



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:10 AM UTC

PDB ID : 7ZI0 / pdb_00007zi0
Title : Structure of human Smoothed in complex with cholesterol and SAG
Authors : Byrne, E.F.X.; Woolley, R.E.; Ansell, B.; Sansom, M.S.P.; Newstead, S.; Siebold, C.
Deposited on : 2022-04-07
Resolution : 3.00 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

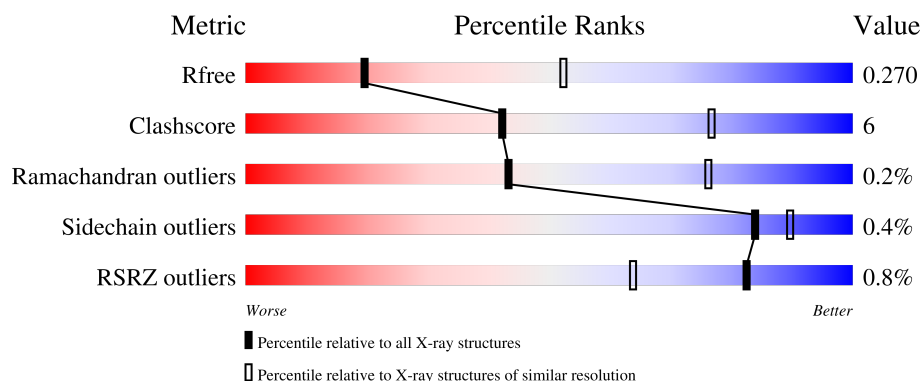
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	638	
1	B	638	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9409 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 Smoothened homolog,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4678	3008	797	840	33			
1	B	578	Total	C	N	O	S	0	0	0
			4567	2936	779	819	33			

There are 52 discrepancies between the modelled and reference sequences:

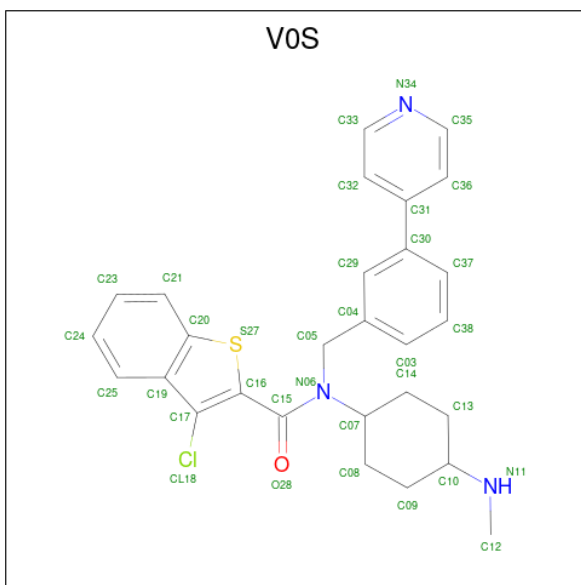
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	PHE	VAL	conflict	UNP Q99835
A	429	ALA	-	linker	UNP Q99835
A	430	ARG	-	linker	UNP Q99835
A	431	ARG	-	linker	UNP Q99835
A	432	GLN	-	linker	UNP Q99835
A	433	LEU	-	linker	UNP Q99835
A	440	TRP	MET	conflict	UNP P0ABE7
A	535	ILE	HIS	conflict	UNP P0ABE7
A	539	LEU	-	linker	UNP P0ABE7
A	540	GLU	-	linker	UNP P0ABE7
A	541	ARG	-	linker	UNP P0ABE7
A	542	ALA	-	linker	UNP P0ABE7
A	543	ARG	-	linker	UNP P0ABE7
A	544	SER	-	linker	UNP P0ABE7
A	545	THR	-	linker	UNP P0ABE7
A	546	LEU	-	linker	UNP P0ABE7
A	660	GLY	-	expression tag	UNP Q99835
A	661	THR	-	expression tag	UNP Q99835
A	662	GLU	-	expression tag	UNP Q99835
A	663	THR	-	expression tag	UNP Q99835
A	664	SER	-	expression tag	UNP Q99835
A	665	GLN	-	expression tag	UNP Q99835
A	666	VAL	-	expression tag	UNP Q99835
A	667	ALA	-	expression tag	UNP Q99835
A	668	PRO	-	expression tag	UNP Q99835

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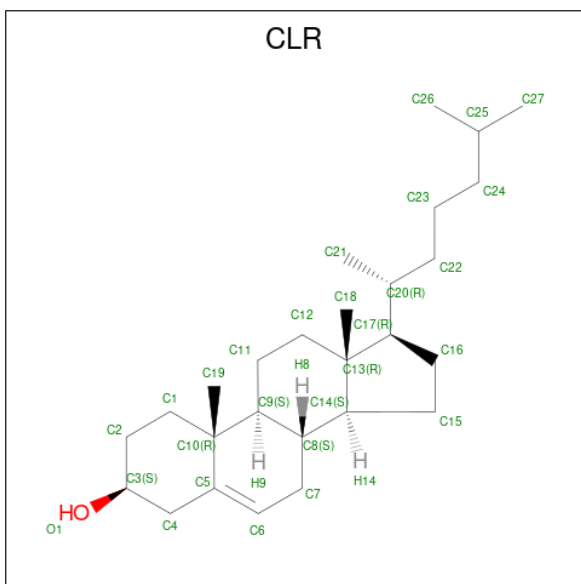
Chain	Residue	Modelled	Actual	Comment	Reference
A	669	ALA	-	expression tag	UNP Q99835
B	329	PHE	VAL	conflict	UNP Q99835
B	429	ALA	-	linker	UNP Q99835
B	430	ARG	-	linker	UNP Q99835
B	431	ARG	-	linker	UNP Q99835
B	432	GLN	-	linker	UNP Q99835
B	433	LEU	-	linker	UNP Q99835
B	440	TRP	MET	conflict	UNP P0ABE7
B	535	ILE	HIS	conflict	UNP P0ABE7
B	539	LEU	-	linker	UNP P0ABE7
B	540	GLU	-	linker	UNP P0ABE7
B	541	ARG	-	linker	UNP P0ABE7
B	542	ALA	-	linker	UNP P0ABE7
B	543	ARG	-	linker	UNP P0ABE7
B	544	SER	-	linker	UNP P0ABE7
B	545	THR	-	linker	UNP P0ABE7
B	546	LEU	-	linker	UNP P0ABE7
B	660	GLY	-	expression tag	UNP Q99835
B	661	THR	-	expression tag	UNP Q99835
B	662	GLU	-	expression tag	UNP Q99835
B	663	THR	-	expression tag	UNP Q99835
B	664	SER	-	expression tag	UNP Q99835
B	665	GLN	-	expression tag	UNP Q99835
B	666	VAL	-	expression tag	UNP Q99835
B	667	ALA	-	expression tag	UNP Q99835
B	668	PRO	-	expression tag	UNP Q99835
B	669	ALA	-	expression tag	UNP Q99835

- Molecule 2 is 3-chloro-N-[trans-4-(methylamino)cyclohexyl]-N-{{[3-(pyridin-4-yl)phenyl]methyl}-1-benzothiophene-2-carboxamide (CCD ID: V0S) (formula: C₂₈H₂₈ClN₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			34	28	1	3	1	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			34	28	1	3	1	1		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

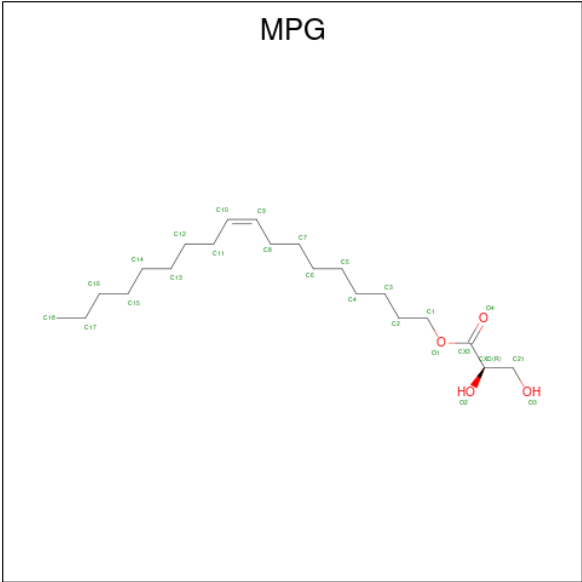


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (CCD ID: MPG) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



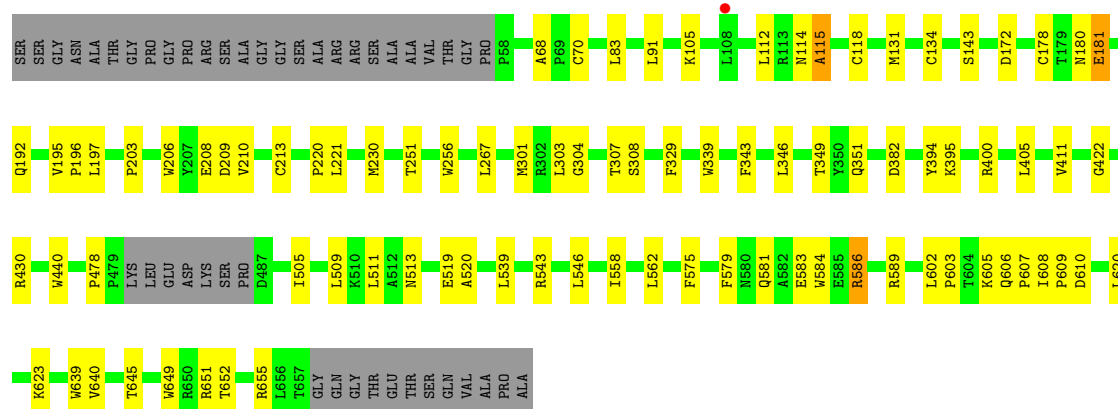
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			24	21	3		

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.

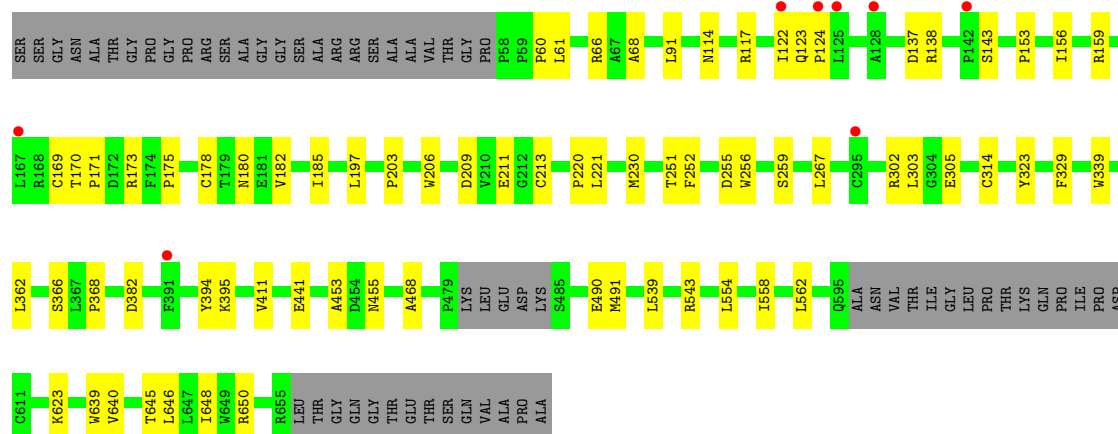
- Molecule 1: Smoothened homolog,Soluble cytochrome b562

Chain A: 



- Molecule 1: Smoothened homolog,Soluble cytochrome b562

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.86Å 63.15Å 208.06Å 90.00° 96.29° 90.00°	Depositor
Resolution (Å)	60.00 – 3.00 60.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (60.00-3.00) 96.9 (60.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.231 , 0.275 0.232 , 0.270	Depositor DCC
R_{free} test set	1480 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	87.7	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9409	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: MPG, NAG, VOS, NA, CLR

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	0.98	2/4797 (0.0%)	1.11	4/6524 (0.1%)
1	B	0.95	1/4683 (0.0%)	1.07	6/6364 (0.1%)
All	All	0.96	3/9480 (0.0%)	1.09	10/12888 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	GLU	CA-CB	5.63	1.61	1.54
1	B	468	ALA	CA-C	-5.59	1.45	1.52
1	A	478	PRO	CA-C	5.56	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	SER	N-CA-C	6.40	117.95	110.97
1	B	114	ASN	N-CA-C	6.37	118.31	111.36
1	B	137	ASP	N-CA-C	5.93	119.73	111.90
1	A	256	TRP	N-CA-C	5.59	118.10	111.33
1	A	505	ILE	N-CA-C	-5.55	105.11	110.72
1	B	256	TRP	N-CA-C	5.43	117.91	111.33
1	B	455	ASN	N-CA-C	5.37	116.44	108.60
1	B	122	ILE	N-CA-C	5.09	115.86	110.72
1	A	180	ASN	N-CA-C	5.05	116.86	111.36
1	B	453	ALA	N-CA-C	5.01	117.81	110.30

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	4678	0	4616	66	1
1	B	4567	0	4494	53	0
2	A	34	0	0	2	0
2	B	34	0	0	0	0
3	A	28	0	46	2	0
3	B	28	0	46	0	0
4	A	14	0	13	0	0
5	A	2	0	0	0	0
6	A	24	0	40	0	0
All	All	9409	0	9255	118	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 (118) 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:602:LEU:HD12	1:A:603:PRO:CD	1.75	1.15
1:A:602:LEU:HD12	1:A:603:PRO:HD2	1.12	1.11
1:B:153:PRO:HA	1:B:211:GLU:OE2	1.59	1.02
1:A:509:LEU:HD23	1:A:513:ASN:ND2	1.75	1.01
1:A:602:LEU:CD1	1:A:603:PRO:HD2	1.99	0.93
1:B:640:VAL:HG13	1:B:645:THR:HG21	1.50	0.90
1:B:153:PRO:CA	1:B:211:GLU:OE2	2.23	0.87
1:A:400:ARG:NH2	1:A:581:GLN:OE1	2.10	0.85
1:A:509:LEU:CD2	1:A:513:ASN:HD21	1.91	0.83
1:A:209:ASP:OD2	1:A:589:ARG:NH2	2.13	0.82
1:B:490:GLU:N	1:B:490:GLU:OE1	2.13	0.81
1:B:305:GLU:HG2	1:B:314:CYS:HB3	1.64	0.79
1:B:156:ILE:HG22	1:B:209:ASP:CG	2.07	0.79
1:B:305:GLU:HG2	1:B:314:CYS:SG	2.22	0.79
1:A:511:LEU:HD13	1:A:519:GLU:C	2.08	0.78
1:A:509:LEU:CD2	1:A:513:ASN:ND2	2.47	0.78
1:B:558:ILE:O	1:B:562:LEU:HD13	1.86	0.75
1:A:606:GLN:HB3	1:A:607:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ILE:O	1:A:562:LEU:HD13	1.90	0.72
1:B:61:LEU:O	1:B:138:ARG:NH2	2.24	0.70
1:B:117:ARG:HB2	1:B:211:GLU:HG3	1.72	0.70
1:B:382:ASP:HB2	1:B:394:TYR:HB2	1.74	0.70
1:B:305:GLU:HG2	1:B:314:CYS:CB	2.21	0.69
1:B:175:PRO:HB2	1:B:178:CYS:SG	2.35	0.67
1:A:382:ASP:HB2	1:A:394:TYR:HB2	1.76	0.67
1:A:303:LEU:HD13	1:A:395:LYS:HD2	1.78	0.66
1:B:170:THR:N	1:B:171:PRO:HD2	2.11	0.66
1:A:586:ARG:HH11	1:B:441:GLU:HG3	1.62	0.64
1:A:267:LEU:HD22	1:A:639:TRP:CD2	2.33	0.64
1:A:509:LEU:HD21	1:A:513:ASN:HD21	1.63	0.63
1:A:267:LEU:HD22	1:A:639:TRP:CG	2.35	0.62
1:A:349:THR:HG23	1:A:351:GLN:HG3	1.80	0.62
1:B:255:ASP:HB2	1:B:648:ILE:HD13	1.82	0.61
1:B:143:SER:HB3	1:B:178:CYS:HB2	1.83	0.60
1:B:153:PRO:CB	1:B:211:GLU:OE2	2.48	0.60
1:B:267:LEU:HD22	1:B:639:TRP:CD2	2.36	0.60
1:A:181:GLU:O	1:A:181:GLU:HG3	2.03	0.58
1:A:620:LEU:HD22	1:B:554:LEU:HD13	1.87	0.57
1:B:302:ARG:NH1	1:B:305:GLU:OE1	2.36	0.56
1:A:509:LEU:HD23	1:A:513:ASN:HD22	1.66	0.56
1:B:252:PHE:HD1	1:B:259:SER:HB3	1.69	0.56
1:B:646:LEU:O	1:B:650:ARG:HG3	2.06	0.56
1:B:61:LEU:C	1:B:138:ARG:HH22	2.13	0.56
1:A:581:GLN:HA	1:A:584:TRP:CE3	2.41	0.56
2:A:701:V0S:C04	2:A:701:V0S:C16	2.81	0.56
1:B:267:LEU:HD22	1:B:639:TRP:CG	2.41	0.55
1:A:210:VAL:HG22	3:A:702:CLR:H262	1.89	0.55
1:A:197:LEU:HB3	1:A:213:CYS:HB3	1.89	0.55
1:B:60:PRO:HB2	1:B:138:ARG:NH1	2.24	0.53
1:A:440:TRP:CD2	1:A:539:LEU:HD13	2.44	0.53
1:B:159:ARG:NH2	1:B:209:ASP:OD2	2.42	0.53
1:A:114:ASN:HA	1:A:192:GLN:O	2.09	0.52
1:A:511:LEU:HD13	1:A:519:GLU:CB	2.39	0.52
1:A:105:LYS:HD2	3:A:702:CLR:H21	1.90	0.52
1:A:511:LEU:HD12	1:A:520:ALA:HA	1.91	0.52
1:B:303:LEU:HD13	1:B:395:LYS:HD2	1.93	0.51
1:A:511:LEU:HD13	1:A:520:ALA:N	2.25	0.51
1:B:175:PRO:HG2	1:B:178:CYS:SG	2.51	0.50
1:A:143:SER:HB3	1:A:178:CYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LEU:HD13	1:A:519:GLU:HB3	1.93	0.50
1:A:579:PHE:C	1:A:579:PHE:CD1	2.90	0.49
1:A:511:LEU:CD1	1:A:519:GLU:C	2.83	0.49
1:B:558:ILE:O	1:B:562:LEU:CD1	2.59	0.48
1:B:197:LEU:HB3	1:B:213:CYS:HB3	1.95	0.48
1:A:602:LEU:HD21	1:A:609:PRO:HD3	1.95	0.47
1:B:491:MET:HA	1:B:491:MET:HE2	1.96	0.47
1:A:114:ASN:O	1:A:115:ALA:HB3	2.14	0.47
1:A:649:TRP:O	1:A:652:THR:OG1	2.24	0.47
1:B:640:VAL:HG13	1:B:645:THR:CG2	2.35	0.47
1:A:602:LEU:HD23	1:A:608:ILE:HG23	1.97	0.46
1:B:170:THR:N	1:B:171:PRO:CD	2.77	0.46
1:B:329:PHE:HB3	1:B:411:VAL:HG11	1.97	0.46
1:A:640:VAL:HB	1:A:645:THR:HG21	1.97	0.46
1:A:203:PRO:HA	1:A:206:TRP:CD2	2.50	0.46
1:A:195:VAL:HG13	1:A:196:PRO:HA	1.98	0.46
1:A:610:ASP:OD1	1:A:610:ASP:N	2.41	0.45
1:A:208:GLU:OE1	1:A:589:ARG:HG3	2.15	0.45
1:B:66:ARG:HH22	1:B:173:ARG:HG2	1.82	0.45
1:A:304:GLY:O	1:A:307:THR:HG23	2.17	0.45
1:A:301:MET:HE1	2:A:701:VOS:C37	2.46	0.45
1:A:339:TRP:CZ3	1:A:422:GLY:HA3	2.52	0.45
1:A:602:LEU:CD2	1:A:609:PRO:HD2	2.47	0.44
1:B:323:TYR:CE1	1:B:368:PRO:HB2	2.52	0.44
1:B:230:MET:HE1	1:B:623:LYS:HG3	1.99	0.44
1:A:220:PRO:HG2	1:A:221:LEU:HD12	2.00	0.44
1:A:405:LEU:HD11	1:A:575:PHE:HA	1.99	0.44
1:A:343:PHE:O	1:A:346:LEU:HG	2.17	0.44
1:B:182:VAL:HA	1:B:185:ILE:HD12	1.99	0.44
1:A:267:LEU:HD12	1:A:267:LEU:N	2.32	0.43
1:A:230:MET:HE1	1:A:623:LYS:HG3	1.99	0.43
1:A:539:LEU:HD23	1:A:543:ARG:HD3	2.00	0.43
1:B:68:ALA:HB2	1:B:91:LEU:HD22	2.01	0.43
1:A:114:ASN:O	1:A:115:ALA:CB	2.66	0.43
1:B:539:LEU:HD23	1:B:543:ARG:HD3	2.00	0.43
1:B:123:GLN:HB2	1:B:124:PRO:HD3	2.01	0.43
1:B:251:THR:OG1	1:B:640:VAL:HG11	2.18	0.43
1:B:490:GLU:N	1:B:490:GLU:CD	2.76	0.43
1:B:255:ASP:CB	1:B:648:ILE:HD13	2.48	0.43
1:A:651:ARG:O	1:A:655:ARG:HG3	2.18	0.43
1:A:602:LEU:HD21	1:A:609:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HG23	1:A:349:THR:O	2.19	0.42
1:A:430:ARG:HA	1:A:546:LEU:HD21	2.01	0.42
1:A:329:PHE:HB3	1:A:411:VAL:HG11	2.01	0.42
1:B:305:GLU:CG	1:B:314:CYS:HB3	2.40	0.42
1:A:558:ILE:O	1:A:562:LEU:CD1	2.64	0.42
1:A:70:CYS:SG	1:A:134:CYS:C	3.03	0.42
1:B:143:SER:OG	1:B:180:ASN:ND2	2.51	0.42
1:A:83:LEU:HD11	1:A:131:MET:HE2	2.02	0.42
1:A:251:THR:HG22	1:A:649:TRP:NE1	2.36	0.41
1:B:153:PRO:HB3	1:B:211:GLU:OE2	2.20	0.41
1:A:68:ALA:HB2	1:A:91:LEU:HD22	2.02	0.41
1:B:175:PRO:CB	1:B:178:CYS:SG	3.07	0.41
1:B:220:PRO:HG2	1:B:221:LEU:HD12	2.02	0.41
1:A:251:THR:CG2	1:A:649:TRP:HE1	2.33	0.41
1:B:203:PRO:HA	1:B:206:TRP:CD2	2.55	0.41
1:B:267:LEU:HD12	1:B:267:LEU:N	2.36	0.41
1:A:112:LEU:HD23	1:A:118:CYS:SG	2.60	0.41
1:B:362:LEU:O	1:B:366:SER: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)
1:A:172:ASP:OD1	1:A:192:GLN:NE2[4_446]	1.55	0.65

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	589/638 (92%)	567 (96%)	20 (3%)	2 (0%)	36	70
1	B	572/638 (90%)	551 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1161/1276 (91%)	1118 (96%)	41 (4%)	2 (0%)	43 76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	605	LYS
1	A	115	ALA

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	499/529 (94%)	497 (100%)	2 (0%)	84 90
1	B	486/529 (92%)	484 (100%)	2 (0%)	84 90
All	All	985/1058 (93%)	981 (100%)	4 (0%)	84 90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	583	GLU
1	A	586	ARG
1	B	169	CYS
1	B	339	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	148	GLN
1	A	380	GLN
1	A	396	ASN
1	A	513	ASN
1	B	63	HIS
1	B	180	ASN

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Mol	Chain	Res	Type
1	B	380	GLN
1	B	396	ASN
1	B	513	ASN
1	B	536	GLN
1	B	550	ASN
1	B	581	GLN

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	V0S	B	701	-	38,38,38	0.64	1 (2%)	48,53,53	0.87	3 (6%)
4	NAG	A	703	1	14,14,15	0.64	0	17,19,21	0.90	1 (5%)
3	CLR	B	702	-	31,31,31	0.66	0	48,48,48	1.16	3 (6%)
6	MPG	A	706	-	23,23,24	0.51	0	23,23,25	1.09	1 (4%)
2	V0S	A	701	-	38,38,38	0.65	1 (2%)	48,53,53	0.68	1 (2%)
3	CLR	A	702	-	31,31,31	0.65	1 (3%)	48,48,48	1.07	4 (8%)

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	V0S	B	701	-	-	8/22/32/32	0/5/5/5
4	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	CLR	B	702	-	-	4/10/68/68	0/4/4/4
6	MPG	A	706	-	-	10/22/22/25	-
2	V0S	A	701	-	-	5/22/32/32	0/5/5/5
3	CLR	A	702	-	-	5/10/68/68	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	V0S	C31-C30	-2.43	1.43	1.49
2	A	701	V0S	C31-C30	-2.29	1.43	1.49
3	A	702	CLR	C13-C14	-2.19	1.51	1.55

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	706	MPG	O1-CX3-CXD	4.37	122.98	109.56
2	B	701	V0S	C05-N06-C07	-3.77	114.62	118.34
3	B	702	CLR	C1-C2-C3	3.47	115.08	110.48
2	B	701	V0S	C05-N06-C15	2.80	124.75	116.97
3	B	702	CLR	C14-C8-C9	2.78	112.72	109.09
3	A	702	CLR	C14-C8-C9	2.73	112.65	109.09
3	A	702	CLR	C1-C2-C3	2.64	113.98	110.48
2	A	701	V0S	C05-N06-C07	-2.57	115.81	118.34
3	A	702	CLR	C23-C22-C20	-2.34	108.52	115.08
4	A	703	NAG	C2-N2-C7	2.27	125.94	122.90
3	B	702	CLR	C8-C7-C6	-2.27	109.62	112.76
2	B	701	V0S	C21-C20-C19	-2.12	119.24	121.47
3	A	702	CLR	C7-C8-C9	-2.10	107.30	109.72

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	V0S	O28-C15-N06-C07

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Mol	Chain	Res	Type	Atoms
3	A	702	CLR	C17-C20-C22-C23
3	A	702	CLR	C21-C20-C22-C23
6	A	706	MPG	C5-C6-C7-C8
6	A	706	MPG	O1-CX3-CXD-O2
3	A	702	CLR	C22-C23-C24-C25
6	A	706	MPG	O1-CX3-CXD-C21
3	B	702	CLR	C20-C22-C23-C24
2	A	701	V0S	C13-C10-N11-C12
2	A	701	V0S	C09-C10-N11-C12
2	B	701	V0S	C13-C10-N11-C12
2	B	701	V0S	C09-C10-N11-C12
6	A	706	MPG	C4-C5-C6-C7
2	B	701	V0S	C04-C05-N06-C15
6	A	706	MPG	O1-C1-C2-C3
6	A	706	MPG	C3-C4-C5-C6
2	B	701	V0S	C04-C05-N06-C07
6	A	706	MPG	C11-C12-C13-C14
6	A	706	MPG	C14-C15-C16-C17
3	A	702	CLR	C23-C24-C25-C26
6	A	706	MPG	CXD-CX3-O1-C1
2	A	701	V0S	C04-C05-N06-C15
3	B	702	CLR	C23-C24-C25-C27
3	B	702	CLR	C22-C23-C24-C25
2	A	701	V0S	C04-C05-N06-C07
2	B	701	V0S	N06-C15-C16-S27
3	B	702	CLR	C23-C24-C25-C26
6	A	706	MPG	O3-C21-CXD-O2
2	B	701	V0S	C16-C15-N06-C07
3	A	702	CLR	C23-C24-C25-C27
2	A	701	V0S	O28-C15-C16-S27
2	B	701	V0S	O28-C15-C16-S27

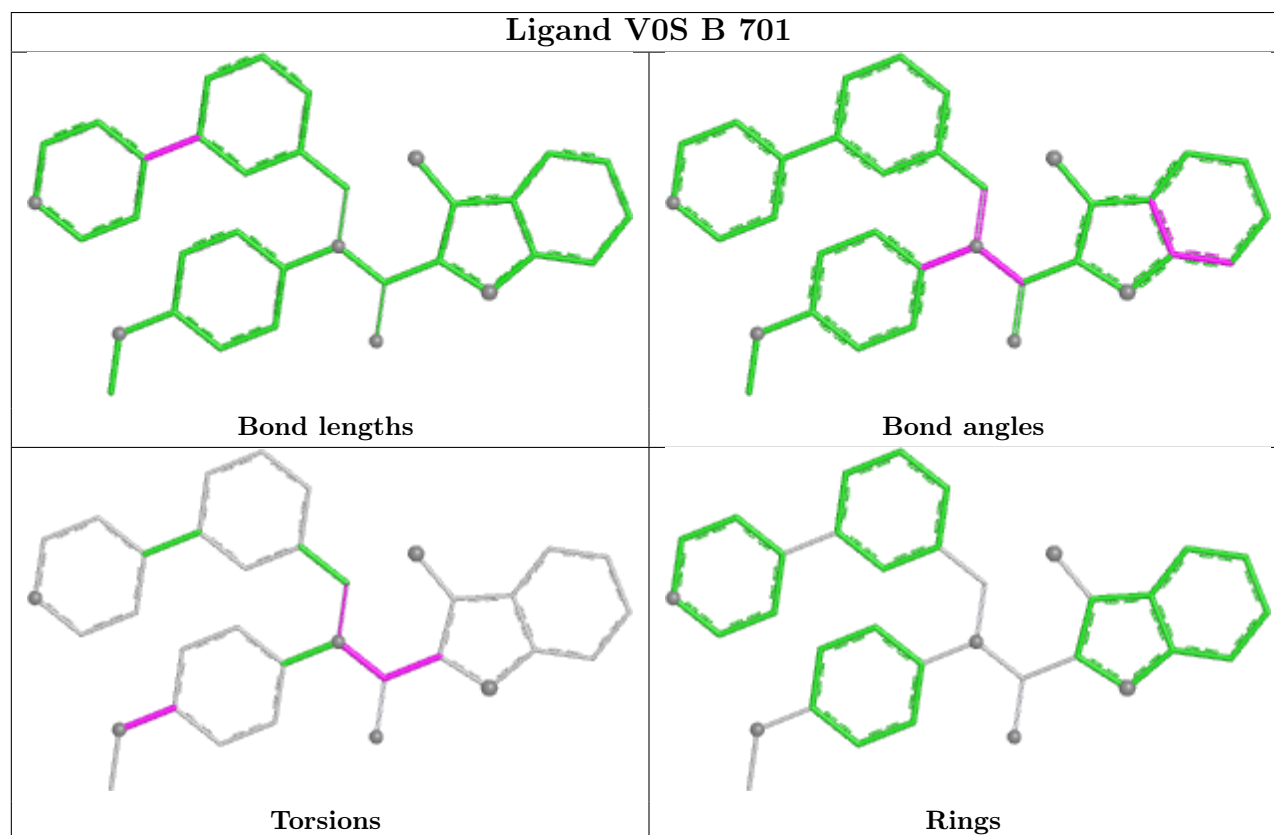
There are no ring outliers.

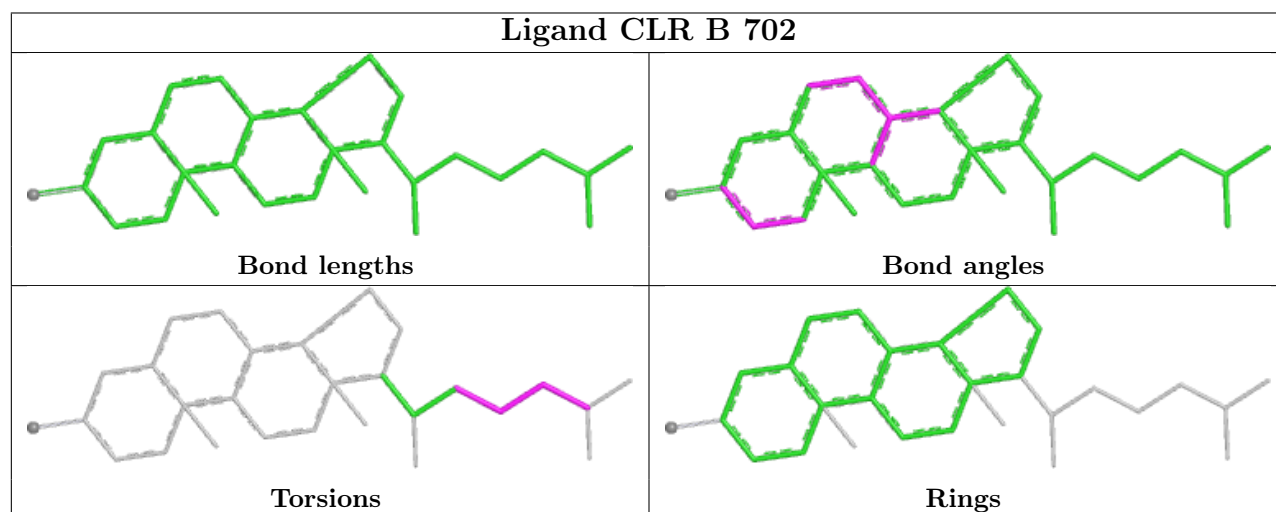
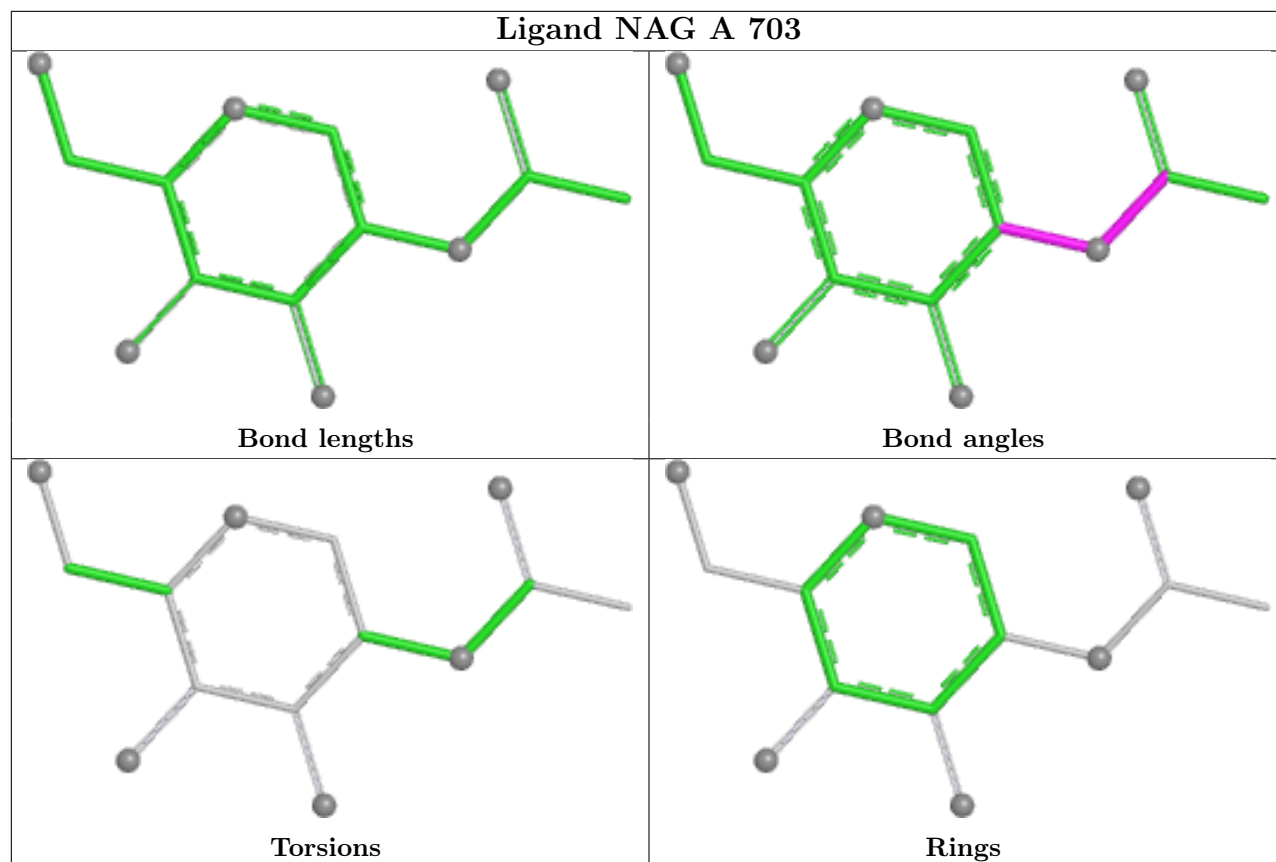
2 monomers are involved in 4 short contacts:

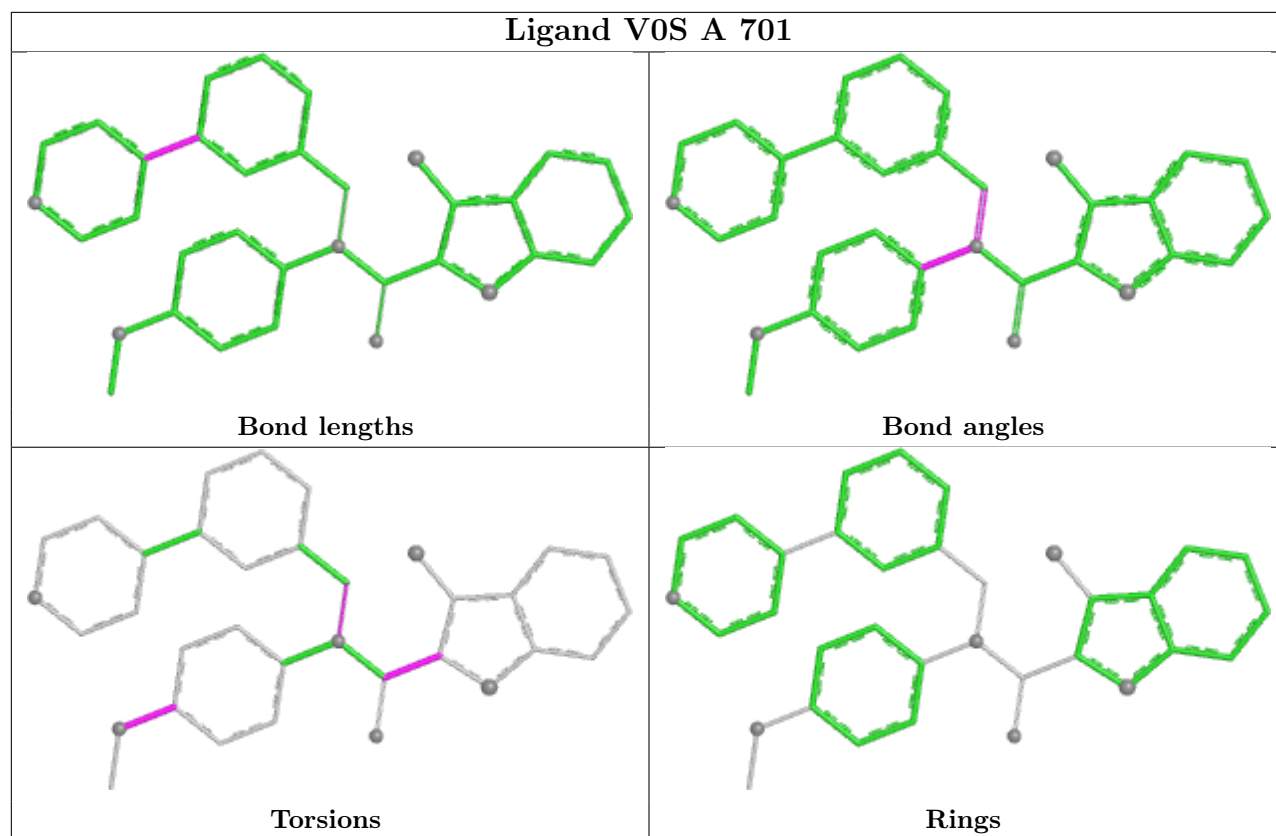
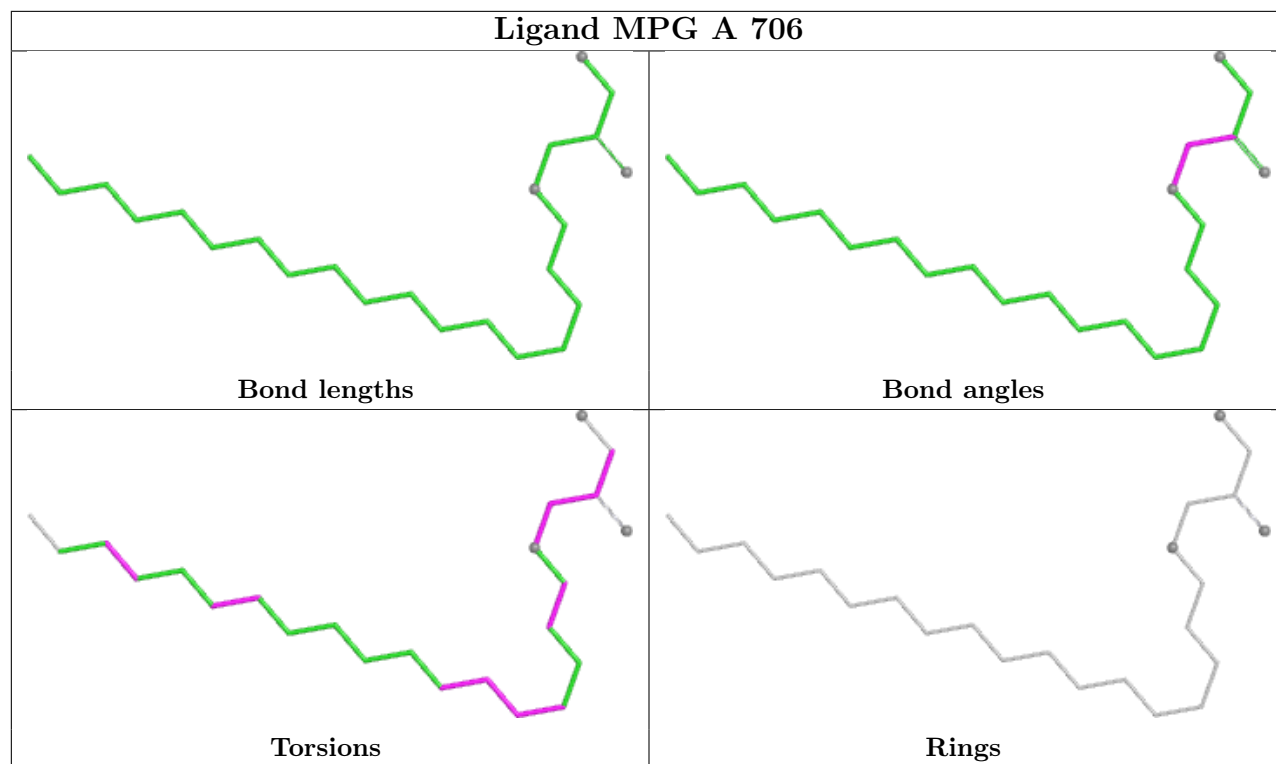
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	V0S	2	0
3	A	702	CLR	2	0

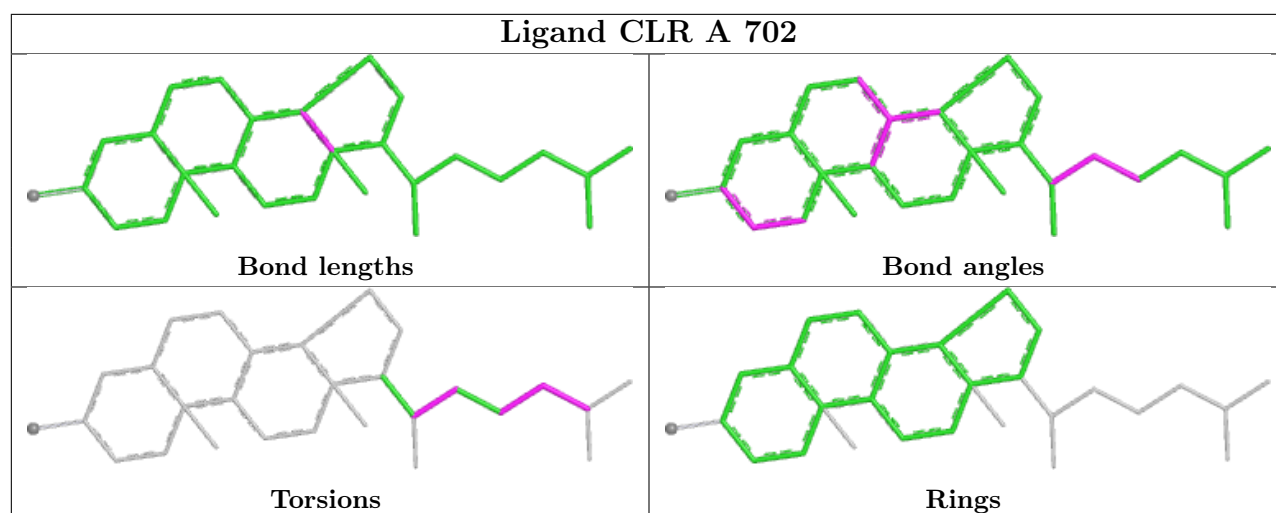
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	593/638 (92%)	-0.25	1 (0%)	91 83	65, 112, 218, 260	0
1	B	578/638 (90%)	-0.21	8 (1%)	73 51	65, 128, 200, 240	0
All	All	1171/1276 (91%)	-0.23	9 (0%)	82 64	65, 120, 211, 260	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	125	LEU	3.3
1	B	142	PRO	3.2
1	B	167	LEU	2.8
1	B	391	PHE	2.5
1	B	128	ALA	2.5
1	B	122	ILE	2.4
1	B	295	CYS	2.4
1	A	108	LEU	2.3
1	B	124	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

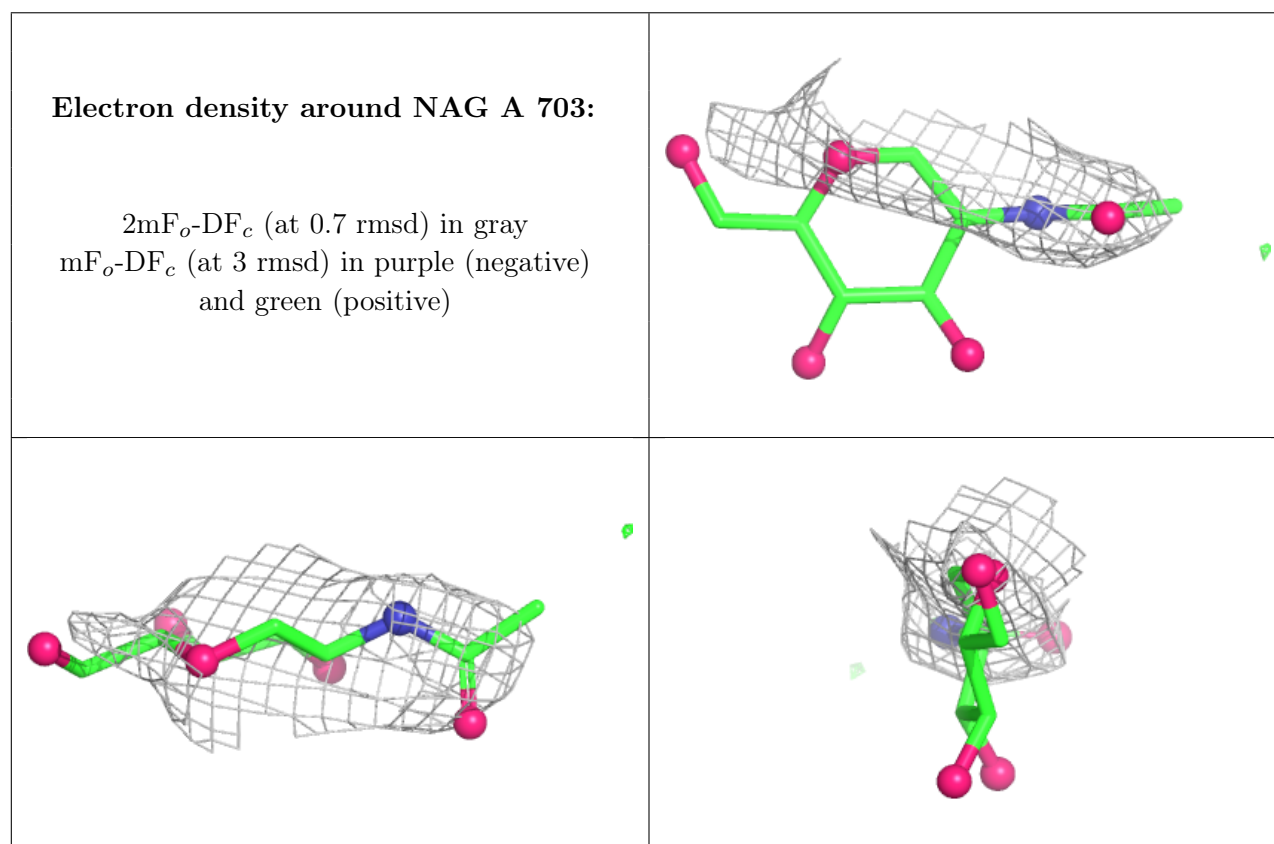
6.4 Ligands [i](#)

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.

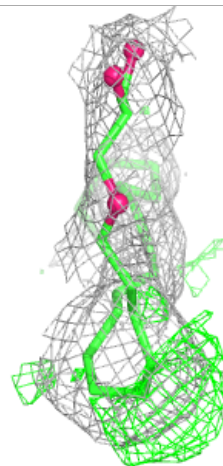
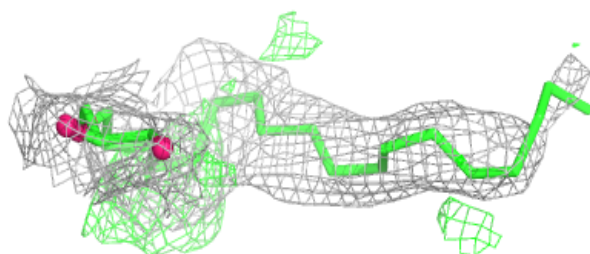
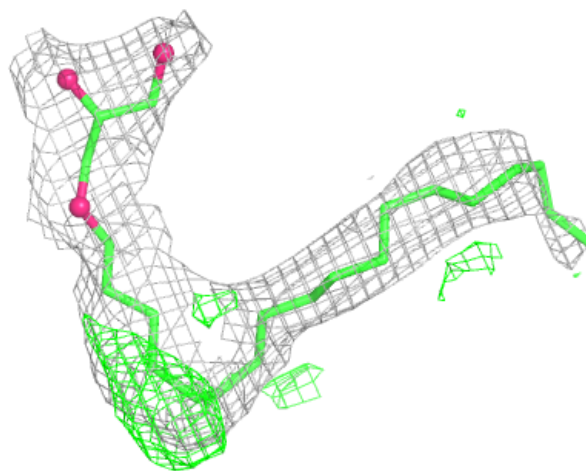
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	703	14/15	0.61	0.14	121,157,197,221	0
6	MPG	A	706	24/25	0.81	0.18	117,136,164,169	0
5	NA	A	705	1/1	0.86	0.23	85,85,85,85	0
3	CLR	B	702	28/28	0.89	0.15	130,145,153,155	0
2	V0S	A	701	34/34	0.91	0.12	72,85,102,114	0
2	V0S	B	701	34/34	0.93	0.12	111,126,165,171	0
5	NA	A	704	1/1	0.93	0.08	91,91,91,91	0
3	CLR	A	702	28/28	0.97	0.08	75,83,94,97	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.



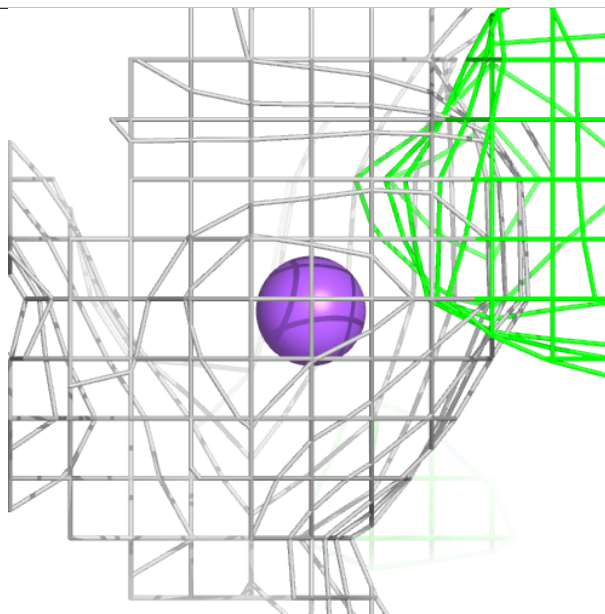
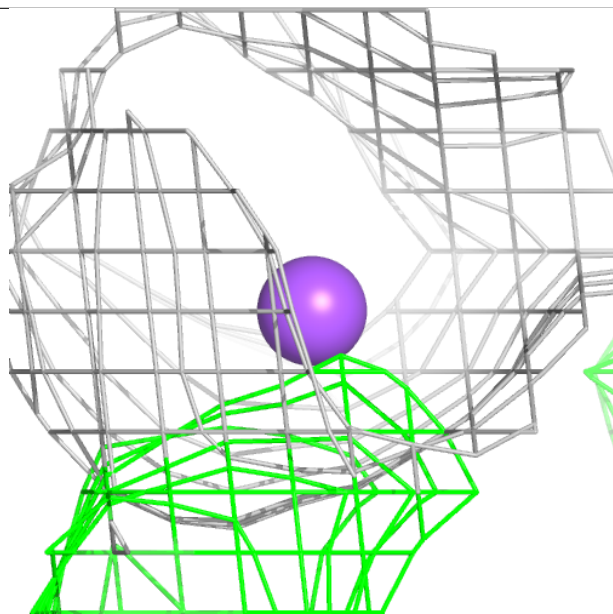
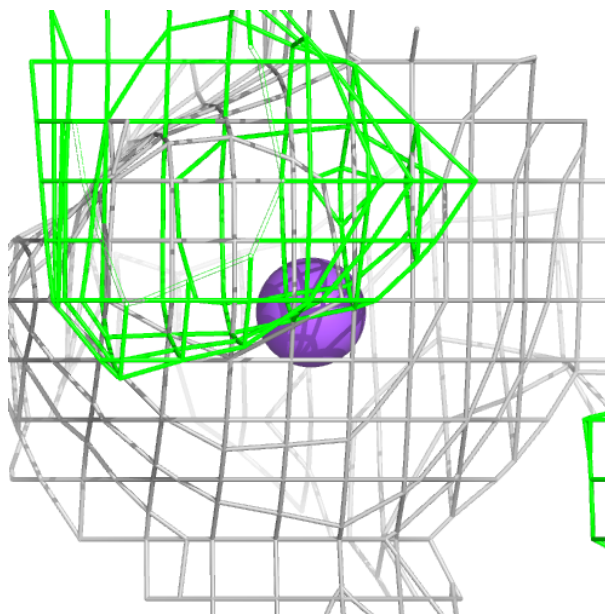
Electron density around MPG A 706:

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



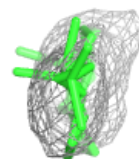
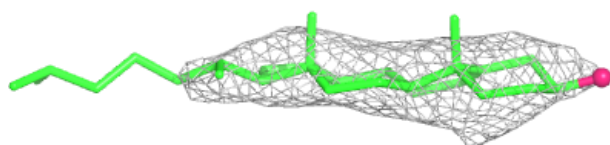
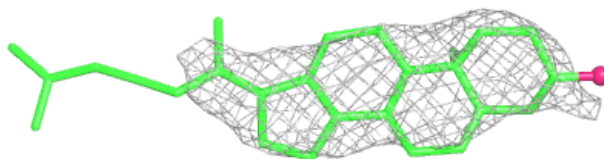
Electron density around NA A 705:

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

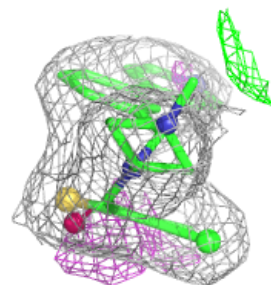
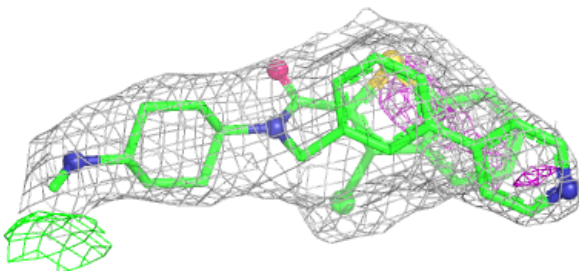
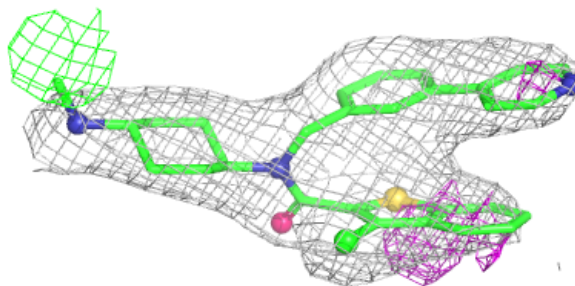


Electron density around CLR B 702:

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

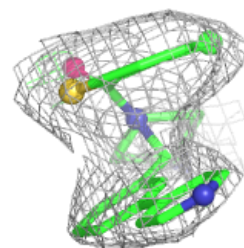
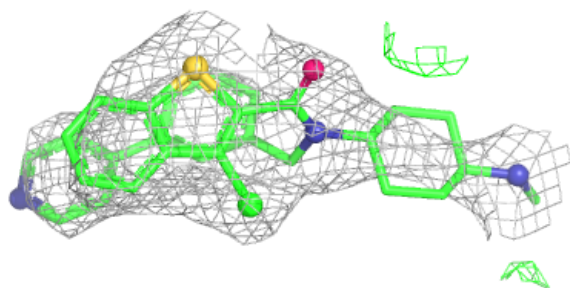
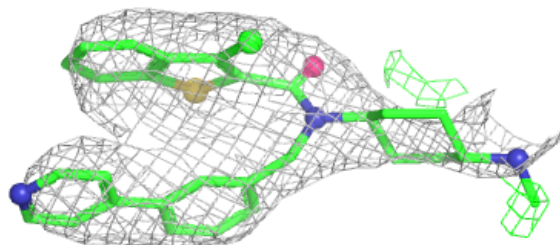
**Electron density around V0S A 701:**

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



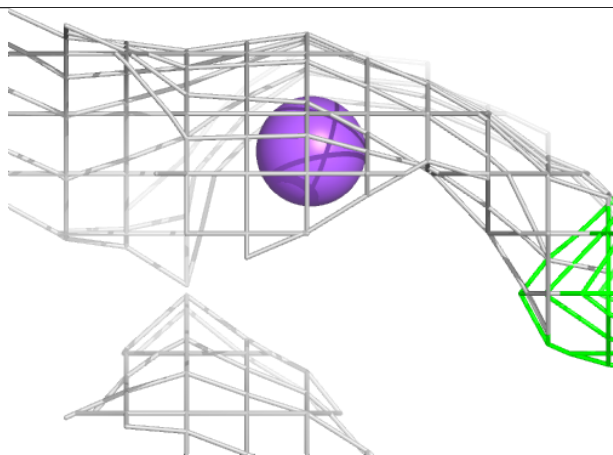
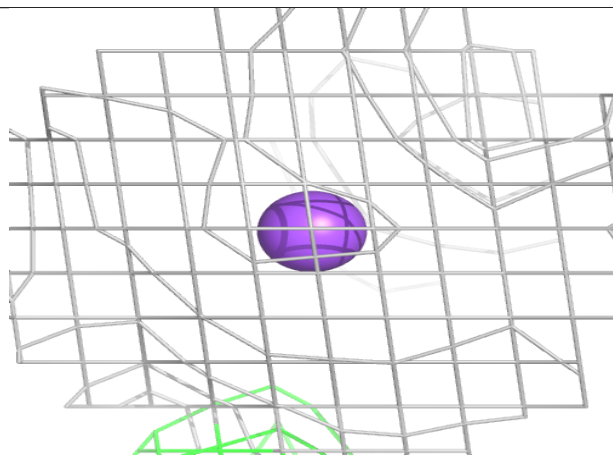
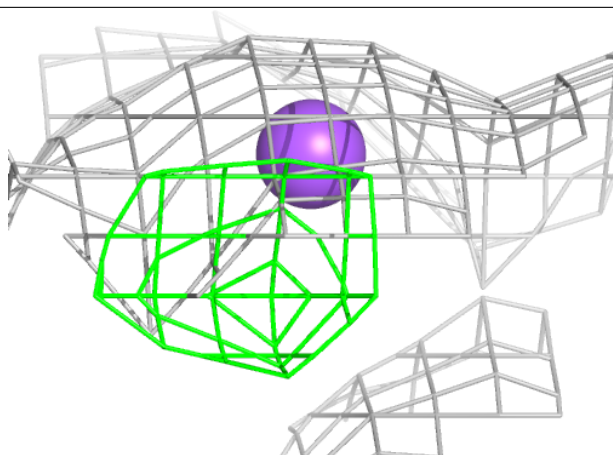
Electron density around V0S B 701:

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

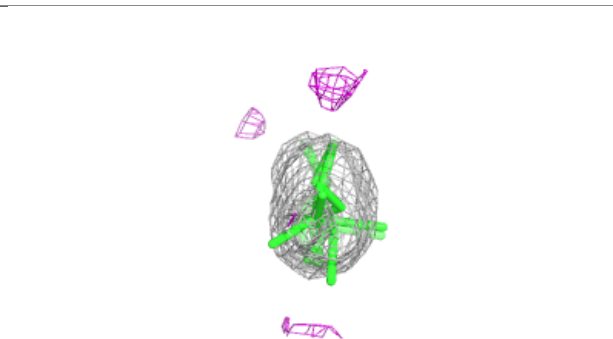
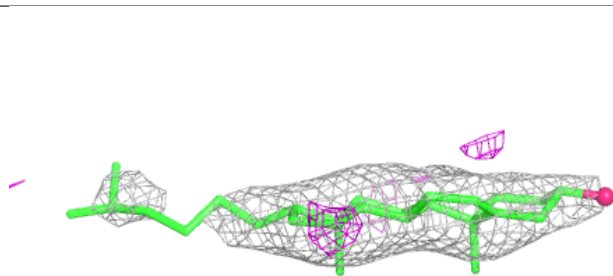
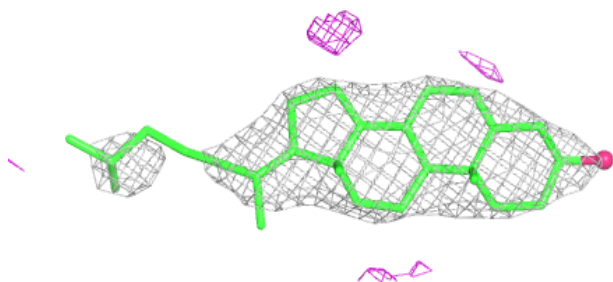


Electron density around NA A 704:

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

**Electron density around CLR 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.