



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:35 AM UTC

PDB ID : 2ZBA / pdb_00002zba
Title : Crystal Structure of F. sporotrichioides TRI101 complexed with Coenzyme A and T-2
Authors : Garvey, G.S.; McCormick, S.P.; Rayment, I.
Deposited on : 2007-10-18
Resolution : 2.00 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

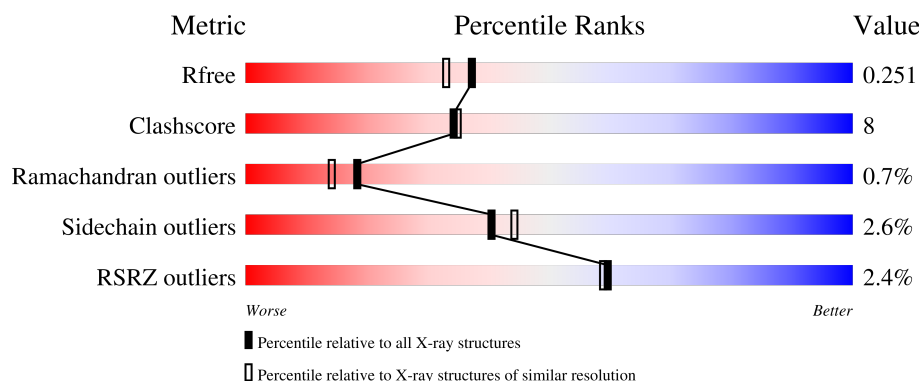
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	459	5% 81% 12% 5%
1	B	459	81% 12% 6%
1	C	459	83% 9% 6%
1	D	459	5% 71% 12% 14%

2 Entry composition [i](#)

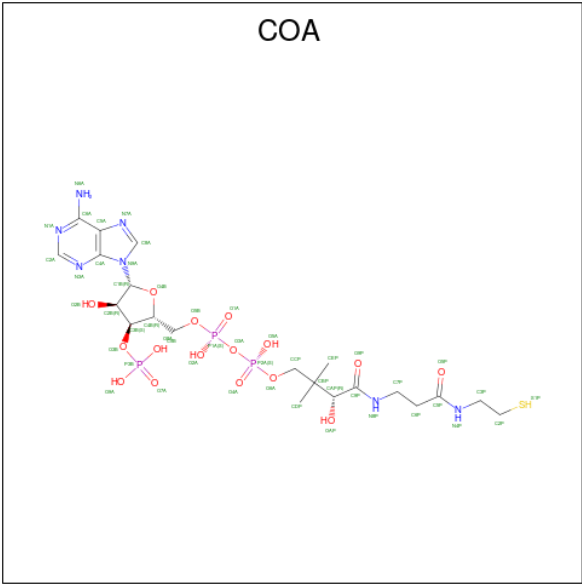
There are 7 unique types of molecules in this entry. The entry contains 14082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Trichothecene 3-O-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	Se	0	4	0
			3315	2109	553	638	3	12			
1	B	430	Total	C	N	O	S	Se	0	1	0
			3264	2070	551	628	3	12			
1	C	431	Total	C	N	O	S	Se	0	4	2
			3299	2100	547	637	3	12			
1	D	393	Total	C	N	O	S	Se	0	1	2
			2959	1892	492	560	3	12			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



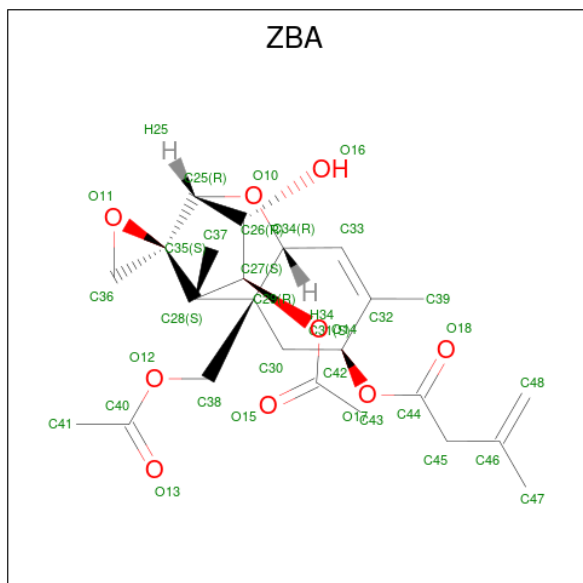
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 12,13-Epoxytrichothec-9-ene-3,4,8,15-tetrol-4,15-diacetate-8-isovalerate (CCD ID: ZBA) (formula: $C_{24}H_{32}O_9$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			30	22 8		
3	B	1	Total	C O	0	0
			33	24 9		
3	C	1	Total	C O	0	0
			33	24 9		
3	D	1	Total	C O	0	0
			33	24 9		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

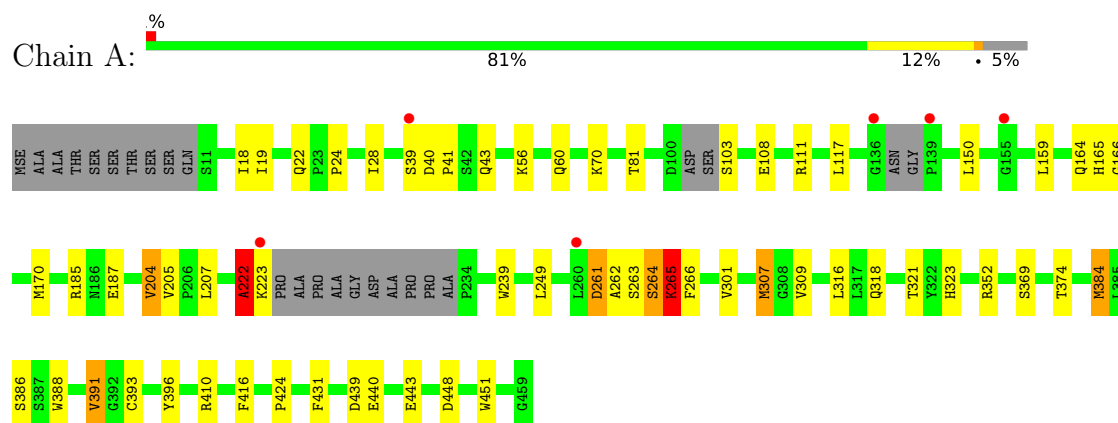
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	220	Total 220	O 220	0	0
7	B	221	Total 221	O 221	0	0
7	C	300	Total 300	O 300	0	0
7	D	171	Total 171	O 171	0	0

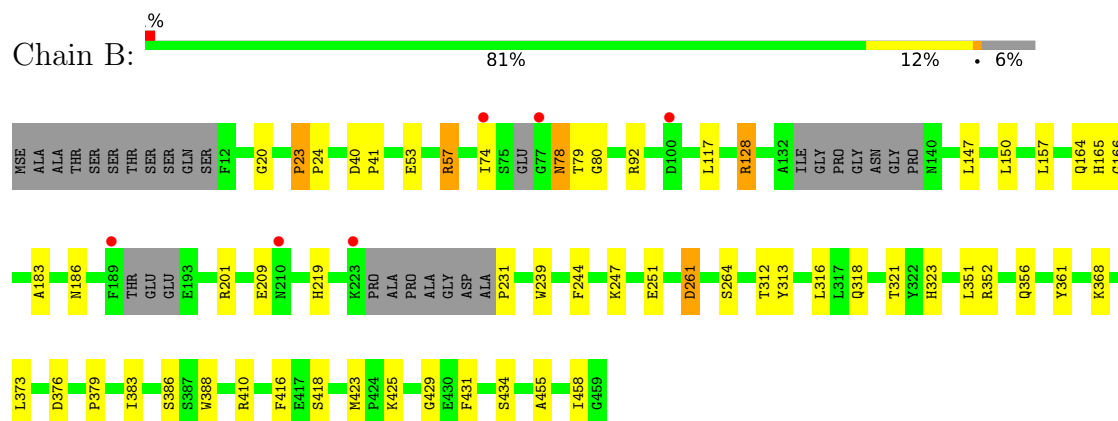
3 Residue-property plots

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.

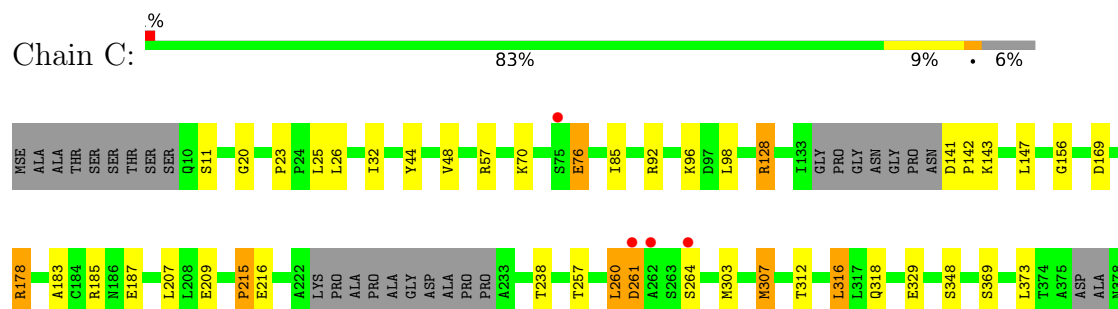
• Molecule 1: Trichothecene 3-O-acetyltransferase

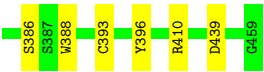


• Molecule 1: Trichothecene 3-O-acetyltransferase

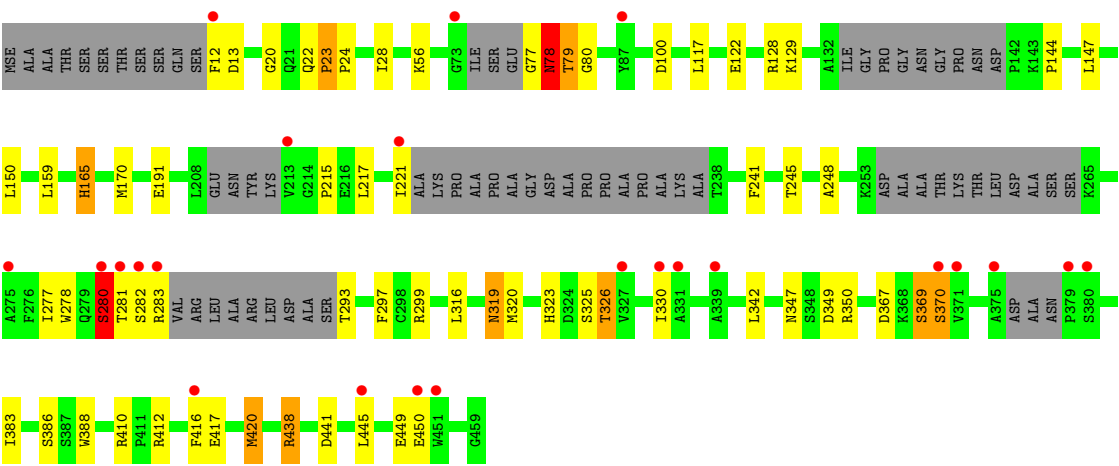


• Molecule 1: Trichothecene 3-O-acetyltransferase





● Molecule 1: Trichothecene 3-O-acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.97Å 81.97Å 113.51Å 90.00° 109.15° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.6 (30.00-2.00) 88.5 (30.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.251 0.199 , 0.251	Depositor DCC
R_{free} test set	5206 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14082	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: GOL, COA, ZBA, CA, DMS

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	0.75	2/3385 (0.1%)	0.92	6/4570 (0.1%)
1	B	0.75	0/3321	0.91	4/4474 (0.1%)
1	C	0.82	1/3369 (0.0%)	0.95	7/4550 (0.2%)
1	D	0.71	0/3011	0.95	8/4048 (0.2%)
All	All	0.76	3/13086 (0.0%)	0.93	25/17642 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	307	MSE	SE-CE	-8.36	1.70	1.95
1	A	384	MSE	SE-CE	-7.64	1.72	1.95
1	A	307	MSE	SE-CE	-7.08	1.74	1.95

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	THR	N-CA-C	8.30	128.49	110.80
1	D	280	SER	N-CA-C	8.10	123.59	111.04
1	C	215	PRO	N-CA-C	7.71	128.36	112.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	PRO	CA-C-N	6.84	126.88	119.90
1	B	231	PRO	C-N-CA	6.84	126.88	119.90
1	C	141	ASP	CA-C-N	-6.64	113.14	119.85
1	C	141	ASP	C-N-CA	-6.64	113.14	119.85
1	A	264	SER	CA-C-N	5.85	132.23	121.70
1	A	264	SER	C-N-CA	5.85	132.23	121.70
1	C	209	GLU	N-CA-C	5.84	117.45	111.14
1	D	78	ASN	CA-C-N	5.71	132.46	121.54
1	D	78	ASN	C-N-CA	5.71	132.46	121.54
1	C	76	GLU	N-CA-C	-5.53	99.03	110.80
1	C	156	GLY	N-CA-C	5.49	119.97	111.08
1	C	260	LEU	N-CA-C	5.43	118.12	111.82
1	A	222	ALA	CA-C-N	5.42	131.45	121.70
1	A	222	ALA	C-N-CA	5.42	131.45	121.70
1	B	458	ILE	N-CA-C	-5.42	107.51	111.90
1	D	78	ASN	N-CA-C	5.22	121.93	110.80
1	A	222	ALA	O-C-N	-5.12	117.94	123.42
1	D	22	GLN	CA-C-N	5.08	125.61	120.38
1	D	22	GLN	C-N-CA	5.08	125.61	120.38
1	D	165	HIS	N-CA-C	5.07	118.56	112.38
1	B	23	PRO	N-CA-C	5.03	116.83	110.70
1	A	369	SER	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ALA	Peptide
1	C	215	PRO	Peptide
1	D	280	SER	Peptide
1	D	78	ASN	Peptide

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	3315	0	3228	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3264	0	3156	47	0
1	C	3299	0	3226	35	0
1	D	2959	0	2812	57	0
2	A	48	0	32	2	0
2	B	48	0	32	5	0
2	C	48	0	32	4	0
2	D	48	0	32	3	0
3	A	30	0	29	7	0
3	B	33	0	32	4	0
3	C	33	0	32	0	0
3	D	33	0	32	1	0
4	A	2	0	0	0	0
5	B	4	0	6	0	0
6	C	6	0	8	0	0
7	A	220	0	0	6	0
7	B	221	0	0	2	0
7	C	300	0	0	6	0
7	D	171	0	0	4	0
All	All	14082	0	12689	197	0

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 8.

All (197) 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:261:ASP:HB2	1:A:262:ALA:HA	1.40	1.03
1:B:373:LEU:CD1	3:B:461:ZBA:H43	1.90	1.01
1:A:222:ALA:HB1	1:A:223:LYS:CB	1.91	1.01
1:A:261:ASP:CB	1:A:262:ALA:HA	1.92	0.96
1:A:264:SER:HA	1:A:265:LYS:HB2	1.44	0.96
1:D:282:SER:HA	1:D:283:ARG:C	1.96	0.91
1:D:277:ILE:HG21	1:D:420:MSE:HE1	1.52	0.91
1:D:245:THR:HG23	1:D:248:ALA:H	1.36	0.89
1:B:373:LEU:HD13	3:B:461:ZBA:H43	1.53	0.89
1:D:319:ASN:HD22	1:D:320:MSE:H	1.20	0.88
1:B:79:THR:HG23	7:B:1141:HOH:O	1.71	0.88
1:D:369:SER:CA	1:D:370:SER:CB	2.53	0.87
1:C:185:ARG:NH1	1:C:187:GLU:OE2	2.08	0.87
1:D:412:ARG:HG2	1:D:412:ARG:HH11	1.40	0.85
1:D:78:ASN:N	1:D:80:GLY:H	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:HG22	1:A:424:PRO:HG3	1.59	0.84
1:B:361:TYR:CZ	1:B:361:TYR:CD1	2.63	0.84
1:A:261:ASP:HB3	1:A:263:SER:H	1.43	0.84
1:D:416:PHE:CE2	1:D:416:PHE:CE1	2.60	0.82
1:C:329:GLU:OE1	7:C:1012:HOH:O	2.01	0.79
1:B:416:PHE:CD1	1:B:416:PHE:CZ	2.69	0.77
1:B:352:ARG:HG2	1:B:356:GLN:HE21	1.48	0.77
1:C:178:ARG:HD2	7:C:1008:HOH:O	1.85	0.76
1:A:18:ILE:HD13	7:A:1007:HOH:O	1.85	0.75
7:C:1202:HOH:O	1:D:191:GLU:HG3	1.87	0.74
1:D:369:SER:CA	1:D:370:SER:HB2	2.17	0.74
1:B:373:LEU:HD12	3:B:461:ZBA:H43	1.68	0.73
1:B:79:THR:HG21	1:B:368:LYS:H	1.55	0.72
1:D:78:ASN:H	1:D:80:GLY:H	1.38	0.71
1:A:261:ASP:HB3	1:A:263:SER:N	2.05	0.70
1:D:221:ILE:HG13	1:D:370:SER:O	1.91	0.70
1:C:169:ASP:HB3	1:C:316:LEU:HD23	1.74	0.70
1:C:25:LEU:HD13	1:C:316:LEU:HD11	1.74	0.70
1:A:261:ASP:CB	1:A:262:ALA:CA	2.69	0.70
1:D:319:ASN:ND2	1:D:320:MSE:H	1.89	0.69
1:B:150:LEU:HD22	1:B:157:LEU:HD11	1.74	0.69
1:B:425:LYS:HD3	1:B:429:GLY:HA2	1.74	0.69
1:C:70:LYS:HG3	1:C:85:ILE:HD11	1.75	0.68
1:A:117:LEU:HD23	1:A:239:TRP:HB3	1.76	0.68
1:D:347:ASN:HD22	1:D:350:ARG:H	1.43	0.67
1:B:201:ARG:HG2	1:B:313:TYR:OH	1.94	0.67
1:A:391:VAL:CG2	1:A:424:PRO:HG3	2.25	0.67
1:D:369:SER:CA	1:D:370:SER:HB3	2.27	0.65
1:A:28:ILE:HD11	3:A:463:ZBA:H47B	1.79	0.65
1:A:264:SER:HA	1:A:265:LYS:CB	2.22	0.65
1:A:352:ARG:NH1	7:A:1004:HOH:O	2.23	0.63
1:C:185:ARG:NH1	1:C:187:GLU:CD	2.56	0.63
1:A:318:GLN:NE2	3:A:463:ZBA:O14	2.33	0.62
1:D:319:ASN:HD22	1:D:320:MSE:N	1.95	0.62
1:A:204:VAL:HG22	1:A:309:VAL:HG21	1.82	0.61
1:C:388:TRP:HE1	2:C:460:COA:H21	1.66	0.61
1:A:164:GLN:HE22	1:A:166:GLY:H	1.47	0.61
1:A:416:PHE:CE1	3:A:463:ZBA:H48	2.35	0.60
1:C:128:ARG:NH2	1:C:142:PRO:O	2.34	0.60
1:D:388:TRP:HE1	2:D:460:COA:H21	1.65	0.60
1:D:165:HIS:O	1:D:165:HIS:HD2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:463:ZBA:H41A	3:A:463:ZBA:H45A	1.84	0.59
1:D:347:ASN:ND2	1:D:350:ARG:H	2.00	0.59
1:A:165:HIS:HD2	1:A:165:HIS:O	1.85	0.59
1:B:79:THR:CG2	1:B:368:LYS:H	2.15	0.59
1:D:128:ARG:HD3	1:D:147:LEU:CD1	2.33	0.58
1:A:222:ALA:CB	1:A:223:LYS:CB	2.76	0.58
1:A:164:GLN:NE2	1:A:166:GLY:H	2.02	0.58
1:B:386:SER:OG	2:B:460:COA:C2P	2.51	0.57
1:D:412:ARG:HG2	1:D:412:ARG:NH1	2.13	0.57
1:A:81:THR:HG22	7:A:1070:HOH:O	2.05	0.57
1:C:96:LYS:HE2	1:C:98:LEU:HD21	1.85	0.57
1:B:165:HIS:O	1:B:165:HIS:HD2	1.87	0.57
1:A:388:TRP:CH2	1:A:410:ARG:HG3	2.41	0.56
1:B:78:ASN:ND2	1:B:80:GLY:H	2.04	0.56
1:A:19:ILE:HG22	1:A:316:LEU:CD2	2.36	0.56
1:C:20:GLY:HA2	1:C:316:LEU:HD12	1.87	0.56
1:D:165:HIS:O	1:D:165:HIS:CD2	2.59	0.56
1:A:388:TRP:HE1	2:A:462:COA:H21	1.71	0.56
1:D:388:TRP:CH2	1:D:410:ARG:HG3	2.41	0.55
1:C:238:THR:HG23	1:C:439:ASP:OD1	2.07	0.55
1:D:325:SER:HB3	1:D:330:ILE:HD11	1.89	0.55
1:A:391:VAL:HG22	1:A:424:PRO:CG	2.36	0.55
1:B:261:ASP:HB2	7:D:1045:HOH:O	2.06	0.54
1:C:388:TRP:CH2	1:C:410:ARG:HG3	2.43	0.54
1:A:117:LEU:CD2	1:A:239:TRP:HB3	2.37	0.54
1:B:78:ASN:HD22	1:B:80:GLY:H	1.56	0.54
1:D:165:HIS:O	1:D:316:LEU:HD12	2.07	0.54
1:C:44:TYR:O	1:C:48:VAL:HG23	2.08	0.54
1:D:323:HIS:CE1	1:D:342:LEU:HA	2.43	0.54
1:B:321:THR:OG1	1:B:323:HIS:HE1	1.90	0.53
1:B:318:GLN:NE2	2:B:460:COA:S1P	2.80	0.53
1:A:165:HIS:O	1:A:165:HIS:CD2	2.63	0.52
1:B:164:GLN:HE22	1:B:166:GLY:H	1.57	0.52
1:C:92:ARG:HB2	1:C:147:LEU:HD23	1.90	0.52
1:B:53:GLU:O	1:B:57:ARG:HG2	2.10	0.52
1:C:32[A]:ILE:HD13	1:C:388:TRP:CZ3	2.45	0.52
1:B:92:ARG:HB2	1:B:147:LEU:HD23	1.92	0.52
1:C:25:LEU:CD1	1:C:316:LEU:HD11	2.37	0.52
1:C:386:SER:OG	2:C:460:COA:C2P	2.58	0.52
1:A:40:ASP:H	1:A:43:GLN:NE2	2.08	0.51
1:D:78:ASN:N	1:D:80:GLY:N	2.54	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:TRP:CH2	1:B:410:ARG:HG3	2.46	0.51
1:D:386:SER:OG	2:D:460:COA:H22	2.10	0.51
1:C:25:LEU:HD13	1:C:316:LEU:CD1	2.40	0.51
1:D:386:SER:OG	2:D:460:COA:C2P	2.59	0.51
1:B:79:THR:HG21	1:B:368:LYS:HB2	1.93	0.51
1:D:144:PRO:HG2	1:D:147:LEU:HD21	1.94	0.50
1:C:32[A]:ILE:HD13	1:C:388:TRP:HZ3	1.77	0.50
1:B:165:HIS:O	1:B:165:HIS:CD2	2.65	0.49
1:B:57:ARG:HB2	1:B:183:ALA:HB1	1.94	0.49
1:B:23:PRO:N	1:B:24:PRO:HD2	2.27	0.49
1:B:388:TRP:HE1	2:B:460:COA:H21	1.78	0.49
1:A:416:PHE:CZ	3:A:463:ZBA:H48	2.47	0.49
1:B:117:LEU:HD23	1:B:239:TRP:HB3	1.94	0.49
1:A:264:SER:CA	1:A:265:LYS:HB2	2.30	0.49
1:B:219:HIS:HD2	1:B:376:ASP:OD2	1.95	0.49
1:B:312:THR:O	1:B:312:THR:HG22	2.12	0.48
1:D:122:GLU:OE2	1:D:129:LYS:NZ	2.43	0.48
1:C:312:THR:HG22	1:C:312:THR:O	2.13	0.48
1:D:20:GLY:HA2	1:D:316:LEU:HD13	1.95	0.48
1:D:278:TRP:HA	1:D:383:ILE:CD1	2.43	0.48
1:B:74:ILE:H	1:B:74:ILE:HD12	1.79	0.48
1:D:150:LEU:HD13	1:D:159:LEU:HD13	1.96	0.48
1:A:386:SER:OG	2:A:462:COA:C2P	2.61	0.48
1:D:282:SER:CA	1:D:283:ARG:C	2.78	0.48
1:C:261:ASP:N	7:C:1006:HOH:O	2.39	0.47
1:A:22:GLN:HB3	1:A:24:PRO:HD2	1.97	0.47
1:A:249:LEU:HD11	1:A:431:PHE:HB2	1.97	0.47
1:C:178:ARG:NH2	7:C:1009:HOH:O	2.29	0.47
1:D:277:ILE:CG2	1:D:420:MSE:HE1	2.34	0.47
1:A:56:LYS:O	1:A:60:GLN:HG3	2.14	0.47
1:A:261:ASP:HB3	1:A:262:ALA:CA	2.42	0.47
1:B:261:ASP:CB	7:D:1045:HOH:O	2.61	0.47
1:C:23:PRO:HG2	1:C:369:SER:HA	1.96	0.47
1:D:299:ARG:O	1:D:320:MSE:HA	2.15	0.47
1:B:164:GLN:NE2	1:B:166:GLY:H	2.12	0.46
1:A:264:SER:CA	1:A:265:LYS:CB	2.91	0.46
1:C:20:GLY:HA2	1:C:316:LEU:CD1	2.46	0.46
1:B:20:GLY:HA2	1:B:316:LEU:HD13	1.97	0.46
1:A:108:GLU:OE2	1:A:111:ARG:NH1	2.46	0.46
1:D:347:ASN:HD21	1:D:349:ASP:HB2	1.80	0.46
1:D:281:THR:HG21	1:D:383:ILE:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:CD2	1:B:239:TRP:HB3	2.46	0.46
1:B:244:PHE:CE1	1:B:455:ALA:HB2	2.51	0.46
1:B:386:SER:OG	2:B:460:COA:H21	2.15	0.46
1:B:128:ARG:HD3	7:B:1144:HOH:O	2.15	0.46
1:B:425:LYS:HG3	1:B:431:PHE:CE1	2.51	0.46
1:C:393:CYS:HA	1:C:396:TYR:CE2	2.51	0.46
1:A:165:HIS:HE1	3:A:463:ZBA:O16	1.99	0.45
1:B:423:MSE:HE3	1:B:434:SER:HB2	1.99	0.45
1:C:318:GLN:OE1	2:C:460:COA:S1P	2.74	0.45
1:A:393:CYS:HA	1:A:396:TYR:CE2	2.52	0.45
1:C:26:LEU:O	1:C:143:LYS:HE2	2.17	0.45
1:B:386:SER:OG	2:B:460:COA:H22	2.17	0.45
1:B:379:PRO:O	1:B:418:SER:OG	2.35	0.45
1:A:443:GLU:HB3	7:A:1013:HOH:O	2.17	0.44
1:D:412:ARG:NH1	7:D:1159:HOH:O	2.50	0.44
1:C:57:ARG:HD2	1:C:183:ALA:O	2.16	0.44
1:B:247:LYS:O	1:B:251:GLU:HG3	2.18	0.44
1:D:215:PRO:C	1:D:217:LEU:H	2.24	0.44
1:D:77:GLY:O	1:D:78:ASN:HB3	2.18	0.44
1:D:278:TRP:HA	1:D:383:ILE:HD12	1.98	0.44
1:A:40:ASP:HA	1:A:41:PRO:HD3	1.88	0.44
1:B:40:ASP:HA	1:B:41:PRO:HD3	1.90	0.43
1:B:165:HIS:O	1:B:316:LEU:HD12	2.18	0.43
1:B:165:HIS:HE1	3:B:461:ZBA:O16	2.00	0.43
1:D:367:ASP:C	1:D:369:SER:H	2.26	0.43
1:A:205:VAL:HA	1:A:307:MSE:HE2	2.01	0.43
1:D:117:LEU:HD13	1:D:241:PHE:CZ	2.53	0.43
1:D:293:THR:O	1:D:326:THR:HA	2.18	0.43
1:A:374:THR:HB	1:A:384:MSE:HE3	1.99	0.43
1:C:185:ARG:HH11	1:C:185:ARG:HD3	1.65	0.42
1:C:303:MSE:O	1:C:307:MSE:HG2	2.20	0.42
1:D:369:SER:N	1:D:370:SER:HB3	2.35	0.42
1:A:321:THR:OG1	1:A:323:HIS:HE1	2.02	0.42
1:A:150:LEU:HD13	1:A:159:LEU:HD13	2.01	0.42
1:C:388:TRP:CZ3	1:C:410:ARG:HG3	2.53	0.42
1:D:28:ILE:HD11	3:D:461:ZBA:H45A	2.01	0.42
1:A:28:ILE:HD11	3:A:463:ZBA:C47	2.47	0.42
1:A:261:ASP:HA	7:A:1108:HOH:O	2.19	0.42
1:A:265:LYS:HD3	1:A:265:LYS:C	2.45	0.42
1:D:278:TRP:CE2	1:D:297:PHE:HB2	2.54	0.42
1:C:178:ARG:NE	7:C:1009:HOH:O	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:SER:O	1:D:283:ARG:HB3	2.20	0.41
1:D:417:GLU:CG	7:D:1028:HOH:O	2.68	0.41
1:A:264:SER:CB	7:A:1085:HOH:O	2.66	0.41
1:A:440:GLU:HA	1:A:443:GLU:HG2	2.01	0.41
1:C:257:THR:HA	1:C:260:LEU:HG	2.01	0.41
1:C:386:SER:OG	2:C:460:COA:H22	2.19	0.41
1:D:449:GLU:H	1:D:449:GLU:CD	2.28	0.41
1:A:170:MSE:HG2	1:A:388:TRP:CD2	2.55	0.41
1:D:438[A]:ARG:HG3	1:D:441:ASP:HB2	2.01	0.41
1:D:170:MSE:HG2	1:D:388:TRP:CD2	2.55	0.41
1:A:261:ASP:HB3	1:A:262:ALA:HA	1.92	0.41
1:D:215:PRO:C	1:D:217:LEU:N	2.79	0.41
1:A:448:ASP:HB3	1:A:451:TRP:HB3	2.03	0.41
1:A:439:ASP:O	1:A:443:GLU:HG2	2.21	0.41
1:A:185:ARG:HD3	1:A:187:GLU:OE2	2.21	0.41
1:D:23:PRO:N	1:D:24:PRO:HD2	2.37	0.40
1:A:265:LYS:HD2	1:A:266:PHE:HD2	1.85	0.40
1:D:388:TRP:CZ3	1:D:410:ARG:HG3	2.55	0.40

There are no symmetry-related clashes.

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	431/459 (94%)	416 (96%)	13 (3%)	2 (0%)	24	21
1	B	421/459 (92%)	409 (97%)	11 (3%)	1 (0%)	43	42
1	C	427/459 (93%)	410 (96%)	13 (3%)	4 (1%)	14	9
1	D	378/459 (82%)	358 (95%)	15 (4%)	5 (1%)	9	5
All	All	1657/1836 (90%)	1593 (96%)	52 (3%)	12 (1%)	18	14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	LYS
1	B	209	GLU
1	C	11	SER
1	C	216	GLU
1	D	79	THR
1	D	369	SER
1	D	370	SER
1	A	261	ASP
1	D	13	ASP
1	D	78	ASN
1	C	76	GLU
1	C	261	ASP

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	351/377 (93%)	343 (98%)	8 (2%)	44	49
1	B	344/377 (91%)	336 (98%)	8 (2%)	44	49
1	C	352/377 (93%)	345 (98%)	7 (2%)	48	54
1	D	300/377 (80%)	287 (96%)	13 (4%)	26	25
All	All	1347/1508 (89%)	1311 (97%)	36 (3%)	40	42

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	70	LYS
1	A	103	SER
1	A	204	VAL
1	A	207	LEU
1	A	265	LYS
1	A	301	VAL
1	A	391	VAL
1	B	57	ARG
1	B	78	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	128	ARG
1	B	186	ASN
1	B	261	ASP
1	B	264	SER
1	B	351	LEU
1	B	383	ILE
1	C	128	ARG
1	C	178	ARG
1	C	207	LEU
1	C	264	SER
1	C	316	LEU
1	C	348	SER
1	C	373	LEU
1	D	12	PHE
1	D	23	PRO
1	D	56	LYS
1	D	78	ASN
1	D	100	ASP
1	D	280	SER
1	D	319	ASN
1	D	326	THR
1	D	420	MSE
1	D	438[A]	ARG
1	D	438[B]	ARG
1	D	445	LEU
1	D	450	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	123	ASN
1	A	149	GLN
1	A	151	ASN
1	A	164	GLN
1	A	165	HIS
1	A	219	HIS
1	A	318	GLN
1	A	323	HIS
1	A	356	GLN
1	B	43	GLN
1	B	78	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	164	GLN
1	B	165	HIS
1	B	210	ASN
1	B	219	HIS
1	B	323	HIS
1	B	332	ASN
1	B	356	GLN
1	C	43	GLN
1	C	165	HIS
1	C	198	ASN
1	C	220	GLN
1	C	332	ASN
1	C	356	GLN
1	D	149	GLN
1	D	151	ASN
1	D	164	GLN
1	D	165	HIS
1	D	186	ASN
1	D	198	ASN
1	D	319	ASN
1	D	347	ASN
1	D	363	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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
6	GOL	C	462	-	5,5,5	0.49	0	5,5,5	0.45	0
2	COA	C	460	-	47,50,50	1.53	4 (8%)	69,75,75	1.75	15 (21%)
3	ZBA	D	461	-	36,36,36	1.45	6 (16%)	48,58,58	1.89	13 (27%)
3	ZBA	A	463	-	33,33,36	1.35	6 (18%)	44,54,58	1.83	12 (27%)
2	COA	A	462	-	47,50,50	1.70	6 (12%)	69,75,75	1.62	9 (13%)
2	COA	D	460	-	47,50,50	1.79	6 (12%)	69,75,75	1.57	13 (18%)
5	DMS	B	462	-	3,3,3	2.66	1 (33%)	3,3,3	0.80	0
3	ZBA	C	461	-	36,36,36	1.51	7 (19%)	48,58,58	1.74	10 (20%)
2	COA	B	460	-	47,50,50	1.60	5 (10%)	69,75,75	1.71	11 (15%)
3	ZBA	B	461	-	36,36,36	1.31	3 (8%)	48,58,58	1.90	13 (27%)

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	GOL	C	462	-	-	2/4/4/4	-
2	COA	C	460	-	-	6/48/64/64	0/3/3/3
3	ZBA	D	461	-	-	10/18/83/83	0/5/4/4
3	ZBA	A	463	-	-	3/14/79/83	0/5/4/4
2	COA	A	462	-	-	9/48/64/64	0/3/3/3
2	COA	D	460	-	-	6/48/64/64	0/3/3/3
3	ZBA	C	461	-	-	9/18/83/83	0/5/4/4
2	COA	B	460	-	-	5/48/64/64	0/3/3/3
3	ZBA	B	461	-	-	9/18/83/83	0/5/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	460	COA	O9P-C9P	9.41	1.41	1.23
2	A	462	COA	O9P-C9P	8.74	1.40	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	460	COA	O9P-C9P	8.42	1.39	1.23
2	C	460	COA	O9P-C9P	8.06	1.38	1.23
5	B	462	DMS	O-S	4.47	1.79	1.50
3	B	461	ZBA	C48-C46	4.22	1.45	1.33
3	D	461	ZBA	C48-C46	4.18	1.45	1.33
3	C	461	ZBA	C48-C46	4.14	1.45	1.33
3	A	463	ZBA	C48-C46	4.09	1.44	1.33
3	C	461	ZBA	C28-C27	3.98	1.60	1.55
2	A	462	COA	P1A-O3A	3.58	1.63	1.59
3	D	461	ZBA	C28-C27	3.53	1.60	1.55
2	D	460	COA	P1A-O3A	3.51	1.63	1.59
2	D	460	COA	P2A-O3A	3.15	1.62	1.59
2	B	460	COA	C2A-N3A	3.07	1.39	1.33
2	D	460	COA	C2A-N3A	3.06	1.39	1.33
3	B	461	ZBA	C28-C27	3.04	1.59	1.55
2	A	462	COA	C2A-N3A	3.00	1.39	1.33
3	D	461	ZBA	C29-C28	2.89	1.62	1.59
2	A	462	COA	C2A-N1A	2.85	1.39	1.33
2	C	460	COA	C2A-N3A	2.84	1.39	1.33
3	C	461	ZBA	C29-C34	2.71	1.58	1.55
2	D	460	COA	C2A-N1A	2.70	1.38	1.33
2	C	460	COA	P1A-O3A	2.67	1.62	1.59
2	C	460	COA	C2A-N1A	2.59	1.38	1.33
3	C	461	ZBA	C29-C28	2.54	1.62	1.59
2	B	460	COA	C2A-N1A	2.51	1.38	1.33
3	A	463	ZBA	O10-C34	2.45	1.48	1.44
3	D	461	ZBA	C29-C34	2.43	1.58	1.55
3	C	461	ZBA	O10-C34	2.42	1.48	1.44
3	D	461	ZBA	O14-C42	2.35	1.40	1.35
3	C	461	ZBA	O14-C42	2.34	1.40	1.35
3	B	461	ZBA	C30-C29	2.28	1.57	1.54
3	A	463	ZBA	C29-C34	2.28	1.57	1.55
2	D	460	COA	C8A-N7A	2.25	1.36	1.31
2	A	462	COA	C8A-N7A	2.23	1.36	1.31
3	C	461	ZBA	C30-C29	2.23	1.57	1.54
3	D	461	ZBA	C30-C29	2.22	1.57	1.54
2	A	462	COA	P2A-O3A	2.20	1.61	1.59
3	A	463	ZBA	C30-C29	2.15	1.57	1.54
2	B	460	COA	P3B-O3B	2.13	1.63	1.59
3	A	463	ZBA	C28-C27	2.09	1.60	1.56
2	B	460	COA	C8A-N7A	2.06	1.35	1.31
3	A	463	ZBA	C29-C28	2.02	1.61	1.59

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	460	COA	N3A-C2A-N1A	-6.37	118.93	128.58
2	C	460	COA	N3A-C2A-N1A	-6.09	119.37	128.58
2	A	462	COA	N3A-C2A-N1A	-6.02	119.47	128.58
3	D	461	ZBA	C31-O17-C44	5.69	124.76	116.25
2	D	460	COA	N3A-C2A-N1A	-5.23	120.66	128.58
2	B	460	COA	C5A-C4A-N3A	-4.88	119.99	126.72
3	B	461	ZBA	C35-C28-C29	4.80	109.77	106.94
2	A	462	COA	C5A-C4A-N3A	-4.79	120.12	126.72
2	D	460	COA	C5A-C4A-N3A	-4.50	120.52	126.72
3	D	461	ZBA	O14-C42-C43	4.32	118.80	111.09
2	C	460	COA	C5A-C4A-N3A	-4.16	120.99	126.72
3	A	463	ZBA	C30-C29-C34	-4.14	104.72	107.75
3	B	461	ZBA	C31-O17-C44	4.10	122.39	116.25
3	B	461	ZBA	C30-C29-C34	-4.05	104.79	107.75
3	C	461	ZBA	C47-C46-C48	-4.04	112.06	122.23
3	A	463	ZBA	C47-C46-C48	-3.95	112.30	122.23
3	B	461	ZBA	O10-C34-C29	-3.94	107.69	112.61
3	C	461	ZBA	O14-C42-C43	3.80	117.87	111.09
3	B	461	ZBA	C29-C34-C33	3.75	116.69	113.33
3	C	461	ZBA	C31-O17-C44	3.74	121.84	116.25
3	C	461	ZBA	O12-C38-C29	3.72	116.97	109.58
3	A	463	ZBA	O10-C34-C29	-3.71	107.97	112.61
2	B	460	COA	C2A-N3A-C4A	3.68	120.83	111.83
2	A	462	COA	C2A-N3A-C4A	3.66	120.76	111.83
2	C	460	COA	CEP-CBP-CAP	3.58	114.87	108.77
3	A	463	ZBA	C31-O17-C44	3.56	121.57	116.25
2	A	462	COA	N9A-C8A-N7A	-3.54	108.91	113.94
2	D	460	COA	N9A-C8A-N7A	-3.52	108.94	113.94
2	B	460	COA	C5A-N7A-C8A	3.52	108.98	103.45
3	C	461	ZBA	C30-C29-C34	-3.51	105.18	107.75
2	C	460	COA	N9A-C8A-N7A	-3.46	109.03	113.94
2	C	460	COA	C5A-N7A-C8A	3.43	108.84	103.45
3	D	461	ZBA	C29-C34-C33	3.41	116.39	113.33
2	B	460	COA	N9A-C8A-N7A	-3.38	109.14	113.94
3	D	461	ZBA	C30-C29-C34	-3.35	105.30	107.75
3	D	461	ZBA	C47-C46-C48	-3.34	113.83	122.23
2	A	462	COA	C5A-N7A-C8A	3.29	108.63	103.45
3	B	461	ZBA	C27-O14-C42	3.26	122.41	117.79
3	B	461	ZBA	C47-C46-C48	-3.24	114.08	122.23
2	C	460	COA	C2A-N3A-C4A	3.23	119.72	111.83
2	B	460	COA	O5A-P2A-O3A	3.23	116.00	107.27
2	D	460	COA	C2A-N3A-C4A	3.20	119.65	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	463	ZBA	C29-C28-C27	3.18	111.52	108.33
2	D	460	COA	C5A-N7A-C8A	3.16	108.42	103.45
3	C	461	ZBA	C29-C34-C33	3.11	116.12	113.33
2	C	460	COA	O5A-P2A-O3A	3.10	115.66	107.27
2	B	460	COA	N3A-C4A-N9A	3.09	132.43	127.17
3	D	461	ZBA	C29-C30-C31	3.07	118.69	112.47
2	C	460	COA	N3A-C4A-N9A	3.06	132.37	127.17
3	B	461	ZBA	C38-C29-C28	-3.05	109.99	112.68
2	A	462	COA	N3A-C4A-N9A	3.05	132.36	127.17
2	A	462	COA	O5A-P2A-O3A	3.05	115.52	107.27
3	B	461	ZBA	C37-C28-C27	3.00	116.93	111.52
2	B	460	COA	O2A-P1A-O3A	2.88	115.06	107.27
3	B	461	ZBA	C37-C28-C29	-2.85	110.42	113.86
2	D	460	COA	N3A-C4A-N9A	2.84	131.99	127.17
3	A	463	ZBA	C29-C34-C33	2.83	115.88	113.33
3	A	463	ZBA	C35-C25-C26	-2.79	96.93	101.90
2	B	460	COA	C4A-C5A-N7A	-2.78	107.41	110.58
2	C	460	COA	O2A-P1A-O3A	2.76	114.73	107.27
2	C	460	COA	O6A-CCP-CBP	-2.75	106.12	110.55
2	D	460	COA	CEP-CBP-CAP	2.74	113.44	108.77
3	C	461	ZBA	C29-C30-C31	2.70	117.94	112.47
3	A	463	ZBA	C29-C30-C31	2.64	117.82	112.47
2	B	460	COA	O4B-C1B-N9A	2.62	113.11	108.09
3	C	461	ZBA	C29-C28-C27	2.59	110.93	108.33
2	C	460	COA	O4B-C1B-N9A	2.58	113.05	108.09
3	C	461	ZBA	C27-O14-C42	2.58	121.44	117.79
2	B	460	COA	O3A-P1A-O1A	-2.57	102.97	110.70
2	A	462	COA	C4A-C5A-N7A	-2.55	107.66	110.58
3	D	461	ZBA	C37-C28-C27	2.55	116.11	111.52
2	D	460	COA	O2A-P1A-O3A	2.51	114.05	107.27
3	D	461	ZBA	C27-O14-C42	2.50	121.34	117.79
2	A	462	COA	O3A-P1A-O1A	-2.48	103.25	110.70
2	C	460	COA	CAP-C9P-N8P	2.47	121.16	116.48
3	A	463	ZBA	C38-C29-C28	-2.44	110.53	112.68
2	D	460	COA	C7P-C6P-C5P	-2.44	108.33	112.39
2	D	460	COA	O5A-P2A-O3A	2.42	113.81	107.27
2	C	460	COA	O3A-P1A-O1A	-2.42	103.43	110.70
3	D	461	ZBA	O10-C34-C29	-2.42	109.59	112.61
2	D	460	COA	O4B-C1B-N9A	2.40	112.69	108.09
2	D	460	COA	C4A-C5A-N7A	-2.35	107.90	110.58
3	A	463	ZBA	O17-C44-C45	2.34	113.86	110.24
3	D	461	ZBA	C30-C29-C28	2.32	113.41	111.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	463	ZBA	C37-C28-C29	-2.30	111.10	113.86
3	D	461	ZBA	C38-O12-C40	-2.29	112.49	116.96
3	C	461	ZBA	C37-C28-C27	2.29	115.66	111.52
3	B	461	ZBA	O14-C42-C43	2.26	115.11	111.09
3	B	461	ZBA	C29-C30-C31	2.20	116.93	112.47
3	D	461	ZBA	C29-C28-C27	2.19	110.53	108.33
2	C	460	COA	C4A-C5A-N7A	-2.14	108.14	110.58
2	D	460	COA	C6A-C5A-C4A	2.08	120.02	117.18
3	D	461	ZBA	C35-C25-C26	-2.07	98.22	101.90
2	C	460	COA	C6A-C5A-C4A	2.00	119.92	117.18
3	A	463	ZBA	O14-C27-C28	2.00	117.03	112.60
3	B	461	ZBA	C28-C29-C34	2.00	110.83	109.28

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	462	COA	S1P-C2P-C3P-N4P
2	B	460	COA	S1P-C2P-C3P-N4P
2	C	460	COA	S1P-C2P-C3P-N4P
2	D	460	COA	S1P-C2P-C3P-N4P
3	A	463	ZBA	C44-C45-C46-C48
3	B	461	ZBA	C44-C45-C46-C47
3	C	461	ZBA	C44-C45-C46-C47
3	C	461	ZBA	C30-C29-C38-O12
3	C	461	ZBA	C34-C29-C38-O12
3	C	461	ZBA	C28-C29-C38-O12
3	D	461	ZBA	C44-C45-C46-C48
3	D	461	ZBA	C30-C31-O17-C44
3	D	461	ZBA	C32-C31-O17-C44
6	C	462	GOL	O1-C1-C2-C3
3	D	461	ZBA	C43-C42-O14-C27
3	D	461	ZBA	C41-C40-O12-C38
3	B	461	ZBA	C43-C42-O14-C27
2	C	460	COA	O5P-C5P-N4P-C3P
2	C	460	COA	C6P-C5P-N4P-C3P
2	D	460	COA	C6P-C5P-N4P-C3P
3	D	461	ZBA	O13-C40-O12-C38
2	D	460	COA	O5P-C5P-N4P-C3P
2	A	462	COA	C6P-C5P-N4P-C3P
3	D	461	ZBA	O15-C42-O14-C27
2	A	462	COA	O5P-C5P-N4P-C3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	461	ZBA	O15-C42-O14-C27
3	C	461	ZBA	C43-C42-O14-C27
2	B	460	COA	O5P-C5P-N4P-C3P
3	B	461	ZBA	C41-C40-O12-C38
6	C	462	GOL	O1-C1-C2-O2
2	B	460	COA	C6P-C5P-N4P-C3P
2	C	460	COA	P1A-O3A-P2A-O4A
2	D	460	COA	P1A-O3A-P2A-O4A
3	B	461	ZBA	C44-C45-C46-C48
3	D	461	ZBA	O17-C44-C45-C46
3	B	461	ZBA	C28-C27-O14-C42
3	A	463	ZBA	C44-C45-C46-C47
3	D	461	ZBA	C44-C45-C46-C47
3	B	461	ZBA	O13-C40-O12-C38
3	D	461	ZBA	O18-C44-C45-C46
3	B	461	ZBA	O17-C44-C45-C46
2	B	460	COA	P1A-O3A-P2A-O4A
2	A	462	COA	CDP-CBP-CCP-O6A
2	A	462	COA	CAP-CBP-CCP-O6A
3	C	461	ZBA	O15-C42-O14-C27
3	C	461	ZBA	O17-C44-C45-C46
2	A	462	COA	P1A-O3A-P2A-O5A
3	B	461	ZBA	O18-C44-C45-C46
3	C	461	ZBA	C28-C27-O14-C42
2	A	462	COA	P1A-O3A-P2A-O4A
2	C	460	COA	P1A-O3A-P2A-O5A
3	A	463	ZBA	C30-C31-O17-C44
2	D	460	COA	P1A-O3A-P2A-O5A
2	A	462	COA	CEP-CBP-CCP-O6A
3	C	461	ZBA	C44-C45-C46-C48
2	A	462	COA	N8P-C9P-CAP-OAP
2	B	460	COA	N8P-C9P-CAP-OAP
2	C	460	COA	N8P-C9P-CAP-OAP
2	D	460	COA	N8P-C9P-CAP-OAP

There are no ring outliers.

7 monomers are involved in 26 short contacts:

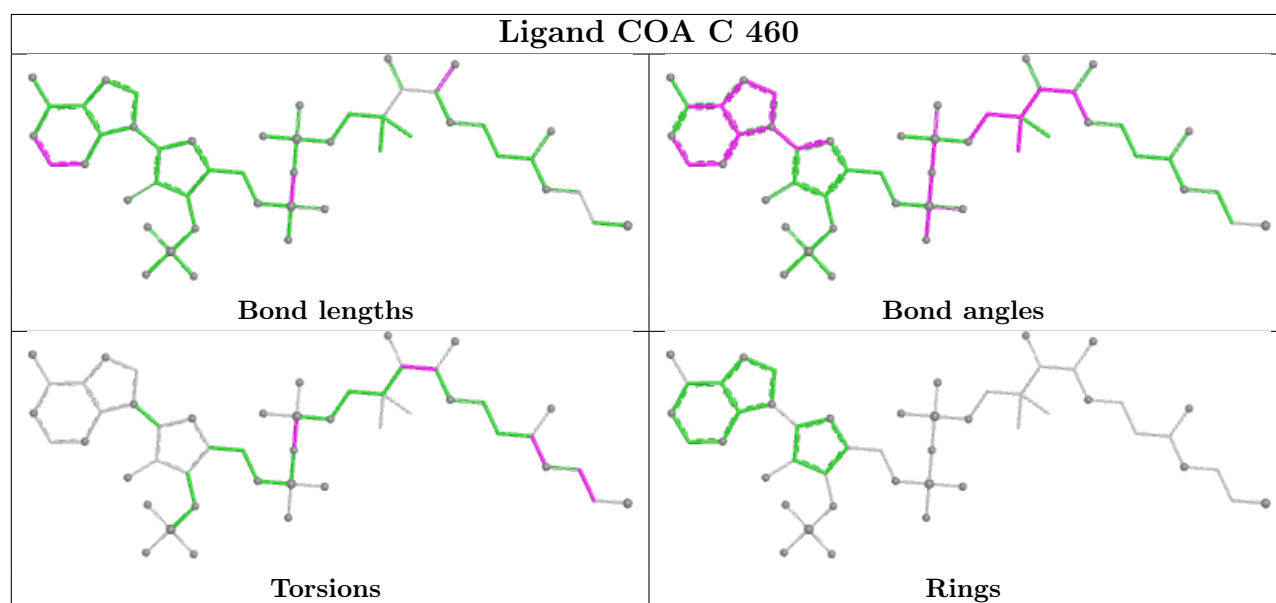
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	460	COA	4	0
3	D	461	ZBA	1	0
3	A	463	ZBA	7	0

Continued on next page...

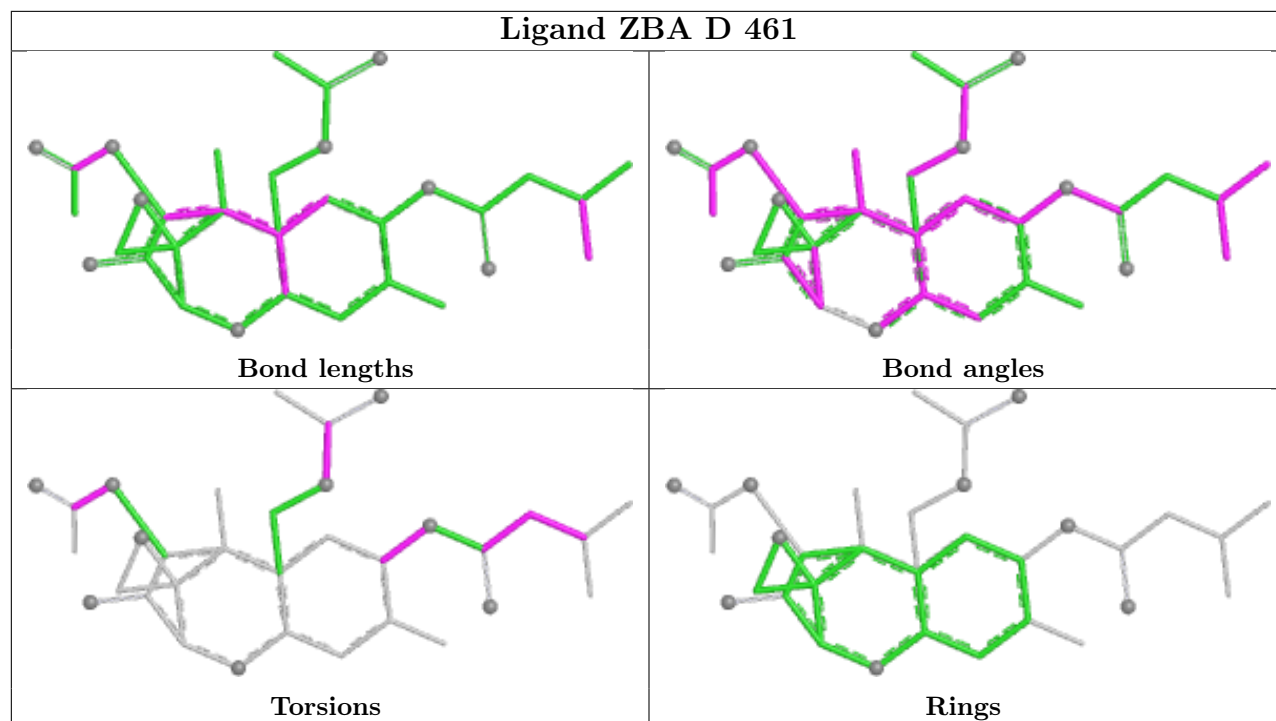
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	462	COA	2	0
2	D	460	COA	3	0
2	B	460	COA	5	0
3	B	461	ZBA	4	0

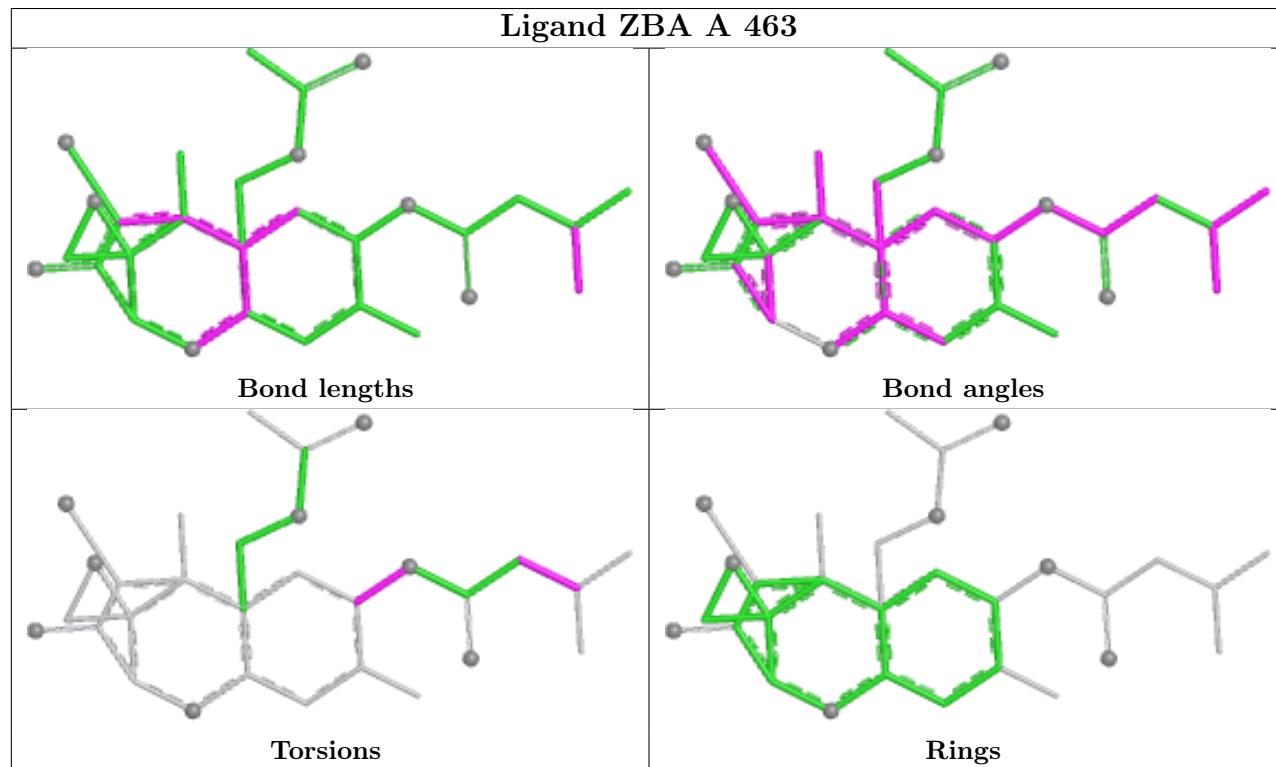
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

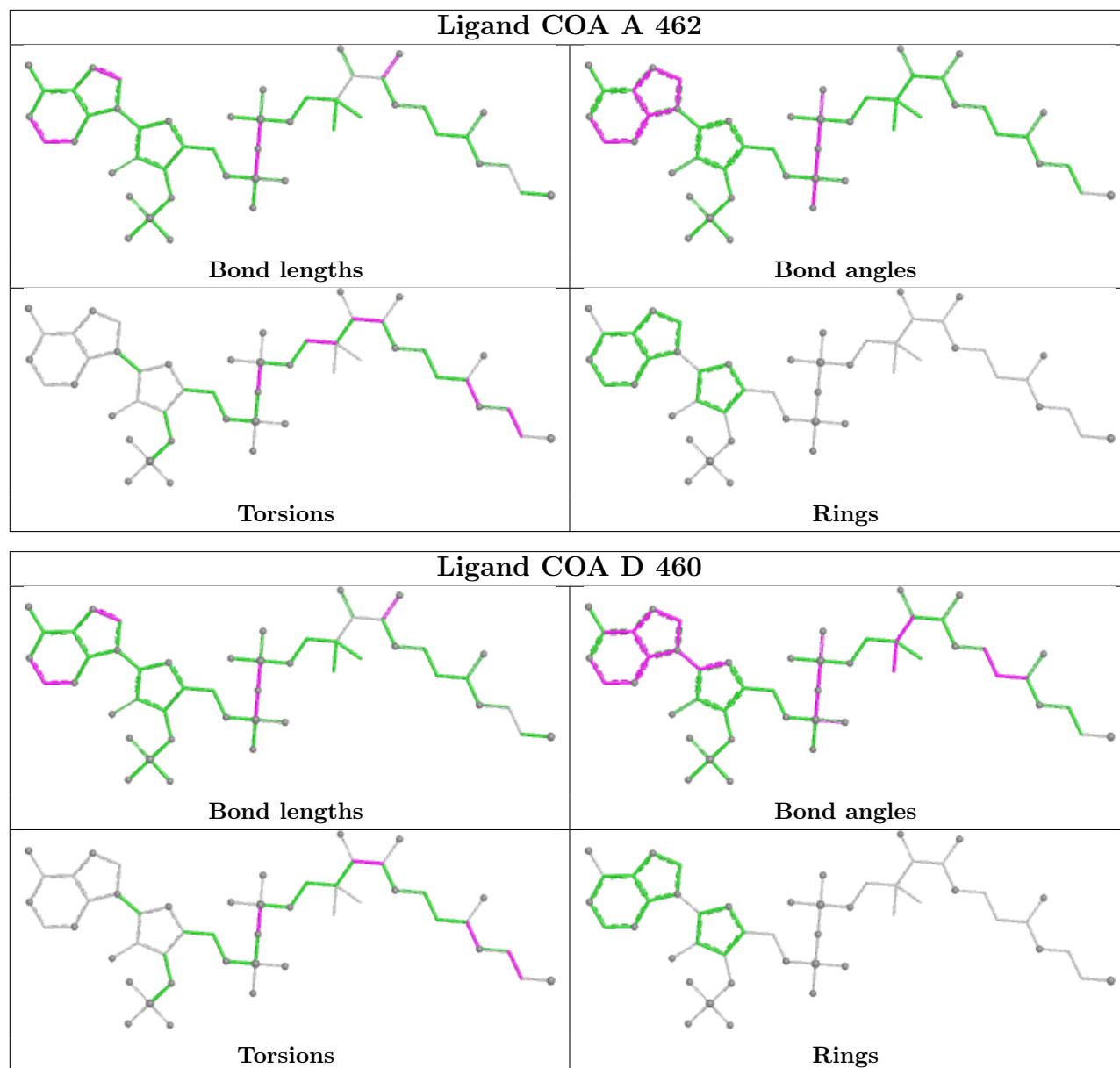


Ligand ZBA D 461

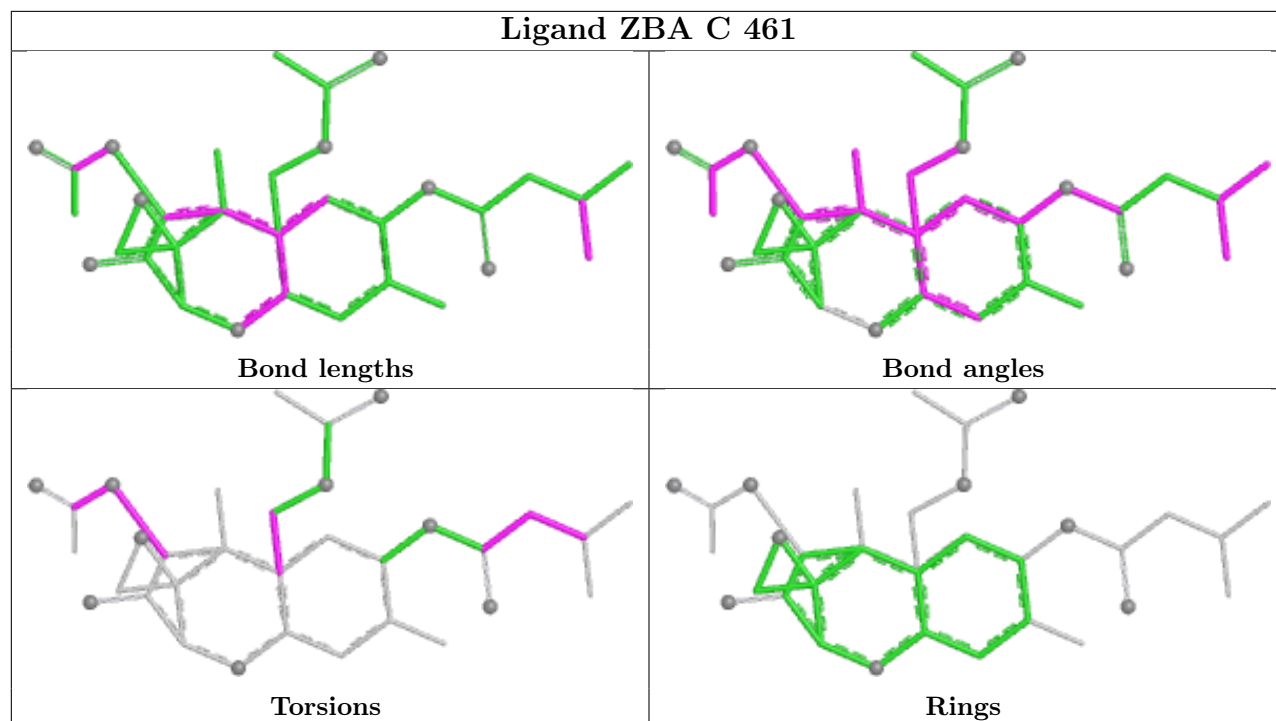


Ligand ZBA A 463

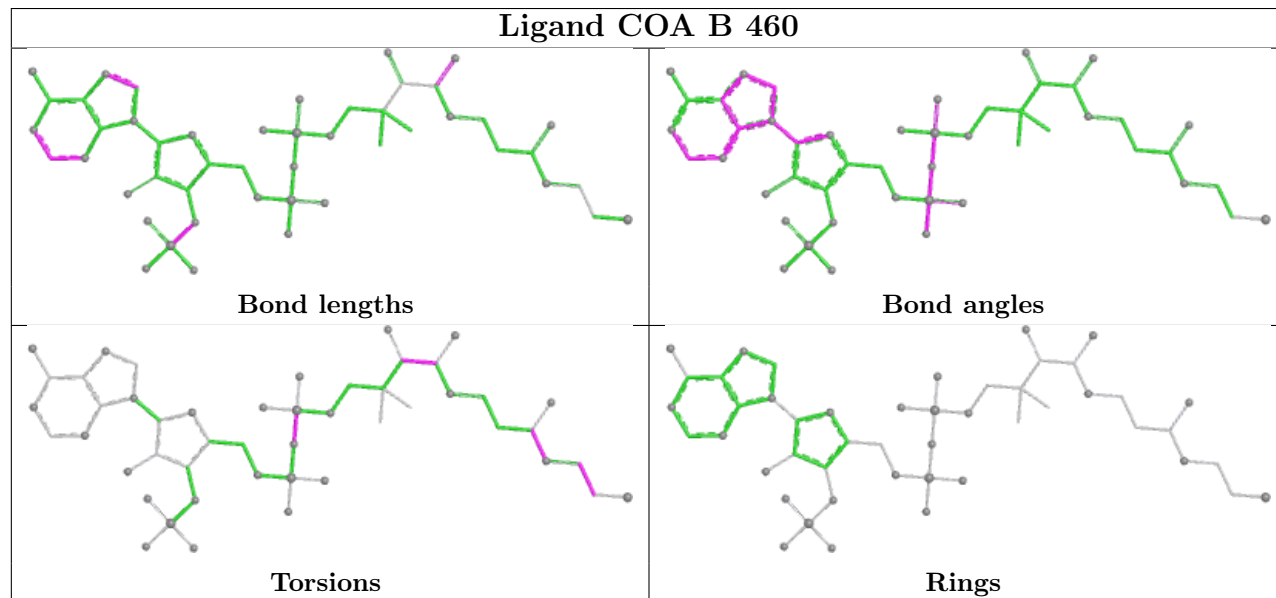


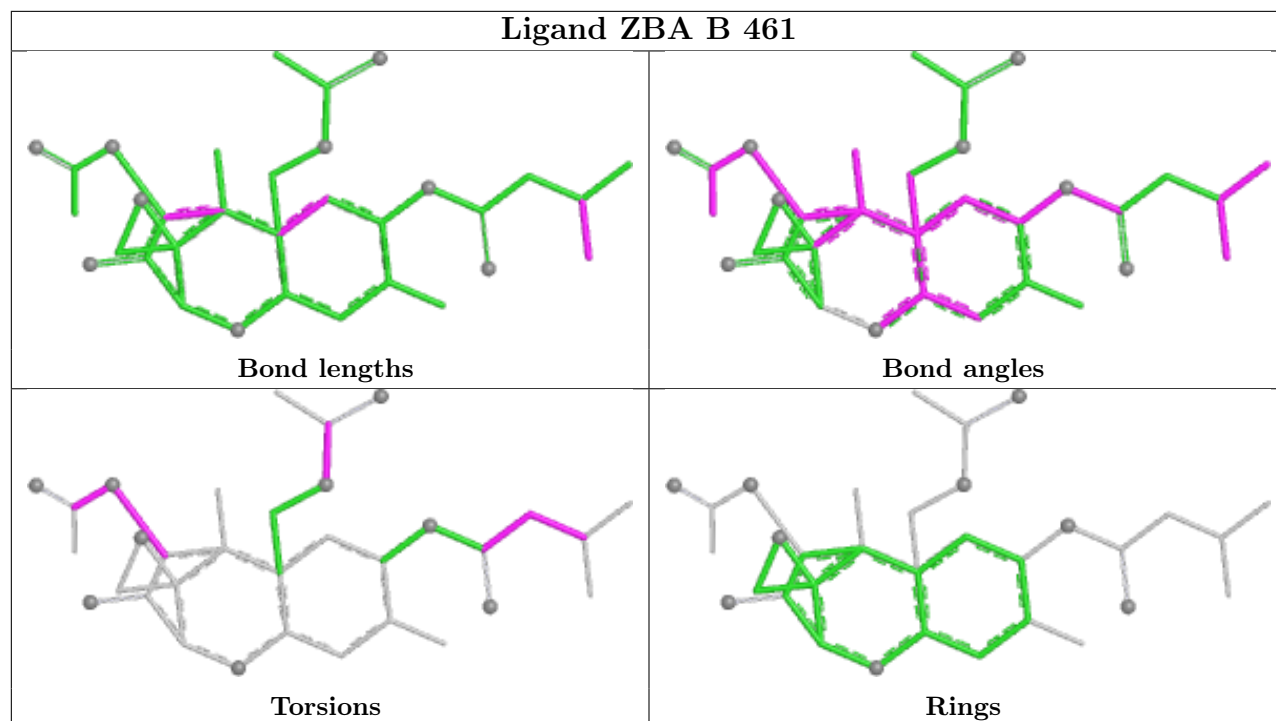


Ligand ZBA C 461



Ligand COA B 460





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	423/459 (92%)	0.05	6 (1%) 73 73	10, 24, 36, 47	6 (1%)
1	B	418/459 (91%)	-0.04	6 (1%) 73 73	9, 21, 36, 44	5 (1%)
1	C	419/459 (91%)	-0.34	4 (0%) 79 79	5, 16, 32, 41	8 (1%)
1	D	381/459 (83%)	0.43	23 (6%) 27 26	12, 27, 42, 45	14 (3%)
All	All	1641/1836 (89%)	0.02	39 (2%) 59 59	5, 22, 38, 47	33 (2%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	371	VAL	7.1
1	D	375	ALA	6.3
1	D	282	SER	4.6
1	D	450	GLU	4.3
1	D	283	ARG	4.1
1	D	370	SER	4.1
1	D	281	THR	3.9
1	D	87	TYR	3.7
1	D	445	LEU	3.6
1	D	379	PRO	3.4
1	D	12	PHE	3.2
1	B	210	ASN	3.0
1	D	213	VAL	3.0
1	A	136	GLY	2.9
1	B	100	ASP	2.8
1	D	280	SER	2.8
1	D	330	ILE	2.8
1	B	74	ILE	2.7
1	C	262	ALA	2.6
1	D	221	ILE	2.6
1	A	223	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	189	PHE	2.6
1	D	331	ALA	2.6
1	A	139	PRO	2.5
1	D	327	VAL	2.5
1	C	264	SER	2.4
1	C	261	ASP	2.3
1	A	260	LEU	2.3
1	D	451	TRP	2.3
1	D	339	ALA	2.2
1	C	75	SER	2.2
1	B	223	LYS	2.2
1	B	77	GLY	2.2
1	D	73	GLY	2.2
1	A	155	GLY	2.1
1	D	275	ALA	2.1
1	D	416	PHE	2.1
1	A	39	SER	2.1
1	D	380	SER	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.

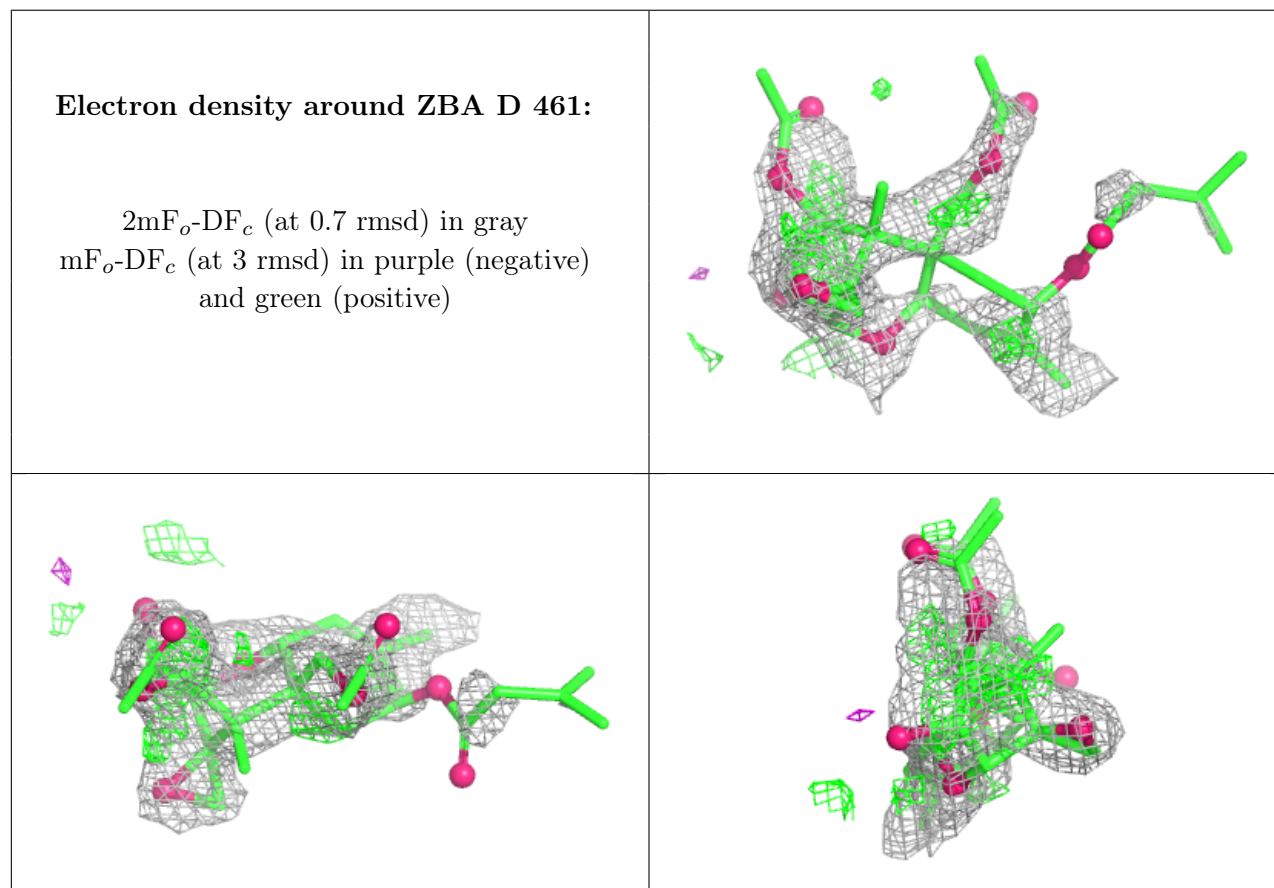
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZBA	D	461	33/33	0.69	0.31	27,29,32,33	33
3	ZBA	B	461	33/33	0.77	0.18	21,24,29,30	33
3	ZBA	C	461	33/33	0.80	0.16	18,23,28,31	33
3	ZBA	A	463	30/33	0.85	0.13	17,20,26,27	30
6	GOL	C	462	6/6	0.87	0.13	30,33,33,34	0

Continued on next page...

Continued from previous page...

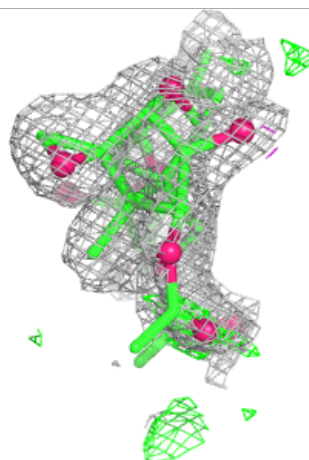
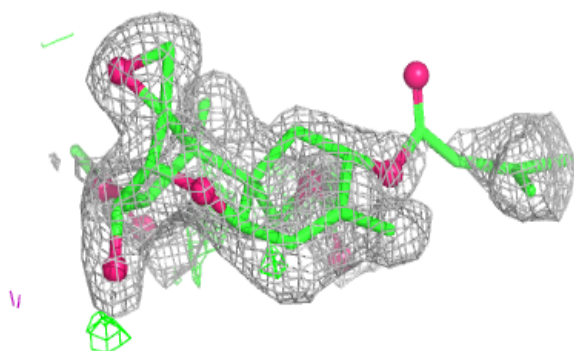
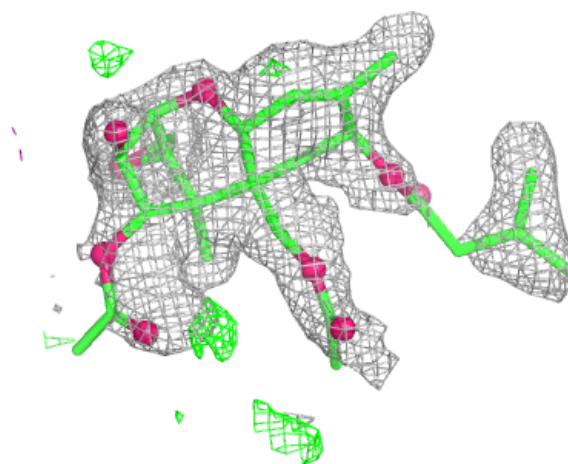
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	COA	D	460	48/48	0.94	0.09	22,30,37,44	0
2	COA	A	462	48/48	0.94	0.08	20,27,30,31	3
5	DMS	B	462	4/4	0.95	0.12	31,32,32,32	0
2	COA	C	460	48/48	0.96	0.06	8,17,27,39	0
2	COA	B	460	48/48	0.96	0.07	11,17,31,42	0
4	CA	A	460	1/1	0.99	0.03	23,23,23,23	0
4	CA	A	461	1/1	1.00	0.01	15,15,15,15	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.



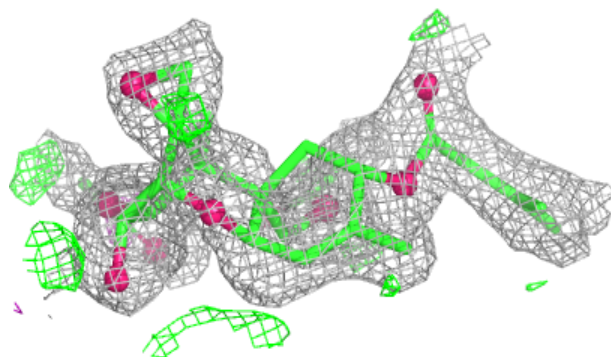
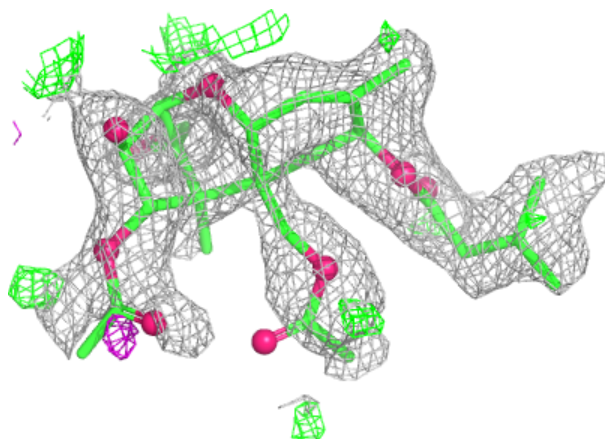
Electron density around ZBA B 461:

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



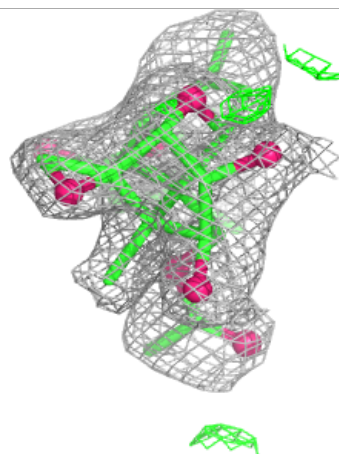
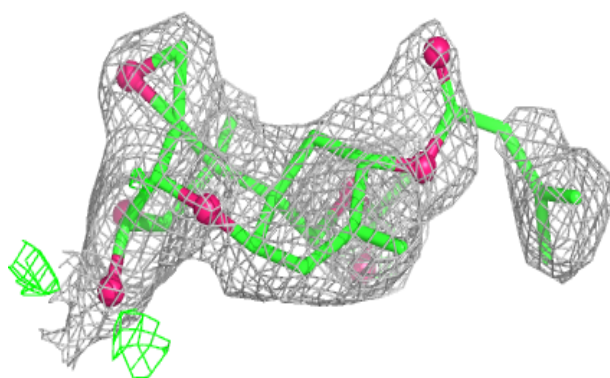
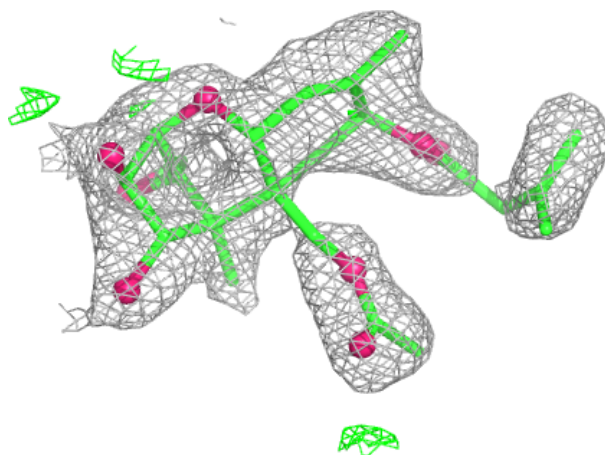
Electron density around ZBA C 461:

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



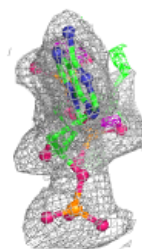
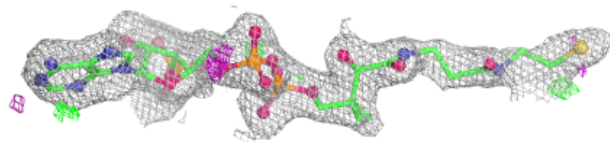
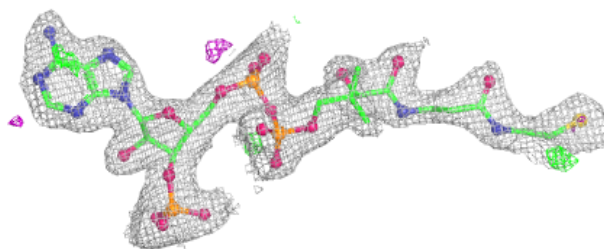
Electron density around ZBA A 463:

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

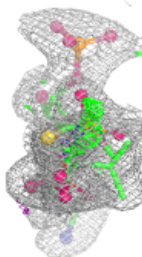
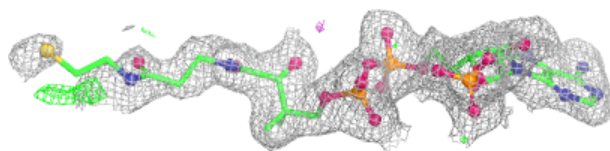
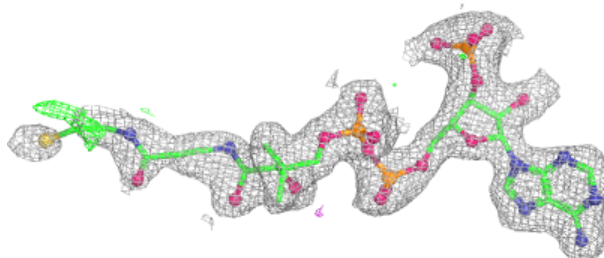


Electron density around COA D 460:

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

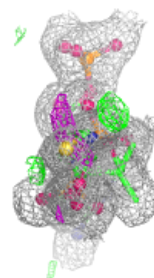
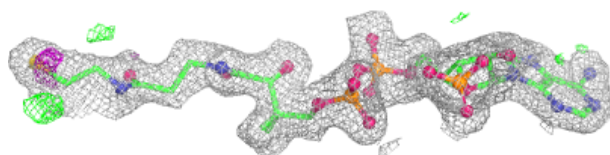
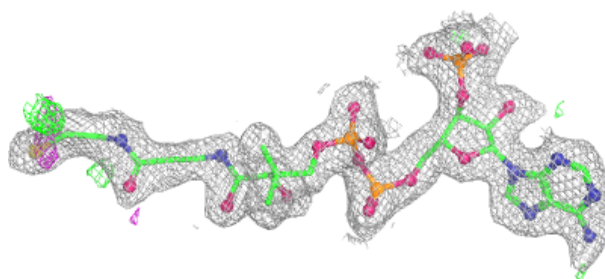
**Electron density around COA A 462:**

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

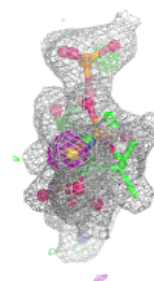
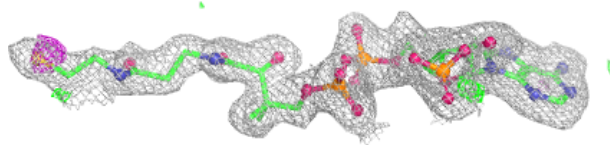
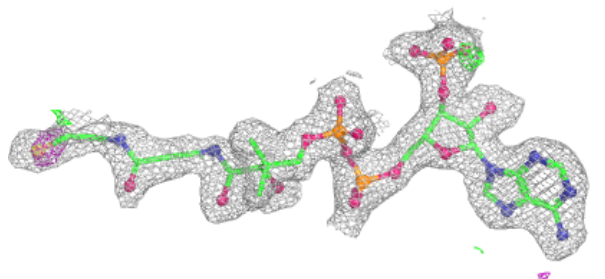


Electron density around COA C 460:

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

**Electron density around COA B 460:**

$2mF_o-DF_c$ (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.