



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:44 AM UTC

PDB ID : 6TI1 / pdb_00006ti1
Title : SHMT from Streptococcus thermophilus Tyr55Ser variant in complex with P
LP/L-Threonine/Lys230 gem diamine complex
Authors : Petrillo, G.; Hernandez, K.; Bujons, J.; Clapes, P.; Uson, I.
Deposited on : 2019-11-21
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

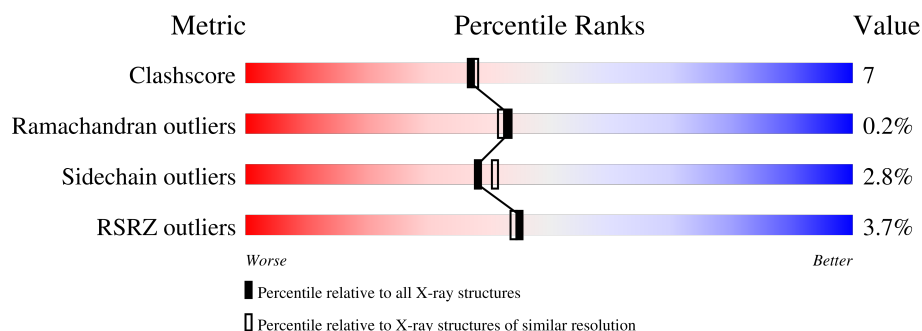
1 Overall quality at a glance

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))
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	416	
1	C	416	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2BO	C	501	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6673 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 Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	1	0
			3127	1978	538	602	9			
1	C	410	Total	C	N	O	S	0	1	0
			3119	1974	536	600	9			

There are 2 discrepancies between the modelled and reference sequences:

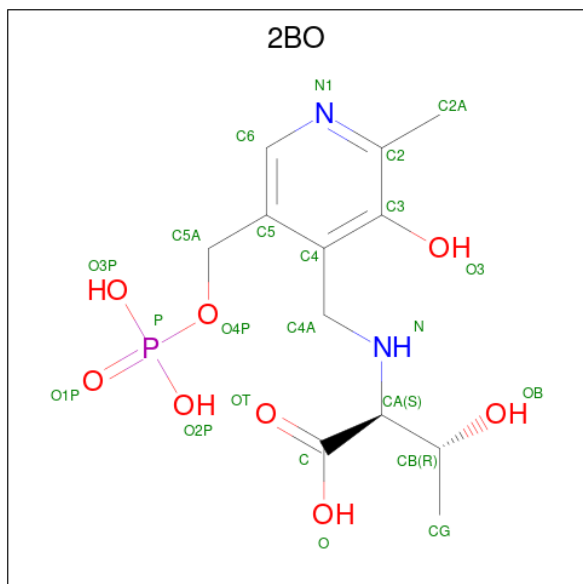
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	SER	TYR	engineered mutation	UNP Q5MCK9
C	55	SER	TYR	engineered mutation	UNP Q5MCK9

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is N-({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methyl)-L-threonine (CCD ID: 2BO) (formula: $C_{12}H_{19}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	12	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			23	12	2	8	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

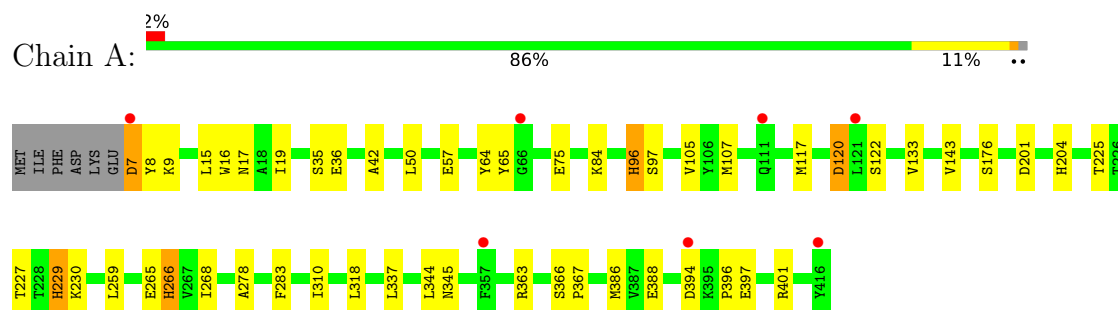
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	0
			215	215		
5	C	159	Total	O	0	0
			159	159		

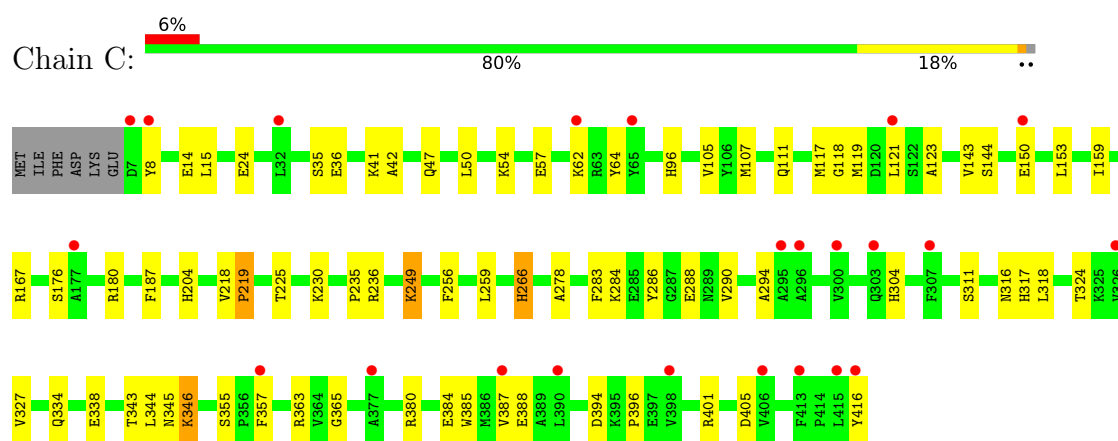
3 Residue-property plots [i](#)

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

• Molecule 1: Serine hydroxymethyltransferase



• Molecule 1: Serine hydroxymethyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.71Å 114.71Å 192.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.48 – 2.00 98.48 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (98.48-2.00) 100.0 (98.48-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: 2BO, GOL, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.24	6/3189 (0.2%)	1.38	6/4330 (0.1%)
1	C	1.22	3/3188 (0.1%)	1.48	12/4328 (0.3%)
All	All	1.23	9/6377 (0.1%)	1.43	18/8658 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	219	PRO	C-O	-6.18	1.16	1.24
1	A	133	VAL	C-O	5.93	1.31	1.24
1	A	97	SER	C-O	5.45	1.30	1.23
1	A	268	ILE	C-O	5.42	1.30	1.24
1	A	229	HIS	CE1-NE2	5.42	1.38	1.32
1	A	36	GLU	C-O	5.35	1.30	1.23
1	A	96	HIS	C-O	5.31	1.30	1.24
1	C	343	THR	C-O	5.27	1.30	1.24
1	C	235	PRO	C-O	5.06	1.29	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	ARG	CG-CD-NE	-7.62	95.25	112.00
1	C	416	TYR	CA-C-O	-6.63	109.53	120.80
1	C	111	GLN	CB-CG-CD	-6.54	101.47	112.60
1	A	64	TYR	CA-C-O	-6.11	113.95	120.42
1	C	64	TYR	CA-C-O	-5.93	113.40	120.10
1	C	54	LYS	CB-CA-C	5.92	119.78	110.19
1	A	120	ASP	CA-C-N	5.85	128.40	120.38
1	A	120	ASP	C-N-CA	5.85	128.40	120.38
1	A	397	GLU	CB-CG-CD	5.82	122.50	112.60
1	C	316	ASN	CA-CB-CG	5.78	118.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	PHE	CA-CB-CG	-5.58	108.22	113.80
1	A	17	ASN	CA-CB-CG	5.54	118.14	112.60
1	C	187	PHE	CA-C-O	-5.51	114.71	120.55
1	C	159	ILE	CA-C-O	-5.24	115.30	120.85
1	A	7	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	294	ALA	CA-C-N	5.13	127.11	120.44
1	C	294	ALA	C-N-CA	5.13	127.11	120.44
1	C	47	GLN	CB-CA-C	5.08	119.47	109.72

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	3127	0	3104	43	0
1	C	3119	0	3091	47	0
2	A	6	0	8	0	0
3	A	23	0	14	4	0
3	C	23	0	14	9	0
4	A	1	0	0	0	0
5	A	215	0	0	4	0
5	C	159	0	0	6	0
All	All	6673	0	6231	89	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 7.

All (89) 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:57:GLU:OE1	3:C:501:2BO:H19	1.63	0.99
1:C:107:MET:HE1	1:C:259:LEU:HG	1.44	0.97
1:A:107:MET:HE1	1:A:259:LEU:HG	1.52	0.92
1:C:107:MET:HE1	1:C:259:LEU:CG	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:GLU:OE2	1:C:401:ARG:NH1	2.08	0.86
1:A:337:LEU:HD13	1:A:386:MET:HE3	1.56	0.86
1:A:57:GLU:OE1	3:C:501:2BO:CG	2.26	0.82
1:C:334:GLN:HE21	1:C:346:LYS:H	1.27	0.79
1:C:249:LYS:HE3	5:C:703:HOH:O	1.84	0.78
1:A:107:MET:HE1	1:A:259:LEU:CG	2.14	0.77
1:A:57:GLU:CD	3:C:501:2BO:H18	2.15	0.71
1:C:204:HIS:NE2	3:C:501:2BO:O	2.23	0.70
1:C:14:GLU:HG3	5:C:705:HOH:O	1.92	0.70
1:C:107:MET:CE	1:C:259:LEU:HG	2.22	0.68
1:C:119:MET:HE2	1:C:123:ALA:O	1.95	0.65
1:A:345:ASN:HD21	1:A:363:ARG:HH21	1.44	0.65
1:C:334:GLN:NE2	1:C:346:LYS:H	1.95	0.63
1:A:266:HIS:H	1:A:266:HIS:CD2	2.17	0.63
3:A:502:2BO:CG	1:C:57:GLU:OE1	2.47	0.62
1:A:337:LEU:CD1	1:A:386:MET:HE3	2.28	0.60
1:A:57:GLU:CD	3:C:501:2BO:CG	2.74	0.60
1:C:107:MET:HE3	1:C:259:LEU:HD11	1.84	0.60
1:C:107:MET:HE1	1:C:259:LEU:CD2	2.32	0.59
1:C:249:LYS:NZ	5:C:602:HOH:O	2.36	0.59
3:A:502:2BO:H18	1:C:57:GLU:OE1	2.04	0.58
1:C:35:SER:HB3	3:C:501:2BO:O	2.04	0.57
1:C:107:MET:CE	1:C:259:LEU:CG	2.82	0.56
1:C:266:HIS:H	1:C:266:HIS:CD2	2.22	0.56
1:A:35:SER:HB3	3:A:502:2BO:O	2.07	0.55
1:A:344:LEU:CD2	1:A:386:MET:HE1	2.35	0.55
1:C:345:ASN:HD21	1:C:363:ARG:HH21	1.54	0.54
1:C:318:LEU:C	1:C:318:LEU:HD12	2.32	0.54
1:A:394:ASP:O	1:A:396:PRO:HD3	2.09	0.52
1:A:344:LEU:HD21	1:A:386:MET:CE	2.40	0.52
1:A:7:ASP:N	5:A:604:HOH:O	2.42	0.52
1:C:107:MET:CE	1:C:259:LEU:HD11	2.41	0.51
1:A:65:TYR:HE2	3:C:501:2BO:H18	1.76	0.50
1:C:380:ARG:O	1:C:384:GLU:HG2	2.12	0.50
1:C:394:ASP:O	1:C:396:PRO:HD3	2.11	0.50
1:C:286:TYR:O	1:C:290:VAL:HG23	2.12	0.49
1:A:345:ASN:ND2	1:A:363:ARG:HH21	2.10	0.47
1:C:107:MET:HE3	1:C:259:LEU:CD1	2.44	0.47
1:A:65:TYR:OH	3:C:501:2BO:H15	2.14	0.47
1:A:15:LEU:HD13	1:A:19:ILE:HD12	1.97	0.47
1:A:176:SER:HA	1:A:204:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:MET:CE	1:A:259:LEU:HG	2.34	0.46
1:C:345:ASN:ND2	5:C:609:HOH:O	2.47	0.46
1:C:345:ASN:ND2	1:C:363:ARG:HH21	2.13	0.46
1:C:105:VAL:HG21	1:C:225:THR:CG2	2.46	0.46
1:C:278:ALA:HA	1:C:283:PHE:CG	2.51	0.46
1:A:8:TYR:HB2	1:C:42:ALA:HB2	1.98	0.46
1:A:344:LEU:CD2	1:A:386:MET:CE	2.93	0.45
1:C:36:GLU:OE2	1:C:36:GLU:HA	2.17	0.45
1:C:107:MET:CE	1:C:259:LEU:CD1	2.95	0.45
1:C:346:LYS:HE2	1:C:357:PHE:O	2.16	0.45
1:A:345:ASN:ND2	5:A:617:HOH:O	2.49	0.45
1:A:42:ALA:HB2	1:C:8:TYR:HB2	1.99	0.45
1:C:176:SER:HA	1:C:204:HIS:CD2	2.52	0.45
1:C:117:MET:HA	1:C:143:VAL:O	2.17	0.44
1:A:9:LYS:HE3	1:A:16:TRP:HB3	1.99	0.44
1:A:366:SER:N	1:A:367:PRO:HD3	2.33	0.44
1:A:117:MET:HA	1:A:143:VAL:O	2.18	0.44
1:A:120:ASP:OD2	1:A:122:SER:HB2	2.18	0.44
1:A:388:GLU:CD	1:A:401:ARG:HH12	2.25	0.43
1:C:218:VAL:N	1:C:219:PRO:CD	2.82	0.43
1:C:317:HIS:O	1:C:365:GLY:HA2	2.19	0.43
1:C:107:MET:HE1	1:C:259:LEU:HD21	2.00	0.43
1:A:278:ALA:HA	1:A:283:PHE:CG	2.54	0.42
1:C:324:THR:HA	1:C:327:VAL:O	2.20	0.42
1:C:385:TRP:CZ2	1:C:405:ASP:HB3	2.55	0.42
1:C:15:LEU:C	1:C:15:LEU:HD13	2.45	0.42
1:A:266:HIS:H	1:A:266:HIS:HD2	1.66	0.42
1:A:105:VAL:HG21	1:A:225:THR:CG2	2.50	0.41
1:A:227:THR:HB	1:A:229:HIS:CE1	2.55	0.41
1:A:366:SER:N	1:A:367:PRO:CD	2.83	0.41
1:A:75:GLU:OE1	1:A:265:GLU:OE2	2.38	0.41
1:A:318:LEU:C	1:A:318:LEU:HD12	2.46	0.41
1:A:96:HIS:HD2	5:A:689:HOH:O	2.03	0.41
1:C:304:HIS:CD2	1:C:387:VAL:HG11	2.56	0.41
1:A:65:TYR:HE2	3:C:501:2BO:CG	2.33	0.41
1:C:153:LEU:CD2	1:C:180:ARG:HG3	2.51	0.41
1:A:84:LYS:HE3	5:A:801:HOH:O	2.21	0.41
1:A:201:ASP:OD2	3:A:502:2BO:N1	2.54	0.41
1:C:96:HIS:HD2	5:C:663:HOH:O	2.04	0.41
1:A:107:MET:HE1	1:A:259:LEU:CD2	2.51	0.41
1:C:118:GLY:O	1:C:144:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:C	1:C:344:LEU:HD12	2.46	0.40
1:A:344:LEU:HD23	1:A:386:MET:HE1	2.02	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	409/416 (98%)	397 (97%)	11 (3%)	1 (0%)	43	42
1	C	409/416 (98%)	398 (97%)	10 (2%)	1 (0%)	43	42
All	All	818/832 (98%)	795 (97%)	21 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	LYS
1	C	230	LYS

5.3.2 Protein sidechains [i](#)

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	328/333 (98%)	325 (99%)	3 (1%)	70	78
1	C	328/333 (98%)	313 (95%)	15 (5%)	24	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	656/666 (98%)	638 (97%)	18 (3%)	38	42

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	266	HIS
1	A	310	ILE
1	C	24	GLU
1	C	41	LYS
1	C	50	LEU
1	C	62	LYS
1	C	121	LEU
1	C	150	GLU
1	C	167	ARG
1	C	249	LYS
1	C	266	HIS
1	C	284	LYS
1	C	288	GLU
1	C	311	SER
1	C	338	GLU
1	C	346	LYS
1	C	355	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	266	HIS
1	A	341	ASN
1	A	345	ASN
1	A	347	ASN
1	A	381	GLN
1	A	393	HIS
1	C	17	ASN
1	C	96	HIS
1	C	111	GLN
1	C	266	HIS
1	C	334	GLN
1	C	345	ASN
1	C	347	ASN

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Mol	Chain	Res	Type
1	C	381	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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$
3	2BO	C	501	1	23,23,23	1.18	2 (8%)	30,33,33	2.12	11 (36%)
2	GOL	A	501	-	5,5,5	0.34	0	5,5,5	0.31	0
3	2BO	A	502	1	23,23,23	1.30	3 (13%)	30,33,33	2.42	11 (36%)

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
3	2BO	C	501	1	-	11/19/19/19	0/1/1/1
2	GOL	A	501	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2BO	A	502	1	-	10/19/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	2BO	O-C	-4.47	1.16	1.30
3	C	501	2BO	O-C	-3.63	1.19	1.30
3	A	502	2BO	C3-C4	-2.36	1.36	1.40
3	C	501	2BO	P-O4P	2.13	1.67	1.60
3	A	502	2BO	C4A-N	2.12	1.53	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	2BO	C4A-N-CA	-6.14	100.66	114.63
3	C	501	2BO	O4P-C5A-C5	5.28	119.25	109.36
3	A	502	2BO	O4P-C5A-C5	4.88	118.50	109.36
3	A	502	2BO	O4P-P-O1P	-4.67	93.81	106.44
3	A	502	2BO	C5A-C5-C6	4.25	126.29	119.36
3	C	501	2BO	C5A-C5-C6	3.52	125.09	119.36
3	C	501	2BO	OB-CB-CG	3.44	119.98	109.68
3	A	502	2BO	C5A-C5-C4	-3.29	115.73	122.67
3	C	501	2BO	C4A-C4-C5	3.23	123.27	119.75
3	A	502	2BO	C4A-C4-C5	3.17	123.20	119.75
3	A	502	2BO	OB-CB-CG	3.05	118.80	109.68
3	C	501	2BO	CG-CB-CA	-3.01	106.35	112.29
3	C	501	2BO	O3P-P-O4P	-3.00	98.85	106.67
3	C	501	2BO	C4A-N-CA	-2.99	107.84	114.63
3	A	502	2BO	O3-C3-C2	2.98	123.75	117.58
3	C	501	2BO	O3-C3-C2	2.75	123.28	117.58
3	C	501	2BO	C5A-C5-C4	-2.67	117.05	122.67
3	C	501	2BO	CB-CA-C	-2.66	105.40	110.03
3	A	502	2BO	O3P-P-O4P	2.38	112.87	106.67
3	A	502	2BO	C4A-C4-C3	-2.33	116.88	119.98
3	C	501	2BO	O3P-P-O2P	2.30	116.42	107.80
3	A	502	2BO	O3P-P-O2P	2.05	115.47	107.80

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	2BO	C5A-O4P-P-O2P
3	A	502	2BO	C5A-O4P-P-O3P
3	A	502	2BO	CB-CA-N-C4A
3	A	502	2BO	N-CA-CB-OB
3	A	502	2BO	N-CA-CB-CG
3	A	502	2BO	C-CA-CB-OB
3	A	502	2BO	C-CA-CB-CG
3	A	502	2BO	OT-C-CA-N
3	C	501	2BO	C5A-O4P-P-O2P
3	C	501	2BO	C5A-O4P-P-O3P
3	C	501	2BO	N-CA-CB-OB
3	C	501	2BO	N-CA-CB-CG
3	C	501	2BO	C-CA-CB-OB
3	C	501	2BO	C-CA-CB-CG
3	C	501	2BO	OT-C-CA-CB
3	A	502	2BO	O-C-CA-N
3	C	501	2BO	OT-C-CA-N
3	A	502	2BO	C5A-O4P-P-O1P
3	C	501	2BO	O-C-CA-N
3	C	501	2BO	O-C-CA-CB
3	C	501	2BO	C5A-O4P-P-O1P

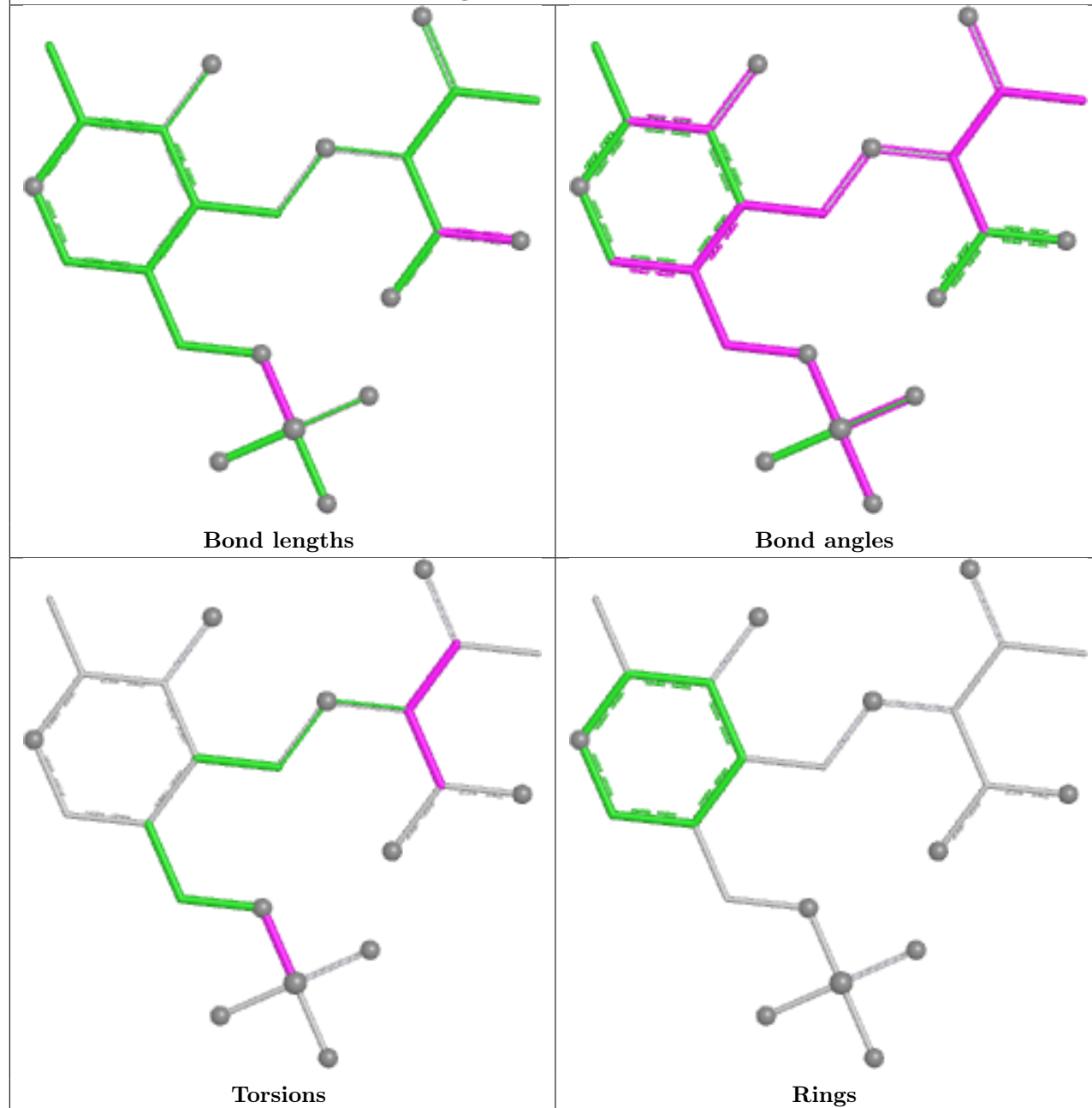
There are no ring outliers.

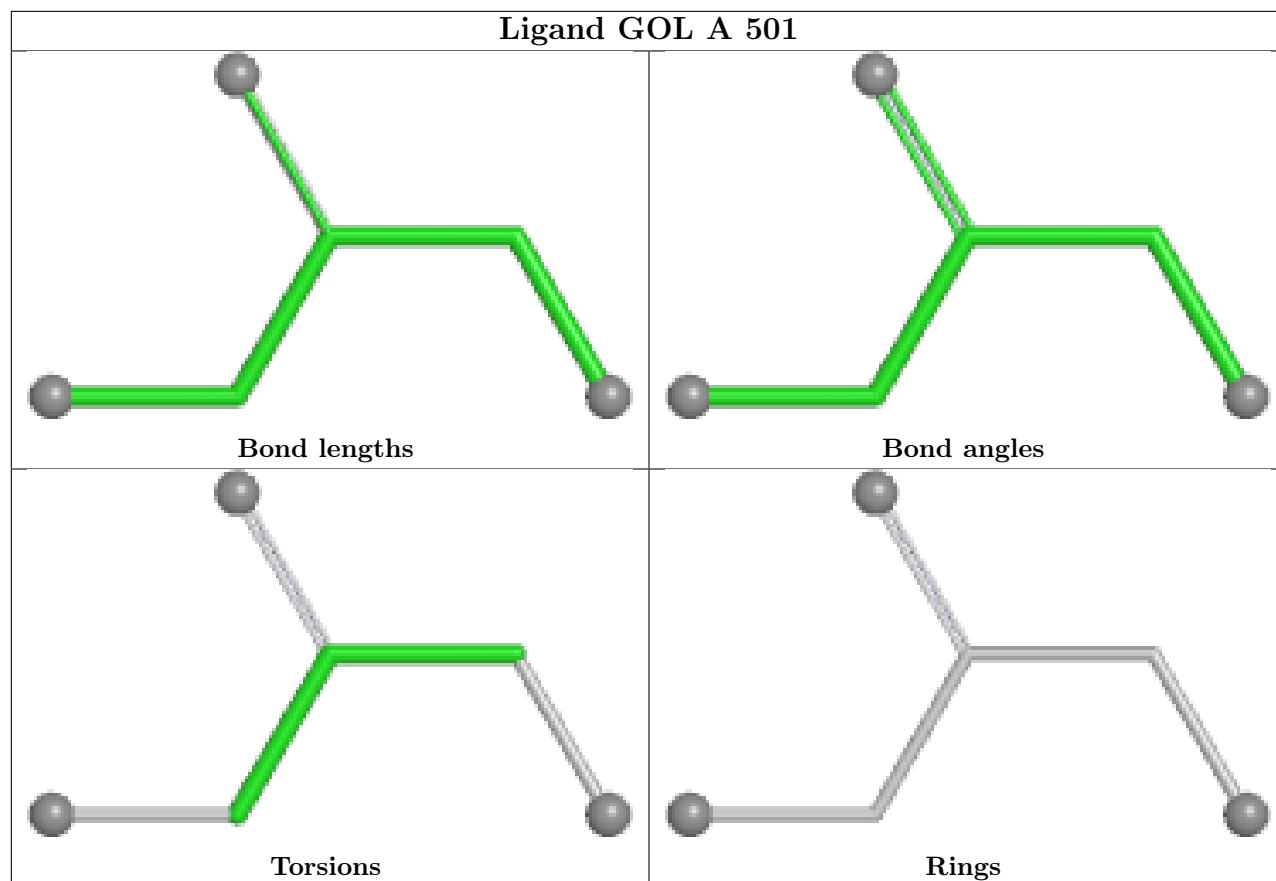
2 monomers are involved in 13 short contacts:

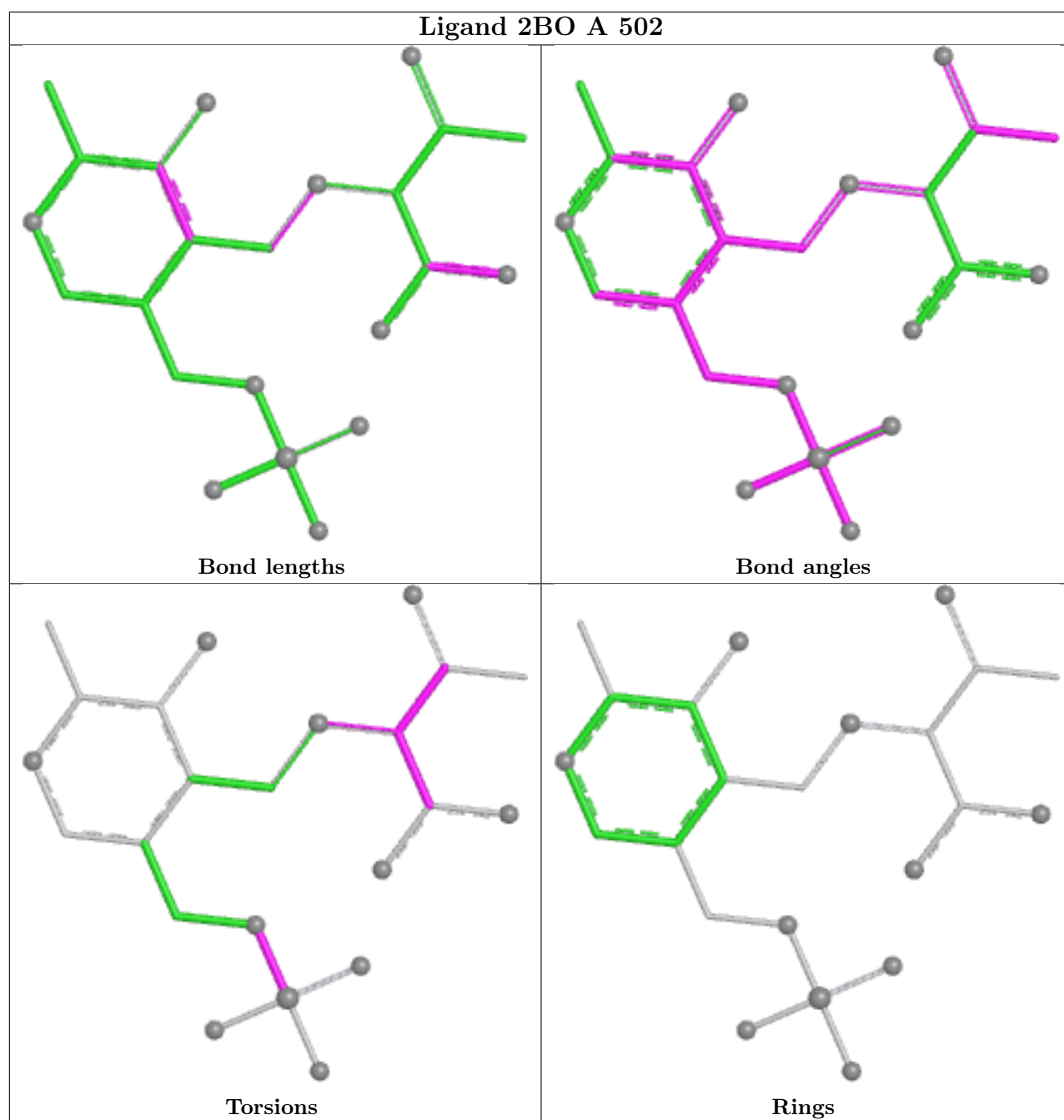
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	2BO	9	0
3	A	502	2BO	4	0

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 2BO C 501







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	410/416 (98%)	0.12	7 (1%) 69 68	23, 42, 62, 91	1 (0%)
1	C	410/416 (98%)	0.56	23 (5%) 30 29	34, 50, 78, 96	1 (0%)
All	All	820/832 (98%)	0.34	30 (3%) 45 44	23, 45, 72, 96	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	300	VAL	3.5
1	C	121	LEU	2.9
1	A	121	LEU	2.8
1	A	111[A]	GLN	2.7
1	A	416	TYR	2.7
1	C	377	ALA	2.6
1	A	394	ASP	2.6
1	C	357	PHE	2.5
1	C	295	ALA	2.5
1	C	390	LEU	2.5
1	C	296	ALA	2.4
1	C	7	ASP	2.4
1	C	65	TYR	2.3
1	C	326	VAL	2.3
1	C	307	PHE	2.3
1	C	387	VAL	2.3
1	C	398	VAL	2.3
1	A	7	ASP	2.2
1	C	416	TYR	2.2
1	C	32	LEU	2.2
1	C	8	TYR	2.2
1	C	150	GLU	2.1
1	C	413	PHE	2.1
1	C	406	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	62	LYS	2.1
1	C	177	ALA	2.1
1	C	303	GLN	2.0
1	A	357	PHE	2.0
1	C	415	LEU	2.0
1	A	66	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

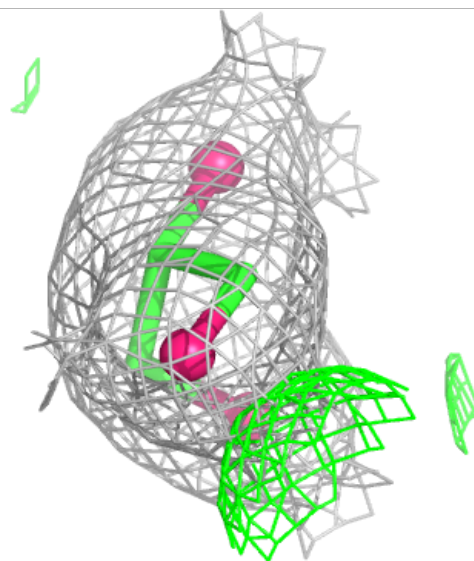
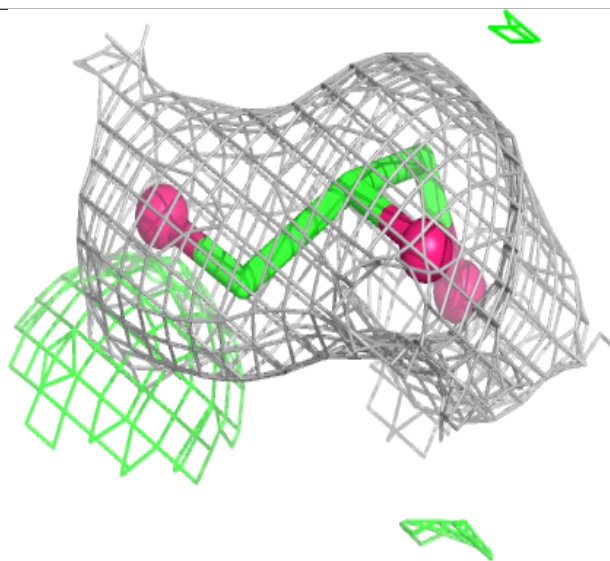
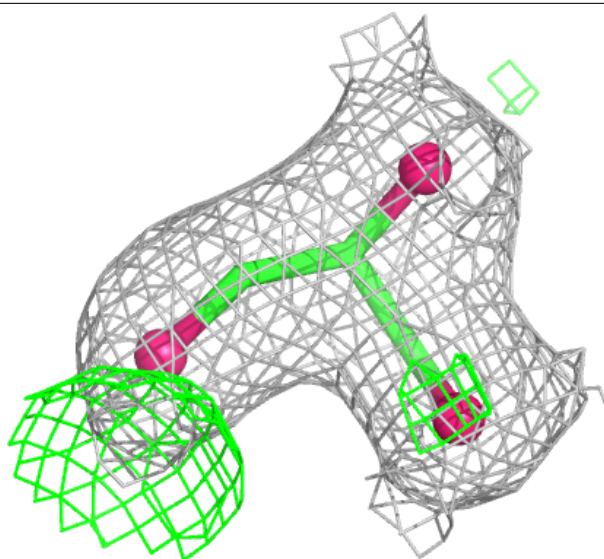
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	501	6/6	0.95	0.09	38,44,46,48	0
3	2BO	A	502	23/23	0.95	0.11	30,40,73,109	0
3	2BO	C	501	23/23	0.95	0.10	39,47,72,95	0
4	NA	A	503	1/1	0.98	0.22	48,48,48,48	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.

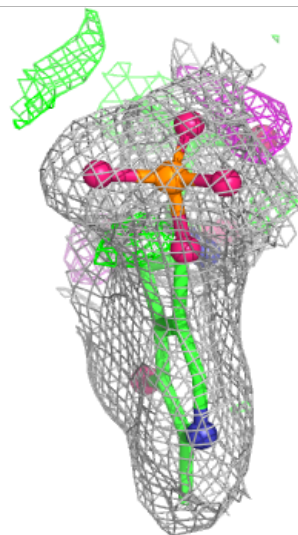
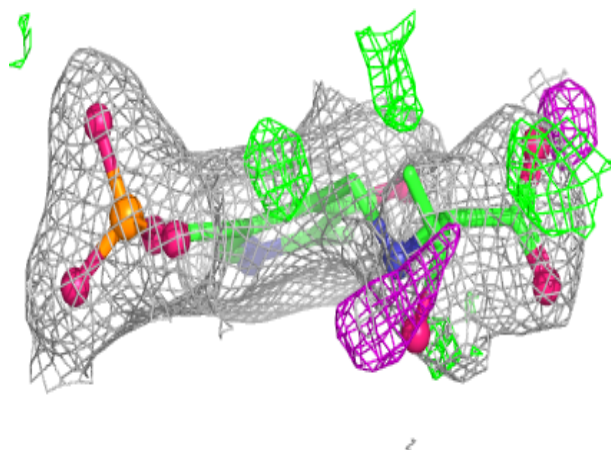
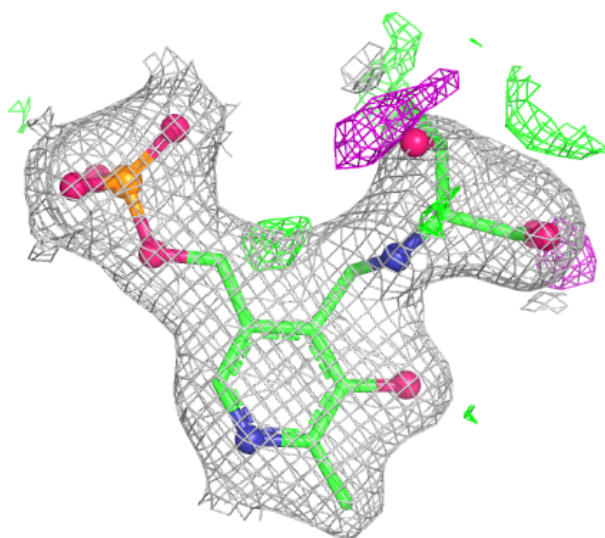
Electron density around GOL A 501:

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



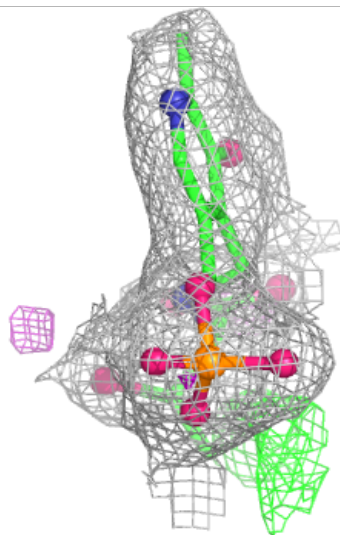
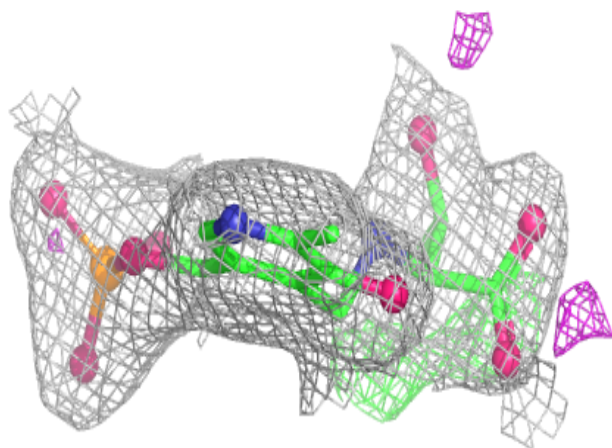
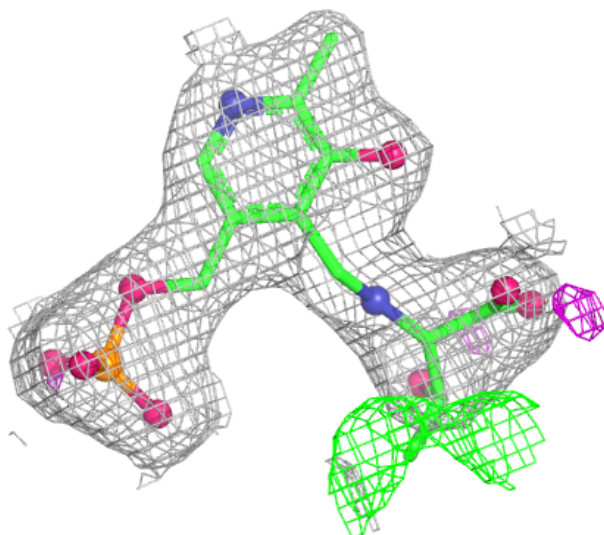
Electron density around 2BO A 502:

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



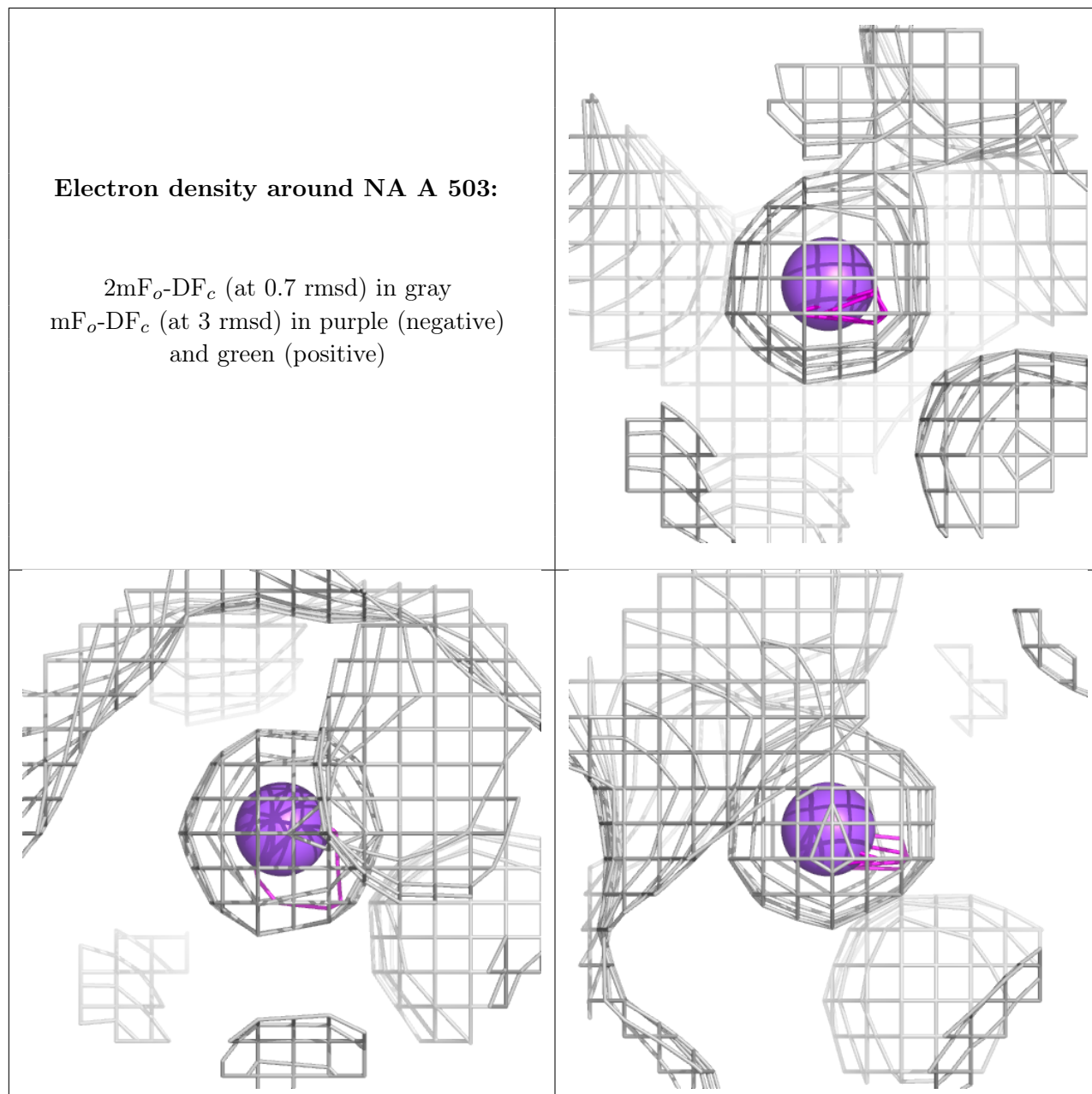
Electron density around 2BO C 501:

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



Electron density around NA A 503:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.