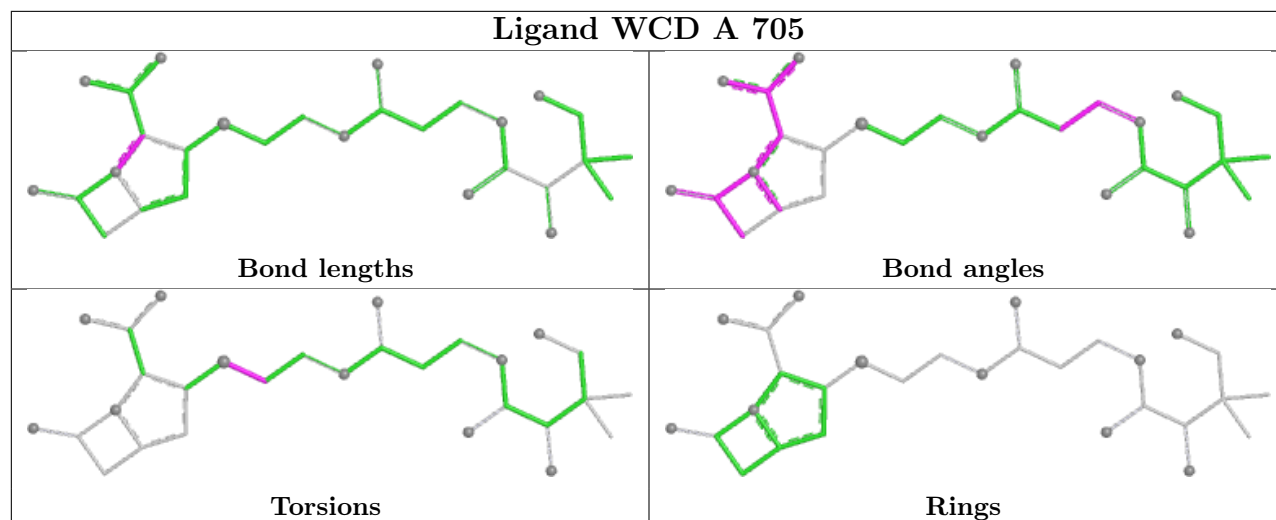
2 monomers are involved in 11 short contacts:

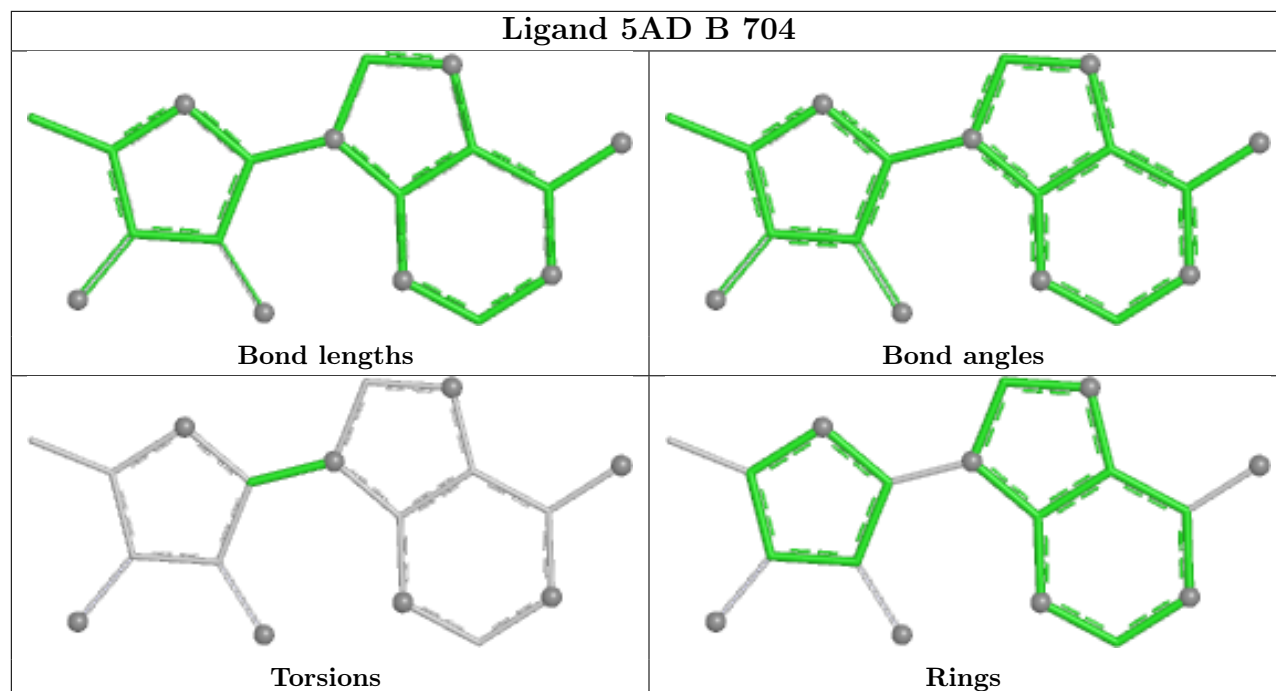
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	B12	5	0
3	B	702	B12	6	0

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 B12 A 702**Ligand B12 B 702**





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	661/681 (97%)	0.06	39 (5%)	28 31	9, 25, 53, 98	4 (0%)
1	B	664/681 (97%)	-0.35	13 (1%)	65 72	9, 18, 36, 82	3 (0%)
All	All	1325/1362 (97%)	-0.15	52 (3%)	43 49	9, 21, 48, 98	7 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	LEU	5.8
1	B	414	PRO	5.3
1	B	415	GLY	5.0
1	A	566	LEU	4.7
1	A	672	LEU	4.5
1	B	416	THR	4.3
1	A	565	GLY	4.1
1	A	414	PRO	3.8
1	A	8	ARG	3.6
1	B	417	PRO	3.6
1	A	142	PRO	3.6
1	B	663	ARG	3.5
1	A	615	PRO	3.5
1	A	415	GLY	3.3
1	A	413	ARG	3.3
1	B	534	ARG	3.2
1	B	418	ASP	3.2
1	A	666	SER	3.1
1	A	141	HIS	3.0
1	A	663	ARG	2.9
1	A	90	GLU	2.8
1	A	559	GLU	2.8
1	A	563	THR	2.8
1	A	614	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	417	PRO	2.7
1	B	413	ARG	2.7
1	A	612	LEU	2.7
1	A	509	PRO	2.7
1	A	616	ARG	2.7
1	A	571	ASP	2.6
1	B	664	PHE	2.6
1	A	665	GLU	2.6
1	B	609	ALA	2.5
1	A	488	ASP	2.5
1	A	664	PHE	2.5
1	A	154	ARG	2.5
1	A	564	LEU	2.4
1	A	416	THR	2.4
1	A	532	ARG	2.4
1	A	562	ALA	2.4
1	A	558	ARG	2.3
1	A	143	ASP	2.3
1	B	665	GLU	2.3
1	A	139	SER	2.3
1	A	560	TYR	2.2
1	B	666	SER	2.2
1	A	638	GLY	2.2
1	A	671	SER	2.2
1	A	510	ALA	2.2
1	A	140	ASP	2.2
1	A	572	ALA	2.1
1	A	555	THR	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.

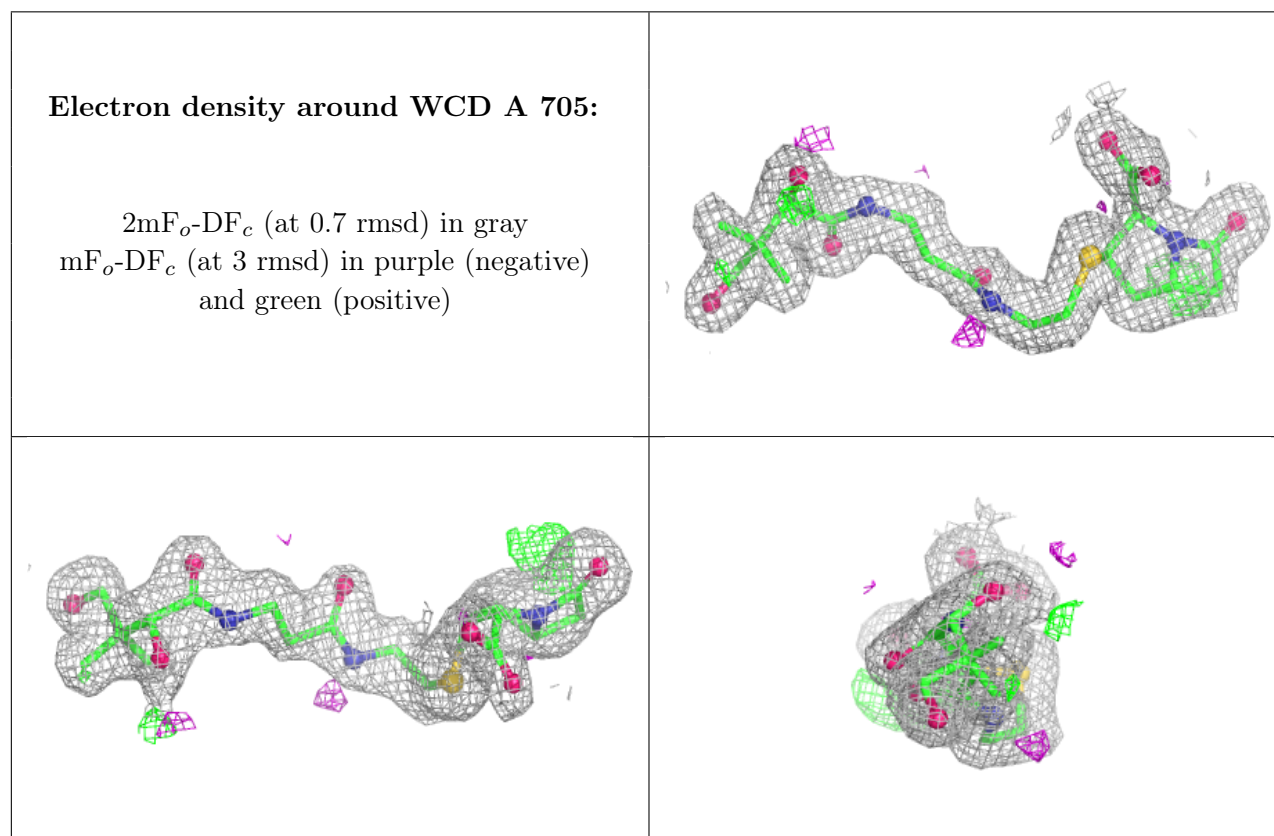
6.4 Ligands [i](#)

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.

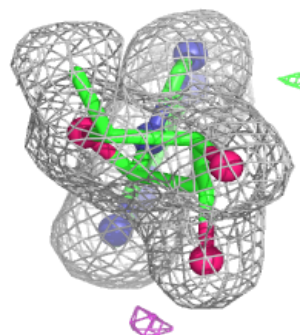
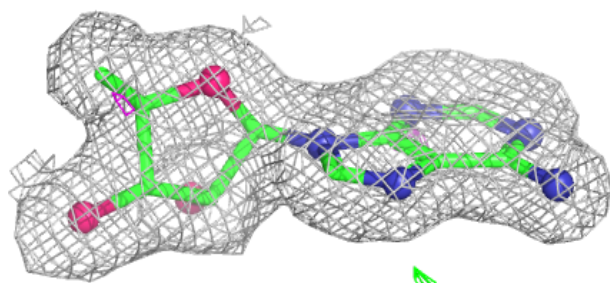
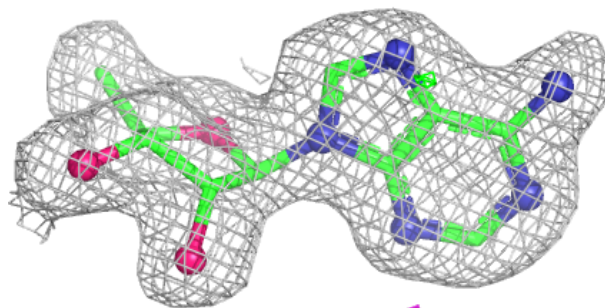
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	WCD	A	705	29/29	0.91	0.11	27,32,36,40	0
7	GOL	A	706	6/6	0.93	0.08	22,29,29,31	0
7	GOL	B	705	6/6	0.93	0.10	16,26,29,30	0
5	5AD	A	704	18/18	0.97	0.05	13,16,18,21	0
3	B12	A	702	91/91	0.98	0.05	7,14,25,37	0
5	5AD	B	704	18/18	0.98	0.04	10,12,14,14	0
3	B12	B	702	91/91	0.98	0.06	6,12,26,43	0
4	MET	A	703	9/9	0.98	0.05	9,13,15,16	0
4	MET	B	703	9/9	0.98	0.05	8,9,13,13	0
8	K	B	707	1/1	0.98	0.04	31,31,31,31	0
2	SF4	A	701	8/8	0.99	0.03	13,13,14,15	0
8	K	A	707	1/1	0.99	0.03	18,18,18,18	0
8	K	A	708	1/1	0.99	0.06	27,27,27,27	0
8	K	B	706	1/1	0.99	0.02	23,23,23,23	0
2	SF4	B	701	8/8	0.99	0.03	10,11,12,12	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.

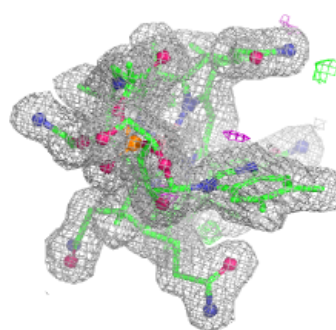
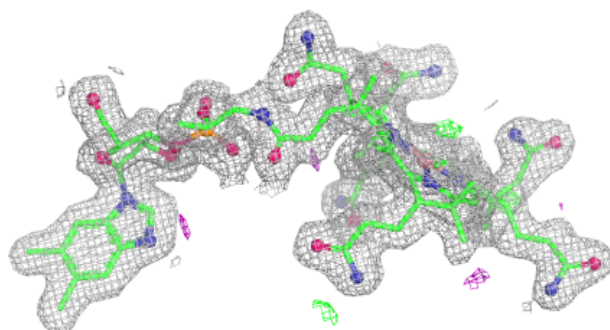
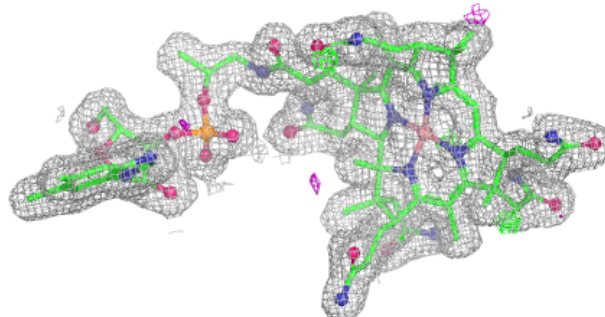


Electron density around 5AD A 704:

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

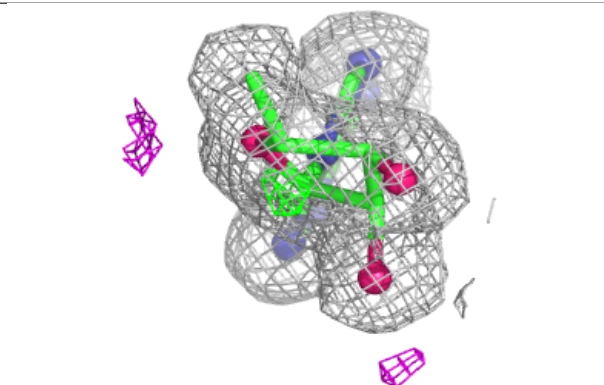
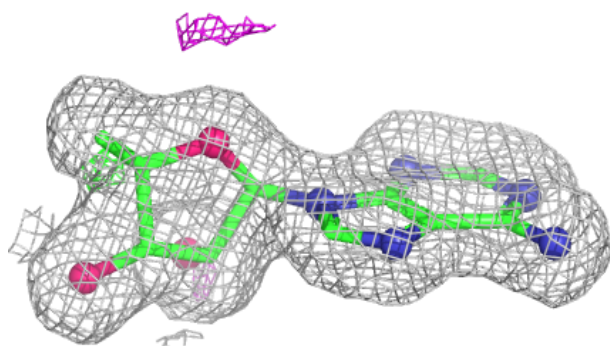
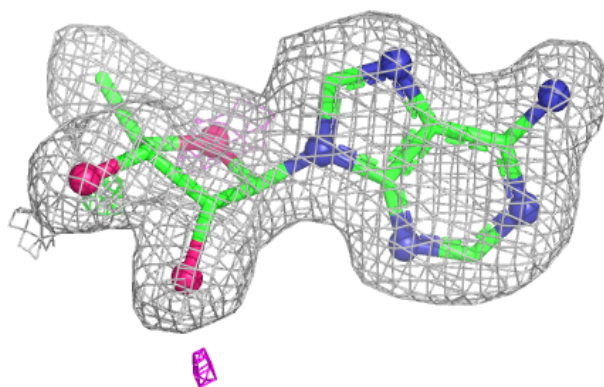
**Electron density around B12 A 702:**

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

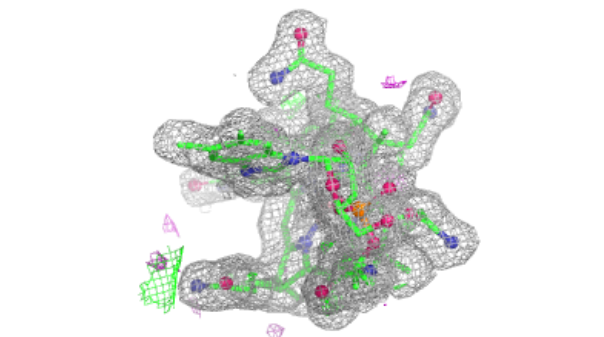
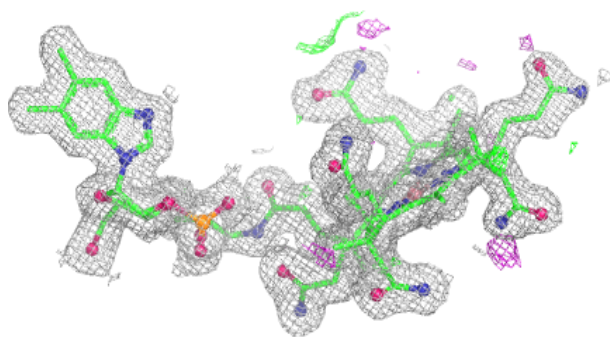
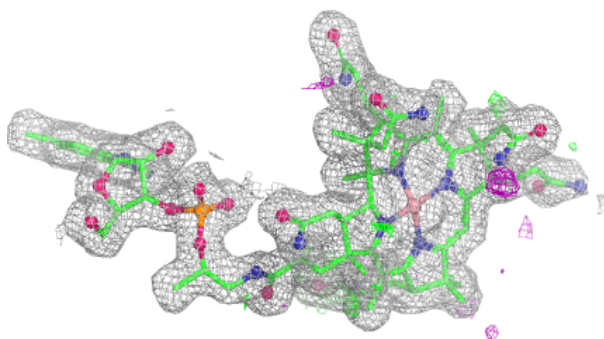


Electron density around 5AD B 704:

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

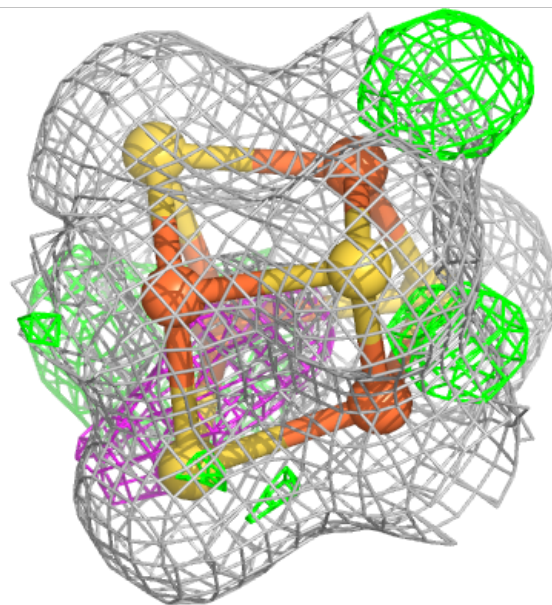
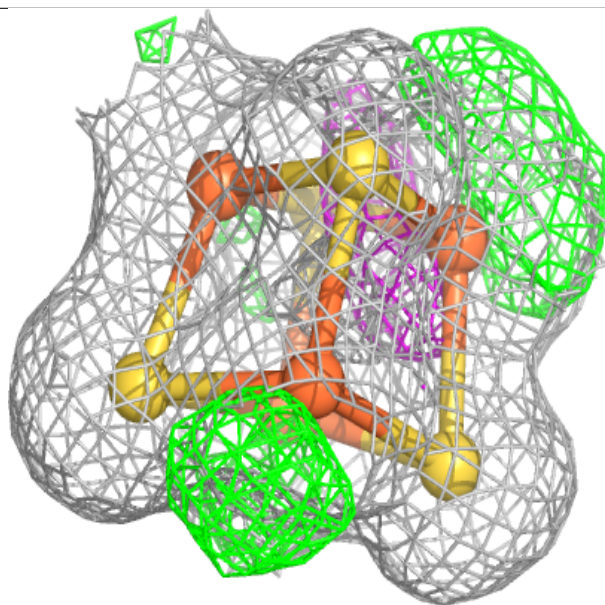
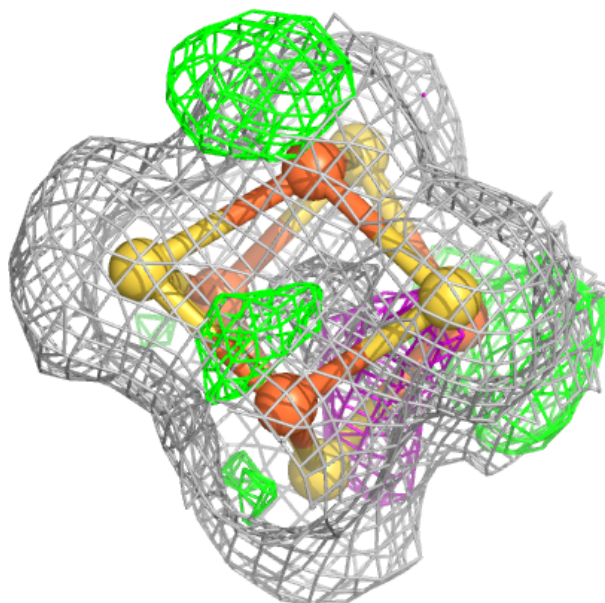
**Electron density around B12 B 702:**

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



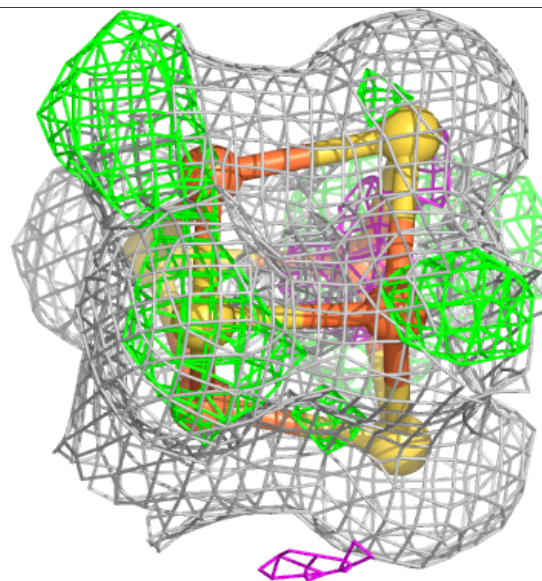
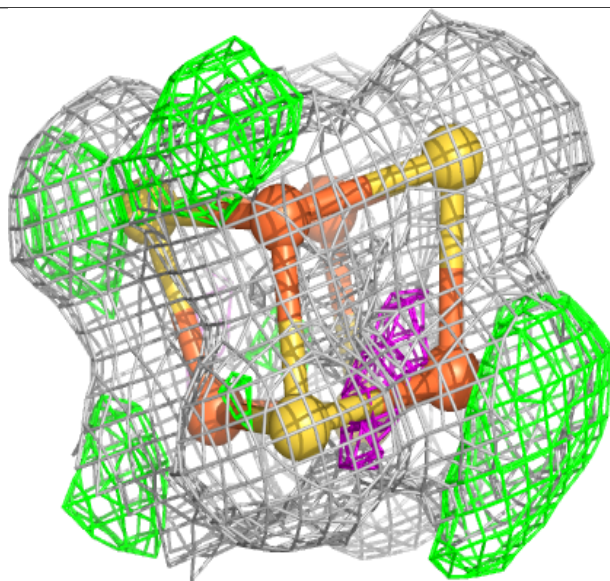
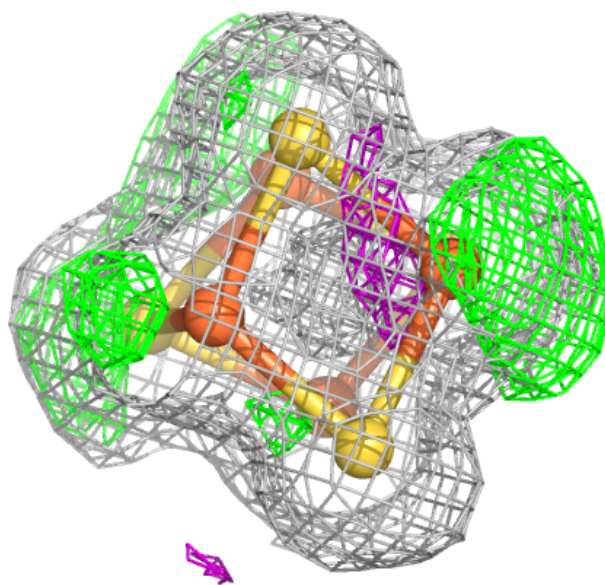
Electron density around SF4 A 701:

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



Electron density around SF4 B 701:

$2mF_o-DF_c$ (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.