



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:14 PM UTC

PDB ID : 7ZEH / pdb_00007zeh
Title : Human cytosolic 5' nucleotidase IIIB in complex with 3,4-diF-Bn7Guanine
Authors : Kubacka, D.; Kozarski, M.; Baranowski, M.R.; Wojcik, R.; Jemielity, J.;
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Deposited on : 2022-03-31
Resolution : 1.50 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

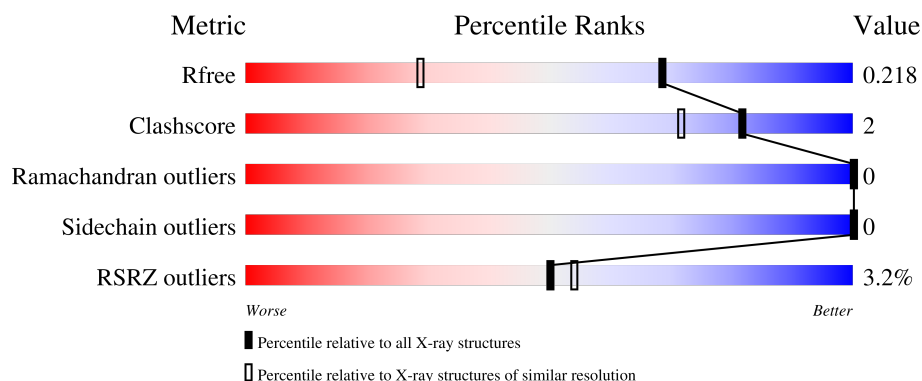
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	302	2% 86% 9%
1	B	302	3% 87% 9%
1	C	302	3% 85% 7% 8%
1	D	302	3% 85% 6% 8%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10071 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.

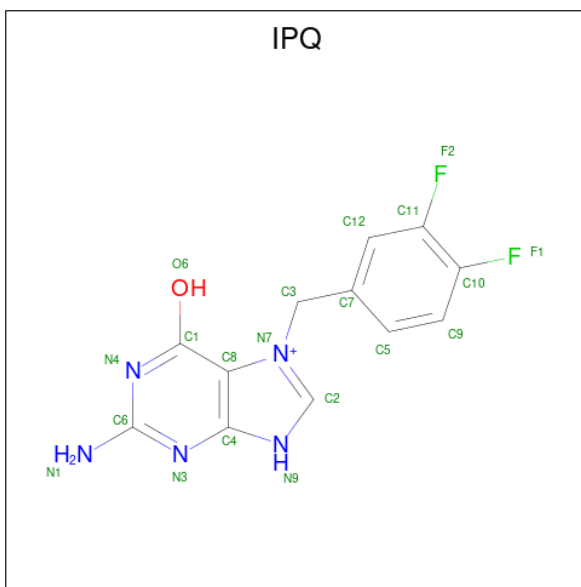
- Molecule 1 is a protein called 7-methylguanosine phosphate-specific 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	1	0
			2168	1379	376	400	13			
1	B	275	Total	C	N	O	S	0	1	0
			2152	1368	374	397	13			
1	C	278	Total	C	N	O	S	0	3	0
			2220	1410	391	407	12			
1	D	277	Total	C	N	O	S	0	4	0
			2201	1402	382	404	13			

There are 8 discrepancies between the modelled and reference sequences:

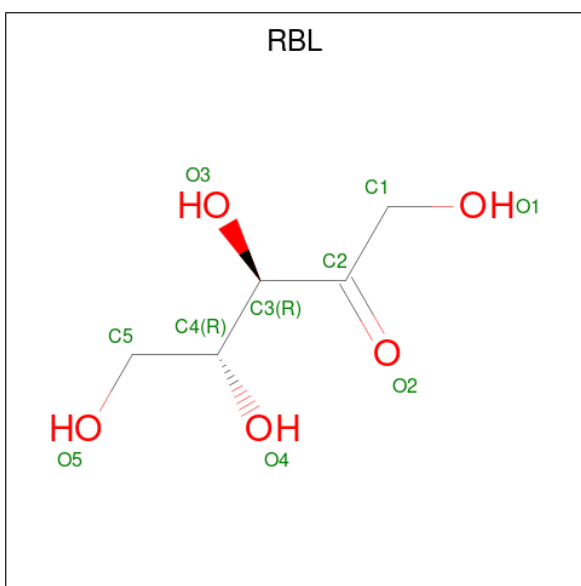
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP Q969T7
A	0	SER	-	expression tag	UNP Q969T7
B	-1	ARG	-	expression tag	UNP Q969T7
B	0	SER	-	expression tag	UNP Q969T7
C	-1	ARG	-	expression tag	UNP Q969T7
C	0	SER	-	expression tag	UNP Q969T7
D	-1	ARG	-	expression tag	UNP Q969T7
D	0	SER	-	expression tag	UNP Q969T7

- Molecule 2 is N7-(3,4-difluorobenzyl) guanine (CCD ID: IPQ) (formula: C₁₂H₁₀F₂N₅O) (labeled as "Ligand of Interest" by depositor).



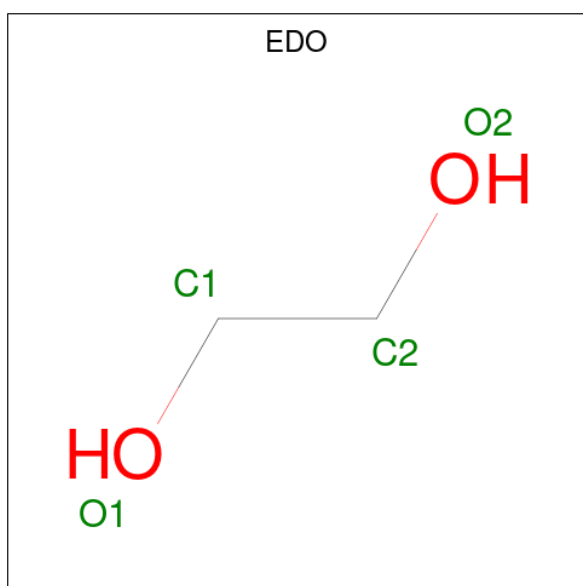
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			20	12	2	5	1		
2	B	1	Total	C	F	N	O	0	0
			20	12	2	5	1		
2	C	1	Total	C	F	N	O	0	0
			20	12	2	5	1		
2	D	1	Total	C	F	N	O	0	0
			20	12	2	5	1		

- Molecule 3 is D-ribulose (CCD ID: RBL) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 5 4	0	0
3	B	1	Total C O 9 5 4	0	0
3	C	1	Total C O 9 5 4	0	0
3	D	1	Total C O 9 5 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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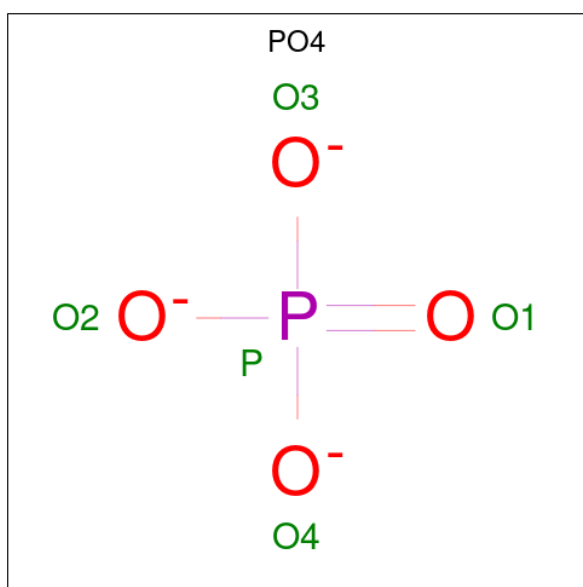
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

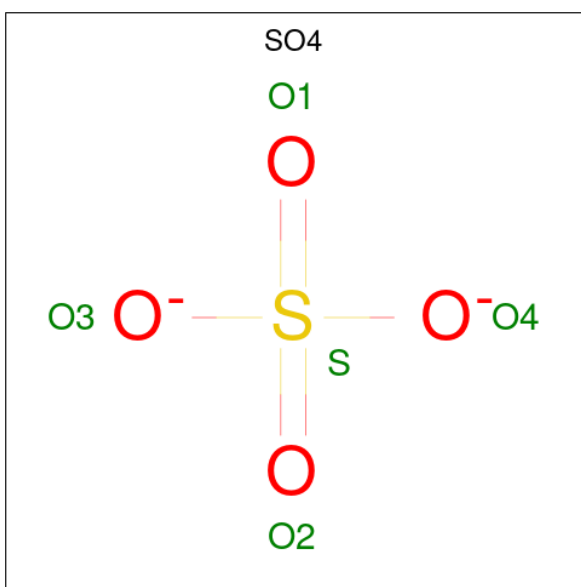
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

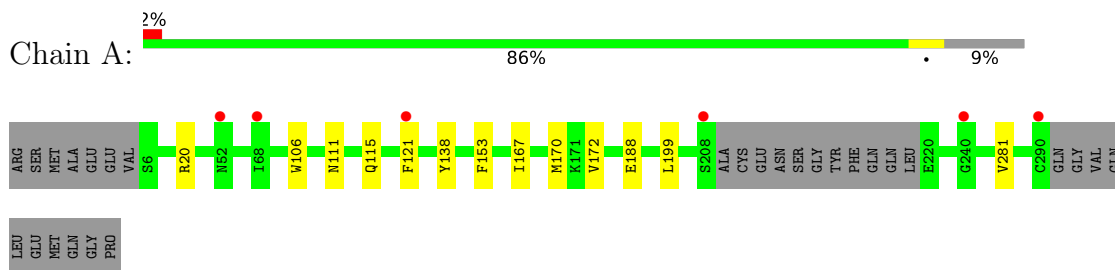
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	267	Total	O	0	0
			267	267		
8	B	260	Total	O	0	0
			260	260		
8	C	263	Total	O	0	0
			263	263		
8	D	264	Total	O	0	0
			264	264		

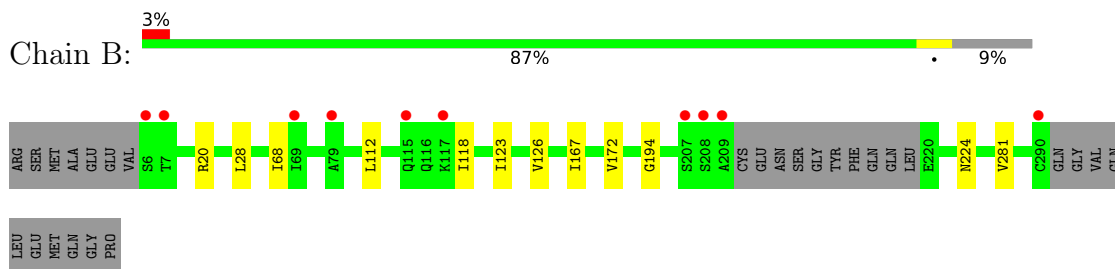
3 Residue-property plots [i](#)

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.

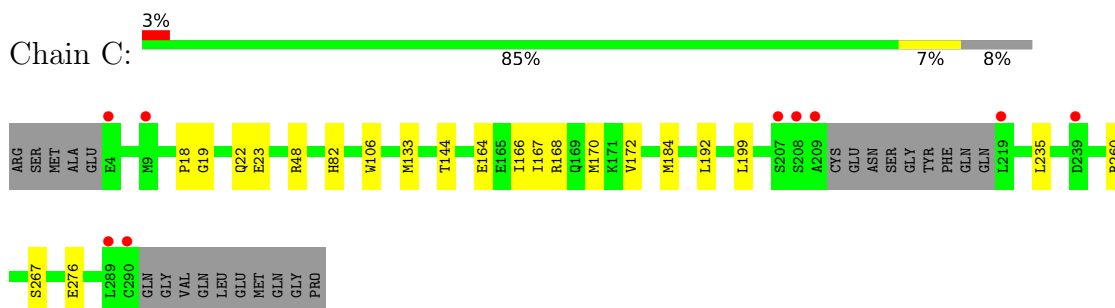
- Molecule 1: 7-methylguanosine phosphate-specific 5'-nucleotidase



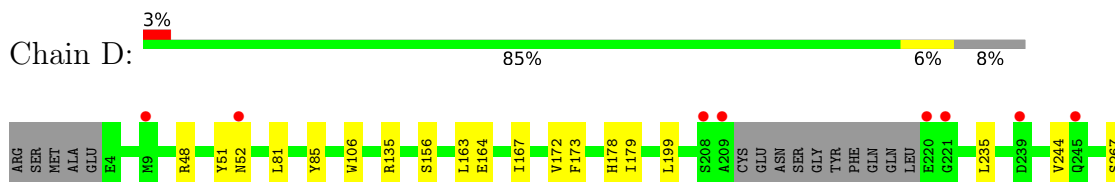
- Molecule 1: 7-methylguanosine phosphate-specific 5'-nucleotidase



- Molecule 1: 7-methylguanosine phosphate-specific 5'-nucleotidase



- Molecule 1: 7-methylguanosine phosphate-specific 5'-nucleotidase



L289	GLN
C290	GLY
	VAL
	GLN
	LEU
	MET
	GLN
	GLY
	PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.59Å 80.89Å 83.17Å 82.22° 72.46° 68.20°	Depositor
Resolution (Å)	75.08 – 1.50 75.08 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (75.08-1.50) 97.6 (75.08-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.188 , 0.220 0.185 , 0.218	Depositor DCC
R_{free} test set	10920 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10071	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% 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: SO4, PO4, IPQ, EDO, RBL, MG

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	0.58	0/2210	0.71	0/2990
1	B	0.58	0/2196	0.72	0/2974
1	C	0.58	0/2265	0.70	0/3062
1	D	0.58	0/2252	0.72	2/3047 (0.1%)
All	All	0.58	0/8923	0.71	2/12073 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	244	VAL	CA-C-N	-5.18	113.46	122.36
1	D	244	VAL	C-N-CA	-5.18	113.46	122.36

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	2168	0	2109	11	0
1	B	2152	0	2087	8	0
1	C	2220	0	2175	13	0
1	D	2201	0	2155	10	0
2	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
3	A	9	0	1	0	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
4	A	24	0	36	3	0
4	B	20	0	30	1	0
4	C	40	0	60	2	0
4	D	32	0	48	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	A	267	0	0	3	0
8	B	260	0	0	2	0
8	C	263	0	0	1	0
8	D	264	0	0	2	0
All	All	10071	0	8701	44	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 2.

All (44) 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:C:144:THR:HA	4:C:411:EDO:H21	1.82	0.59
1:B:20:ARG:HD2	8:B:568:HOH:O	2.03	0.58
1:B:281:VAL:HG23	8:B:671:HOH:O	2.04	0.57
1:A:281:VAL:HG23	8:A:667:HOH:O	2.04	0.56
1:D:48:ARG:HG3	1:D:135:ARG:HA	1.89	0.55
1:A:20:ARG:HD3	8:A:651:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:PRO:O	1:C:22:GLN:HG3	2.06	0.54
1:D:163[B]:LEU:HD22	1:D:179:ILE:HD13	1.93	0.51
4:D:410:EDO:H12	8:D:2669:HOH:O	2.11	0.51
1:A:170:MET:HE3	1:A:170:MET:HA	1.91	0.51
1:C:82:HIS:HA	4:C:407:EDO:H22	1.93	0.51
1:C:235:LEU:HD11	1:C:267:SER:HB3	1.94	0.50
1:A:167:ILE:HG23	1:A:172:VAL:HG23	1.93	0.50
1:D:81:LEU:HD12	1:D:85:TYR:HB2	1.94	0.50
1:C:106:TRP:HB3	1:C:199:LEU:HD11	1.93	0.49
1:D:106:TRP:HB3	1:D:199:LEU:HD11	1.94	0.48
1:B:167:ILE:HG23	1:B:172:VAL:HG23	1.95	0.48
1:C:133:MET:HE2	1:C:133:MET:HB3	1.75	0.48
1:C:164:GLU:HG2	1:C:168[B]:ARG:HE	1.78	0.48
1:D:178:HIS:HB3	4:D:404:EDO:H21	1.96	0.48
4:D:410:EDO:H21	8:D:2827:HOH:O	2.14	0.47
1:A:106:TRP:HB3	1:A:199:LEU:HD11	1.97	0.47
1:A:153:PHE:CD2	4:A:408:EDO:H22	2.51	0.46
1:C:166:ILE:O	1:C:170:MET:HG2	2.17	0.45
1:C:48:ARG:HG3	1:C:276:GLU:OE1	2.16	0.45
1:A:188:GLU:HG3	8:A:612:HOH:O	2.17	0.45
1:B:194:GLY:HA2	4:B:405:EDO:H12	1.98	0.44
1:D:167:ILE:HG23	1:D:172:VAL:HG23	1.98	0.44
1:A:111:ASN:O	1:A:115:GLN:HG2	2.18	0.44
1:D:51:TYR:CD2	1:D:52:ASN:HB2	2.53	0.43
1:A:138:TYR:OH	1:A:170:MET:HE2	2.18	0.43
1:D:156:SER:HB2	1:D:163[A]:LEU:HD21	1.98	0.43
1:B:68:ILE:HD12	1:B:118:ILE:HG12	2.01	0.43
1:C:184:MET:HB3	1:C:192:LEU:HD13	2.01	0.43
1:D:235:LEU:HD11	1:D:267:SER:HB3	2.00	0.43
1:D:164:GLU:HG3	1:D:173:PHE:CE2	2.54	0.43
1:C:19:GLY:O	1:C:23:GLU:HG3	2.19	0.42
1:C:167:ILE:HG23	1:C:172:VAL:HG23	2.01	0.42
1:B:28:LEU:CD2	1:B:224:ASN:HB3	2.49	0.41
1:B:123:ILE:O	1:B:126:VAL:HG22	2.20	0.41
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.87	0.40
1:C:260:ARG:NH1	8:C:512:HOH:O	2.53	0.40
1:A:121:PHE:CE1	4:A:407:EDO:H11	2.56	0.40
1:A:153:PHE:CG	4:A:408:EDO:H22	2.57	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	271/302 (90%)	267 (98%)	4 (2%)	0	100	100
1	B	272/302 (90%)	266 (98%)	6 (2%)	0	100	100
1	C	277/302 (92%)	272 (98%)	5 (2%)	0	100	100
1	D	277/302 (92%)	273 (99%)	4 (1%)	0	100	100
All	All	1097/1208 (91%)	1078 (98%)	19 (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	232/269 (86%)	232 (100%)	0	100	100
1	B	228/269 (85%)	228 (100%)	0	100	100
1	C	238/269 (88%)	238 (100%)	0	100	100
1	D	236/269 (88%)	236 (100%)	0	100	100
All	All	934/1076 (87%)	934 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	GLN
1	A	246	ASN
1	B	115	GLN
1	B	119	GLN
1	B	246	ASN
1	C	17	GLN
1	C	22	GLN
1	C	37	GLN
1	C	246	ASN
1	D	101	HIS
1	D	198	GLN
1	D	246	ASN

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 49 ligands modelled in this entry, 4 are monoatomic - leaving 45 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	EDO	C	409	-	3,3,3	0.40	0	2,2,2	0.62	0
4	EDO	B	406	-	3,3,3	0.59	0	2,2,2	0.14	0
4	EDO	D	405	-	3,3,3	0.38	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	D	413	-	4,4,4	0.56	0	6,6,6	0.61	0
4	EDO	C	405	-	3,3,3	0.34	0	2,2,2	0.44	0
4	EDO	C	404	-	3,3,3	0.41	0	2,2,2	0.63	0
4	EDO	A	403	-	3,3,3	0.42	0	2,2,2	0.40	0
4	EDO	C	412	-	3,3,3	0.41	0	2,2,2	0.53	0
4	EDO	B	404	-	3,3,3	0.56	0	2,2,2	0.11	0
3	RBL	C	402	1	8,8,9	1.32	1 (12%)	6,9,11	0.35	0
6	PO4	A	410	-	4,4,4	1.99	2 (50%)	6,6,6	1.23	1 (16%)
3	RBL	D	402	1	8,8,9	1.15	1 (12%)	6,9,11	0.82	0
4	EDO	D	408	-	3,3,3	0.42	0	2,2,2	0.46	0
2	IPQ	A	401	-	21,22,22	0.66	0	26,32,32	0.86	1 (3%)
4	EDO	C	406	-	3,3,3	0.51	0	2,2,2	0.35	0
4	EDO	D	409	-	3,3,3	0.44	0	2,2,2	0.37	0
6	PO4	D	412	-	4,4,4	1.29	1 (25%)	6,6,6	2.05	2 (33%)
4	EDO	B	403	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	C	410	-	3,3,3	0.51	0	2,2,2	0.20	0
7	SO4	C	415	-	4,4,4	0.58	0	6,6,6	0.61	0
4	EDO	C	408	-	3,3,3	0.44	0	2,2,2	0.30	0
2	IPQ	D	401	-	21,22,22	0.67	0	26,32,32	0.89	2 (7%)
4	EDO	A	406	-	3,3,3	0.42	0	2,2,2	0.39	0
6	PO4	C	414	-	4,4,4	1.77	1 (25%)	6,6,6	1.17	1 (16%)
4	EDO	C	403	-	3,3,3	0.40	0	2,2,2	0.54	0
4	EDO	D	404	-	3,3,3	0.41	0	2,2,2	0.41	0
7	SO4	B	410	-	4,4,4	0.59	0	6,6,6	0.86	0
6	PO4	B	409	-	4,4,4	1.86	2 (50%)	6,6,6	1.58	1 (16%)
4	EDO	A	405	-	3,3,3	0.42	0	2,2,2	0.47	0
4	EDO	A	404	-	3,3,3	0.67	0	2,2,2	0.09	0
4	EDO	C	411	-	3,3,3	0.48	0	2,2,2	0.35	0
4	EDO	D	407	-	3,3,3	0.39	0	2,2,2	0.41	0
7	SO4	A	411	-	4,4,4	0.35	0	6,6,6	0.70	0
2	IPQ	C	401	-	21,22,22	0.74	1 (4%)	26,32,32	0.76	1 (3%)
4	EDO	A	407	-	3,3,3	0.47	0	2,2,2	0.33	0
2	IPQ	B	401	-	21,22,22	0.62	0	26,32,32	0.82	2 (7%)
4	EDO	B	405	-	3,3,3	0.60	0	2,2,2	0.17	0
4	EDO	A	408	-	3,3,3	0.35	0	2,2,2	0.41	0
4	EDO	D	406	-	3,3,3	0.46	0	2,2,2	0.11	0
3	RBL	B	402	1	8,8,9	1.27	1 (12%)	6,9,11	0.69	0
4	EDO	C	407	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	D	403	-	3,3,3	0.40	0	2,2,2	0.41	0
4	EDO	B	407	-	3,3,3	0.43	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	410	-	3,3,3	0.62	0	2,2,2	0.53	0
3	RBL	A	402	1	8,8,9	0.82	0	6,9,11	0.86	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
4	EDO	C	409	-	-	0/1/1/1	-
4	EDO	B	406	-	-	0/1/1/1	-
4	EDO	D	405	-	-	0/1/1/1	-
4	EDO	C	405	-	-	0/1/1/1	-
4	EDO	C	404	-	-	0/1/1/1	-
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	C	412	-	-	1/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
3	RBL	C	402	1	-	3/8/8/12	-
3	RBL	D	402	1	-	3/8/8/12	-
4	EDO	D	408	-	-	1/1/1/1	-
2	IPQ	A	401	-	-	0/4/4/4	0/3/3/3
4	EDO	C	406	-	-	1/1/1/1	-
4	EDO	D	409	-	-	1/1/1/1	-
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	C	410	-	-	0/1/1/1	-
4	EDO	C	408	-	-	0/1/1/1	-
2	IPQ	D	401	-	-	0/4/4/4	0/3/3/3
4	EDO	A	406	-	-	1/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-
4	EDO	D	404	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	C	411	-	-	0/1/1/1	-
4	EDO	D	407	-	-	1/1/1/1	-
2	IPQ	C	401	-	-	0/4/4/4	0/3/3/3
4	EDO	A	407	-	-	0/1/1/1	-
2	IPQ	B	401	-	-	0/4/4/4	0/3/3/3
4	EDO	B	405	-	-	0/1/1/1	-
4	EDO	A	408	-	-	0/1/1/1	-
4	EDO	D	406	-	-	0/1/1/1	-
3	RBL	B	402	1	-	4/8/8/12	-
4	EDO	C	407	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	403	-	-	0/1/1/1	-
4	EDO	B	407	-	-	1/1/1/1	-
4	EDO	D	410	-	-	1/1/1/1	-
3	RBL	A	402	1	-	2/8/8/12	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	RBL	C3-C2	3.20	1.55	1.51
6	A	410	PO4	P-O2	-2.85	1.46	1.54
6	B	409	PO4	P-O3	-2.72	1.46	1.54
6	A	410	PO4	P-O3	-2.54	1.47	1.54
3	C	402	RBL	C3-C2	2.53	1.54	1.51
6	B	409	PO4	P-O2	-2.48	1.47	1.54
6	D	412	PO4	P-O2	-2.45	1.47	1.54
6	C	414	PO4	P-O1	-2.41	1.45	1.50
2	C	401	IPQ	C8-C1	-2.20	1.38	1.42
3	D	402	RBL	C1-C2	2.18	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	412	PO4	O3-P-O2	3.59	119.09	107.91
2	D	401	IPQ	C7-C3-N7	-2.64	108.67	112.15
2	A	401	IPQ	C4-N9-C2	2.54	109.63	106.88
2	B	401	IPQ	C7-C3-N7	-2.39	109.00	112.15
2	B	401	IPQ	C4-N9-C2	2.35	109.42	106.88
6	B	409	PO4	O4-P-O1	-2.30	102.82	110.95
6	C	414	PO4	O4-P-O1	2.29	119.04	110.95
6	D	412	PO4	O3-P-O1	-2.25	102.98	110.95
6	A	410	PO4	O4-P-O1	-2.21	103.15	110.95
2	D	401	IPQ	C4-N9-C2	2.15	109.21	106.88
2	C	401	IPQ	C4-N9-C2	2.10	109.15	106.88

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	RBL	O1-C1-C2-O2
3	C	402	RBL	O1-C1-C2-O2
3	D	402	RBL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	407	EDO	O1-C1-C2-O2
4	C	406	EDO	O1-C1-C2-O2
4	D	408	EDO	O1-C1-C2-O2
4	D	407	EDO	O1-C1-C2-O2
3	B	402	RBL	O1-C1-C2-C3
3	C	402	RBL	O1-C1-C2-C3
3	D	402	RBL	O1-C1-C2-C3
4	C	412	EDO	O1-C1-C2-O2
3	B	402	RBL	C1-C2-C3-C4
4	A	406	EDO	O1-C1-C2-O2
3	A	402	RBL	C1-C2-C3-C4
3	B	402	RBL	O2-C2-C3-C4
3	C	402	RBL	C1-C2-C3-C4
3	D	402	RBL	C1-C2-C3-C4
4	D	404	EDO	O1-C1-C2-O2
4	D	409	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2
3	A	402	RBL	O2-C2-C3-C4
4	D	410	EDO	O1-C1-C2-O2

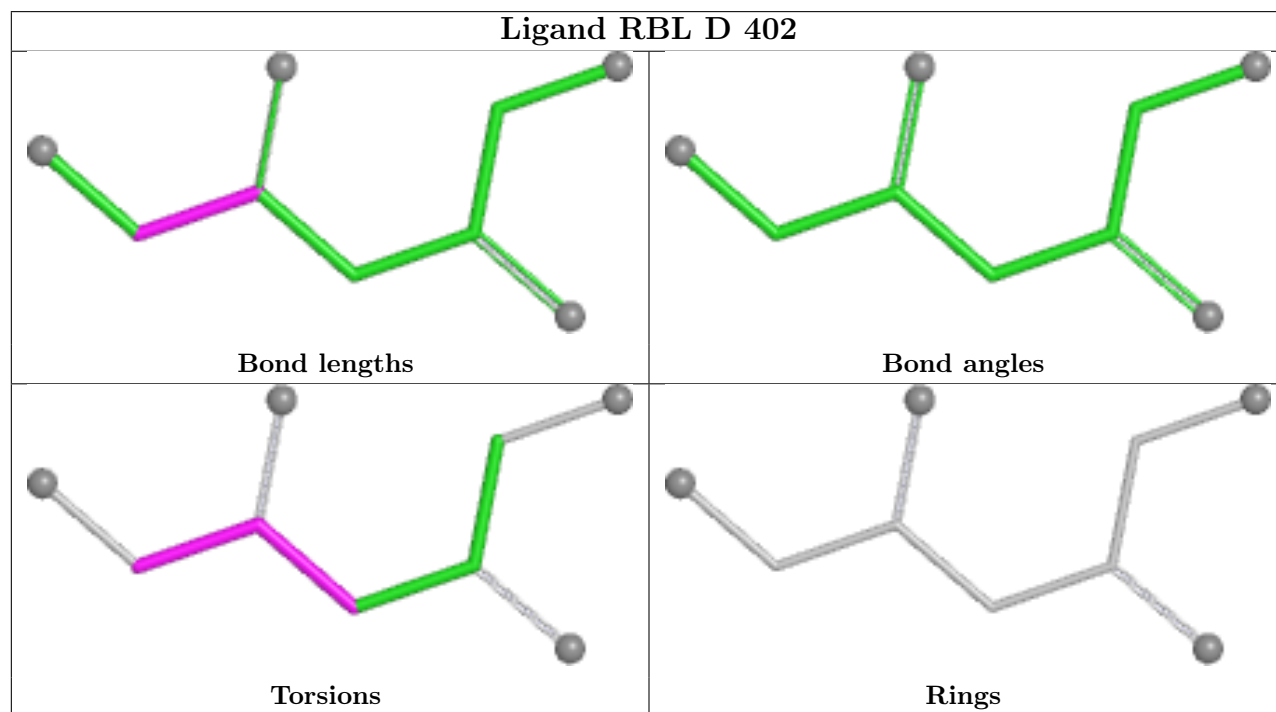
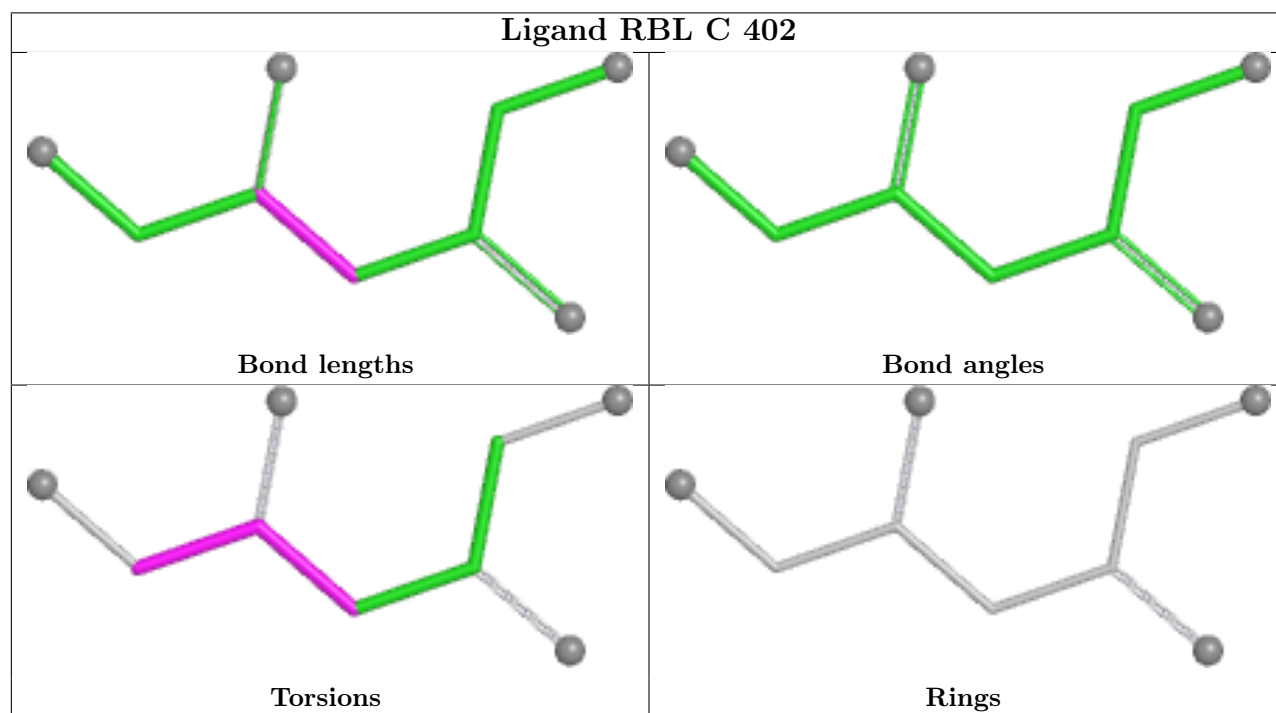
There are no ring outliers.

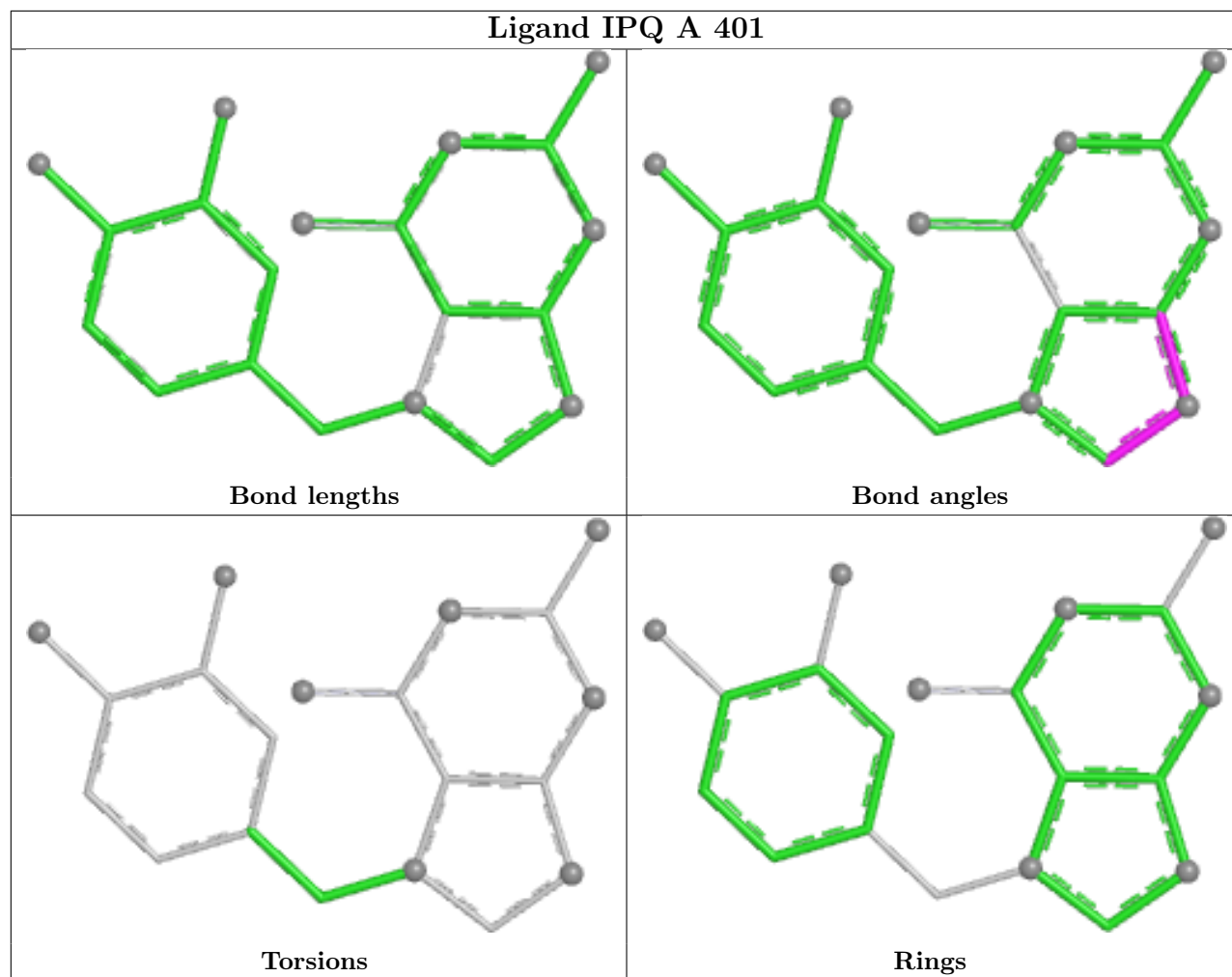
7 monomers are involved in 9 short contacts:

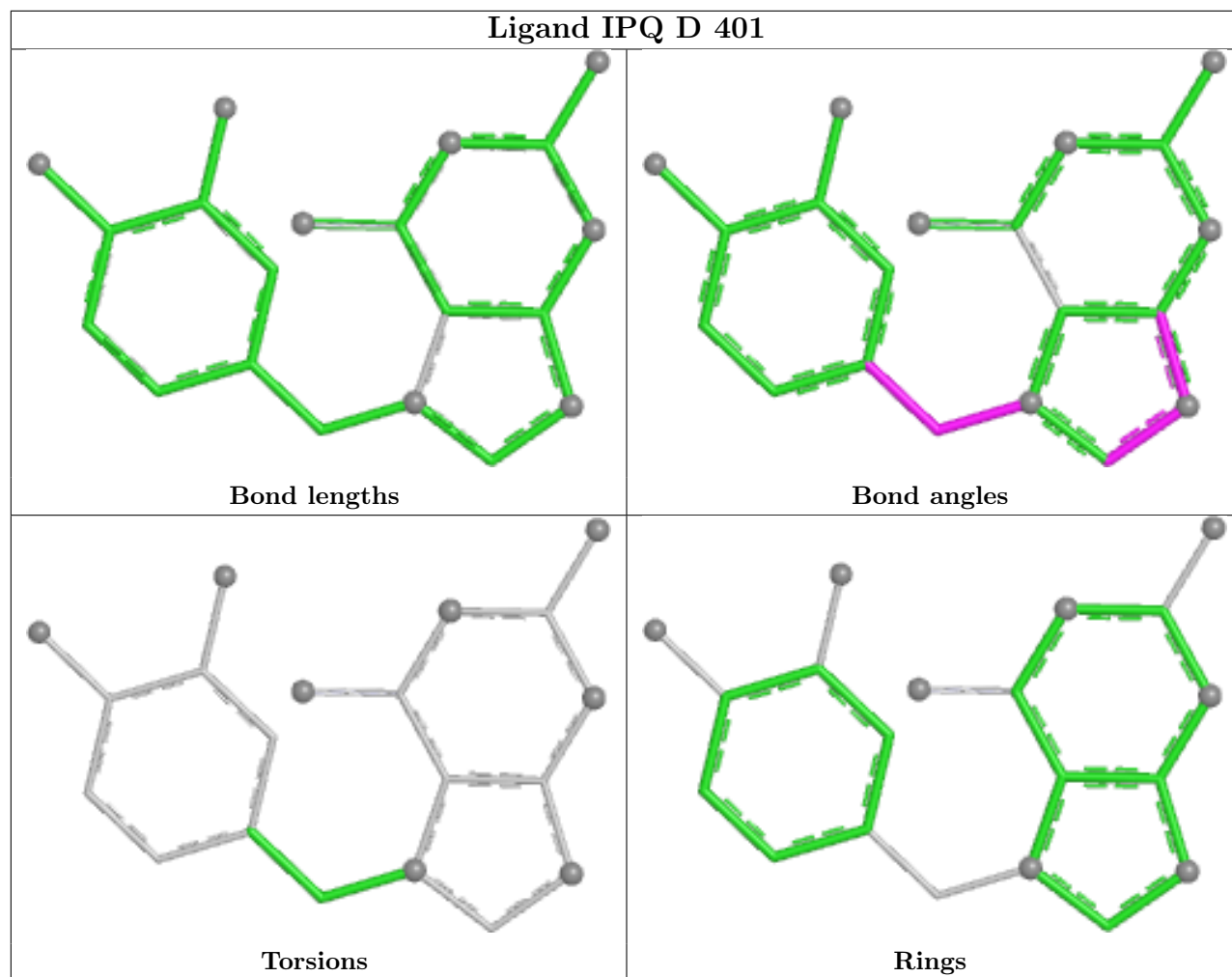
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	404	EDO	1	0
4	C	411	EDO	1	0
4	A	407	EDO	1	0
4	B	405	EDO	1	0
4	A	408	EDO	2	0
4	C	407	EDO	1	0
4	D	410	EDO	2	0

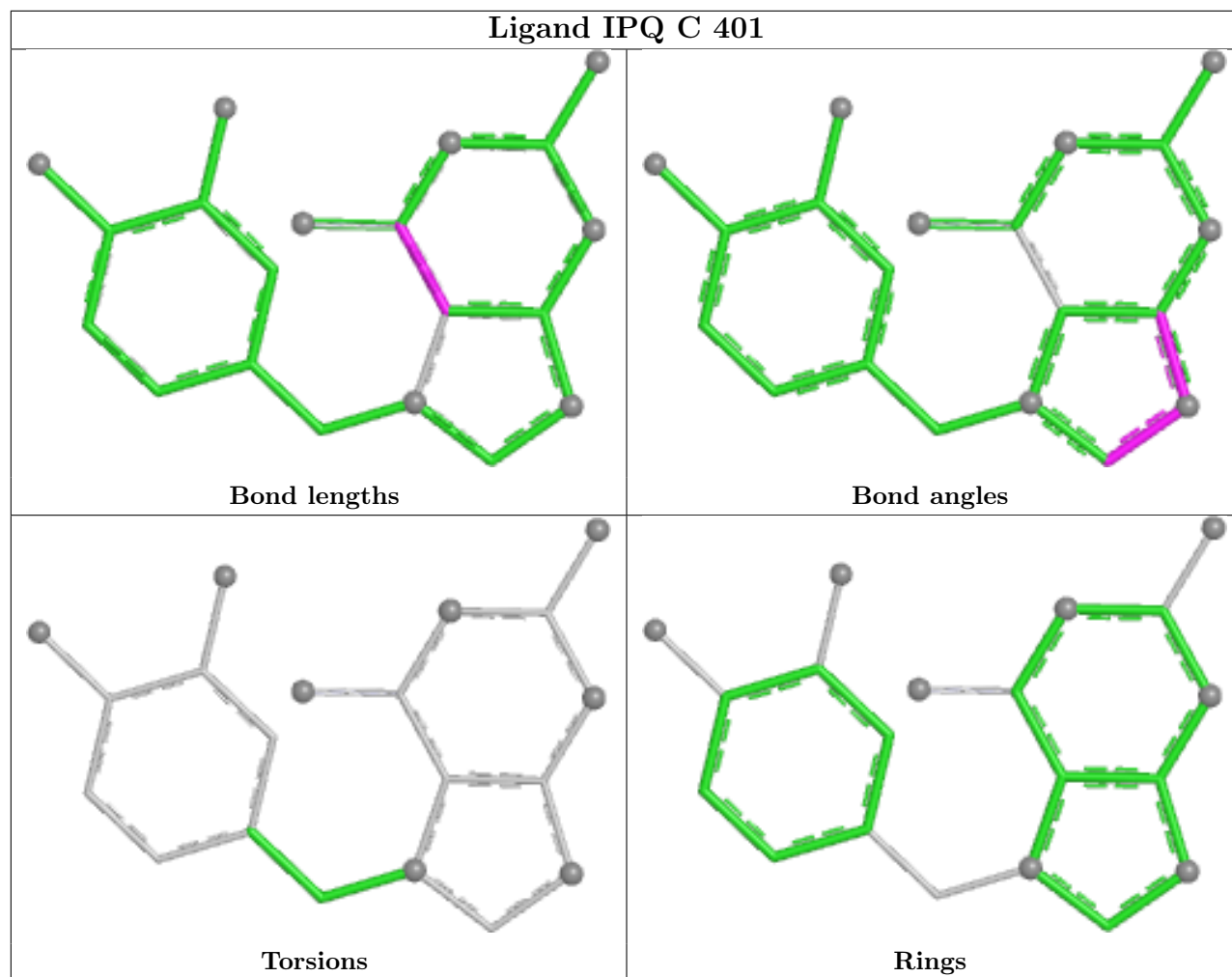
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

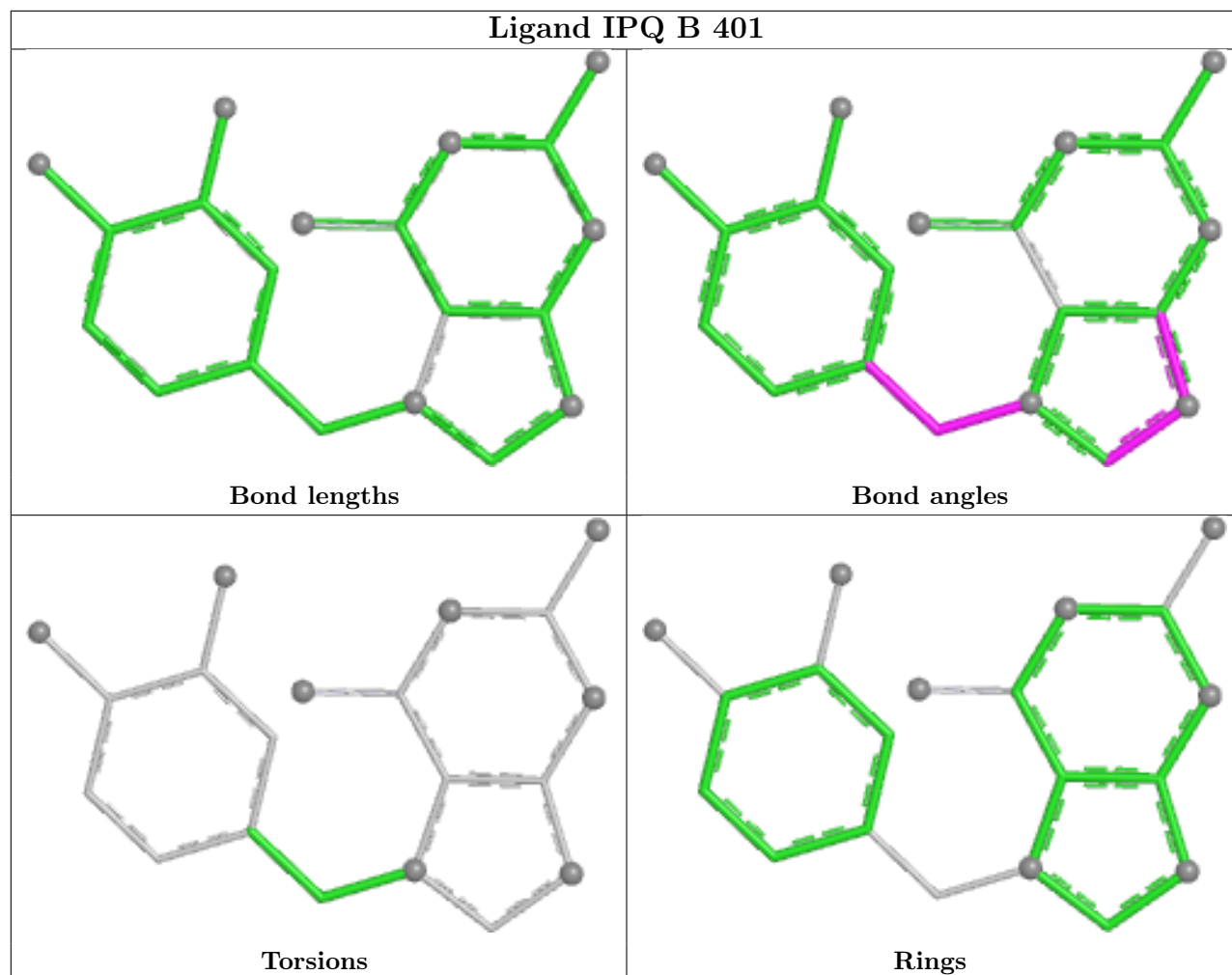




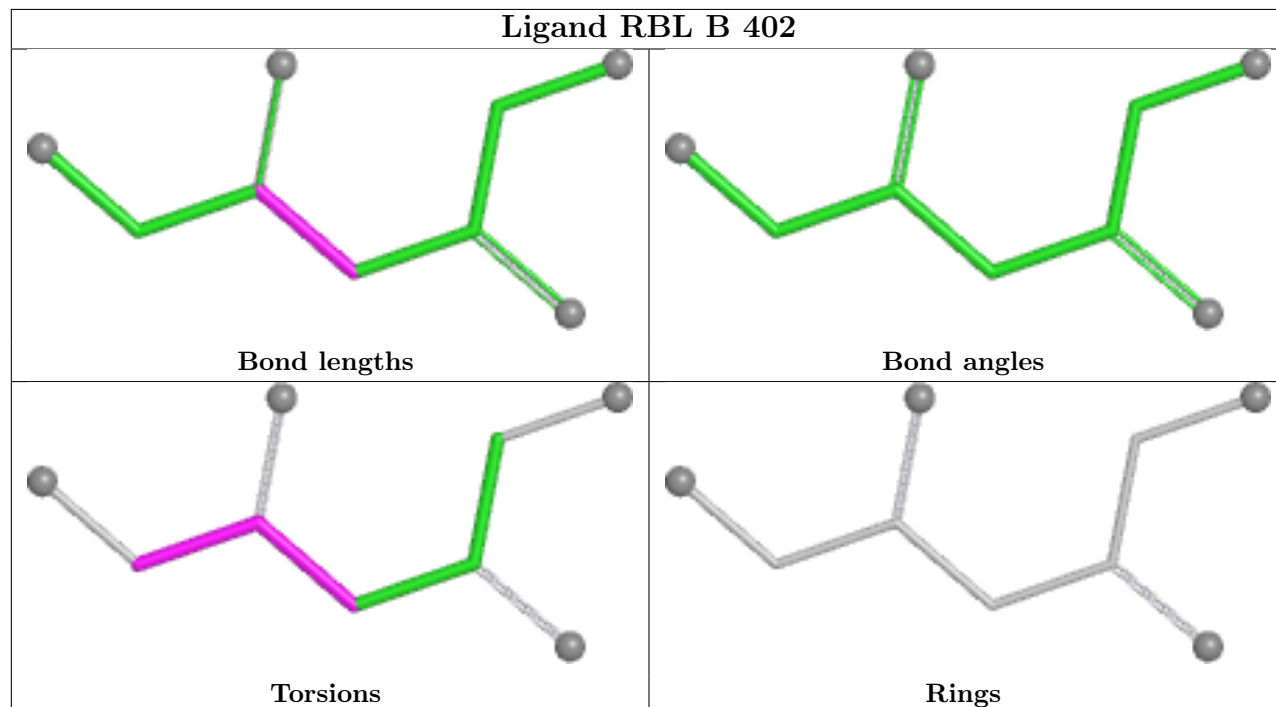


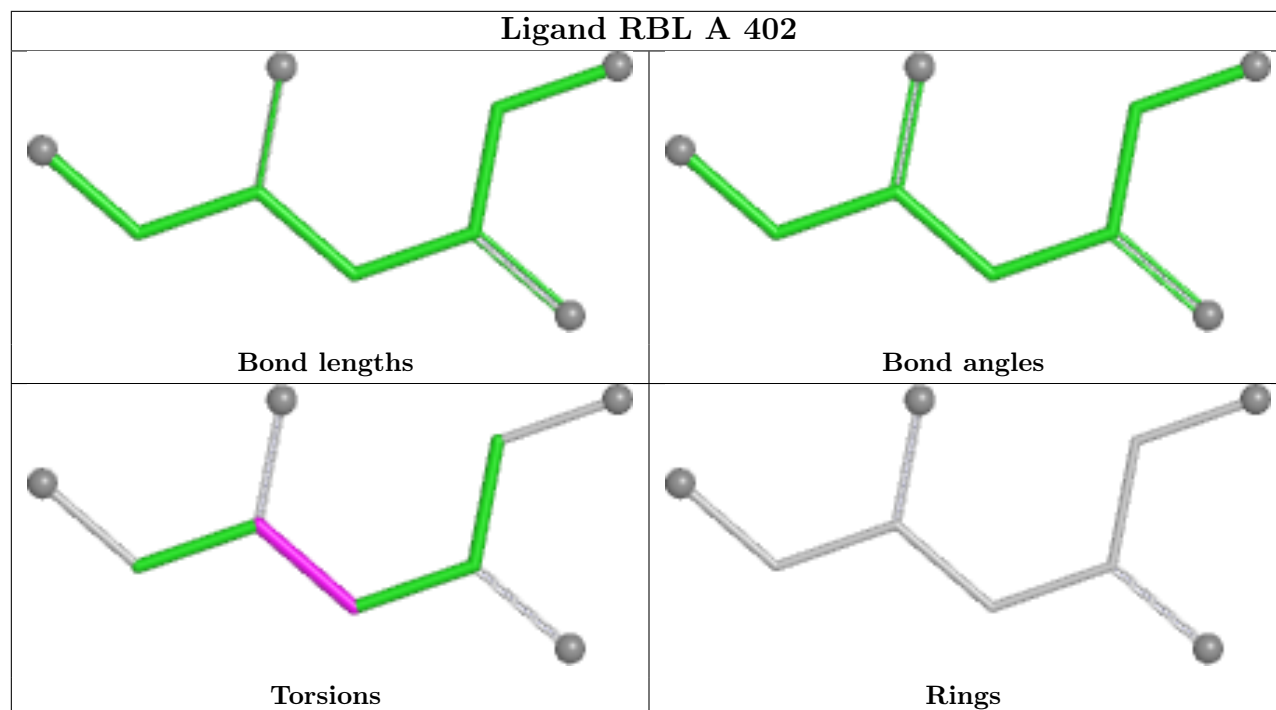


Ligand IPQ B 401



Ligand RBL B 402





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	274/302 (90%)	0.14	6 (2%) 62 66	10, 26, 41, 60	1 (0%)
1	B	275/302 (91%)	0.16	10 (3%) 46 50	12, 25, 43, 62	1 (0%)
1	C	278/302 (92%)	0.20	9 (3%) 50 54	9, 26, 43, 63	3 (1%)
1	D	277/302 (91%)	0.24	10 (3%) 46 50	10, 26, 41, 61	4 (1%)
All	All	1104/1208 (91%)	0.19	35 (3%) 50 54	9, 26, 42, 63	9 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	CYS	6.4
1	D	208	SER	5.2
1	B	209	ALA	4.6
1	C	209	ALA	4.6
1	D	290	CYS	4.5
1	B	290	CYS	4.4
1	D	209	ALA	4.2
1	C	208	SER	4.2
1	A	208	SER	4.1
1	C	219	LEU	3.9
1	B	208	SER	3.2
1	A	290	CYS	3.1
1	D	245	GLN	2.8
1	B	6	SER	2.7
1	C	289	LEU	2.6
1	C	9	MET	2.6
1	B	207	SER	2.6
1	A	121	PHE	2.5
1	B	117	LYS	2.5
1	A	240	GLY	2.4
1	B	115	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	9	MET	2.3
1	D	239	ASP	2.3
1	A	68	ILE	2.3
1	D	52	ASN	2.2
1	B	7	THR	2.2
1	C	4	GLU	2.2
1	B	69	ILE	2.1
1	A	52	ASN	2.1
1	D	220	GLU	2.1
1	D	221	GLY	2.1
1	C	207	SER	2.0
1	C	239	ASP	2.0
1	B	79	ALA	2.0
1	D	289	LEU	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($\text{\AA}^2$)	Q<0.9
3	RBL	D	402	9/10	0.69	0.17	34,41,57,61	0
3	RBL	C	402	9/10	0.73	0.17	38,45,57,63	0
4	EDO	C	412	4/4	0.76	0.18	45,49,52,60	0
4	EDO	D	406	4/4	0.79	0.17	51,51,59,62	0
4	EDO	D	404	4/4	0.80	0.16	50,54,58,60	0
4	EDO	C	408	4/4	0.80	0.19	53,55,58,63	0
4	EDO	D	409	4/4	0.81	0.16	46,50,51,56	0
4	EDO	A	407	4/4	0.83	0.15	46,52,55,57	0
4	EDO	C	406	4/4	0.83	0.17	47,50,50,54	0

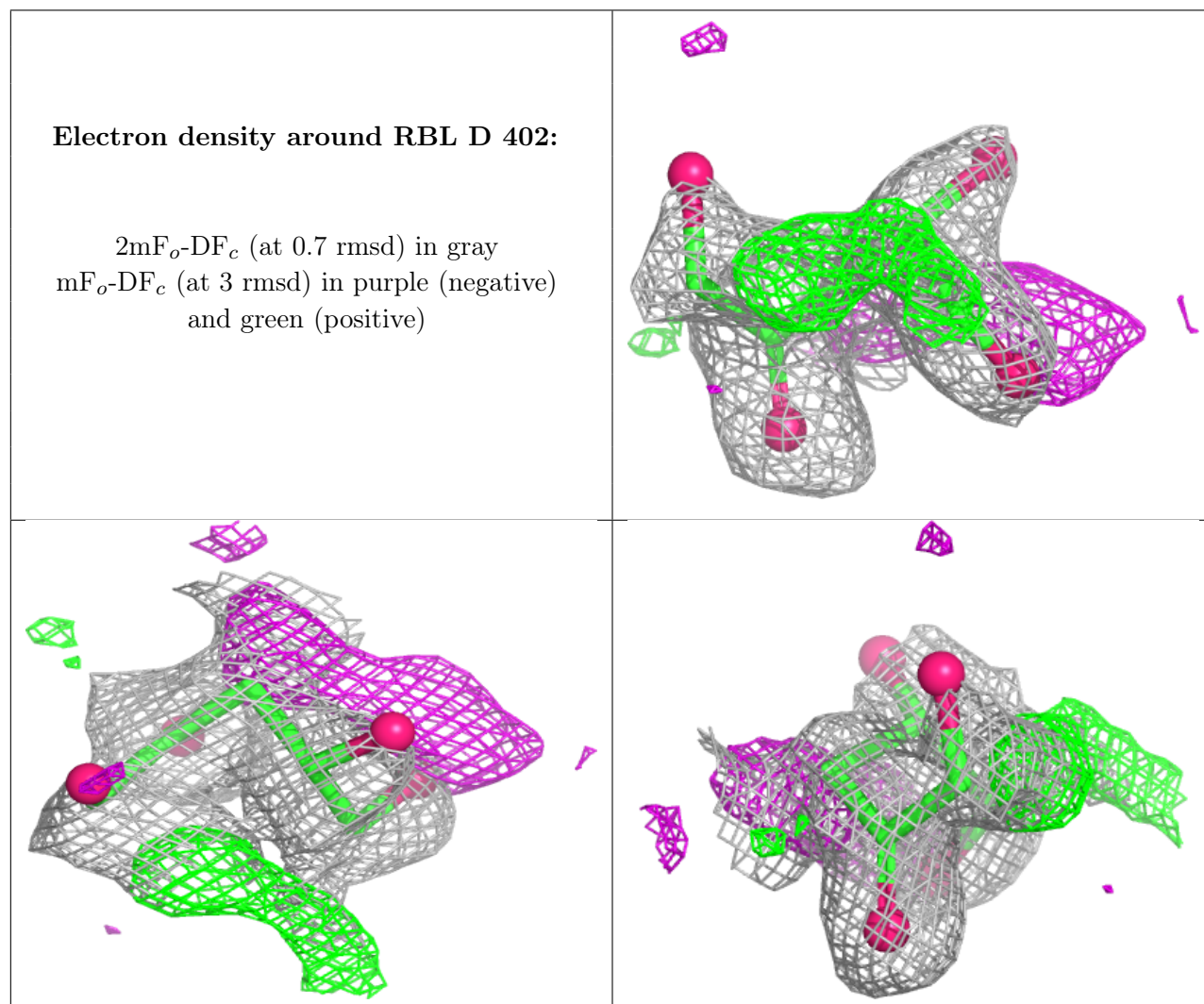
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	407	4/4	0.83	0.14	49,50,56,58	0
3	RBL	B	402	9/10	0.83	0.16	35,38,51,55	0
4	EDO	D	410	4/4	0.84	0.16	32,34,39,44	0
3	RBL	A	402	9/10	0.85	0.12	28,36,43,59	0
4	EDO	A	403	4/4	0.86	0.15	46,48,59,60	0
4	EDO	A	408	4/4	0.86	0.16	42,48,53,60	0
4	EDO	D	407	4/4	0.86	0.16	44,47,52,55	0
4	EDO	C	411	4/4	0.86	0.17	52,54,58,59	0
4	EDO	A	404	4/4	0.86	0.15	38,44,47,48	0
4	EDO	B	404	4/4	0.87	0.13	43,46,49,56	0
4	EDO	C	404	4/4	0.87	0.13	37,45,47,51	0
4	EDO	D	403	4/4	0.88	0.13	37,38,44,47	0
4	EDO	B	405	4/4	0.88	0.14	34,45,46,50	0
4	EDO	C	403	4/4	0.88	0.18	52,54,57,63	0
4	EDO	A	405	4/4	0.89	0.12	48,51,54,59	0
4	EDO	B	403	4/4	0.90	0.14	31,39,52,62	0
4	EDO	C	405	4/4	0.90	0.14	42,47,47,51	0
4	EDO	D	408	4/4	0.90	0.14	37,44,49,60	0
4	EDO	A	406	4/4	0.90	0.14	32,44,48,58	0
4	EDO	D	405	4/4	0.90	0.16	43,54,55,57	0
4	EDO	B	406	4/4	0.91	0.15	22,26,46,70	0
4	EDO	B	407	4/4	0.91	0.14	37,37,49,54	0
7	SO4	D	413	5/5	0.92	0.10	27,29,39,42	0
4	EDO	C	409	4/4	0.93	0.11	47,47,50,56	0
4	EDO	C	410	4/4	0.94	0.10	31,38,39,64	0
2	IPQ	C	401	20/20	0.95	0.09	18,23,47,50	0
2	IPQ	D	401	20/20	0.95	0.08	17,21,39,42	0
2	IPQ	A	401	20/20	0.95	0.07	20,26,35,41	0
7	SO4	C	415	5/5	0.95	0.08	25,28,36,39	0
2	IPQ	B	401	20/20	0.95	0.08	20,25,40,43	0
6	PO4	C	414	5/5	0.98	0.07	20,21,28,29	0
6	PO4	D	412	5/5	0.98	0.07	18,22,28,34	0
7	SO4	A	411	5/5	0.98	0.05	24,26,38,38	0
7	SO4	B	410	5/5	0.98	0.08	23,25,36,37	0
6	PO4	A	410	5/5	0.98	0.07	20,22,22,23	0
6	PO4	B	409	5/5	0.98	0.07	19,20,25,25	0
5	MG	A	409	1/1	0.99	0.05	17,17,17,17	0
5	MG	B	408	1/1	0.99	0.05	17,17,17,17	0
5	MG	C	413	1/1	1.00	0.04	14,14,14,14	0
5	MG	D	411	1/1	1.00	0.05	14,14,14,14	0

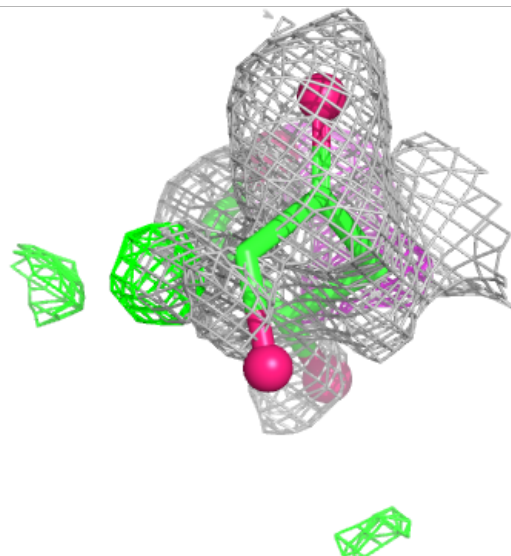
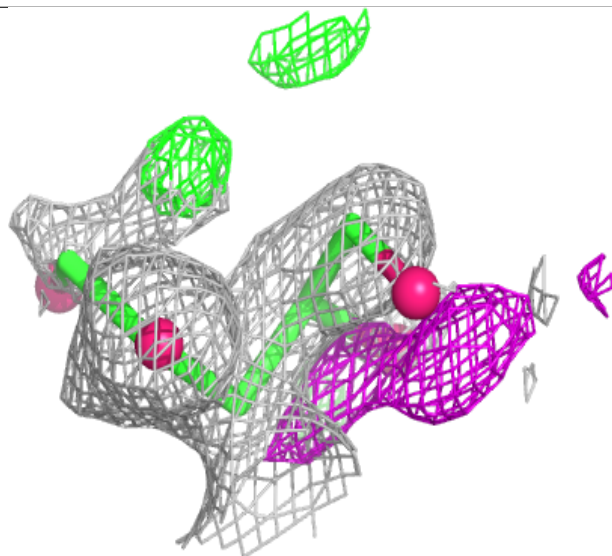
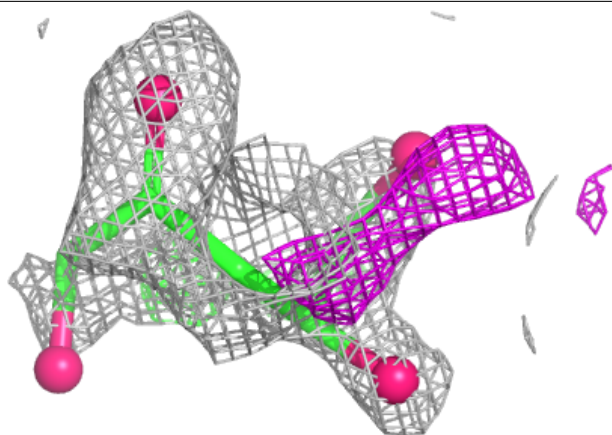
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



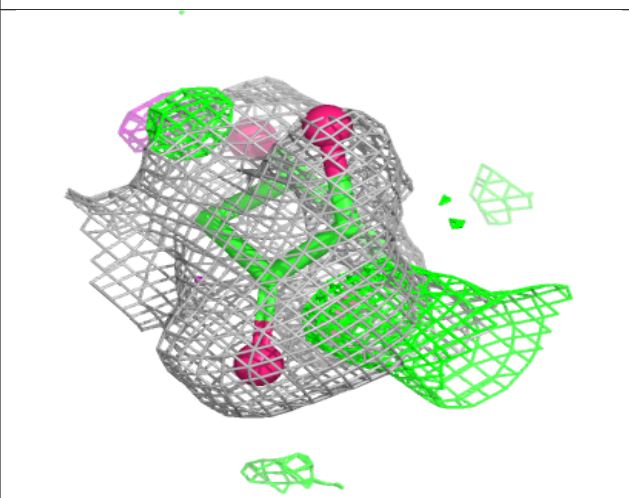
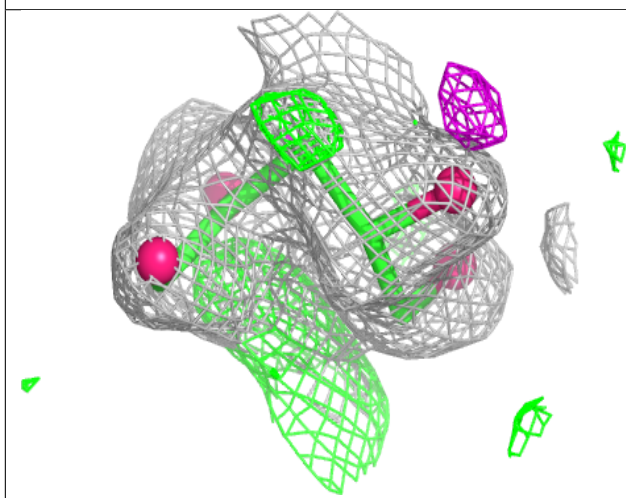
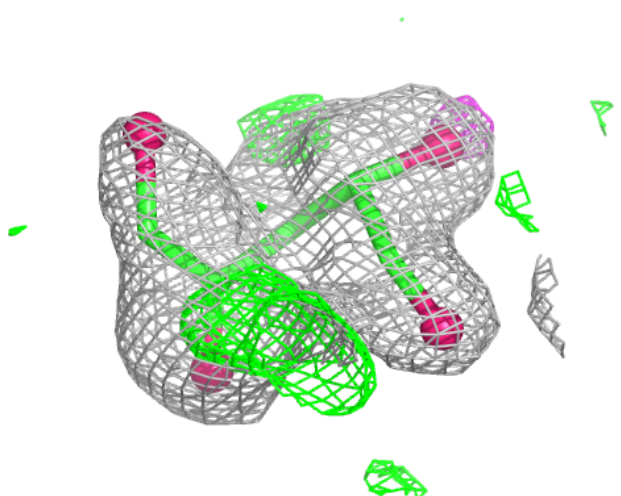
Electron density around RBL C 402:

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



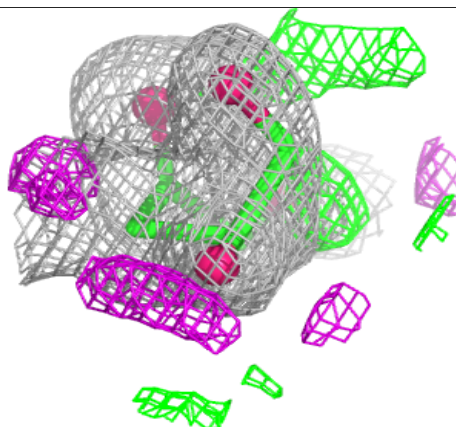
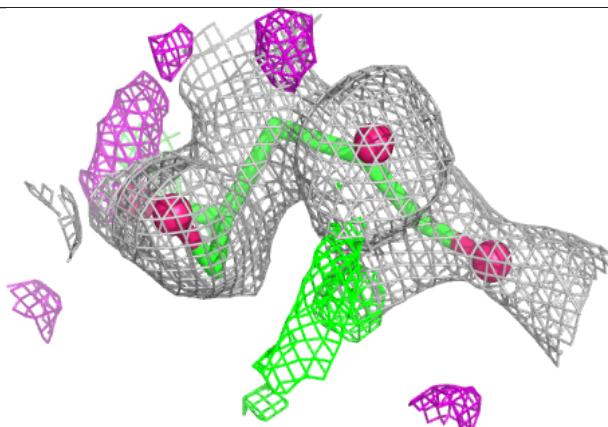
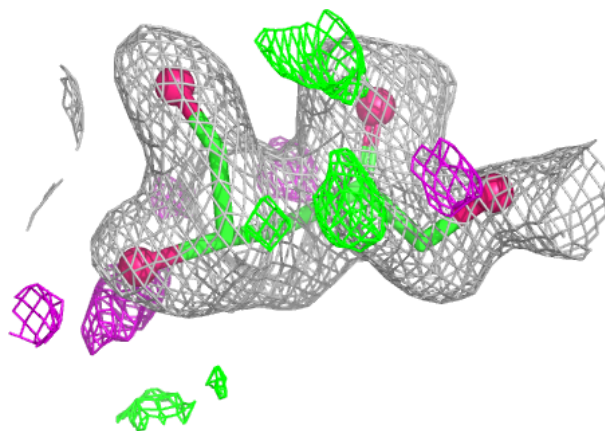
Electron density around RBL B 402:

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

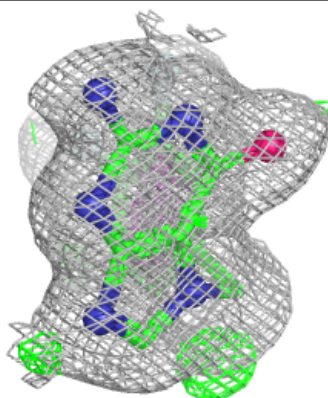
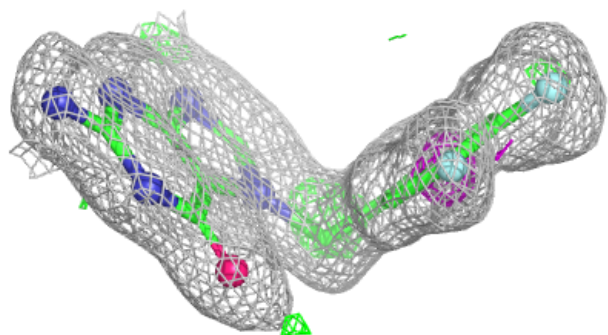
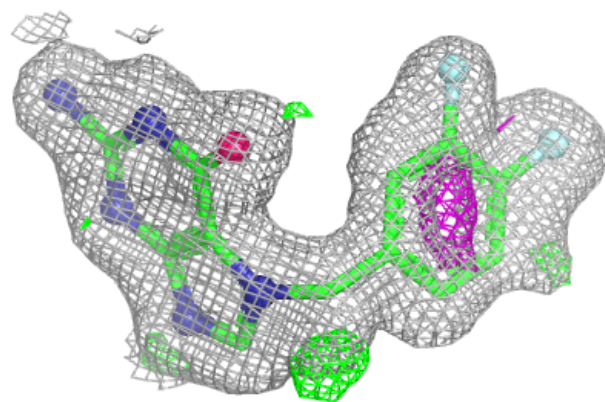


Electron density around RBL A 402:

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

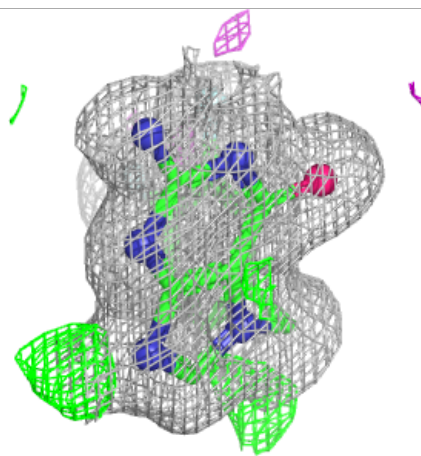
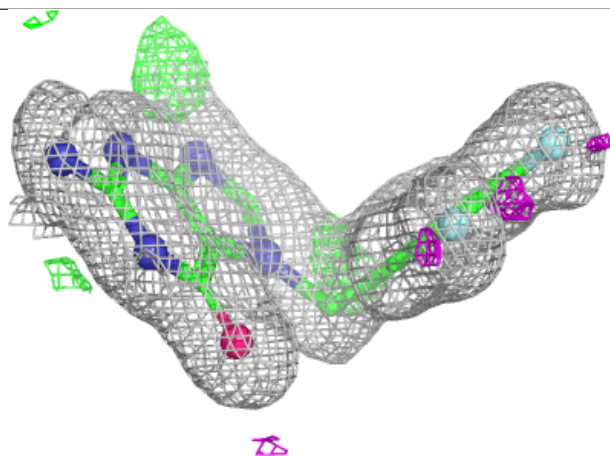
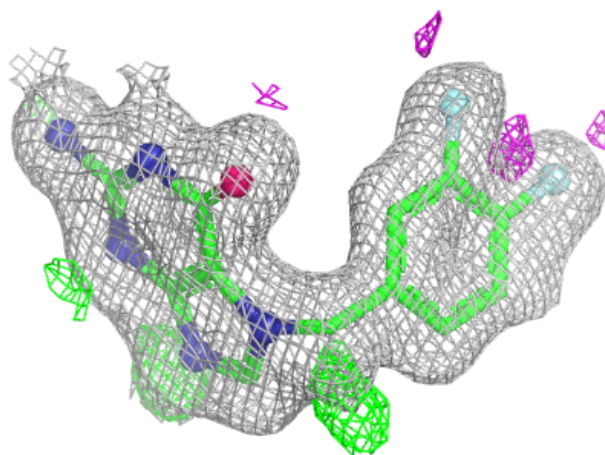
**Electron density around IPQ C 401:**

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



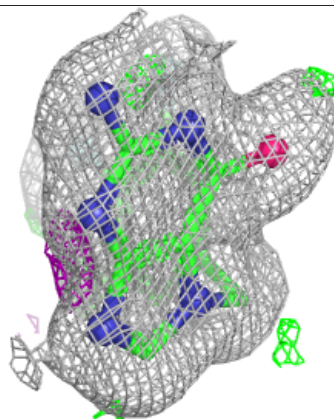
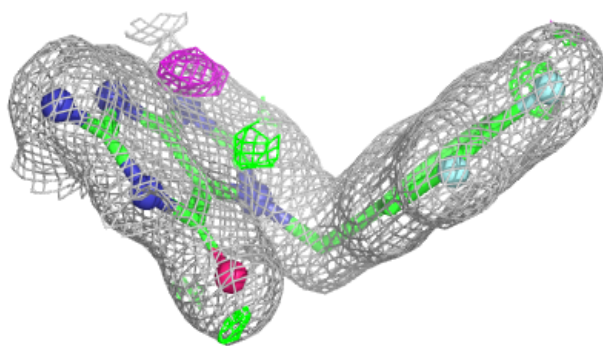
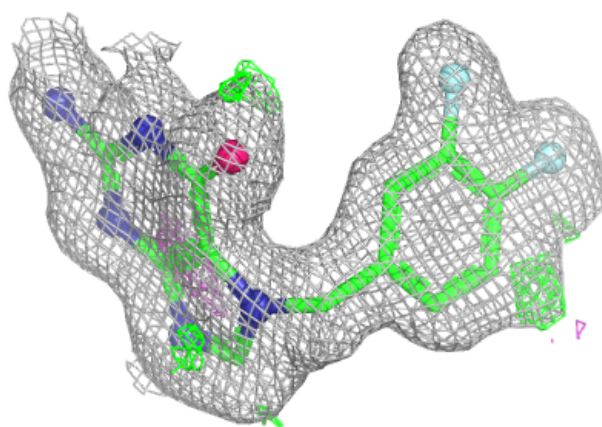
Electron density around IPQ D 401:

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

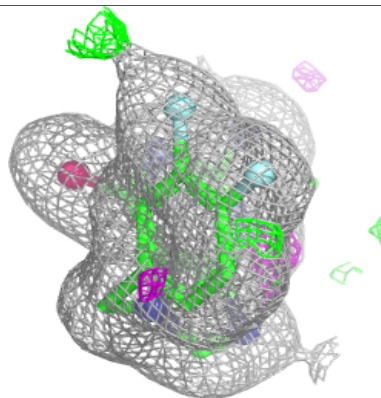
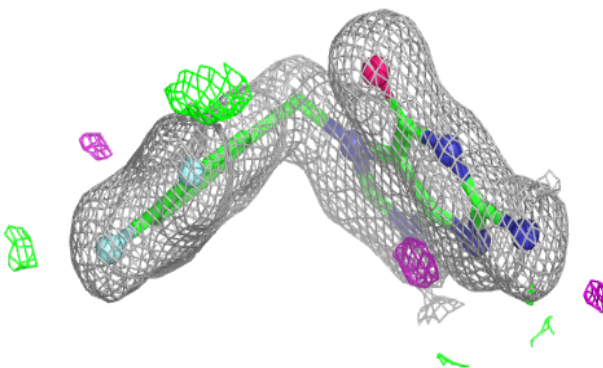
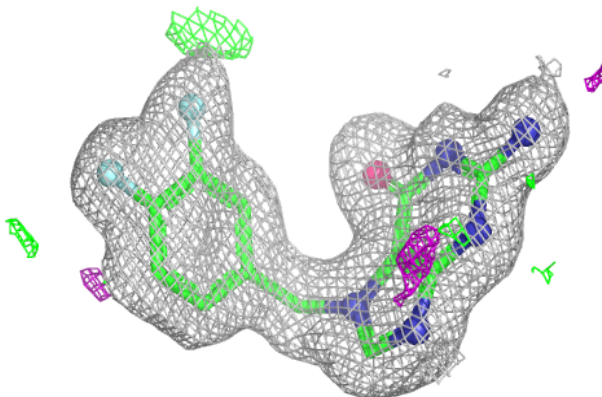


Electron density around IPQ A 401:

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

**Electron density around IPQ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.