



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:49 AM UTC

PDB ID : 8W5Z / pdb_00008w5z
Title : Crystal structure of tick tyrosylprotein sulfotransferase reveals the activation mechanism of tick anticoagulant protein madanin
Authors : Yoshimura, M.; Teramoto, T.; Nishimoto, E.; Kakuta, Y.
Deposited on : 2023-08-28
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

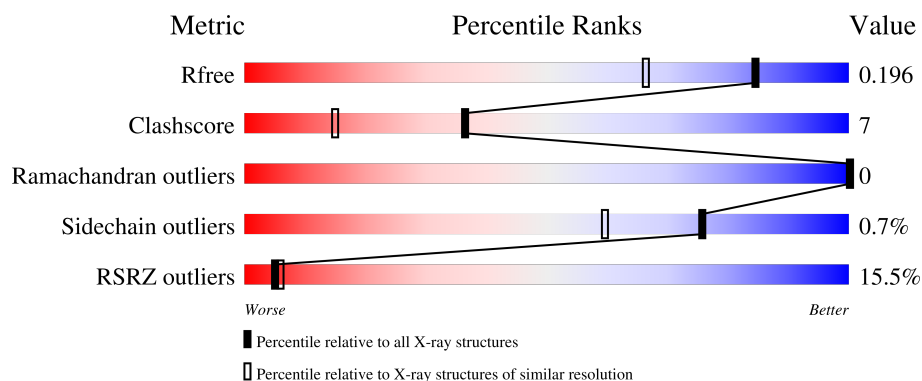
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	393	13% 70% 15% 15%
1	C	393	13% 73% 12% 15%
2	B	11	27% 55% 45%
2	D	11	18% 55% 45%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6467 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 Protein-tyrosine sulfotransferase (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	29	0
			2891	1843	516	510	22			
1	C	333	Total	C	N	O	S	0	21	0
			2834	1805	506	501	22			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A147BHN3
A	2	ARG	-	expression tag	UNP A0A147BHN3
A	3	GLY	-	expression tag	UNP A0A147BHN3
A	4	MET	-	expression tag	UNP A0A147BHN3
A	5	VAL	-	expression tag	UNP A0A147BHN3
A	6	ALA	-	expression tag	UNP A0A147BHN3
A	7	HIS	-	expression tag	UNP A0A147BHN3
A	8	ARG	-	expression tag	UNP A0A147BHN3
A	9	LEU	-	expression tag	UNP A0A147BHN3
A	10	THR	-	expression tag	UNP A0A147BHN3
A	11	ARG	-	expression tag	UNP A0A147BHN3
A	12	ARG	-	expression tag	UNP A0A147BHN3
A	13	TRP	-	expression tag	UNP A0A147BHN3
A	14	PHE	-	expression tag	UNP A0A147BHN3
A	15	LEU	-	expression tag	UNP A0A147BHN3
A	16	LEU	-	expression tag	UNP A0A147BHN3
A	17	SER	-	expression tag	UNP A0A147BHN3
A	18	ALA	-	expression tag	UNP A0A147BHN3
A	19	LEU	-	expression tag	UNP A0A147BHN3
A	20	SER	-	expression tag	UNP A0A147BHN3
A	21	LEU	-	expression tag	UNP A0A147BHN3
A	22	PHE	-	expression tag	UNP A0A147BHN3
A	23	GLY	-	expression tag	UNP A0A147BHN3
A	24	LEU	-	expression tag	UNP A0A147BHN3
A	25	VAL	-	expression tag	UNP A0A147BHN3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	LEU	-	expression tag	UNP A0A147BHN3
A	27	LEU	-	expression tag	UNP A0A147BHN3
A	28	TYR	-	expression tag	UNP A0A147BHN3
A	29	SER	-	expression tag	UNP A0A147BHN3
A	30	LEU	-	expression tag	UNP A0A147BHN3
A	31	LEU	-	expression tag	UNP A0A147BHN3
A	32	GLY	-	expression tag	UNP A0A147BHN3
A	33	SER	-	expression tag	UNP A0A147BHN3
A	34	CYS	-	expression tag	UNP A0A147BHN3
A	35	ARG	-	expression tag	UNP A0A147BHN3
A	36	GLN	-	expression tag	UNP A0A147BHN3
A	37	ARG	-	expression tag	UNP A0A147BHN3
A	38	ALA	-	expression tag	UNP A0A147BHN3
A	39	SER	-	expression tag	UNP A0A147BHN3
A	40	ASN	-	expression tag	UNP A0A147BHN3
A	41	PHE	-	expression tag	UNP A0A147BHN3
A	42	THR	-	expression tag	UNP A0A147BHN3
A	43	TYR	-	expression tag	UNP A0A147BHN3
A	44	VAL	-	expression tag	UNP A0A147BHN3
A	45	SER	-	expression tag	UNP A0A147BHN3
A	46	PRO	-	expression tag	UNP A0A147BHN3
A	47	ASP	-	expression tag	UNP A0A147BHN3
A	374	ALA	SER	conflict	UNP A0A147BHN3
C	1	MET	-	initiating methionine	UNP A0A147BHN3
C	2	ARG	-	expression tag	UNP A0A147BHN3
C	3	GLY	-	expression tag	UNP A0A147BHN3
C	4	MET	-	expression tag	UNP A0A147BHN3
C	5	VAL	-	expression tag	UNP A0A147BHN3
C	6	ALA	-	expression tag	UNP A0A147BHN3
C	7	HIS	-	expression tag	UNP A0A147BHN3
C	8	ARG	-	expression tag	UNP A0A147BHN3
C	9	LEU	-	expression tag	UNP A0A147BHN3
C	10	THR	-	expression tag	UNP A0A147BHN3
C	11	ARG	-	expression tag	UNP A0A147BHN3
C	12	ARG	-	expression tag	UNP A0A147BHN3
C	13	TRP	-	expression tag	UNP A0A147BHN3
C	14	PHE	-	expression tag	UNP A0A147BHN3
C	15	LEU	-	expression tag	UNP A0A147BHN3
C	16	LEU	-	expression tag	UNP A0A147BHN3
C	17	SER	-	expression tag	UNP A0A147BHN3
C	18	ALA	-	expression tag	UNP A0A147BHN3
C	19	LEU	-	expression tag	UNP A0A147BHN3

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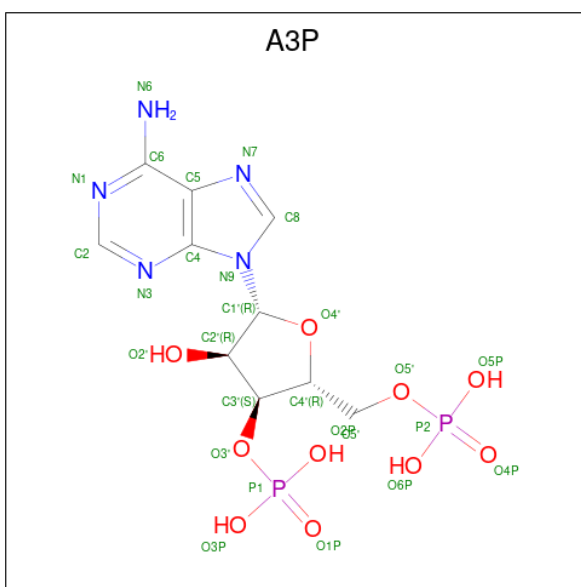
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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	SER	-	expression tag	UNP A0A147BHN3
C	21	LEU	-	expression tag	UNP A0A147BHN3
C	22	PHE	-	expression tag	UNP A0A147BHN3
C	23	GLY	-	expression tag	UNP A0A147BHN3
C	24	LEU	-	expression tag	UNP A0A147BHN3
C	25	VAL	-	expression tag	UNP A0A147BHN3
C	26	LEU	-	expression tag	UNP A0A147BHN3
C	27	LEU	-	expression tag	UNP A0A147BHN3
C	28	TYR	-	expression tag	UNP A0A147BHN3
C	29	SER	-	expression tag	UNP A0A147BHN3
C	30	LEU	-	expression tag	UNP A0A147BHN3
C	31	LEU	-	expression tag	UNP A0A147BHN3
C	32	GLY	-	expression tag	UNP A0A147BHN3
C	33	SER	-	expression tag	UNP A0A147BHN3
C	34	CYS	-	expression tag	UNP A0A147BHN3
C	35	ARG	-	expression tag	UNP A0A147BHN3
C	36	GLN	-	expression tag	UNP A0A147BHN3
C	37	ARG	-	expression tag	UNP A0A147BHN3
C	38	ALA	-	expression tag	UNP A0A147BHN3
C	39	SER	-	expression tag	UNP A0A147BHN3
C	40	ASN	-	expression tag	UNP A0A147BHN3
C	41	PHE	-	expression tag	UNP A0A147BHN3
C	42	THR	-	expression tag	UNP A0A147BHN3
C	43	TYR	-	expression tag	UNP A0A147BHN3
C	44	VAL	-	expression tag	UNP A0A147BHN3
C	45	SER	-	expression tag	UNP A0A147BHN3
C	46	PRO	-	expression tag	UNP A0A147BHN3
C	47	ASP	-	expression tag	UNP A0A147BHN3
C	374	ALA	SER	conflict	UNP A0A147BHN3

- Molecule 2 is a protein called Madanin Y54-peptide.

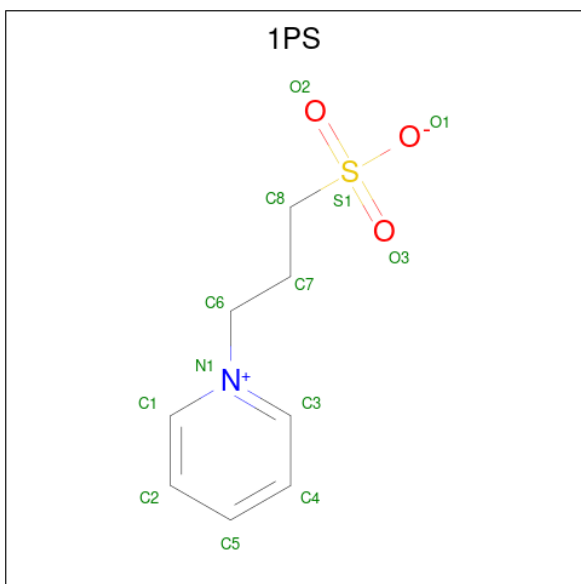
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	0	0	0
			58	37	6	15			
2	D	6	Total	C	N	O	0	0	0
			58	37	6	15			

- Molecule 3 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 3-PYRIDINIUM-1-YLPROPANE-1-SULFONATE (CCD ID: 1PS) (formula: $C_8H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



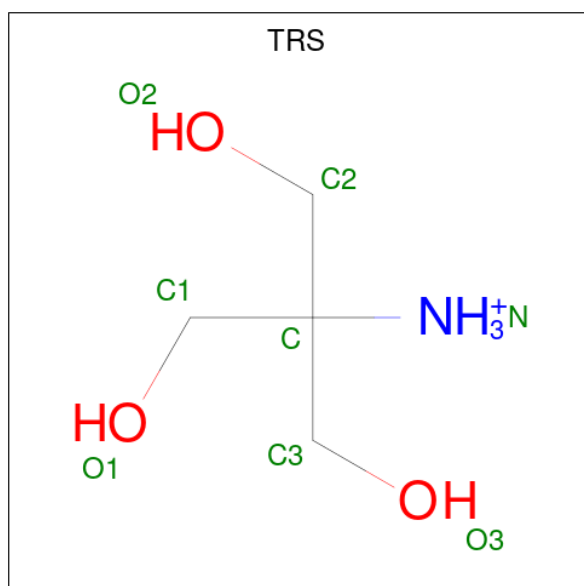
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
4	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	C	2	Total	Mg	0	0
			2	2		

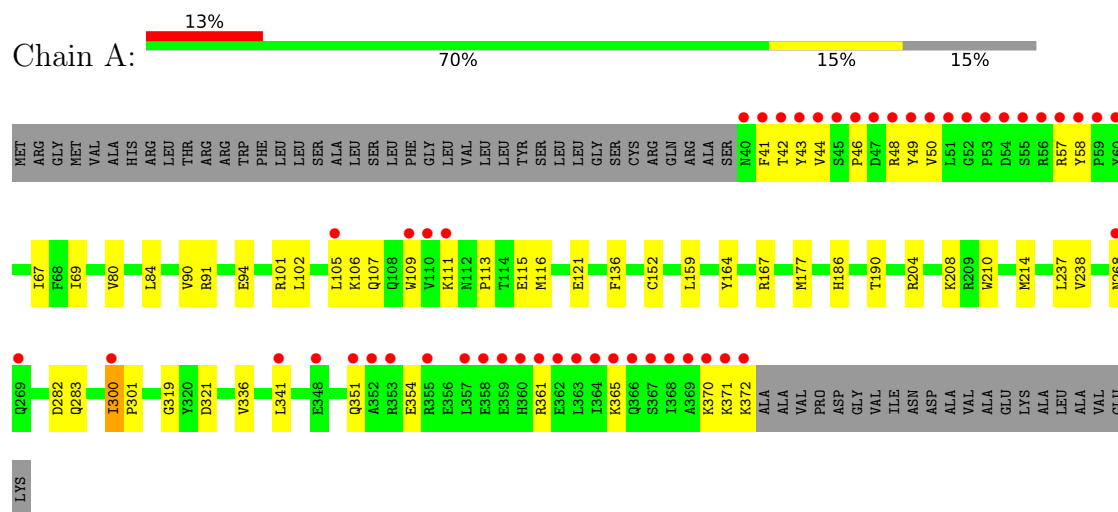
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	245	Total 245	O 245	0	0
7	B	3	Total 3	O 3	0	0
7	C	233	Total 233	O 233	0	0
7	D	3	Total 3	O 3	0	0

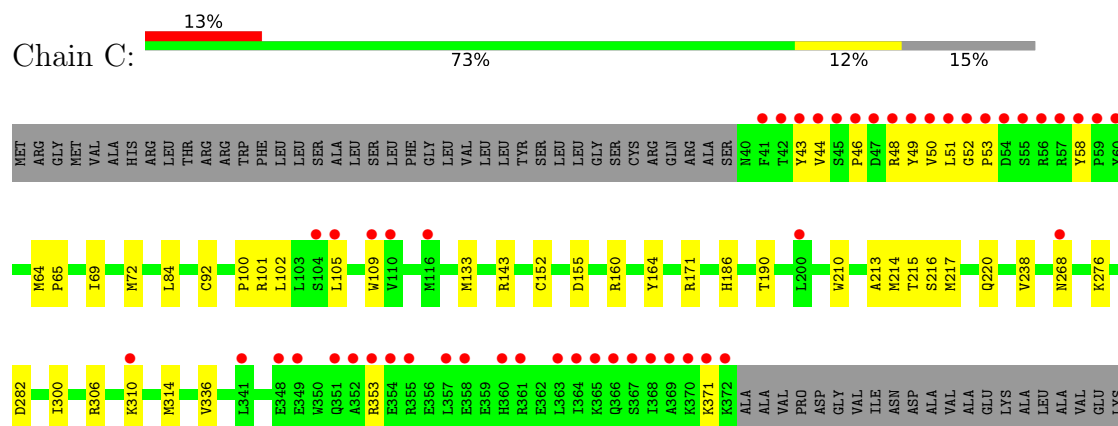
3 Residue-property plots

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: Protein-tyrosine sulfotransferase (Fragment)



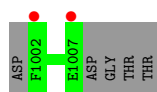
• Molecule 1: Protein-tyrosine sulfotransferase (Fragment)



• Molecule 2: Madanin Y54-peptide



- Molecule 2: Madanin Y54-peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	147.13Å 151.19Å 93.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.68 – 1.55 47.68 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.68-1.55) 99.9 (47.68-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.55Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.173 , 0.195 0.173 , 0.196	Depositor DCC
R_{free} test set	1990 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.084 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6467	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TRS, 1PS, A3P

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	0.69	0/2983	0.74	0/4042
1	C	0.72	0/2913	0.78	0/3950
2	B	0.47	0/59	0.63	0/78
2	D	0.43	0/59	0.55	0/78
All	All	0.70	0/6014	0.76	0/8148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2891	0	2951	58	0
1	C	2834	0	2885	48	0
2	B	58	0	39	0	0
2	D	58	0	39	0	0
3	A	27	0	11	0	0
3	C	27	0	11	0	0
4	A	52	0	44	7	0
5	A	32	0	48	5	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2	0	0	0	0
7	A	245	0	0	3	0
7	B	3	0	0	0	0
7	C	233	0	0	6	0
7	D	3	0	0	0	0
All	All	6467	0	6028	87	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 (87) 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:48:ARG:HA	1:C:46:PRO:HD2	1.59	0.85
1:A:321:ASP:HA	5:A:405:TRS:H12	1.61	0.82
1:A:268:ASN:ND2	7:A:503:HOH:O	2.20	0.75
1:C:220[B]:GLN:NE2	7:C:501:HOH:O	2.13	0.73
1:C:50:VAL:HB	1:C:58:TYR:HB2	1.73	0.70
1:A:80[B]:VAL:HG21	1:A:177:MET:SD	2.33	0.67
1:A:101:ARG:HD2	1:C:109:TRP:NE1	2.09	0.67
1:A:282[A]:ASP:OD1	1:A:283[A]:GLN:NE2	2.27	0.67
1:C:48:ARG:HH11	1:C:48:ARG:HG3	1.60	0.66
1:A:101:ARG:HD2	1:C:109:TRP:HE1	1.62	0.65
1:C:310:LYS:H	1:C:310:LYS:HD2	1.60	0.65
1:A:319:GLY:HA3	4:A:406:1PS:H1	1.80	0.64
1:A:167:ARG:HB2	4:A:407:1PS:H4	1.79	0.63
1:C:310:LYS:HD2	1:C:310:LYS:N	2.13	0.63
1:A:164:TYR:HA	4:A:407:1PS:H3	1.81	0.62
1:A:105:LEU:HD22	1:C:105:LEU:HD22	1.82	0.61
1:A:167:ARG:HD3	4:A:407:1PS:C4	2.30	0.61
1:C:160:ARG:O	1:C:220[B]:GLN:NE2	2.36	0.59
1:A:41:PHE:HD1	1:C:52:GLY:HA2	1.67	0.58
1:C:186:HIS:CE1	1:C:190:THR:HG21	2.42	0.55
1:A:341[A]:LEU:HG	7:A:596:HOH:O	2.07	0.54
1:A:46:PRO:HD2	1:C:48:ARG:HA	1.89	0.54
1:A:69:ILE:HD11	1:A:84:LEU:HD12	1.91	0.53
1:A:282[A]:ASP:OD2	7:A:502:HOH:O	2.19	0.53
1:C:213:ALA:O	1:C:217[B]:MET:HG2	2.07	0.53
1:A:301:PRO:HG2	5:A:408:TRS:H11	1.91	0.53
1:A:115:GLU:OE2	1:C:101:ARG:NH2	2.33	0.52
1:A:210:TRP:CE2	1:A:214[A]:MET:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216[B]:SER:OG	7:C:501:HOH:O	2.19	0.52
1:A:121[B]:GLU:OE2	1:C:276:LYS:HB2	2.10	0.51
1:C:92[B]:CYS:HG	1:C:152[B]:CYS:HG	1.57	0.51
1:A:101:ARG:CD	1:C:109:TRP:HE1	2.23	0.51
1:A:204:ARG:HG2	1:A:208:LYS:HE3	1.93	0.51
1:A:42:THR:HB	1:C:51:LEU:HD12	1.93	0.51
1:A:80[B]:VAL:HG22	1:A:237:LEU:CD2	2.41	0.50
1:A:370:LYS:C	1:A:372:LYS:H	2.19	0.50
1:C:100:PRO:HG3	1:C:155:ASP:HB3	1.93	0.50
1:C:48:ARG:HG3	1:C:48:ARG:NH1	2.27	0.49
1:A:105:LEU:HD21	1:A:109:TRP:CZ2	2.48	0.49
1:A:167:ARG:HD3	4:A:407:1PS:H4	1.94	0.49
1:A:41:PHE:CD1	1:C:52:GLY:HA2	2.47	0.48
1:C:268:ASN:OD1	1:C:353:ARG:NH1	2.47	0.48
1:C:215[B]:THR:HG23	1:C:314:MET:HG2	1.96	0.48
1:A:102[B]:LEU:HD21	1:C:102[B]:LEU:HD21	1.96	0.47
1:A:321:ASP:HB2	5:A:405:TRS:H21	1.96	0.47
1:A:90:VAL:CG1	1:A:152[B]:CYS:SG	3.02	0.47
1:A:50:VAL:HB	1:A:58:TYR:HB2	1.97	0.47
1:A:361:ARG:O	1:A:365:LYS:HD3	2.16	0.46
1:A:109:TRP:NE1	1:C:101:ARG:HE	2.13	0.46
1:C:238:VAL:O	1:C:336[B]:VAL:HG21	2.15	0.46
1:C:44:VAL:HG12	1:C:46:PRO:HD3	1.97	0.45
1:A:106:LYS:HE3	1:A:164:TYR:CZ	2.51	0.45
1:A:351:GLN:HA	1:A:351:GLN:NE2	2.30	0.45
1:A:43:TYR:HB2	1:C:143:ARG:HH12	1.81	0.45
1:C:92[B]:CYS:SG	1:C:152[B]:CYS:SG	3.06	0.45
1:C:214[B]:MET:HE2	1:C:217[B]:MET:HG3	1.98	0.45
1:A:301:PRO:CG	5:A:408:TRS:H11	2.46	0.45
1:C:133:MET:HE3	1:C:133:MET:HB3	1.92	0.44
1:A:113:PRO:HA	1:A:116:MET:HE3	1.99	0.44
1:A:282[B]:ASP:OD2	1:A:354[B]:GLU:HG3	2.17	0.44
1:A:300[B]:ILE:O	4:A:403:1PS:H3	2.18	0.43
1:C:306:ARG:NH1	7:C:508:HOH:O	2.50	0.43
1:A:238:VAL:O	1:A:336[B]:VAL:HG21	2.19	0.43
1:C:171:ARG:NH1	7:C:504:HOH:O	2.43	0.43
1:A:50:VAL:HG22	1:C:43:TYR:HD1	1.84	0.43
1:C:64:MET:HB2	1:C:65:PRO:HD2	1.99	0.43
1:A:43:TYR:HD1	1:C:50:VAL:HG22	1.83	0.42
1:C:160:ARG:NH2	7:C:509:HOH:O	2.51	0.42
1:C:282:ASP:C	1:C:282:ASP:OD1	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102[A]:LEU:HD22	1:A:136:PHE:CD1	2.54	0.42
1:A:44:VAL:HB	1:C:49:TYR:CZ	2.55	0.42
1:A:319:GLY:O	4:A:406:1PS:H81	2.20	0.42
1:A:94:GLU:OE2	5:A:409:TRS:H22	2.19	0.42
1:A:49:TYR:CE1	1:A:57:ARG:HG2	2.55	0.42
1:A:113:PRO:HB3	1:C:371:LYS:HG2	2.02	0.42
1:A:107:GLN:O	1:A:111:LYS:HB2	2.20	0.41
1:A:91:ARG:HD2	1:A:91:ARG:C	2.45	0.41
1:C:72[B]:MET:HG3	1:C:210:TRP:CD1	2.55	0.41
1:C:102[B]:LEU:HD23	1:C:102[B]:LEU:HA	1.81	0.41
1:A:48:ARG:H	1:A:48:ARG:HG3	1.60	0.41
1:A:41:PHE:CE1	1:C:53:PRO:HD3	2.55	0.41
1:C:69:ILE:HD11	1:C:84:LEU:HD12	2.03	0.41
1:A:67:ILE:HB	1:A:152[B]:CYS:HB3	2.02	0.40
1:C:215[B]:THR:HG22	1:C:314:MET:SD	2.61	0.40
1:A:186:HIS:CE1	1:A:190[B]:THR:HG21	2.56	0.40
1:C:164:TYR:OH	7:C:502:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	360/393 (92%)	352 (98%)	8 (2%)	0	100	100
1	C	352/393 (90%)	347 (99%)	5 (1%)	0	100	100
2	B	4/11 (36%)	4 (100%)	0	0	100	100
2	D	4/11 (36%)	4 (100%)	0	0	100	100
All	All	720/808 (89%)	707 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	322/340 (95%)	318 (99%)	4 (1%)	63	40
1	C	314/340 (92%)	312 (99%)	2 (1%)	78	64
2	B	6/10 (60%)	6 (100%)	0	100	100
2	D	6/10 (60%)	6 (100%)	0	100	100
All	All	648/700 (93%)	642 (99%)	6 (1%)	76	51

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LEU
1	A	300[A]	ILE
1	A	300[B]	ILE
1	A	371	LYS
1	C	300[A]	ILE
1	C	300[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS
1	A	331	GLN
1	A	351	GLN
1	C	338	ASN
1	C	366	GLN

5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 4 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$
4	1PS	A	407	-	13,13,13	0.96	1 (7%)	17,17,17	0.99	1 (5%)
3	A3P	C	401	-	29,29,29	0.72	1 (3%)	44,45,45	0.94	2 (4%)
4	1PS	A	403	-	13,13,13	0.84	1 (7%)	17,17,17	0.79	1 (5%)
3	A3P	A	401	-	29,29,29	0.78	2 (6%)	44,45,45	0.86	2 (4%)
5	TRS	A	409	-	7,7,7	0.33	0	9,9,9	0.79	0
4	1PS	A	402	-	13,13,13	0.92	1 (7%)	17,17,17	1.01	0
5	TRS	A	405	-	7,7,7	0.25	0	9,9,9	1.01	1 (11%)
5	TRS	A	404	-	7,7,7	0.37	0	9,9,9	1.15	0
4	1PS	A	406	-	13,13,13	0.73	0	17,17,17	1.15	2 (11%)
5	TRS	A	408	-	7,7,7	0.68	0	9,9,9	1.48	2 (22%)

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
4	1PS	A	407	-	-	4/7/7/7	0/1/1/1
3	A3P	C	401	-	-	1/15/31/31	0/3/3/3
4	1PS	A	403	-	-	4/7/7/7	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A3P	A	401	-	-	0/15/31/31	0/3/3/3
5	TRS	A	409	-	-	7/9/9/9	-
4	1PS	A	402	-	-	2/7/7/7	0/1/1/1
5	TRS	A	405	-	-	6/9/9/9	-
5	TRS	A	404	-	-	3/9/9/9	-
4	1PS	A	406	-	-	7/7/7/7	0/1/1/1
5	TRS	A	408	-	-	6/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	1PS	C8-S1	2.70	1.81	1.77
4	A	407	1PS	C8-S1	2.53	1.81	1.77
3	C	401	A3P	P1-O3'	2.41	1.63	1.59
4	A	403	1PS	C8-S1	2.35	1.80	1.77
3	A	401	A3P	P2-O5P	-2.15	1.46	1.54
3	A	401	A3P	P2-O5'	2.13	1.67	1.60

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	406	1PS	O2-S1-C8	-2.88	102.37	106.73
4	A	406	1PS	C7-C8-S1	-2.67	109.15	113.25
3	A	401	A3P	C2'-C1'-N9	-2.62	106.79	113.30
5	A	405	TRS	C3-C-N	2.53	114.62	108.17
4	A	403	1PS	C7-C8-S1	-2.34	109.66	113.25
5	A	408	TRS	O2-C2-C	2.33	117.37	110.88
5	A	408	TRS	C2-C-C1	-2.26	104.65	110.66
3	C	401	A3P	O6P-P2-O5P	2.18	115.99	107.80
3	C	401	A3P	C2'-C1'-N9	-2.14	107.98	113.30
4	A	407	1PS	O2-S1-C8	2.03	109.79	106.73
3	A	401	A3P	O2'-C2'-C3'	2.01	116.81	111.19

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	1PS	N1-C6-C7-C8
4	A	407	1PS	C7-C8-S1-O1
4	A	407	1PS	C7-C8-S1-O2

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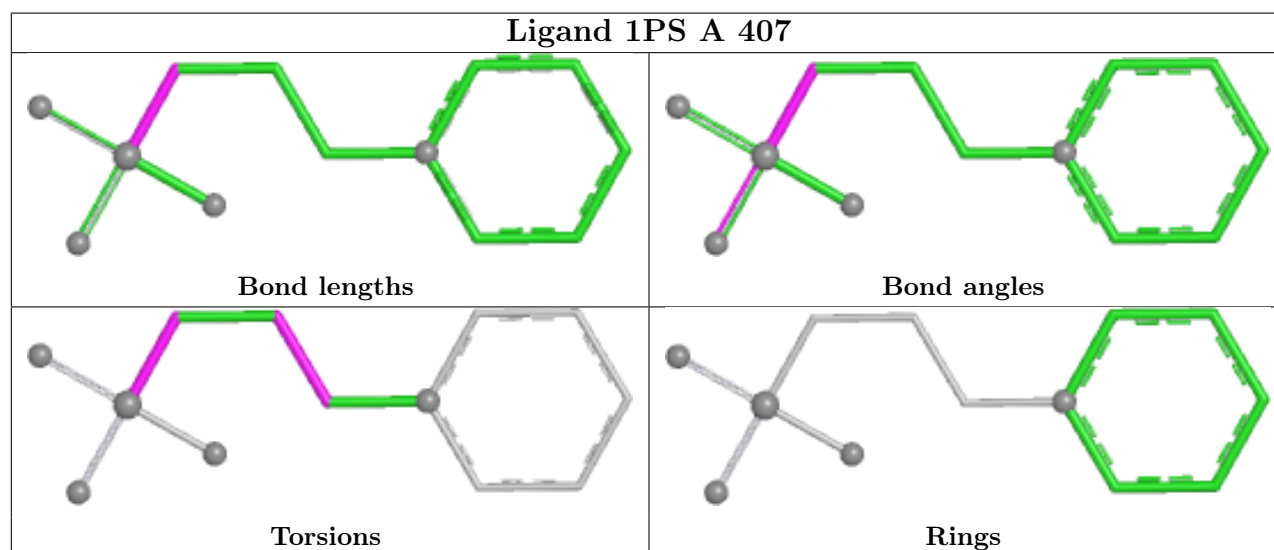
Mol	Chain	Res	Type	Atoms
5	A	404	TRS	N-C-C3-O3
5	A	405	TRS	C2-C-C1-O1
5	A	405	TRS	C3-C-C1-O1
5	A	405	TRS	N-C-C1-O1
5	A	405	TRS	N-C-C2-O2
5	A	408	TRS	N-C-C2-O2
5	A	409	TRS	C1-C-C2-O2
5	A	409	TRS	C3-C-C2-O2
5	A	409	TRS	C1-C-C3-O3
5	A	409	TRS	C2-C-C3-O3
5	A	409	TRS	N-C-C3-O3
5	A	404	TRS	C2-C-C3-O3
5	A	408	TRS	C3-C-C2-O2
5	A	408	TRS	C2-C-C3-O3
4	A	402	1PS	C7-C8-S1-O3
4	A	403	1PS	C7-C8-S1-O2
4	A	406	1PS	C7-C8-S1-O2
4	A	407	1PS	C7-C8-S1-O3
5	A	408	TRS	C1-C-C2-O2
5	A	408	TRS	C1-C-C3-O3
5	A	409	TRS	N-C-C2-O2
4	A	406	1PS	C7-C6-N1-C3
4	A	406	1PS	C6-C7-C8-S1
4	A	406	1PS	C7-C8-S1-O1
4	A	406	1PS	C7-C6-N1-C1
4	A	406	1PS	N1-C6-C7-C8
4	A	407	1PS	N1-C6-C7-C8
5	A	405	TRS	C3-C-C2-O2
3	C	401	A3P	C5'-O5'-P2-O4P
5	A	408	TRS	N-C-C3-O3
4	A	403	1PS	C7-C8-S1-O1
4	A	403	1PS	C7-C8-S1-O3
4	A	406	1PS	C7-C8-S1-O3
5	A	404	TRS	C1-C-C3-O3
5	A	405	TRS	C1-C-C2-O2
5	A	409	TRS	N-C-C1-O1
4	A	402	1PS	C7-C8-S1-O1

There are no ring outliers.

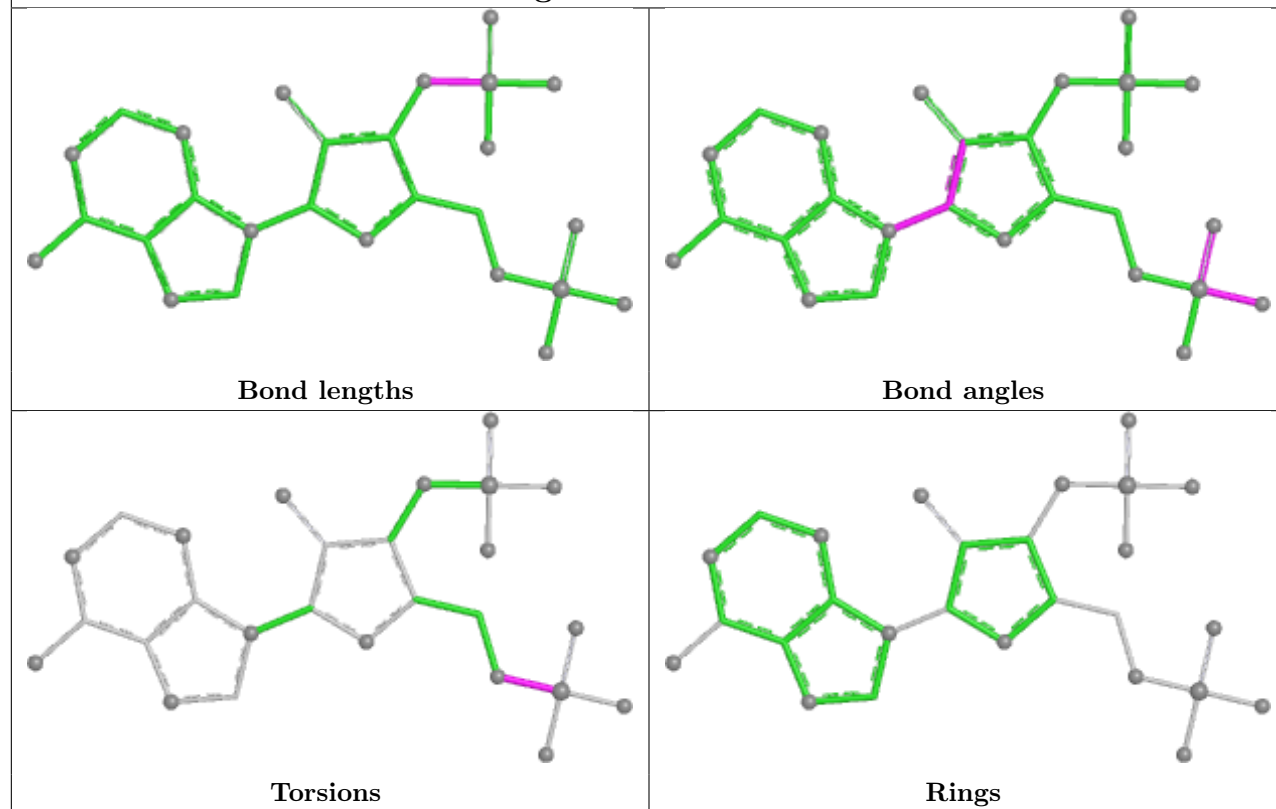
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	407	1PS	4	0
4	A	403	1PS	1	0
5	A	409	TRS	1	0
5	A	405	TRS	2	0
4	A	406	1PS	2	0
5	A	408	TRS	2	0

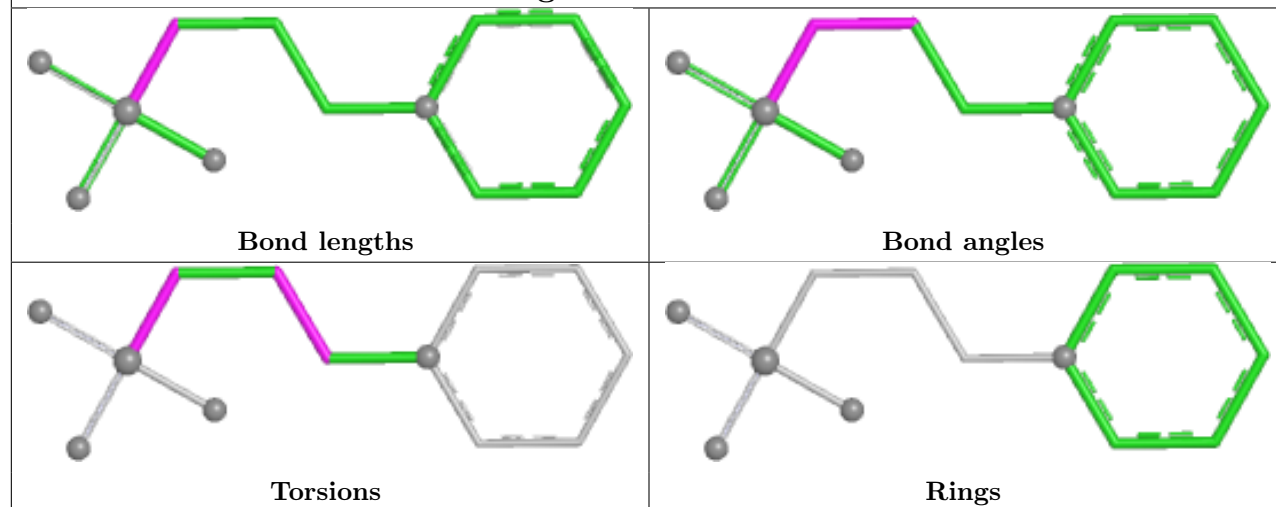
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

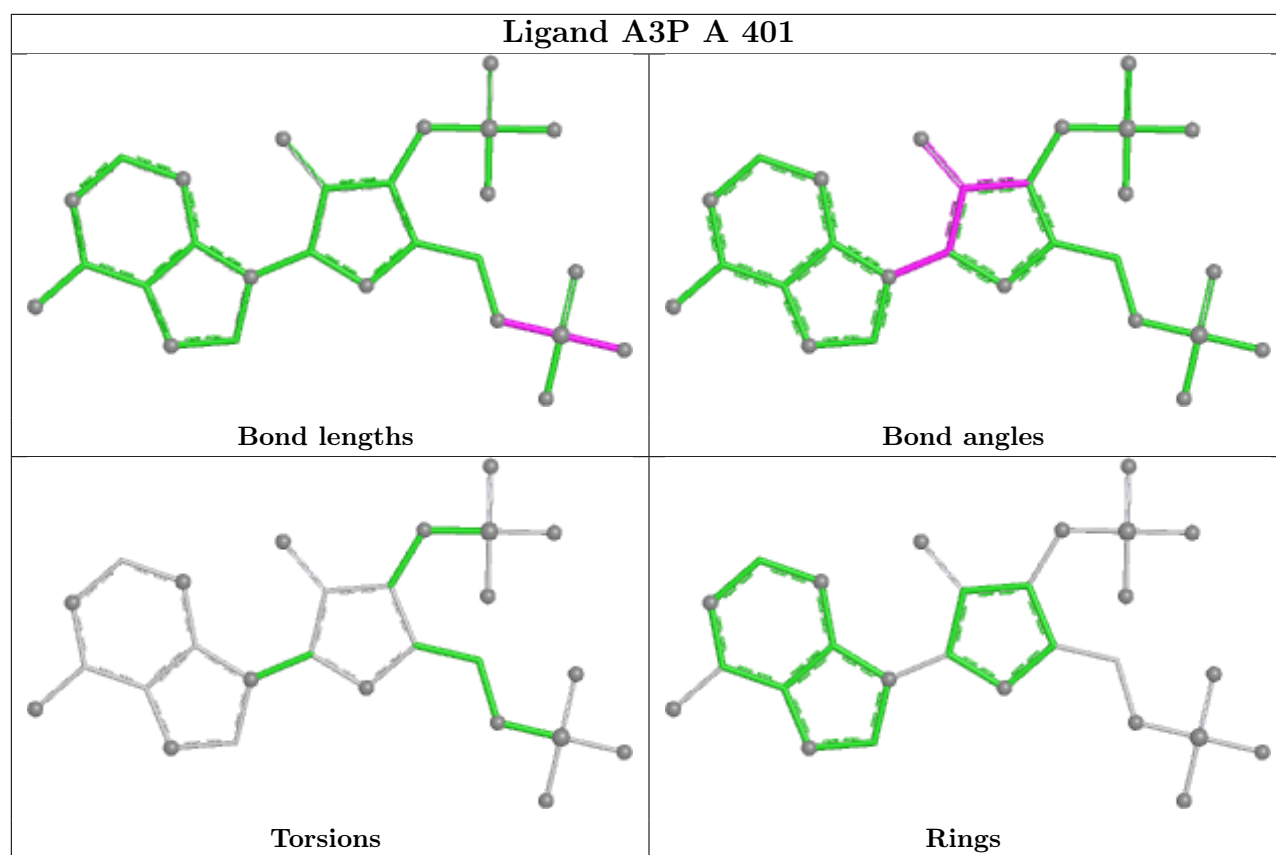


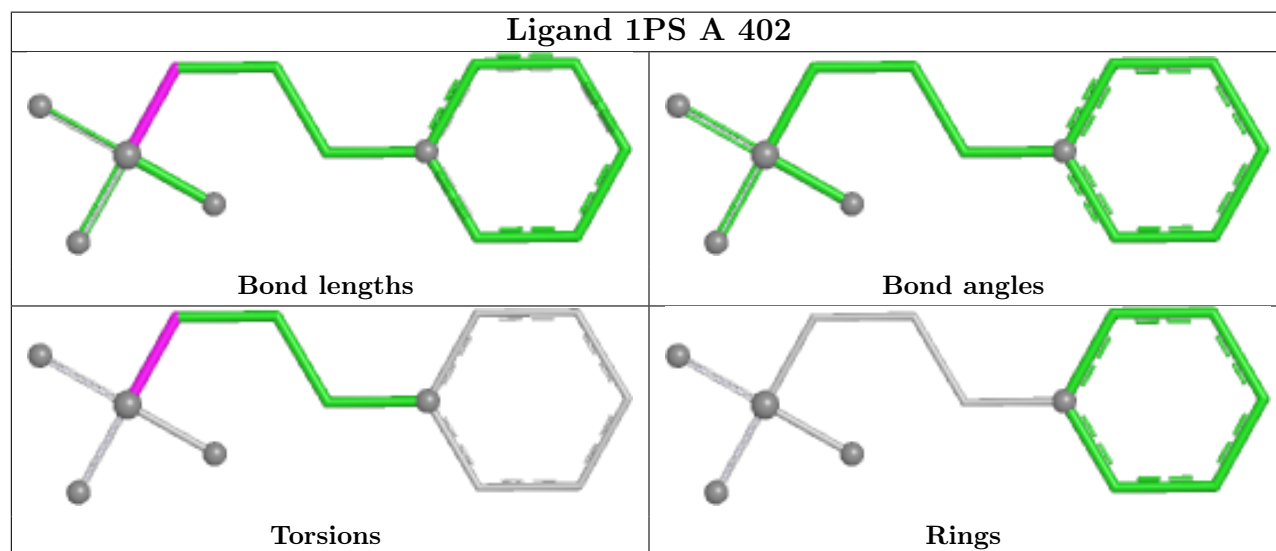
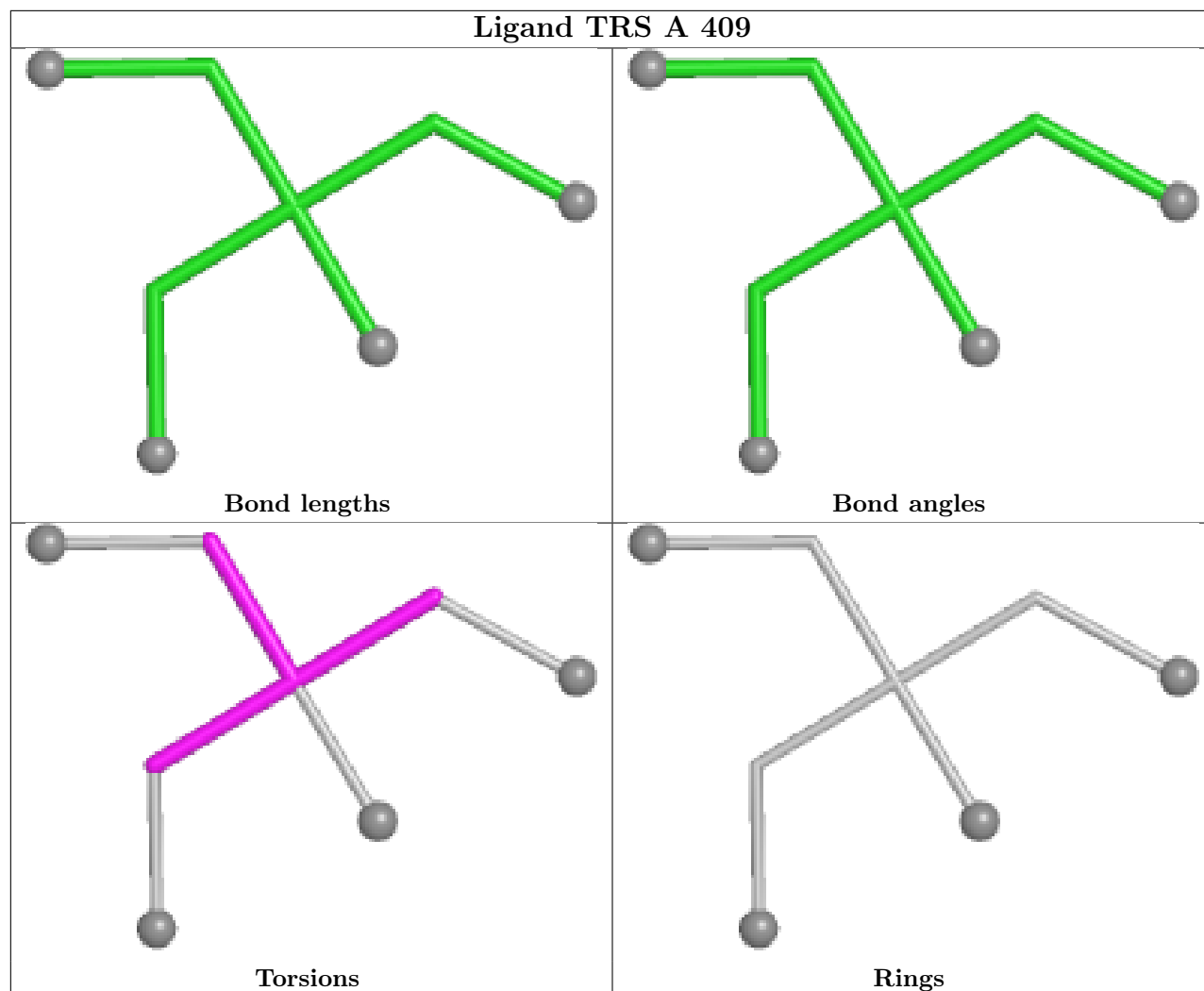
Ligand A3P C 401

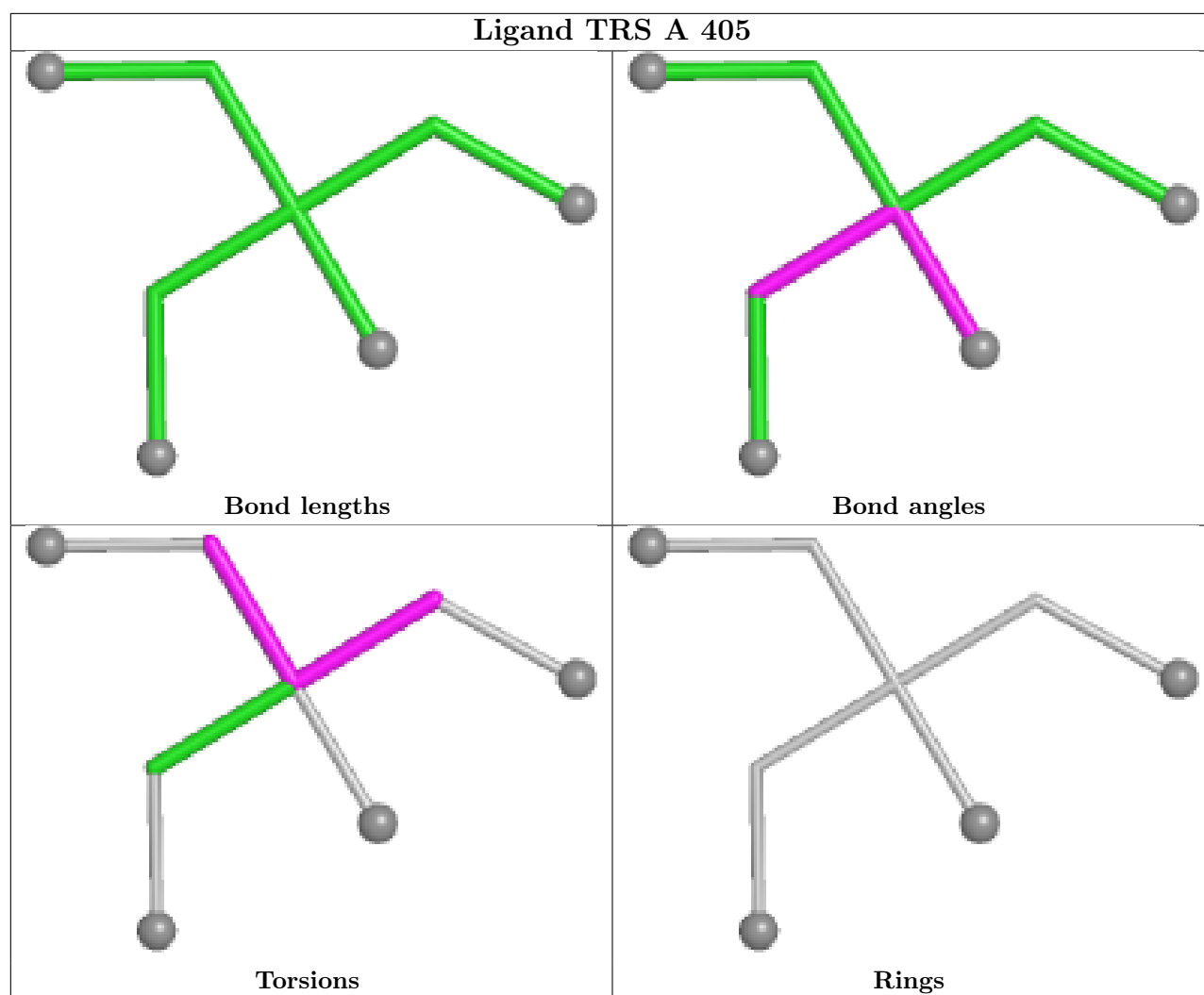


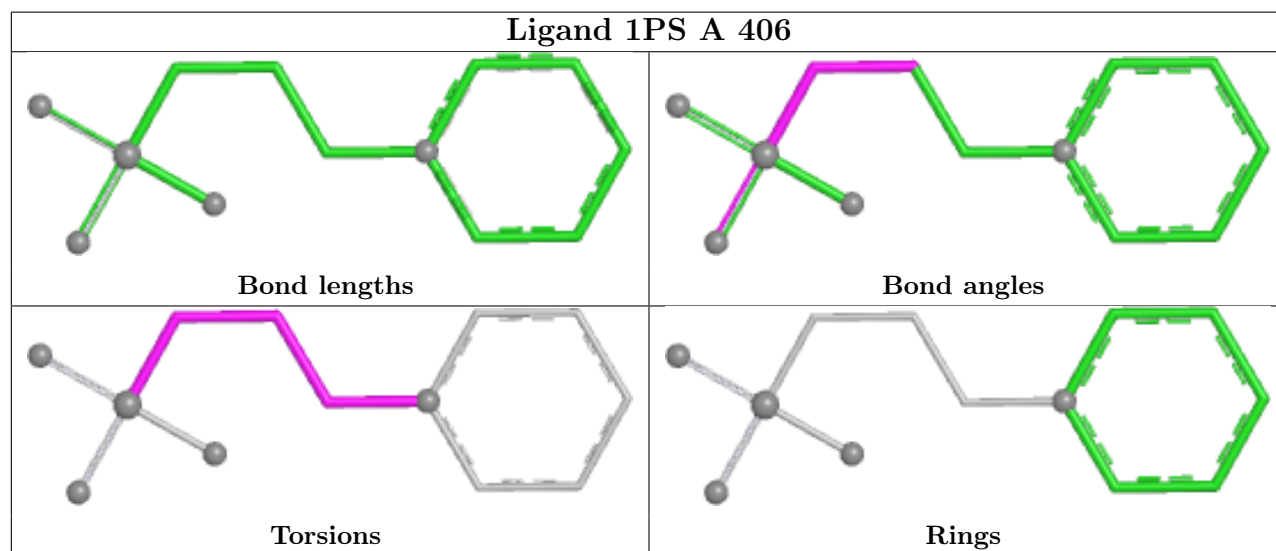
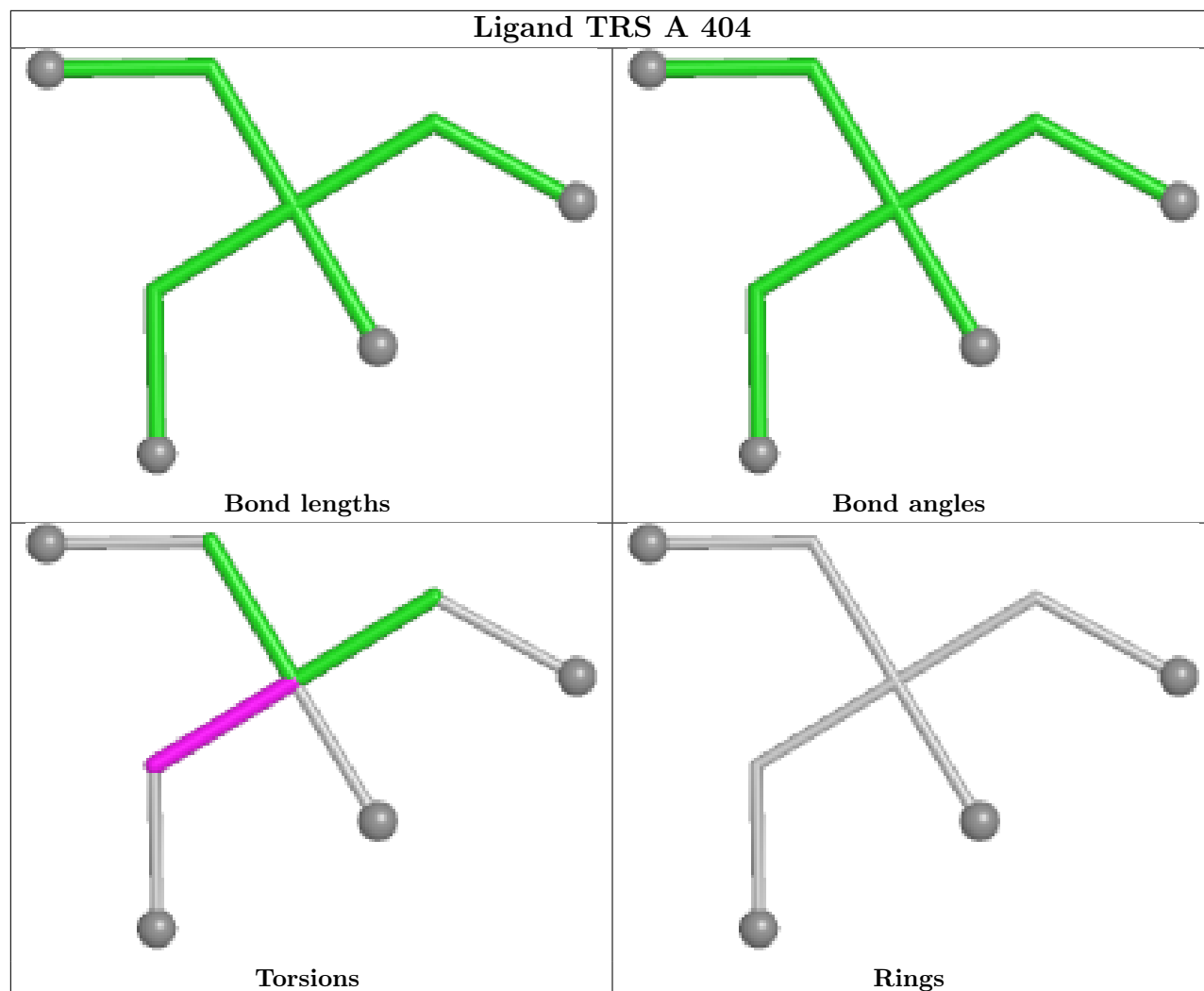
Ligand 1PS A 403

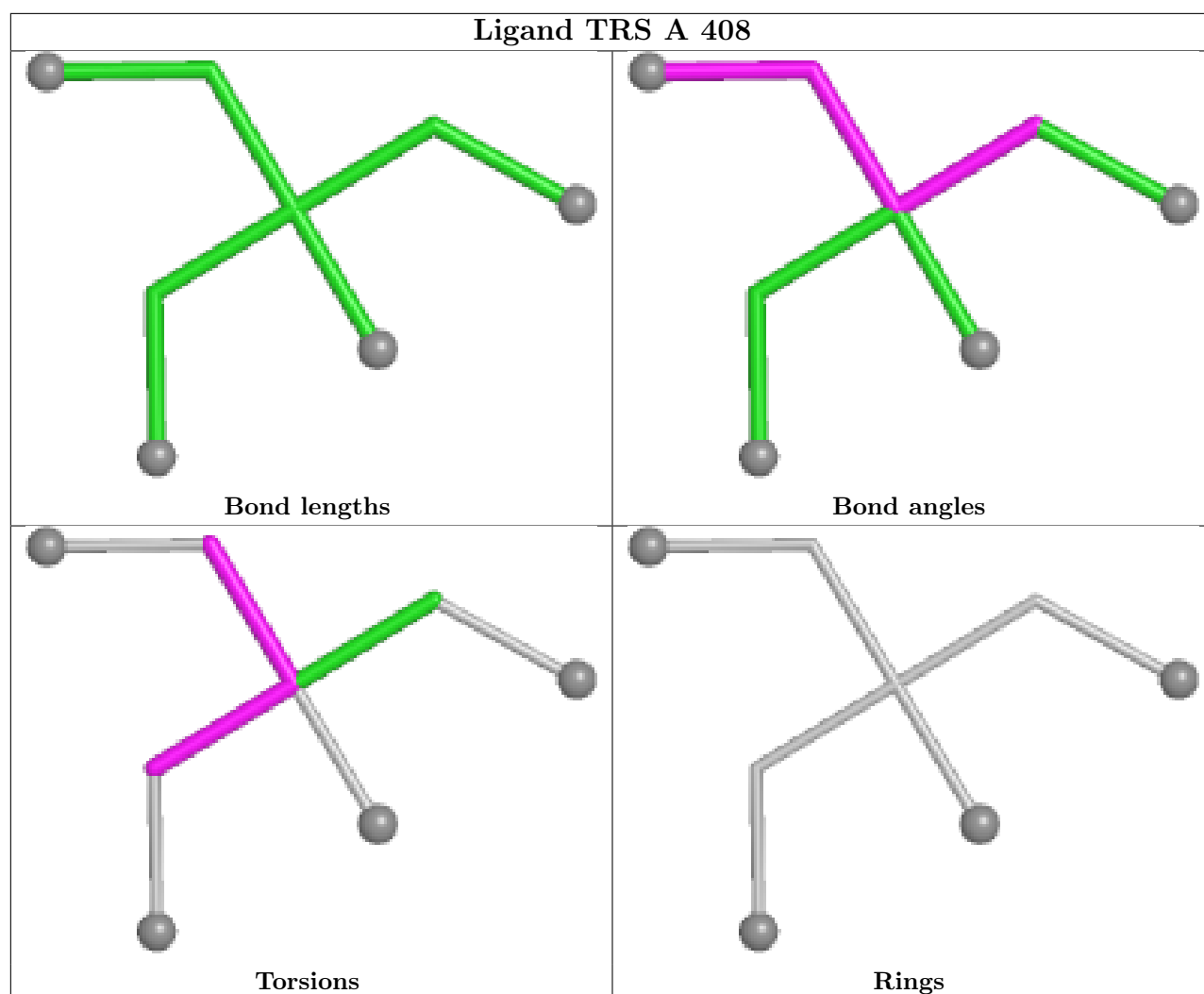












5.7 Other polymers [i](#)

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	333/393 (84%)	0.71	50 (15%) 5 6	10, 27, 105, 154	30 (9%)
1	C	333/393 (84%)	0.69	50 (15%) 5 6	11, 27, 107, 142	21 (6%)
2	B	6/11 (54%)	1.74	3 (50%) 0 0	34, 50, 61, 75	1 (16%)
2	D	6/11 (54%)	1.74	2 (33%) 1 1	35, 60, 67, 71	0
All	All	678/808 (83%)	0.71	105 (15%) 5 6	10, 27, 106, 154	52 (7%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	PHE	7.7
1	A	46	PRO	7.6
1	C	46	PRO	7.3
1	A	363	LEU	6.9
1	A	43	TYR	5.8
1	A	44	VAL	5.8
1	C	41	PHE	5.6
1	A	45	SER	5.5
1	C	44	VAL	5.4
1	C	59	PRO	5.4
1	C	42	THR	5.4
1	A	49	TYR	5.4
1	C	43	TYR	5.4
1	C	363	LEU	5.3
1	C	364	ILE	5.1
1	C	49	TYR	5.1
1	A	364	ILE	5.0
1	A	42	THR	5.0
1	A	51	LEU	4.8
1	A	369	ALA	4.8
1	C	51	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	52	GLY	4.6
1	C	55	SER	4.6
1	C	352	ALA	4.6
1	C	58	TYR	4.5
1	C	368	ILE	4.5
1	C	53	PRO	4.3
1	A	110	VAL	4.1
1	A	47	ASP	4.1
1	A	53	PRO	4.1
1	A	55	SER	4.0
1	A	48	ARG	4.0
1	C	48	ARG	4.0
1	A	52	GLY	4.0
1	A	58	TYR	3.9
1	A	368	ILE	3.9
1	C	45	SER	3.9
1	A	360	HIS	3.7
1	A	371	LYS	3.7
1	A	352	ALA	3.6
1	C	109	TRP	3.5
1	C	357	LEU	3.5
1	A	109	TRP	3.4
2	B	1007	GLU	3.4
1	C	355	ARG	3.4
2	D	1002	PHE	3.2
1	A	341[A]	LEU	3.2
1	A	54	ASP	3.2
1	C	372	LYS	3.2
1	A	355	ARG	3.1
1	A	370	LYS	3.1
1	C	361	ARG	3.1
1	A	359	GLU	3.0
1	A	367	SER	3.0
1	C	56	ARG	3.0
1	C	351	GLN	3.0
1	C	369	ALA	3.0
1	C	50	VAL	3.0
1	A	361	ARG	3.0
1	C	367	SER	3.0
1	C	47	ASP	2.9
1	A	372	LYS	2.9
1	C	370	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	371	LYS	2.9
1	C	57	ARG	2.8
1	C	54	ASP	2.8
1	A	105	LEU	2.8
1	C	360	HIS	2.7
2	D	1007	GLU	2.7
1	C	349	GLU	2.6
1	A	357	LEU	2.6
1	A	268	ASN	2.6
1	A	351	GLN	2.5
1	C	110	VAL	2.5
1	A	269[A]	GLN	2.5
1	A	366	GLN	2.5
1	C	366	GLN	2.5
1	C	353	ARG	2.5
1	A	358	GLU	2.4
1	A	59	PRO	2.4
1	C	105	LEU	2.4
1	C	116[A]	MET	2.4
1	A	365	LYS	2.4
1	A	57	ARG	2.4
1	C	268	ASN	2.4
1	C	310	LYS	2.3
1	A	362	GLU	2.3
1	C	104	SER	2.3
1	C	358	GLU	2.3
1	A	40	ASN	2.3
1	A	50	VAL	2.3
1	A	56	ARG	2.3
1	C	365	LYS	2.2
1	A	353	ARG	2.2
1	C	348	GLU	2.2
2	B	1006	GLU	2.2
2	B	1002	PHE	2.2
1	C	354	GLU	2.1
1	A	111	LYS	2.1
1	A	60	TYR	2.1
1	A	300[A]	ILE	2.1
1	C	60	TYR	2.1
1	A	348	GLU	2.1
1	C	200	LEU	2.0
1	C	341	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

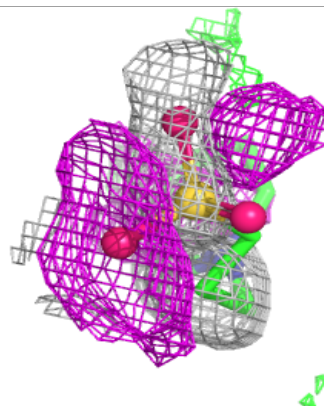
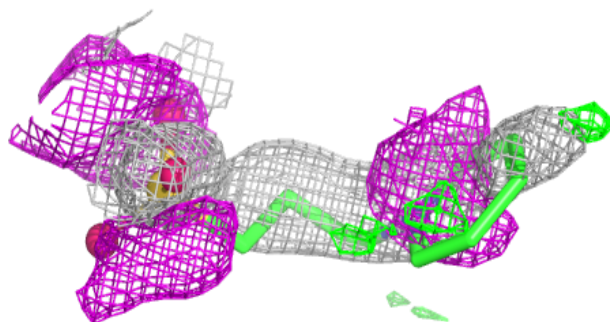
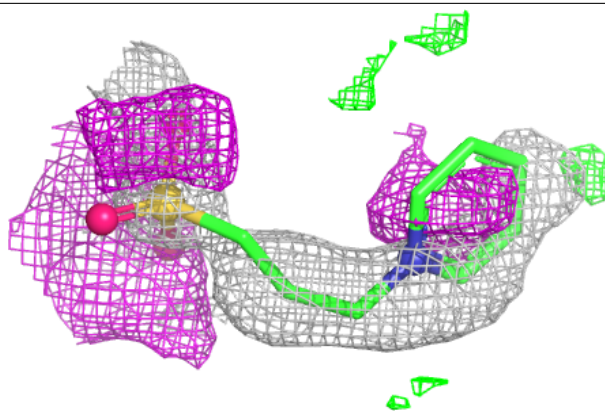
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	1PS	A	407	13/13	0.47	0.28	44,81,129,154	0
4	1PS	A	403	13/13	0.68	0.18	43,71,142,156	0
4	1PS	A	406	13/13	0.73	0.23	35,66,114,141	0
4	1PS	A	402	13/13	0.80	0.19	39,53,70,82	0
5	TRS	A	409	8/8	0.80	0.14	51,57,72,74	0
5	TRS	A	405	8/8	0.84	0.18	50,64,79,81	0
5	TRS	A	404	8/8	0.84	0.15	36,52,60,62	0
5	TRS	A	408	8/8	0.87	0.14	33,46,68,75	0
6	MG	A	411	1/1	0.98	0.15	44,44,44,44	1
3	A3P	C	401	27/27	0.99	0.04	17,21,23,24	0
6	MG	A	410	1/1	0.99	0.03	24,24,24,24	1
3	A3P	A	401	27/27	0.99	0.04	18,20,22,25	0
6	MG	C	402	1/1	0.99	0.03	22,22,22,22	1
6	MG	C	403	1/1	0.99	0.05	29,29,29,29	1

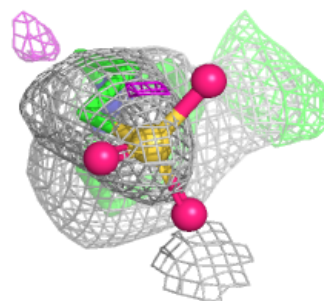
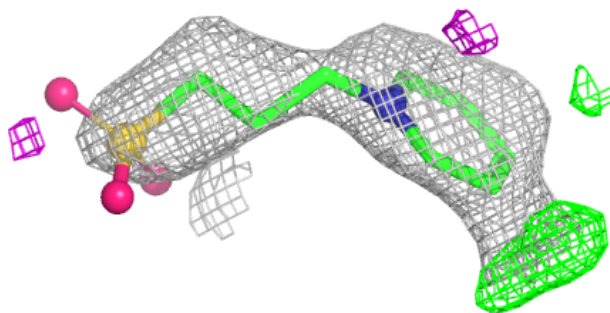
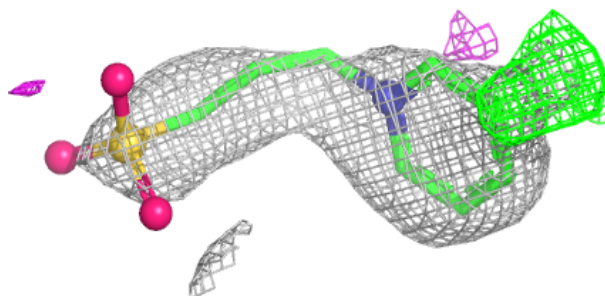
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1PS A 407:

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

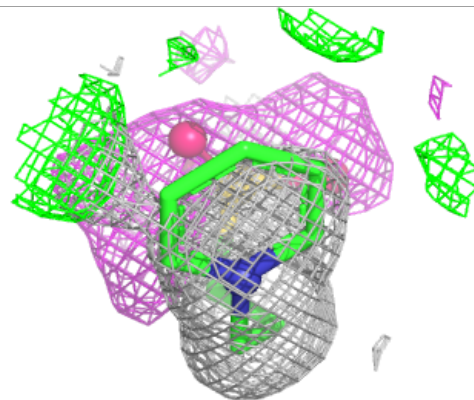
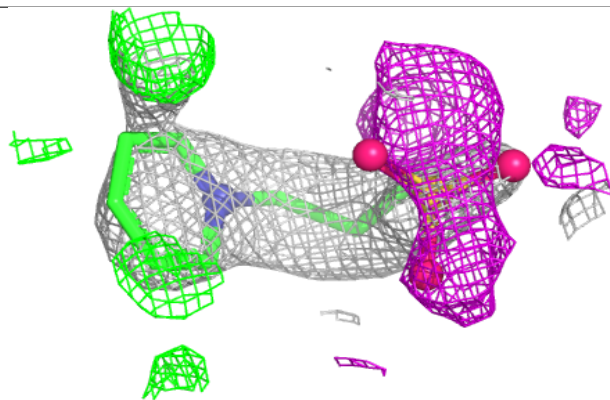
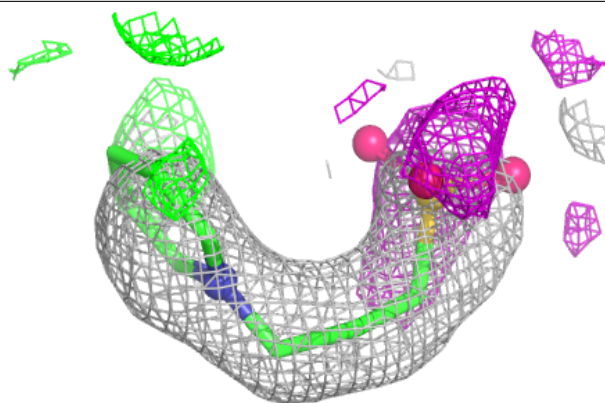
**Electron density around 1PS A 403:**

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

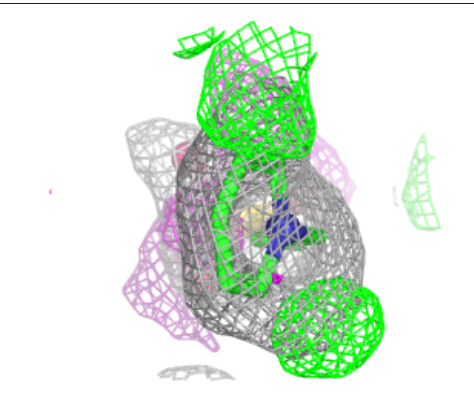
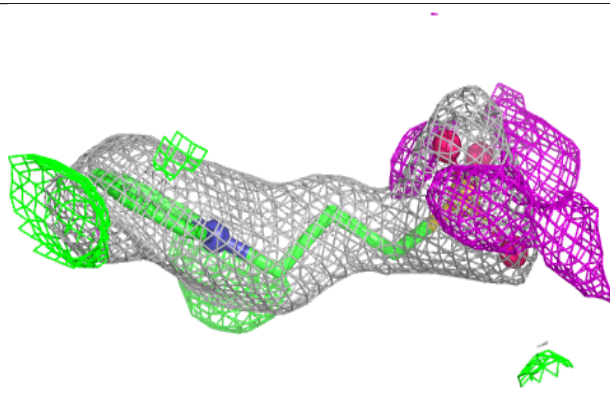
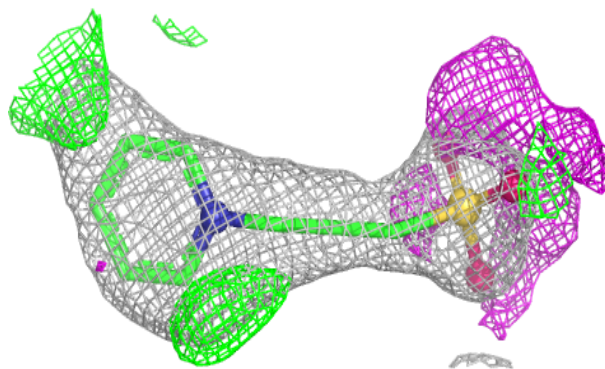


Electron density around 1PS A 406:

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

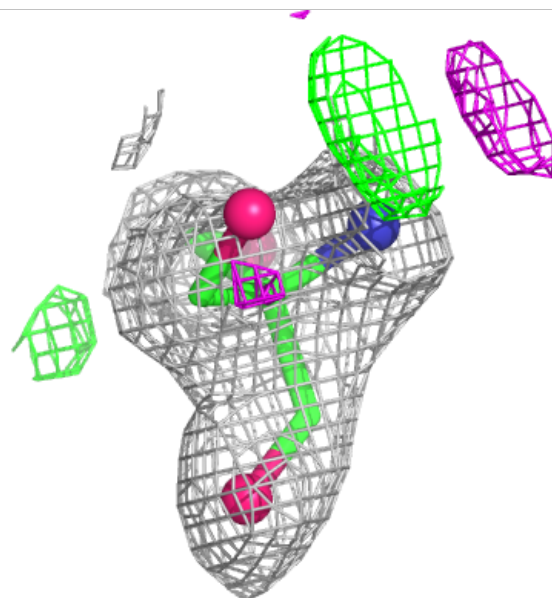
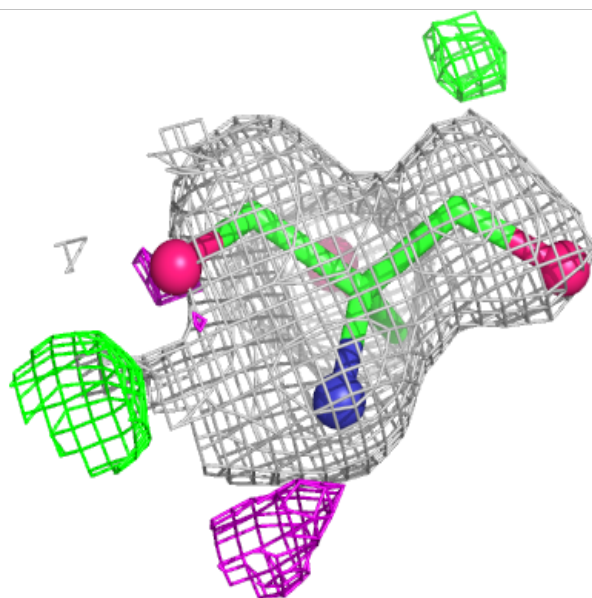
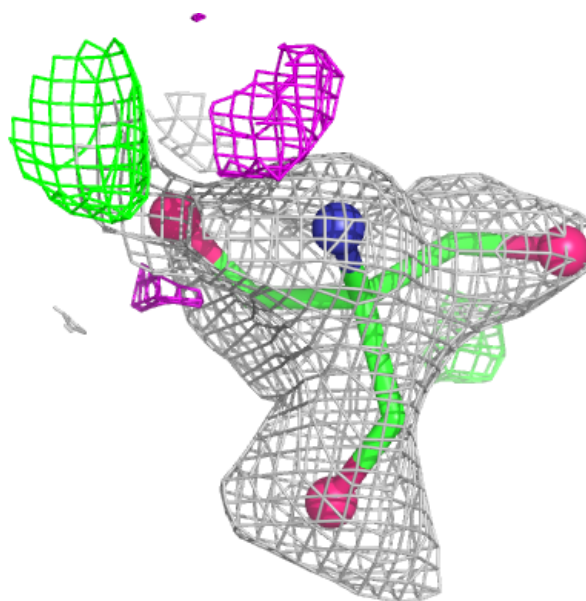
**Electron density around 1PS A 402:**

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



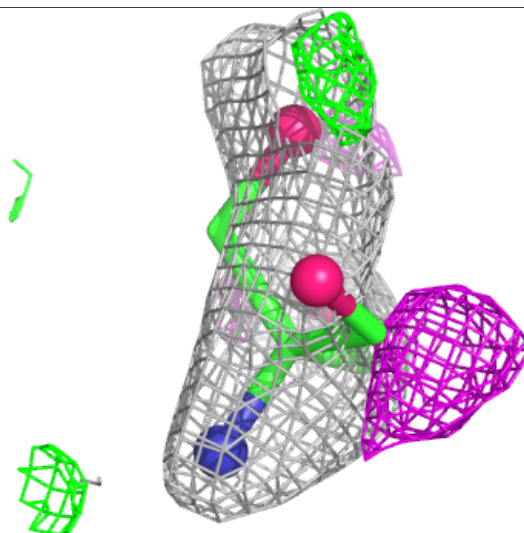
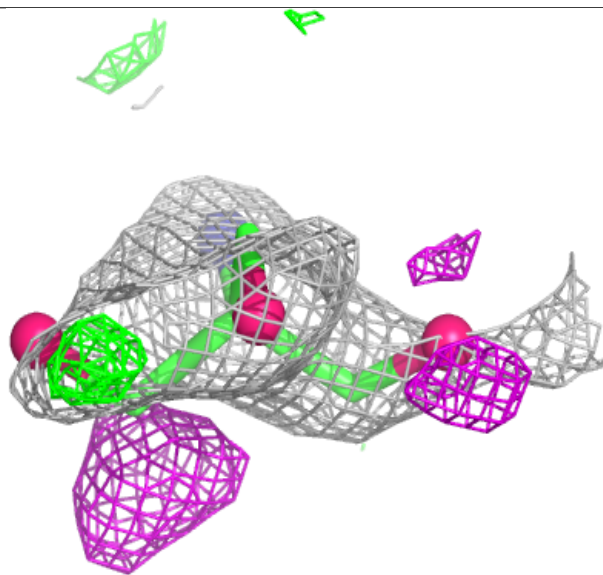
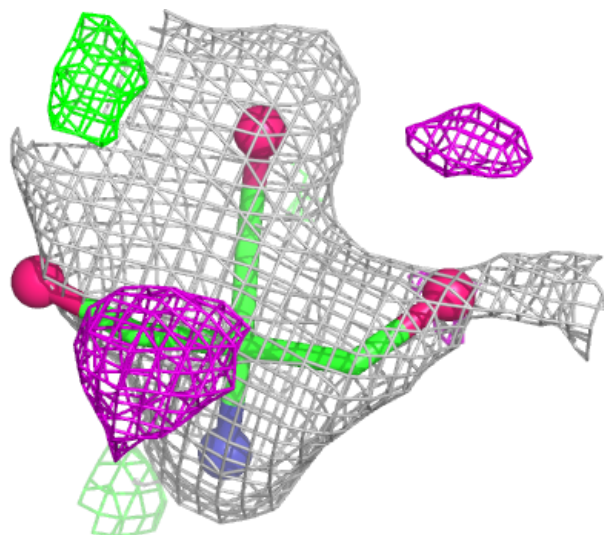
Electron density around TRS A 409:

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



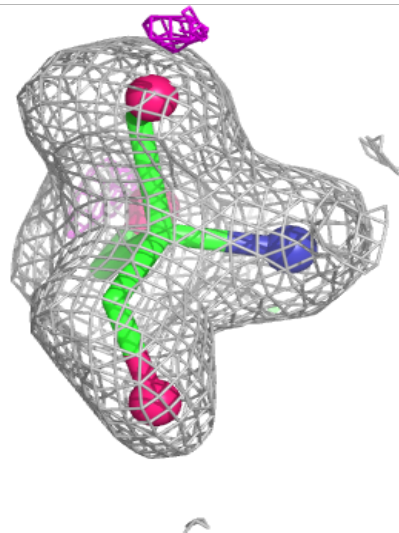
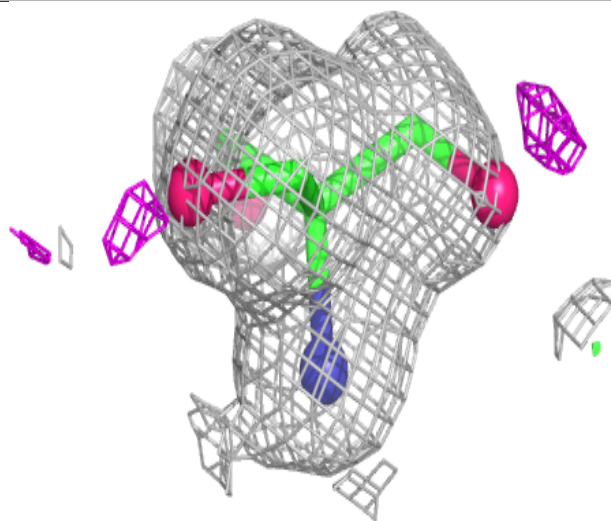
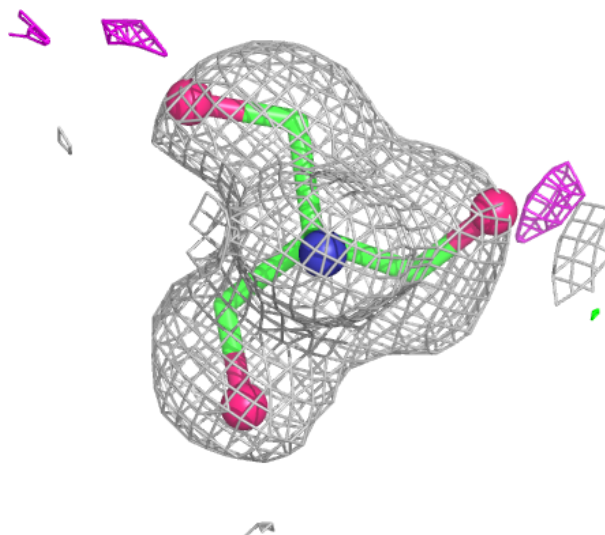
Electron density around TRS A 405:

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



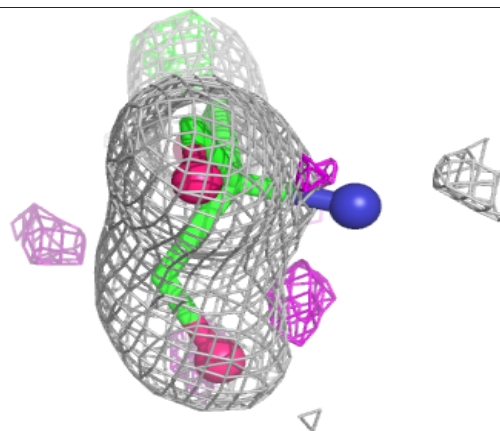
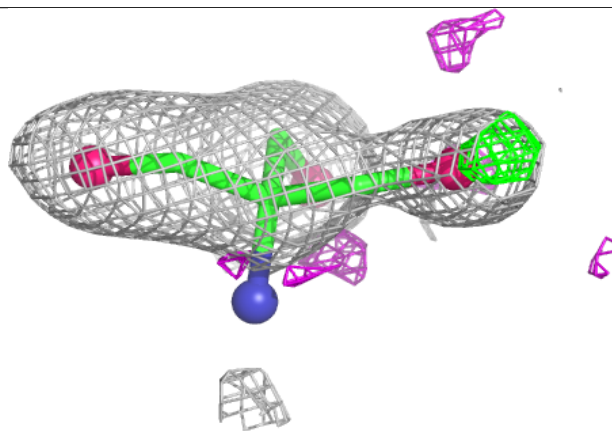
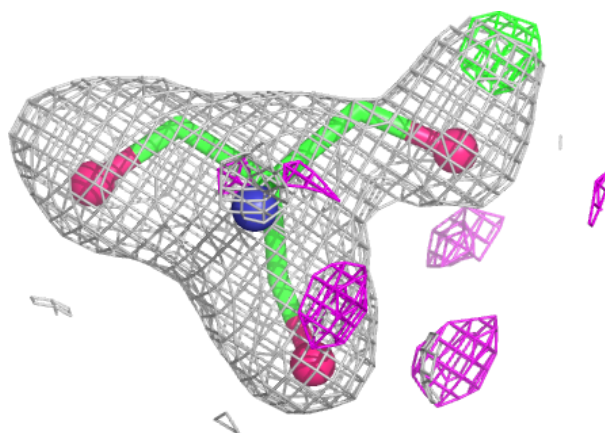
Electron density around TRS A 404:

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



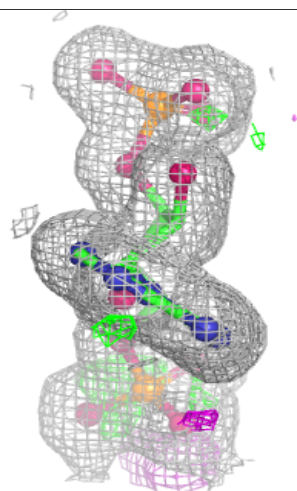
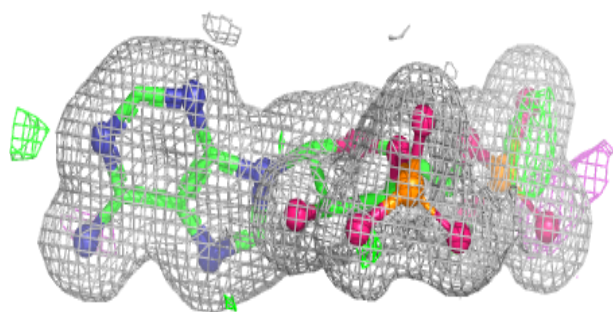
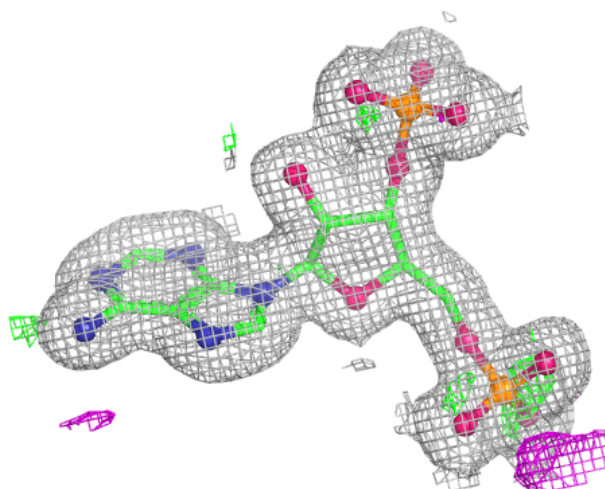
Electron density around TRS A 408:

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



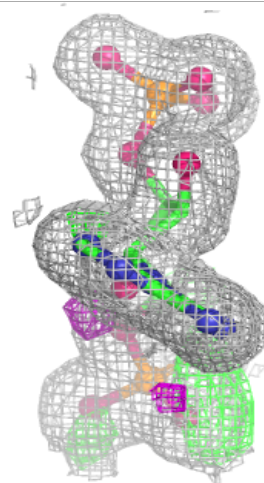
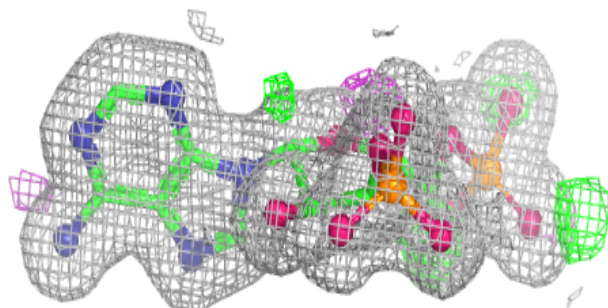
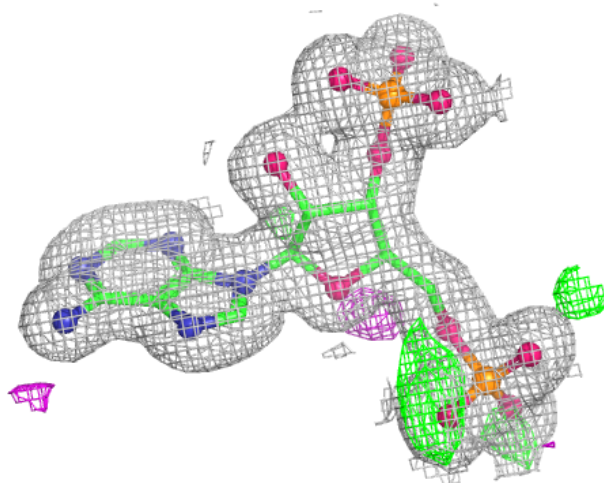
Electron density around A3P C 401:

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



Electron density around A3P A 401:

$2mF_o-DF_c$ (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.