



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:39 PM UTC

PDB ID : 8VR5 / pdb_00008vr5
Title : crystal structure of the Pcryo_0618 aminotransferase from *Psychrobacter cryohalolentis* K5 in the presence of PMP and glutamate
Authors : Bockhaus, N.J.; Thoden, J.B.; Holden, H.M.
Deposited on : 2024-01-20
Resolution : 2.20 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

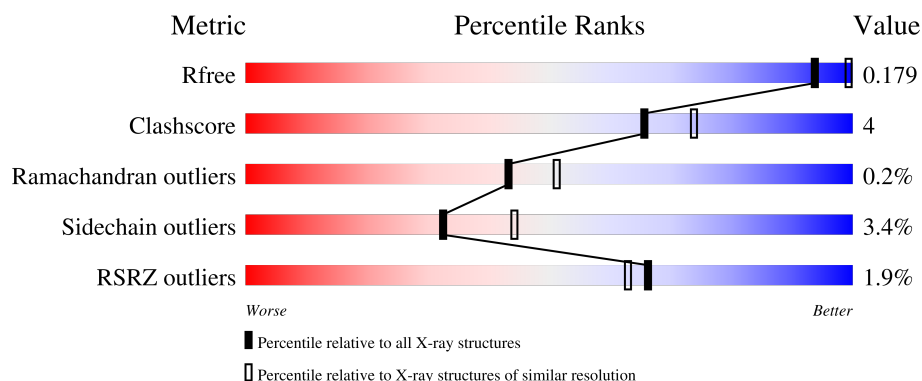
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	380	2% 85% 12% ..
1	B	380	2% 85% 13% ..
1	C	380	2% 89% 8% ..
1	D	380	2% 85% 12% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12658 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 DegT/DnrJ/EryC1/StrS aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	3	0
			2897	1841	490	550	16			
1	B	376	Total	C	N	O	S	0	3	0
			2930	1861	497	556	16			
1	C	374	Total	C	N	O	S	0	1	0
			2896	1840	489	551	16			
1	D	374	Total	C	N	O	S	0	0	0
			2893	1838	489	550	16			

There are 32 discrepancies between the modelled and reference sequences:

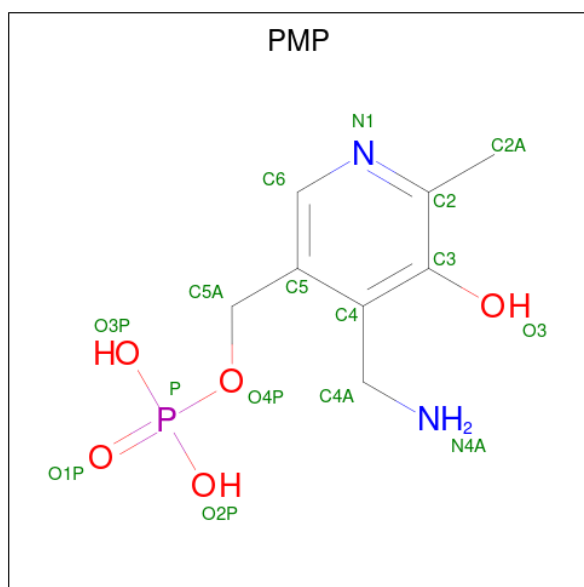
Chain	Residue	Modelled	Actual	Comment	Reference
A	373	LEU	-	expression tag	UNP Q1QD52
A	374	GLU	-	expression tag	UNP Q1QD52
A	375	HIS	-	expression tag	UNP Q1QD52
A	376	HIS	-	expression tag	UNP Q1QD52
A	377	HIS	-	expression tag	UNP Q1QD52
A	378	HIS	-	expression tag	UNP Q1QD52
A	379	HIS	-	expression tag	UNP Q1QD52
A	380	HIS	-	expression tag	UNP Q1QD52
B	373	LEU	-	expression tag	UNP Q1QD52
B	374	GLU	-	expression tag	UNP Q1QD52
B	375	HIS	-	expression tag	UNP Q1QD52
B	376	HIS	-	expression tag	UNP Q1QD52
B	377	HIS	-	expression tag	UNP Q1QD52
B	378	HIS	-	expression tag	UNP Q1QD52
B	379	HIS	-	expression tag	UNP Q1QD52
B	380	HIS	-	expression tag	UNP Q1QD52
C	373	LEU	-	expression tag	UNP Q1QD52
C	374	GLU	-	expression tag	UNP Q1QD52
C	375	HIS	-	expression tag	UNP Q1QD52
C	376	HIS	-	expression tag	UNP Q1QD52
C	377	HIS	-	expression tag	UNP Q1QD52

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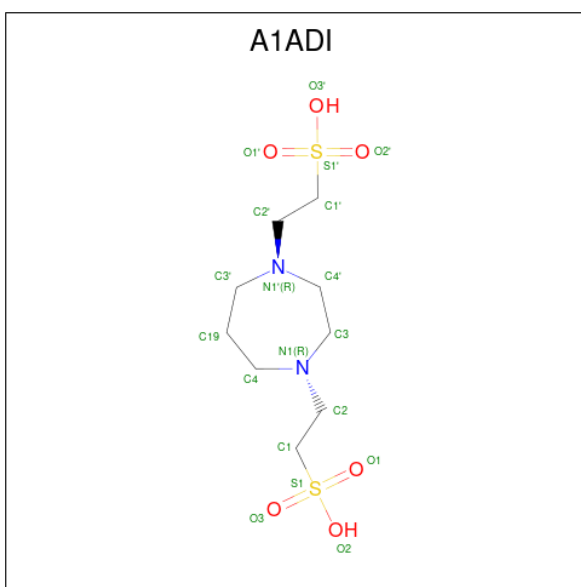
Chain	Residue	Modelled	Actual	Comment	Reference
C	378	HIS	-	expression tag	UNP Q1QD52
C	379	HIS	-	expression tag	UNP Q1QD52
C	380	HIS	-	expression tag	UNP Q1QD52
D	373	LEU	-	expression tag	UNP Q1QD52
D	374	GLU	-	expression tag	UNP Q1QD52
D	375	HIS	-	expression tag	UNP Q1QD52
D	376	HIS	-	expression tag	UNP Q1QD52
D	377	HIS	-	expression tag	UNP Q1QD52
D	378	HIS	-	expression tag	UNP Q1QD52
D	379	HIS	-	expression tag	UNP Q1QD52
D	380	HIS	-	expression tag	UNP Q1QD52

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 2,2'-(1,4-diazepane-1,4-diyl)di(ethane-1-sulfonic acid) (CCD ID: A1ADI) (formula: $C_9H_{20}N_2O_6S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			19	9	2	6	2		
3	B	1	Total	C	N	O	S	0	0
			19	9	2	6	2		
3	B	1	Total	C	N	O	S	0	0
			19	9	2	6	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

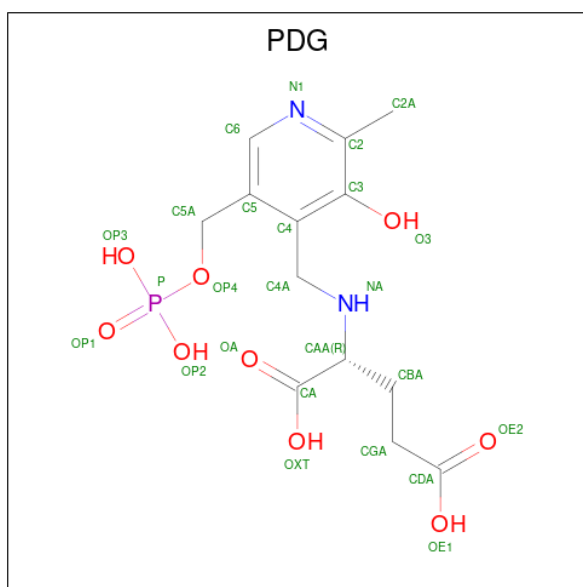


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is N-({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)-D-GLUTAMIC ACID (CCD ID: PDG) (formula: C₁₃H₁₉N₂O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
7	C	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
7	D	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Na	0	0
			1	1		
8	C	1	Total	Na	0	0
			1	1		
8	D	1	Total	Na	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	246	Total	O	0	0
			246	246		
9	B	257	Total	O	0	0
			257	257		
9	C	195	Total	O	0	0
			195	195		

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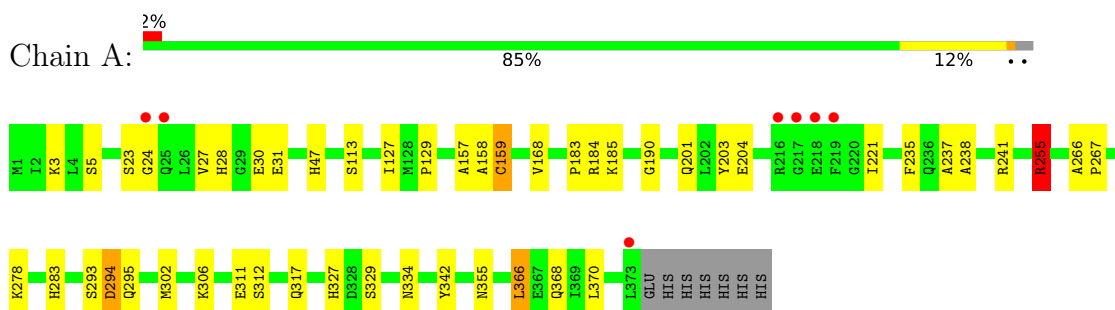
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	159	Total 159	O 159	0	0

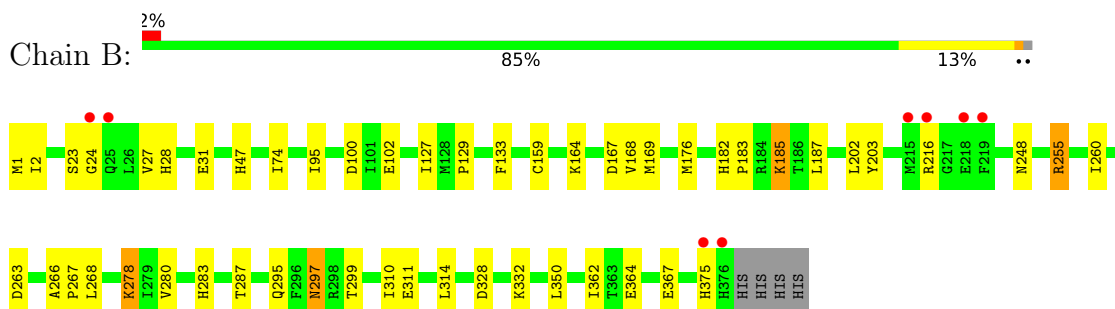
3 Residue-property plots

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.

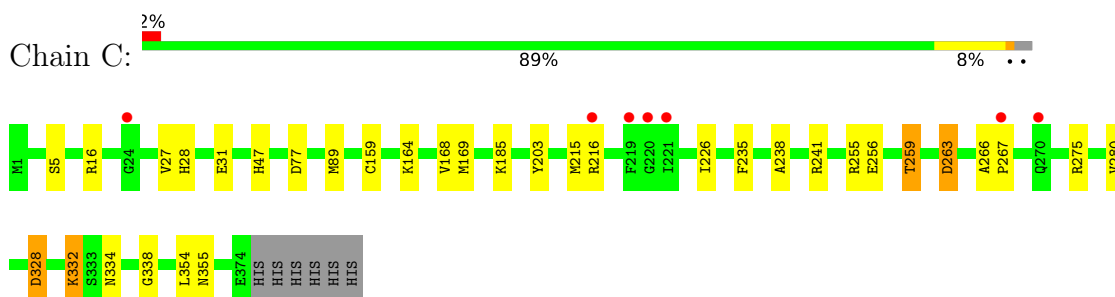
- Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase



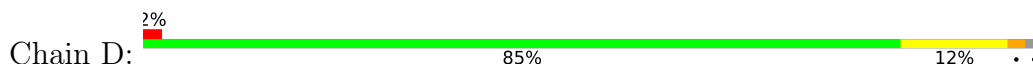
- Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase

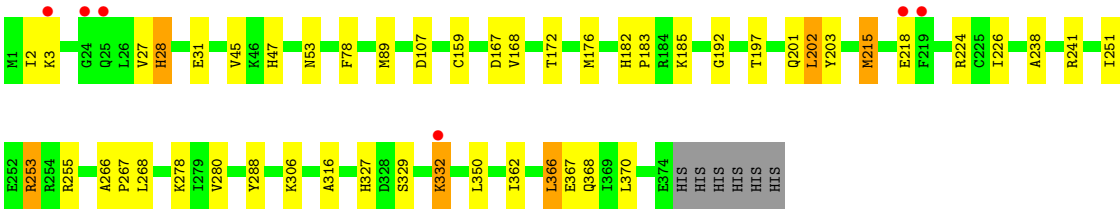


- Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase



- Molecule 1: DegT/DnrJ/EryC1/StrS aminotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.49Å 159.82Å 115.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.89 – 2.20 32.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.89-2.20) 99.6 (32.89-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.178 , 0.213 (Not available) , 0.179	Depositor DCC
R_{free} test set	6297 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12658	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2739e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, MG, A1ADI, PMP, PDG, EDO, 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	0.67	0/2953	1.09	6/3991 (0.2%)
1	B	0.65	0/2988	1.09	5/4038 (0.1%)
1	C	0.61	0/2946	1.05	2/3981 (0.1%)
1	D	0.60	0/2940	1.06	3/3973 (0.1%)
All	All	0.63	0/11827	1.07	16/15983 (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	B	0	1
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	ASP	CA-CB-CG	7.36	119.96	112.60
1	B	263	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	204	GLU	CB-CG-CD	6.19	123.12	112.60
1	D	332	LYS	CB-CA-C	6.15	120.36	110.09
1	A	283	HIS	CA-CB-CG	5.84	119.64	113.80
1	A	235	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	293	SER	CA-C-N	5.80	132.62	121.54
1	A	293	SER	C-N-CA	5.80	132.62	121.54
1	B	295	GLN	CB-CA-C	-5.69	100.10	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	CYS	CB-CA-C	-5.57	101.16	110.56
1	B	100	ASP	CA-CB-CG	5.49	118.09	112.60
1	D	167	ASP	CA-CB-CG	5.42	118.02	112.60
1	B	167	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	107	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	235	PHE	CA-CB-CG	5.08	118.88	113.80
1	B	283	HIS	CA-CB-CG	5.05	118.85	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	255	ARG	Sidechain
1	B	255	ARG	Sidechain
1	C	16	ARG	Sidechain
1	C	275	ARG	Sidechain

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	2897	0	2946	20	0
1	B	2930	0	2969	25	0
1	C	2896	0	2940	16	0
1	D	2893	0	2935	27	0
2	A	16	0	11	1	0
3	A	19	0	0	0	0
3	B	38	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
5	A	16	0	24	0	0
5	B	12	0	18	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	25	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	25	0	15	2	0
7	D	25	0	15	2	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	246	0	0	2	1
9	B	257	0	0	2	0
9	C	195	0	0	1	0
9	D	159	0	0	3	0
All	All	12658	0	11888	91	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (91) 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:159:CYS:SG	1:A:185:LYS:NZ	2.35	0.99
1:B:159:CYS:SG	1:B:185:LYS:NZ	2.36	0.97
1:D:253:ARG:HH11	1:D:253:ARG:HG2	1.37	0.86
1:D:159:CYS:SG	1:D:185:LYS:NZ	2.53	0.81
7:D:401:PDG:H4A1	7:D:401:PDG:HGA1	1.66	0.78
1:A:278:LYS:HE3	9:A:518:HOH:O	1.84	0.76
1:C:159:CYS:SG	1:C:185:LYS:NZ	2.64	0.70
1:A:23:SER:OG	1:A:24:GLY:N	2.22	0.70
1:C:263:ASP:HB2	9:C:584:HOH:O	1.92	0.69
1:C:266:ALA:N	1:C:267:PRO:HD2	2.11	0.65
1:A:3:LYS:HD3	1:A:311:GLU:OE1	1.96	0.65
1:A:334[A]:ASN:OD1	9:A:502:HOH:O	2.13	0.65
1:C:226:ILE:HG22	1:D:89:MET:SD	2.42	0.59
1:D:251:ILE:O	1:D:255:ARG:HG3	2.01	0.59
1:B:255:ARG:NH2	1:B:280:VAL:O	2.36	0.59
1:B:278:LYS:HE2	9:B:722:HOH:O	2.04	0.58
1:A:127:ILE:HG22	1:A:129:PRO:HD3	1.87	0.57
1:D:253:ARG:HH11	1:D:253:ARG:CG	2.16	0.56
1:A:47:HIS:HB3	1:A:203:TYR:CD1	2.41	0.55
1:D:366:LEU:HD22	1:D:370:LEU:HG	1.88	0.55
1:A:355:ASN:HB2	4:A:403:CL:CL	2.45	0.54
1:B:164:LYS:HG3	1:B:169:MET:SD	2.47	0.54
1:B:1:MET:CE	1:B:310:ILE:C	2.81	0.53
1:D:266:ALA:HB3	1:D:267:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:401:PDG:HGA1	7:D:401:PDG:C4A	2.39	0.52
1:B:182:HIS:CE1	7:B:401:PDG:HGA1	2.45	0.51
1:B:248[A]:ASN:ND2	9:B:502:HOH:O	2.23	0.51
1:D:268:LEU:HD21	1:D:367:GLU:HG3	1.93	0.49
1:B:127:ILE:HG22	1:B:129:PRO:HD3	1.94	0.49
1:D:176:MET:HG2	1:D:197:THR:HB	1.94	0.49
1:C:31:GLU:HG2	1:C:238:ALA:HB2	1.94	0.49
1:D:182:HIS:CD2	1:D:183:PRO:HD2	2.49	0.48
1:B:27:VAL:O	1:B:28:HIS:C	2.57	0.48
1:D:327:HIS:ND1	1:D:329:SER:HB3	2.29	0.48
1:C:47:HIS:HB3	1:C:203:TYR:CD1	2.50	0.47
1:A:302:MET:HG2	1:A:312:SER:OG	2.14	0.47
1:D:47:HIS:HB3	1:D:203:TYR:CD1	2.49	0.46
1:B:23:SER:OG	1:B:24:GLY:N	2.48	0.46
1:A:157:ALA:O	1:A:158:ALA:C	2.58	0.46
7:C:401:PDG:H4A1	7:C:401:PDG:HGA2	1.97	0.46
1:B:1:MET:CE	1:B:311:GLU:N	2.79	0.45
1:B:266:ALA:N	1:B:267:PRO:HD2	2.32	0.45
1:B:187:LEU:C	1:B:187:LEU:HD23	2.42	0.45
1:A:183:PRO:HD3	1:A:190:GLY:O	2.17	0.45
7:C:401:PDG:O3	7:C:401:PDG:NA	2.50	0.45
1:B:297:ASN:HD21	1:B:299:THR:HB	1.82	0.44
1:A:27:VAL:O	1:A:28:HIS:C	2.61	0.44
1:A:255:ARG:HH11	1:A:255:ARG:HB3	1.83	0.44
1:B:350:LEU:C	1:B:350:LEU:HD23	2.43	0.44
1:B:74:ILE:HA	1:B:95:ILE:O	2.18	0.44
1:C:77:ASP:OD2	1:C:338:GLY:HA3	2.18	0.44
1:A:266:ALA:N	1:A:267:PRO:CD	2.81	0.43
1:B:268:LEU:HD21	1:B:367:GLU:HG3	2.01	0.43
1:B:133:PHE:HB3	1:B:287:THR:HB	1.99	0.43
1:A:327:HIS:ND1	1:A:329:SER:HB3	2.34	0.43
1:B:2:ILE:HG21	1:B:362:ILE:HD11	2.01	0.43
1:B:182:HIS:CD2	1:B:183:PRO:HD2	2.53	0.43
1:C:266:ALA:N	1:C:267:PRO:CD	2.82	0.42
1:C:255:ARG:NH2	1:C:280:VAL:O	2.52	0.42
1:D:31:GLU:OE2	1:D:241:ARG:NH2	2.46	0.42
1:A:31:GLU:HG2	1:A:238:ALA:HB2	2.00	0.42
1:D:255:ARG:NH2	1:D:280:VAL:O	2.52	0.42
1:C:355:ASN:HB2	4:C:402:CL:CL	2.57	0.42
1:D:53:ASN:HA	1:D:192:GLY:C	2.44	0.42
1:D:182:HIS:HE1	9:D:623:HOH:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:MET:HG3	1:D:224:ARG:CZ	2.49	0.42
1:B:102:GLU:OE1	1:B:278:LYS:NZ	2.38	0.42
1:A:255:ARG:HB3	1:A:255:ARG:NH1	2.35	0.41
1:C:328:ASP:OD2	1:C:332:LYS:HE2	2.20	0.41
1:D:2:ILE:HG21	1:D:362:ILE:HD11	2.01	0.41
1:D:27:VAL:O	1:D:28:HIS:C	2.62	0.41
1:D:182:HIS:CE1	9:D:623:HOH:O	2.74	0.41
1:B:314:LEU:C	1:B:314:LEU:HD12	2.45	0.41
1:C:164:LYS:HG2	1:C:169:MET:SD	2.61	0.41
1:D:202:LEU:HD12	1:D:202:LEU:HA	1.91	0.41
1:D:201:GLN:HG2	9:D:621:HOH:O	2.20	0.41
1:A:317:GLN:HA	1:A:342:TYR:CD2	2.56	0.41
1:B:260:ILE:N	1:B:260:ILE:HD13	2.34	0.41
1:A:237:ALA:O	1:A:241:ARG:HG3	2.21	0.41
2:A:401:PMP:O3	2:A:401:PMP:N4A	2.52	0.41
1:B:47:HIS:HB3	1:B:203:TYR:CD1	2.56	0.41
1:B:176:MET:HE3	1:B:202:LEU:HB3	2.03	0.41
1:C:256:GLU:O	1:C:259:THR:HB	2.20	0.41
1:D:31:GLU:HG2	1:D:238:ALA:HB2	2.02	0.41
1:A:366:LEU:HD22	1:A:370:LEU:HG	2.02	0.40
1:C:27:VAL:O	1:C:28:HIS:C	2.64	0.40
1:C:31:GLU:OE2	1:C:241:ARG:NH2	2.44	0.40
1:D:288:TYR:HB2	1:D:350:LEU:HD13	2.03	0.40
1:D:45:VAL:HB	1:D:172:THR:HG22	2.02	0.40
1:D:78:PHE:CZ	1:D:316:ALA:HB3	2.56	0.40
1:C:89:MET:SD	1:D:226:ILE:HG22	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:724:HOH:O	9:A:724:HOH:O[2_555]	1.25	0.95

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	374/380 (98%)	361 (96%)	12 (3%)	1 (0%)	36	42
1	B	377/380 (99%)	365 (97%)	11 (3%)	1 (0%)	36	42
1	C	373/380 (98%)	362 (97%)	11 (3%)	0	100	100
1	D	372/380 (98%)	360 (97%)	11 (3%)	1 (0%)	36	42
All	All	1496/1520 (98%)	1448 (97%)	45 (3%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	B	375	HIS
1	D	28	HIS

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	314/318 (99%)	301 (96%)	13 (4%)	27	37
1	B	317/318 (100%)	308 (97%)	9 (3%)	38	52
1	C	313/318 (98%)	304 (97%)	9 (3%)	37	51
1	D	312/318 (98%)	301 (96%)	11 (4%)	32	43
All	All	1256/1272 (99%)	1214 (97%)	42 (3%)	32	45

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	30	GLU
1	A	113	SER
1	A	168	VAL
1	A	184	ARG

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Mol	Chain	Res	Type
1	A	201	GLN
1	A	221	ILE
1	A	255	ARG
1	A	294	ASP
1	A	295	GLN
1	A	306	LYS
1	A	366	LEU
1	A	368	GLN
1	B	31	GLU
1	B	168	VAL
1	B	185	LYS
1	B	216	ARG
1	B	278	LYS
1	B	297	ASN
1	B	328	ASP
1	B	332	LYS
1	B	364	GLU
1	C	5	SER
1	C	168	VAL
1	C	215	MET
1	C	216	ARG
1	C	259	THR
1	C	328	ASP
1	C	332	LYS
1	C	334	ASN
1	C	354	LEU
1	D	3	LYS
1	D	168	VAL
1	D	202	LEU
1	D	215	MET
1	D	218	GLU
1	D	253	ARG
1	D	278	LYS
1	D	306	LYS
1	D	332	LYS
1	D	366	LEU
1	D	368	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN

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Mol	Chain	Res	Type
1	A	201	GLN
1	B	150	ASN
1	B	182	HIS
1	B	201	GLN
1	B	297	ASN
1	B	317	GLN
1	B	376	HIS
1	C	147	ASN
1	C	166	GLN
1	C	236	GLN
1	D	6	GLN
1	D	116	GLN
1	D	150	ASN
1	D	182	HIS
1	D	353	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 23 ligands modelled in this entry, 9 are monoatomic - leaving 14 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
5	EDO	A	404	-	3,3,3	0.13	0	2,2,2	0.24	0
5	EDO	B	405	-	3,3,3	0.37	0	2,2,2	0.43	0
5	EDO	B	406	-	3,3,3	0.39	0	2,2,2	0.37	0
7	PDG	C	401	-	25,25,25	0.82	1 (4%)	31,35,35	1.13	2 (6%)
7	PDG	D	401	-	25,25,25	0.96	1 (4%)	31,35,35	1.39	3 (9%)
3	A1ADI	B	402	-	19,19,19	2.21	2 (10%)	21,27,27	2.42	8 (38%)
5	EDO	B	407	-	3,3,3	0.16	0	2,2,2	0.27	0
3	A1ADI	A	402	-	19,19,19	2.19	2 (10%)	21,27,27	2.17	4 (19%)
5	EDO	A	405	-	3,3,3	0.34	0	2,2,2	0.72	0
5	EDO	A	406	-	3,3,3	0.19	0	2,2,2	0.29	0
7	PDG	B	401	-	25,25,25	0.85	0	31,35,35	1.00	1 (3%)
3	A1ADI	B	403	-	19,19,19	2.17	7 (36%)	21,27,27	2.42	8 (38%)
2	PMP	A	401	-	16,16,16	0.56	0	22,23,23	0.80	0
5	EDO	A	407	-	3,3,3	0.43	0	2,2,2	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	404	-	-	0/1/1/1	-
5	EDO	B	405	-	-	0/1/1/1	-
5	EDO	B	406	-	-	0/1/1/1	-
7	PDG	C	401	-	-	10/20/20/20	0/1/1/1
7	PDG	D	401	-	-	6/20/20/20	0/1/1/1
3	A1ADI	B	402	-	-	6/12/23/23	0/1/1/1
5	EDO	B	407	-	-	1/1/1/1	-
3	A1ADI	A	402	-	-	4/12/23/23	0/1/1/1
5	EDO	A	405	-	-	0/1/1/1	-
5	EDO	A	406	-	-	0/1/1/1	-
7	PDG	B	401	-	-	10/20/20/20	0/1/1/1
3	A1ADI	B	403	-	-	10/12/23/23	0/1/1/1
2	PMP	A	401	-	-	1/8/8/8	0/1/1/1
5	EDO	A	407	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1ADI	C1'-S1'	-6.13	1.69	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1ADI	C1-S1	-6.01	1.69	1.77
3	A	402	A1ADI	C1'-S1'	-5.61	1.69	1.77
3	A	402	A1ADI	C1-S1	-5.52	1.69	1.77
3	B	403	A1ADI	C1'-S1'	-5.21	1.70	1.77
3	B	403	A1ADI	C1-S1	-4.48	1.71	1.77
7	C	401	PDG	OE2-CDA	2.53	1.30	1.22
3	B	403	A1ADI	C4'-N1'	2.41	1.52	1.46
3	B	403	A1ADI	C3-N1	2.25	1.52	1.46
7	D	401	PDG	CAA-NA	2.13	1.51	1.46
3	B	403	A1ADI	O3-S1	2.08	1.51	1.45
3	B	403	A1ADI	O1-S1	2.02	1.50	1.45
3	B	403	A1ADI	C2'-C1'	2.01	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	A1ADI	O3-S1-C1	7.68	118.34	106.73
3	B	402	A1ADI	O2'-S1'-C1'	6.45	116.47	106.73
3	A	402	A1ADI	O2'-S1'-C1'	5.97	115.75	106.73
3	B	402	A1ADI	O1-S1-C1	4.72	113.86	106.73
3	B	402	A1ADI	O1'-S1'-C1'	-3.97	100.72	106.73
7	D	401	PDG	C4A-NA-CAA	3.91	121.18	113.84
3	A	402	A1ADI	O3-S1-C1	3.91	112.63	106.73
3	A	402	A1ADI	O1-S1-C1	3.83	112.52	106.73
3	B	403	A1ADI	O2'-S1'-C1'	3.56	112.11	106.73
7	C	401	PDG	CBA-CGA-CDA	3.52	121.88	112.49
7	D	401	PDG	CBA-CGA-CDA	3.36	121.44	112.49
7	D	401	PDG	C4A-C4-C3	3.20	124.23	119.98
3	A	402	A1ADI	O2'-S1'-O1'	-3.19	103.44	113.82
3	B	403	A1ADI	O1'-S1'-C1'	3.17	111.51	106.73
3	B	402	A1ADI	O3'-S1'-C1'	2.94	111.75	106.00
3	B	403	A1ADI	O3-S1-O1	-2.63	105.28	113.82
3	B	402	A1ADI	C19-C3'-N1'	-2.62	110.40	115.35
3	B	403	A1ADI	O2'-S1'-O1'	-2.54	105.55	113.82
7	B	401	PDG	C4A-NA-CAA	2.51	118.56	113.84
3	B	402	A1ADI	C3-C4'-N1'	-2.50	108.83	116.77
3	B	403	A1ADI	C1-C2-N1	2.41	121.48	112.36
3	B	403	A1ADI	C1'-C2'-N1'	2.35	121.26	112.36
7	C	401	PDG	OE2-CDA-CGA	-2.31	115.78	123.09
3	B	402	A1ADI	O3'-S1'-O2'	-2.11	106.13	111.40
3	B	402	A1ADI	O3-S1-C1	2.00	109.75	106.73
3	B	403	A1ADI	C4'-C3-N1	-2.00	110.40	116.77

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	A1ADI	C1-C2-N1-C4
3	A	402	A1ADI	S1-C1-C2-N1
3	B	402	A1ADI	C1'-C2'-N1'-C3'
3	B	403	A1ADI	C2'-C1'-S1'-O1'
3	B	403	A1ADI	S1'-C1'-C2'-N1'
3	B	403	A1ADI	C1'-C2'-N1'-C4'
3	B	403	A1ADI	C1'-C2'-N1'-C3'
3	B	403	A1ADI	C2-C1-S1-O1
3	B	403	A1ADI	C2-C1-S1-O3
7	B	401	PDG	CBA-CAA-NA-C4A
7	C	401	PDG	C5-C4-C4A-NA
7	D	401	PDG	C5-C4-C4A-NA
7	D	401	PDG	CA-CAA-NA-C4A
7	B	401	PDG	NA-CAA-CBA-CGA
7	C	401	PDG	NA-CAA-CBA-CGA
2	A	401	PMP	C3-C4-C4A-N4A
7	C	401	PDG	C4-C4A-NA-CAA
7	C	401	PDG	CA-CAA-CBA-CGA
3	B	402	A1ADI	C2'-C1'-S1'-O3'
7	D	401	PDG	C4-C4A-NA-CAA
7	B	401	PDG	OXT-CA-CAA-NA
7	B	401	PDG	OA-CA-CAA-NA
3	B	403	A1ADI	C2'-C1'-S1'-O3'
3	B	403	A1ADI	C2-C1-S1-O2
7	B	401	PDG	CA-CAA-CBA-CGA
7	B	401	PDG	CAA-CBA-CGA-CDA
3	B	402	A1ADI	C2'-C1'-S1'-O1'
3	B	402	A1ADI	C2'-C1'-S1'-O2'
3	B	403	A1ADI	C2'-C1'-S1'-O2'
3	B	403	A1ADI	S1-C1-C2-N1
7	C	401	PDG	C3-C4-C4A-NA
7	D	401	PDG	C3-C4-C4A-NA
7	C	401	PDG	CBA-CAA-NA-C4A
7	C	401	PDG	CA-CAA-NA-C4A
7	D	401	PDG	CAA-CBA-CGA-CDA
3	A	402	A1ADI	C1-C2-N1-C3
3	B	402	A1ADI	C1-C2-N1-C3
3	B	402	A1ADI	C1'-C2'-N1'-C4'
7	B	401	PDG	C5-C4-C4A-NA
7	C	401	PDG	OE2-CDA-CGA-CBA

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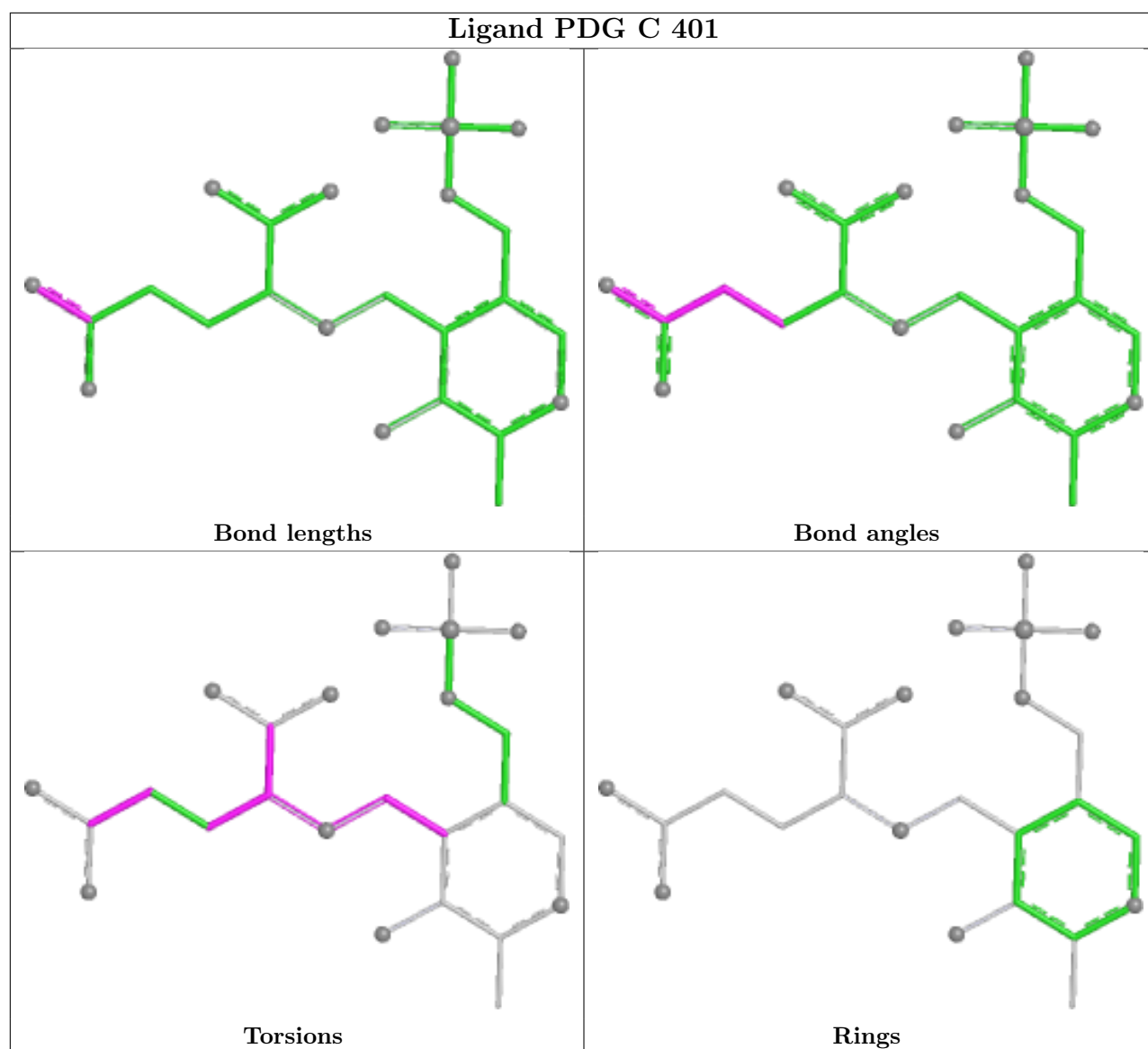
Mol	Chain	Res	Type	Atoms
7	B	401	PDG	OXT-CA-CAA-CBA
7	B	401	PDG	OA-CA-CAA-CBA
7	C	401	PDG	OE1-CDA-CGA-CBA
7	B	401	PDG	C3-C4-C4A-NA
7	D	401	PDG	CBA-CAA-NA-C4A
5	B	407	EDO	O1-C1-C2-O2
7	C	401	PDG	OA-CA-CAA-NA
3	A	402	A1ADI	C2-C1-S1-O2

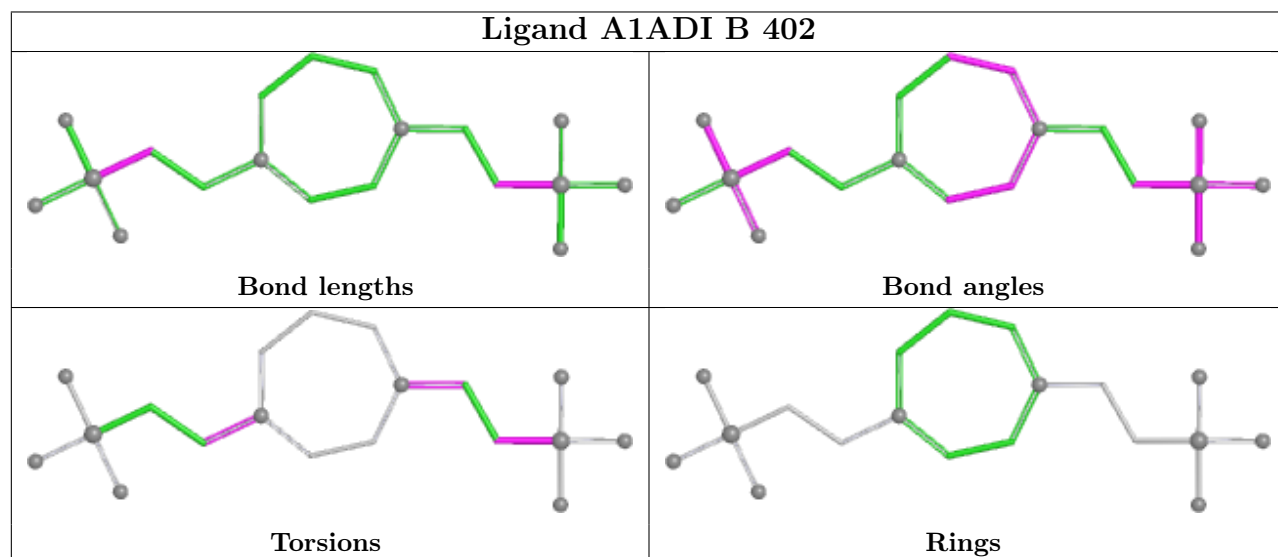
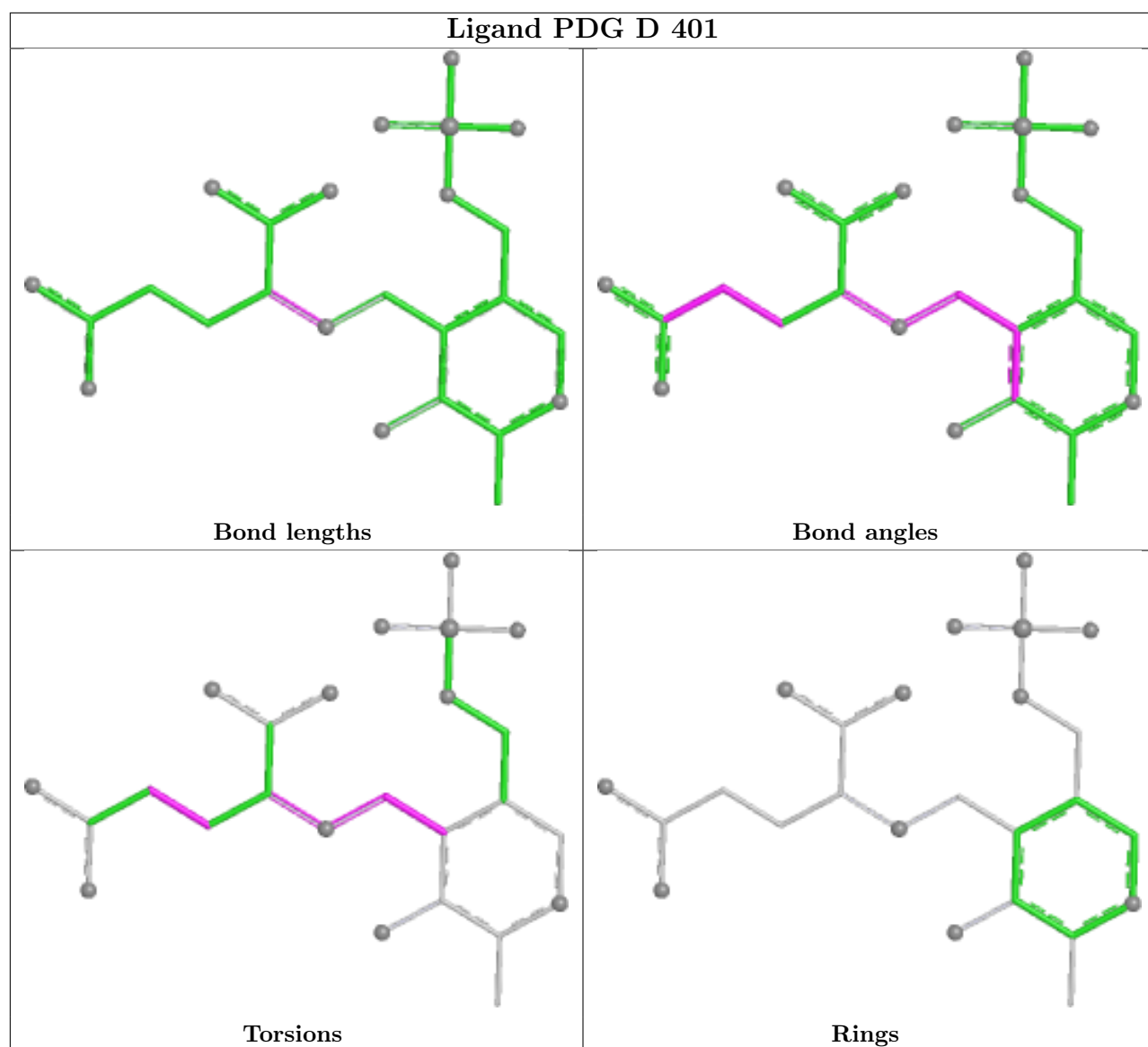
There are no ring outliers.

4 monomers are involved in 6 short contacts:

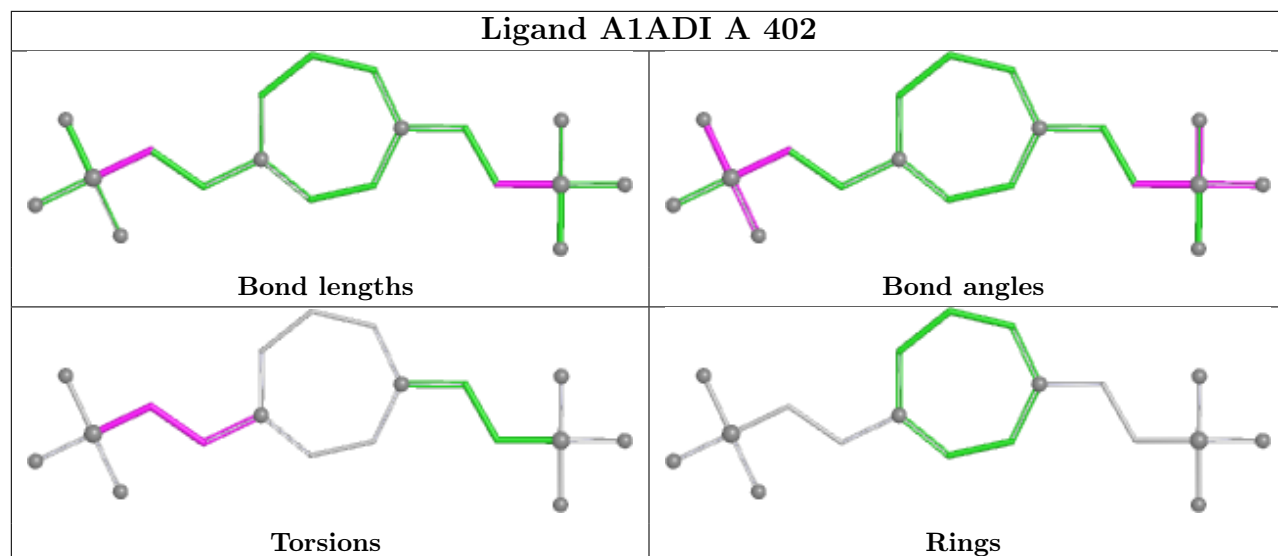
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	401	PDG	2	0
7	D	401	PDG	2	0
7	B	401	PDG	1	0
2	A	401	PMP	1	0

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.

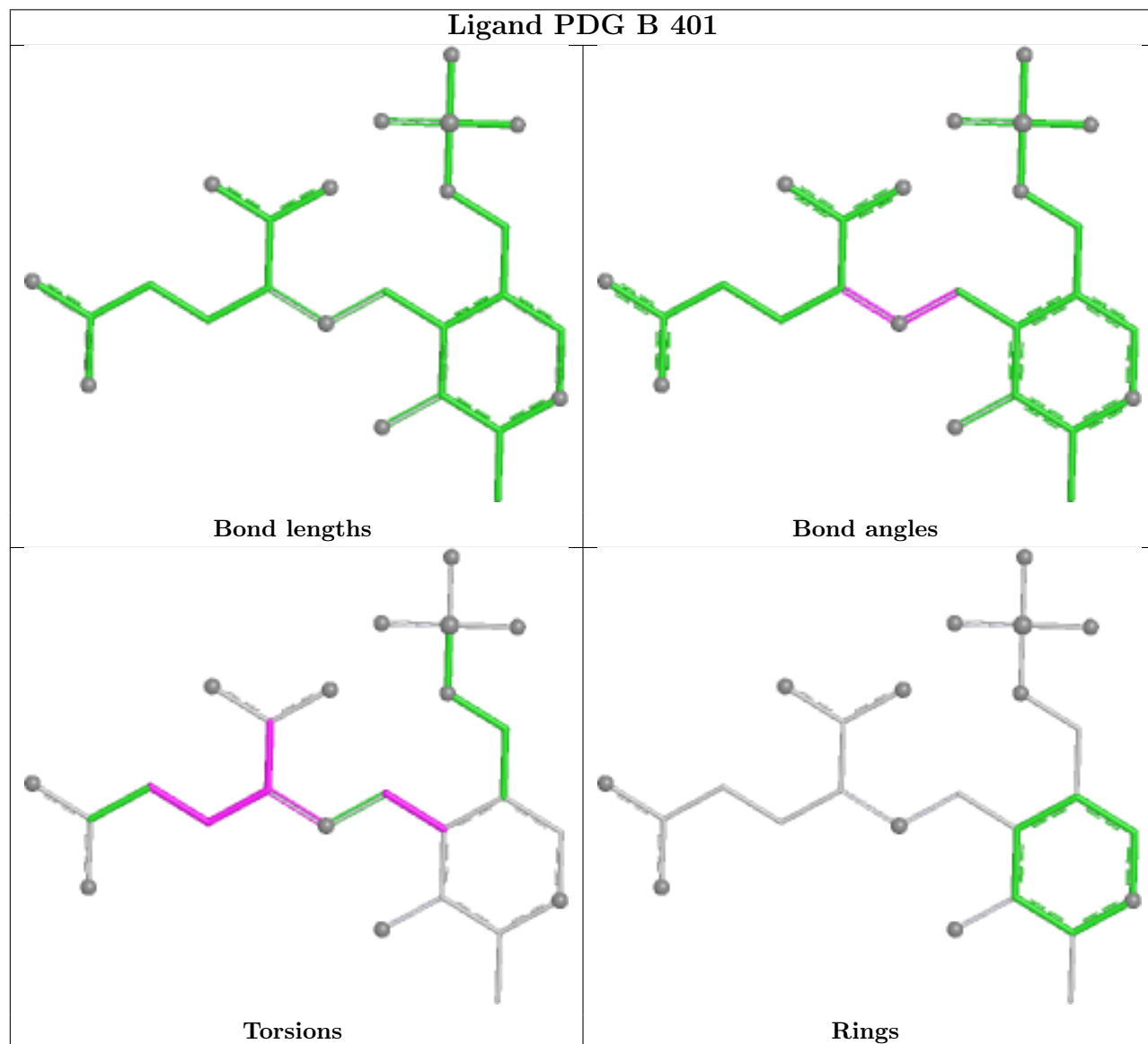


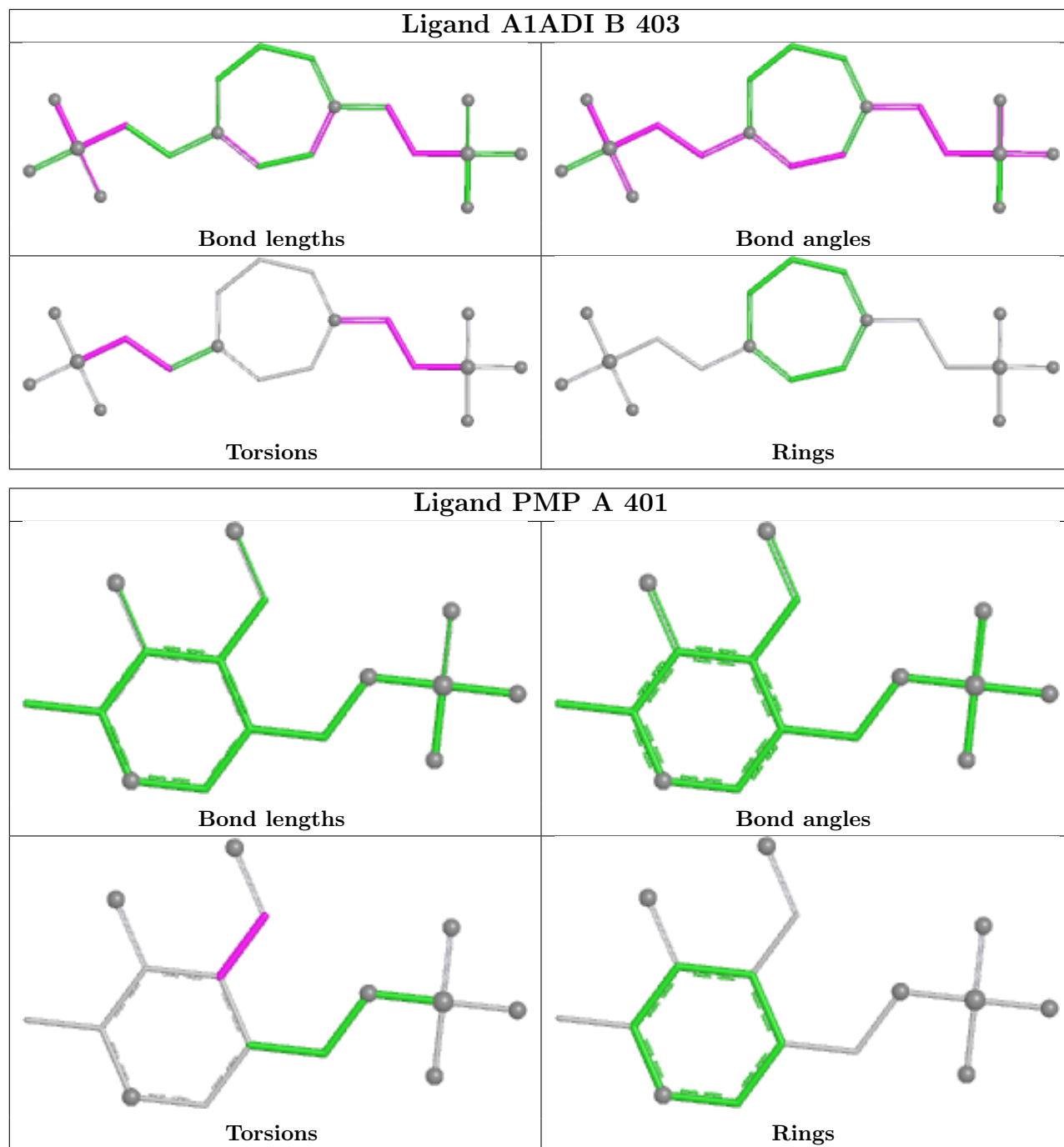


Ligand A1ADI A 402



Ligand PDG B 401





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	373/380 (98%)	-0.48	7 (1%) 66 63	6, 17, 41, 80	3 (0%)
1	B	376/380 (98%)	-0.44	8 (2%) 63 60	9, 18, 40, 95	3 (0%)
1	C	374/380 (98%)	-0.28	7 (1%) 66 63	11, 22, 48, 70	1 (0%)
1	D	374/380 (98%)	-0.21	6 (1%) 70 67	13, 24, 52, 86	0
All	All	1497/1520 (98%)	-0.35	28 (1%) 66 63	6, 21, 47, 95	7 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	376	HIS	7.3
1	D	219	PHE	5.8
1	B	219	PHE	4.7
1	A	219	PHE	4.2
1	B	24	GLY	4.2
1	C	216	ARG	4.1
1	A	216	ARG	3.9
1	A	24	GLY	3.8
1	D	24	GLY	3.8
1	B	375	HIS	3.7
1	B	25	GLN	3.7
1	A	217	GLY	3.7
1	C	24	GLY	3.4
1	B	216	ARG	3.1
1	A	373	LEU	3.1
1	A	218	GLU	2.8
1	A	25	GLN	2.7
1	C	267	PRO	2.6
1	B	215	MET	2.6
1	C	219	PHE	2.6
1	D	25	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	218	GLU	2.4
1	C	270	GLN	2.3
1	D	332	LYS	2.3
1	C	221	ILE	2.2
1	B	218	GLU	2.1
1	C	220	GLY	2.1
1	D	3	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

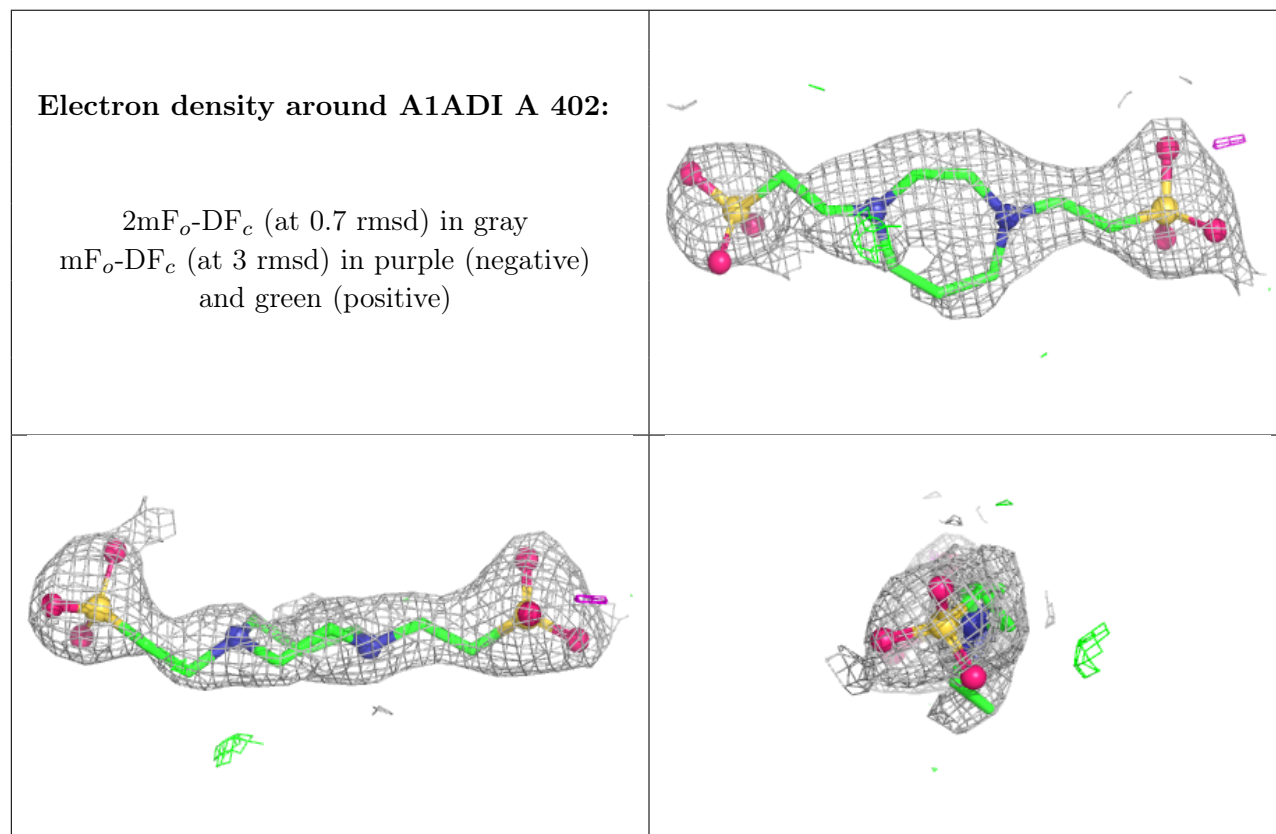
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	406	4/4	0.62	0.31	52,57,60,63	0
5	EDO	A	407	4/4	0.91	0.14	32,33,37,37	4
8	NA	B	409	1/1	0.91	0.15	34,34,34,34	0
3	A1ADI	A	402	19/19	0.92	0.16	41,60,93,104	0
5	EDO	A	404	4/4	0.93	0.13	43,44,45,45	0
6	MG	D	402	1/1	0.93	0.08	41,41,41,41	0
5	EDO	B	405	4/4	0.93	0.10	34,35,35,36	0
3	A1ADI	B	403	19/19	0.94	0.12	32,50,72,74	0
5	EDO	A	406	4/4	0.95	0.07	27,31,34,37	0
3	A1ADI	B	402	19/19	0.96	0.10	27,40,59,62	0
7	PDG	B	401	25/25	0.96	0.11	10,14,61,69	0
5	EDO	A	405	4/4	0.96	0.06	21,21,22,22	0
6	MG	B	408	1/1	0.97	0.05	43,43,43,43	0
4	CL	A	403	1/1	0.97	0.06	32,32,32,32	0
4	CL	C	402	1/1	0.97	0.07	22,22,22,22	0
7	PDG	C	401	25/25	0.97	0.10	11,14,60,65	0

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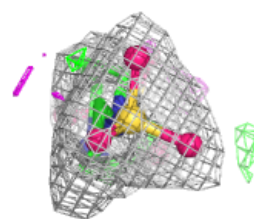
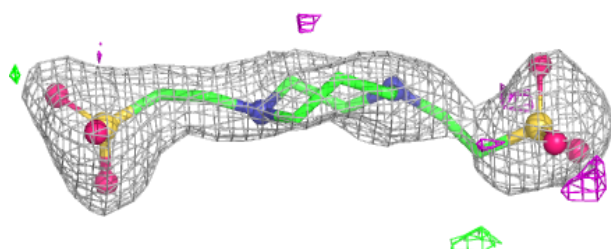
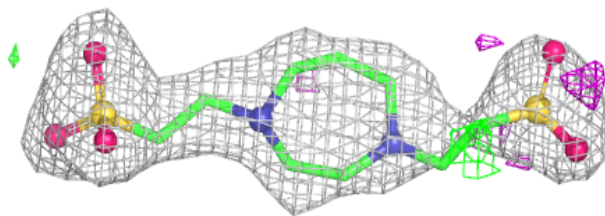
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PDG	D	401	25/25	0.97	0.10	14,20,68,72	0
6	MG	A	408	1/1	0.97	0.04	41,41,41,41	0
8	NA	D	403	1/1	0.97	0.08	33,33,33,33	0
4	CL	B	404	1/1	0.98	0.08	35,35,35,35	0
8	NA	C	403	1/1	0.98	0.07	27,27,27,27	0
5	EDO	B	407	4/4	0.98	0.04	20,21,22,23	0
2	PMP	A	401	16/16	0.99	0.04	8,11,16,21	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.

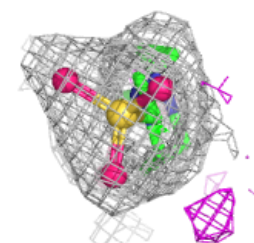
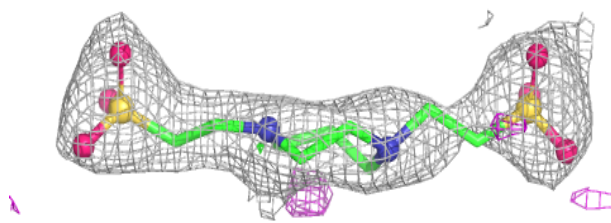
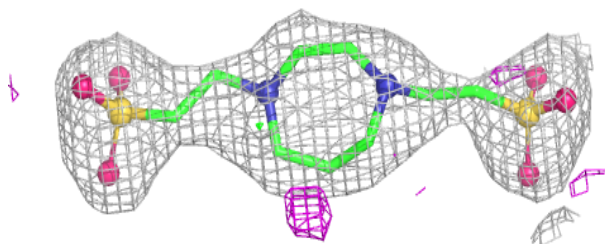


Electron density around A1ADI B 403:

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

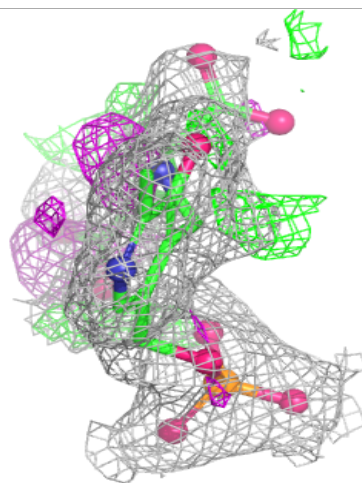
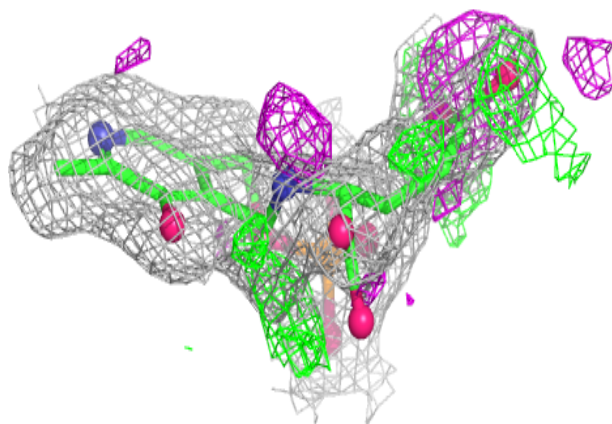
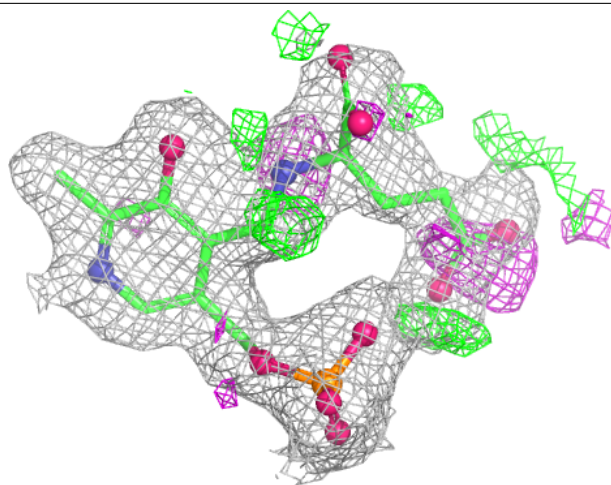
**Electron density around A1ADI B 402:**

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



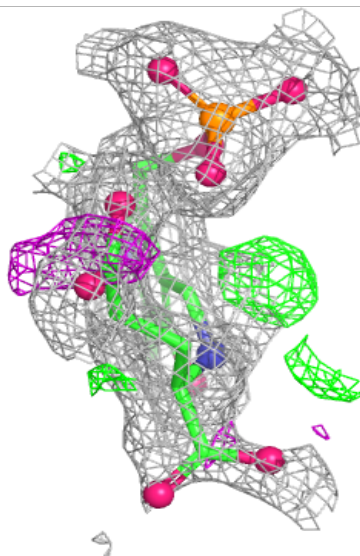
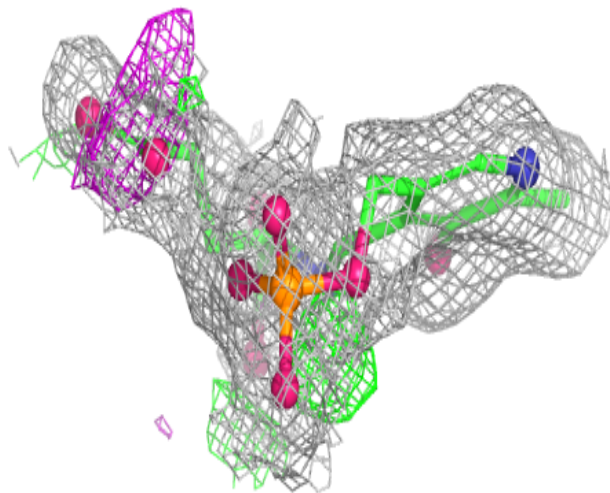
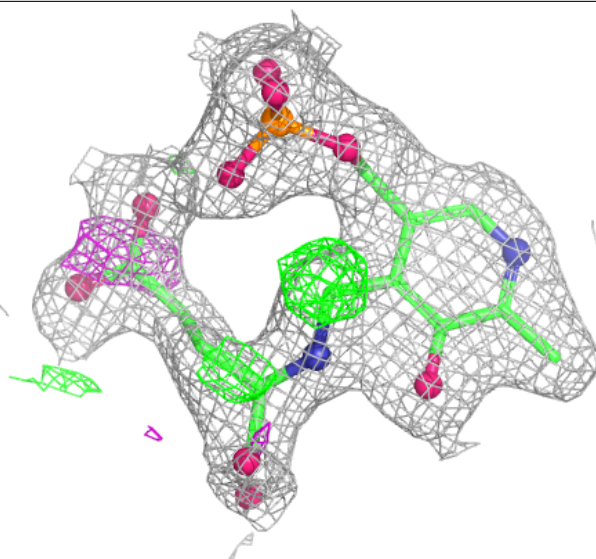
Electron density around PDG B 401:

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



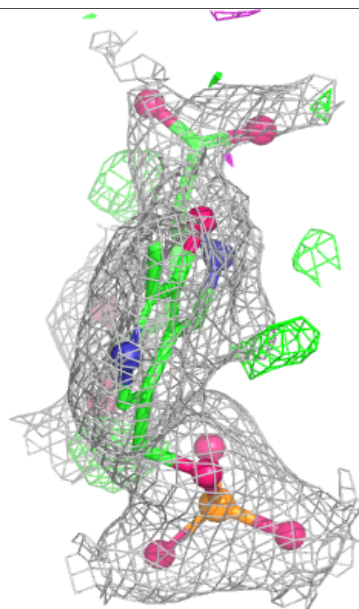
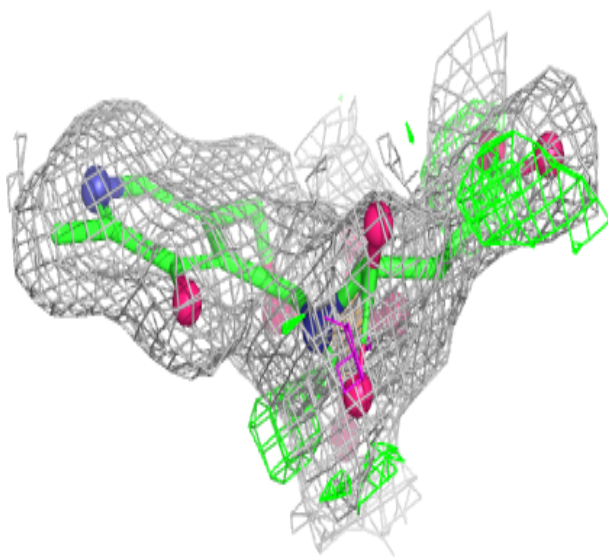
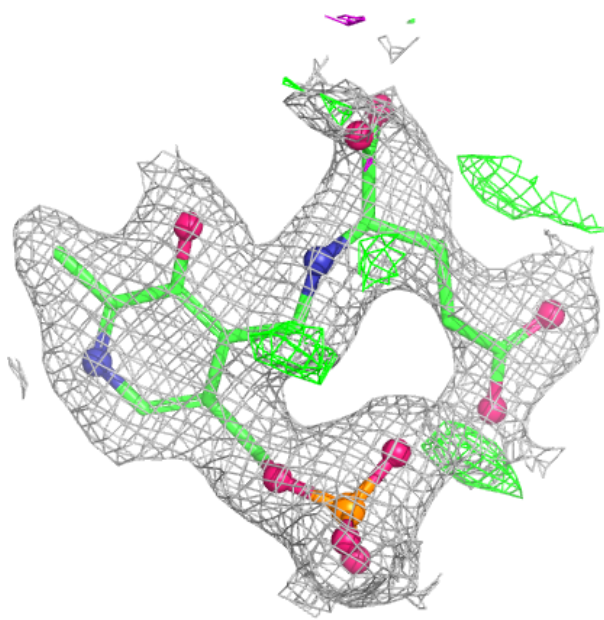
Electron density around PDG C 401:

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



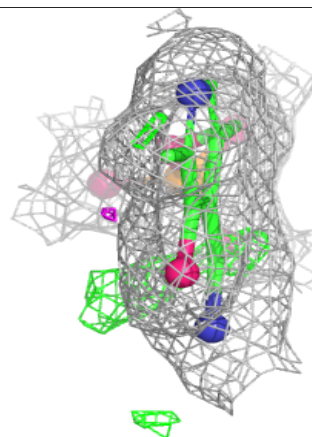
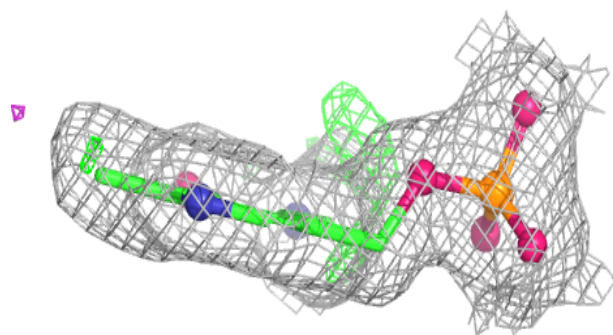
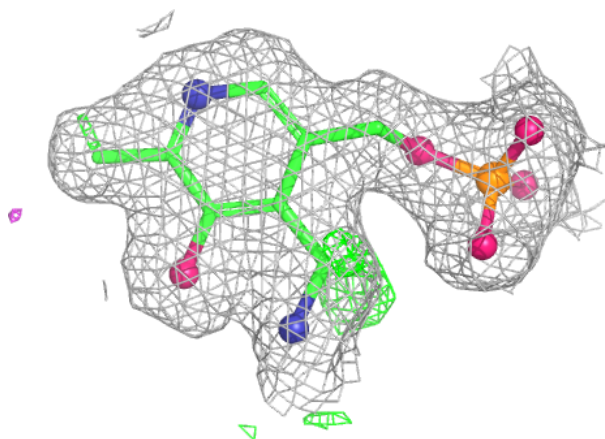
Electron density around PDG D 401:

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



Electron density around PMP 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 [i](#)

There are no such residues in this entry.