



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:34 AM UTC

PDB ID : 7POQ / pdb_00007poq
Title : Crystal structure of profragilysin-3 (proBFT-3) from *Bacteroides fragilis* in complex with foliosidine in P41212.
Authors : Eckhard, U.; Guevara, T.; Gomis-Ruth, F.X.
Deposited on : 2021-09-09
Resolution : 1.85 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

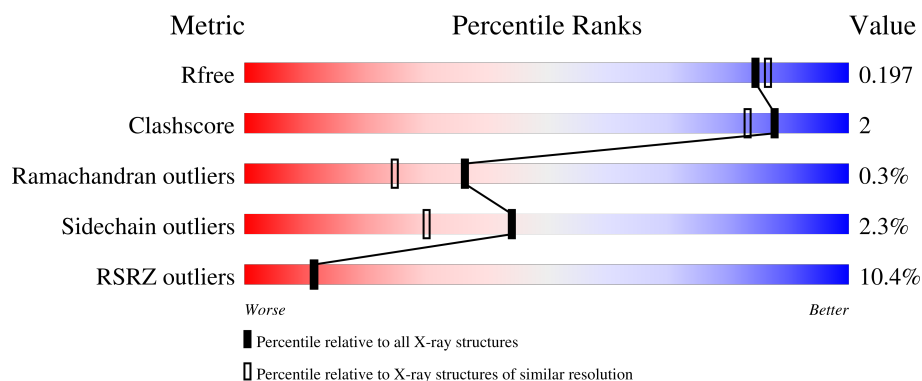
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	402	8% 80% 5% 14%
1	B	402	9% 82% • 13%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6536 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 BFT-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	8	0
			2781	1769	454	544	14			
1	B	348	Total	C	N	O	S	0	10	0
			2820	1794	464	548	14			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP O86049
A	-3	GLY	-	expression tag	UNP O86049
A	-2	SER	-	expression tag	UNP O86049
A	-1	SER	-	expression tag	UNP O86049
A	0	HIS	-	expression tag	UNP O86049
A	1	HIS	-	expression tag	UNP O86049
A	2	HIS	-	expression tag	UNP O86049
A	3	HIS	-	expression tag	UNP O86049
A	4	HIS	-	expression tag	UNP O86049
A	5	HIS	-	expression tag	UNP O86049
A	6	SER	-	expression tag	UNP O86049
A	7	SER	-	expression tag	UNP O86049
A	8	GLY	-	expression tag	UNP O86049
A	9	GLU	-	expression tag	UNP O86049
A	10	ASN	-	expression tag	UNP O86049
A	11	LEU	-	expression tag	UNP O86049
A	12	TYR	-	expression tag	UNP O86049
A	13	PHE	-	expression tag	UNP O86049
A	14	GLN	-	expression tag	UNP O86049
A	15	GLY	-	expression tag	UNP O86049
A	16	ALA	-	expression tag	UNP O86049
A	17	MET	-	expression tag	UNP O86049
B	-4	MET	-	initiating methionine	UNP O86049
B	-3	GLY	-	expression tag	UNP O86049
B	-2	SER	-	expression tag	UNP O86049

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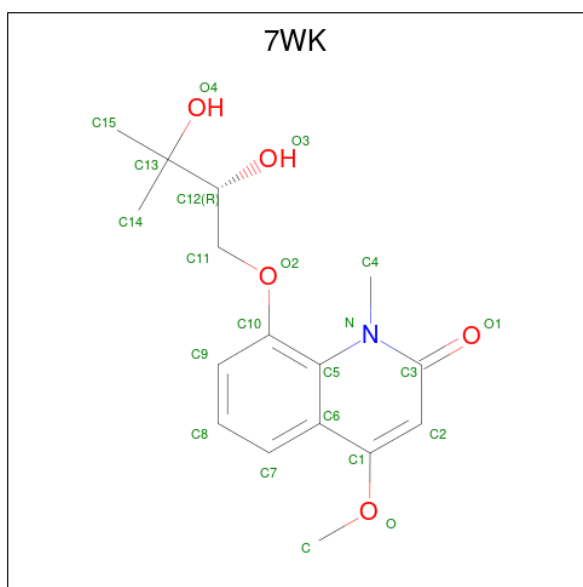
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP O86049
B	0	HIS	-	expression tag	UNP O86049
B	1	HIS	-	expression tag	UNP O86049
B	2	HIS	-	expression tag	UNP O86049
B	3	HIS	-	expression tag	UNP O86049
B	4	HIS	-	expression tag	UNP O86049
B	5	HIS	-	expression tag	UNP O86049
B	6	SER	-	expression tag	UNP O86049
B	7	SER	-	expression tag	UNP O86049
B	8	GLY	-	expression tag	UNP O86049
B	9	GLU	-	expression tag	UNP O86049
B	10	ASN	-	expression tag	UNP O86049
B	11	LEU	-	expression tag	UNP O86049
B	12	TYR	-	expression tag	UNP O86049
B	13	PHE	-	expression tag	UNP O86049
B	14	GLN	-	expression tag	UNP O86049
B	15	GLY	-	expression tag	UNP O86049
B	16	ALA	-	expression tag	UNP O86049
B	17	MET	-	expression tag	UNP O86049

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is foliosidine (CCD ID: 7WK) (formula: C₁₆H₂₁NO₅) (labeled as "Ligand of Interest" by depositor).

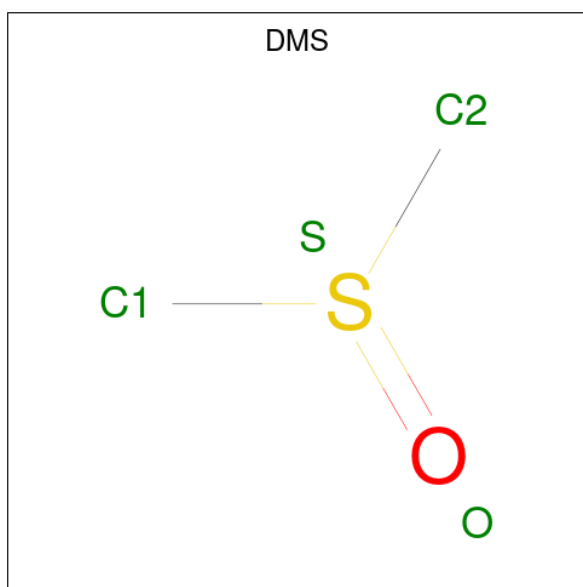


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	16	1	5		
3	B	1	Total	C	N	O	0	0
			22	16	1	5		

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

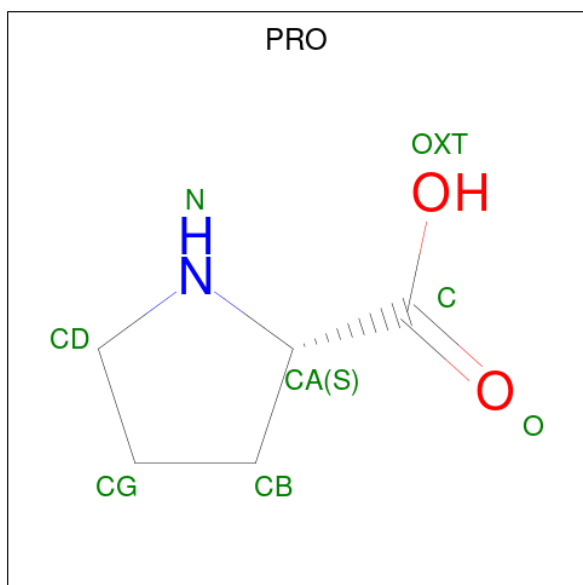
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



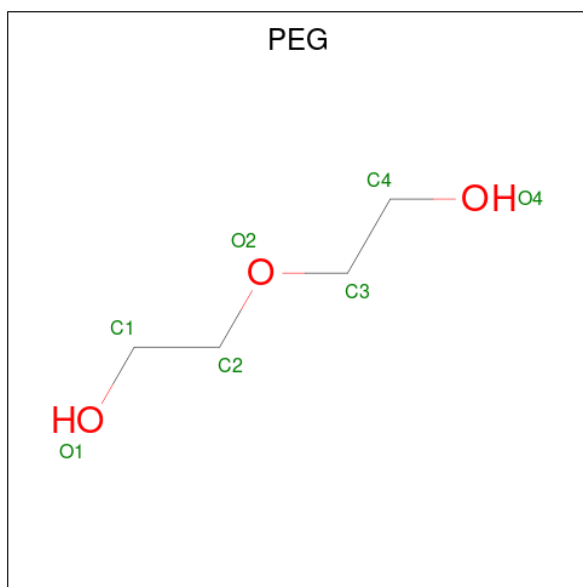
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



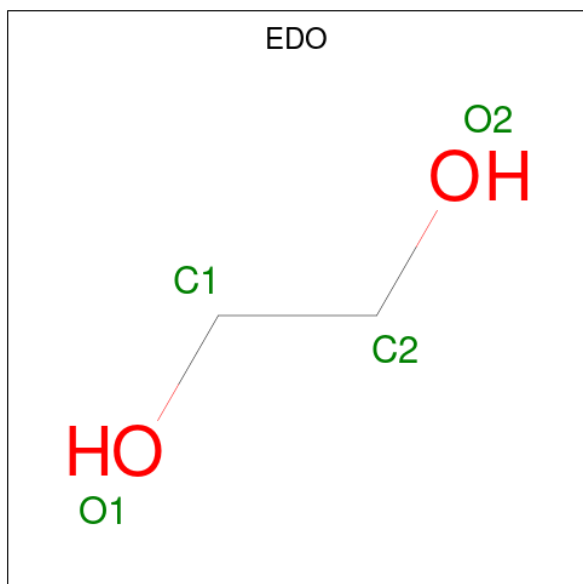
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	5	1	2		
6	A	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



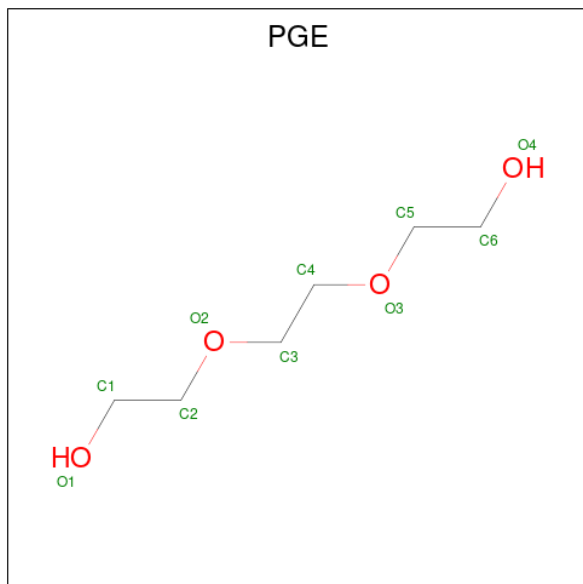
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	383	Total	O	0	17
			400	400		
10	B	394	Total	O	0	19
			413	413		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.83Å 83.83Å 266.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.96 – 1.85 79.96 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (79.96-1.85) 100.0 (79.96-1.85)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.191 , 0.204 0.185 , 0.197	Depositor DCC
R_{free} test set	743 reflections (0.90%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6536	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 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, DMS, EDO, 7WK, ZN, CL, PGE

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	0.68	3/2861 (0.1%)	0.89	1/3872 (0.0%)
1	B	0.69	2/2910 (0.1%)	0.89	1/3936 (0.0%)
All	All	0.68	5/5771 (0.1%)	0.89	2/7808 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	MET	SD-CE	-8.83	1.57	1.79
1	B	192	ILE	CA-C	6.04	1.60	1.52
1	A	192	ILE	CA-C	6.02	1.60	1.52
1	A	382	MET	SD-CE	-5.56	1.65	1.79
1	A	341	MET	SD-CE	-5.11	1.66	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	PHE	CA-CB-CG	5.33	119.12	113.80
1	B	103	PHE	CA-CB-CG	5.25	119.05	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2781	0	2701	8	0
1	B	2820	0	2754	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	0	1	0
3	B	22	0	0	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	6	0	0
5	B	12	0	18	0	0
6	A	16	0	14	0	0
7	A	7	0	10	1	0
8	A	8	0	12	0	0
8	B	16	0	24	3	0
9	B	10	0	14	1	0
10	A	400	0	0	2	0
10	B	413	0	0	0	0
All	All	6536	0	5553	23	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 (23) 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:100:SER:HB2	10:A:539:HOH:O	1.90	0.71
1:B:331:LYS:HA	8:B:409:EDO:H11	1.84	0.60
1:B:230:SER:HA	9:B:407:PGE:H5	1.85	0.58
1:B:379:GLU:HG3	8:B:411:EDO:H21	1.85	0.57
3:B:402:7WK:O2	3:B:402:7WK:C4	2.53	0.56
1:B:192:ILE:HG23	1:B:193:ASN:H	1.72	0.54
1:B:192:ILE:HG23	1:B:193:ASN:N	2.23	0.53
3:A:402:7WK:O2	3:A:402:7WK:C4	2.58	0.51
1:B:192:ILE:CG2	1:B:193:ASN:H	2.27	0.47
1:B:189:CYS:HA	1:B:312:ASN:HB3	1.95	0.47
1:A:341:MET:HG2	10:A:722:HOH:O	2.16	0.45
1:A:184:LEU:HD12	1:A:341:MET:HE2	1.99	0.44
1:A:85:LEU:HA	1:A:264:LEU:HB3	2.00	0.44
1:B:85:LEU:HA	1:B:264:LEU:HB3	2.00	0.43
1:A:181:LYS:HG2	1:A:186:LEU:HD12	2.01	0.43
1:A:93:PHE:HB2	1:A:103:PHE:HB2	2.00	0.43
1:B:93:PHE:HB2	1:B:103:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115[B]:TYR:CZ	1:B:118:GLY:HA2	2.55	0.42
1:B:181:LYS:HG3	1:B:341:MET:HE3	2.02	0.42
1:A:320:ASN:ND2	7:A:408:PEG:O1	2.47	0.42
1:B:192:ILE:CG2	1:B:193:ASN:N	2.82	0.42
1:A:197:LYS:HG2	1:A:319:LEU:HD23	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/402 (86%)	339 (98%)	6 (2%)	1 (0%)	36	25
1	B	352/402 (88%)	343 (97%)	8 (2%)	1 (0%)	36	25
All	All	698/804 (87%)	682 (98%)	14 (2%)	2 (0%)	36	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ILE
1	B	192	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/344 (89%)	297 (97%)	8 (3%)	40	25
1	B	310/344 (90%)	304 (98%)	6 (2%)	50	38
All	All	615/688 (89%)	601 (98%)	14 (2%)	44	30

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	A	147	ARG
1	A	185	ASN
1	A	188	GLU
1	A	198	THR
1	A	213	VAL
1	A	294	GLU
1	A	331	LYS
1	B	145	LYS
1	B	162	ARG
1	B	181	LYS
1	B	192	ILE
1	B	331	LYS
1	B	369	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	B	41	GLN
1	B	130	GLN
1	B	357	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 21 ligands modelled in this entry, 5 are monoatomic - leaving 16 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	$\# Z > 2$
9	PGE	B	407	-	9,9,9	0.18	0	8,8,8	0.15	0
5	DMS	B	406	-	3,3,3	0.28	0	3,3,3	0.37	0
6	PRO	A	407	-	8,8,8	0.93	0	10,10,10	1.25	1 (10%)
8	EDO	A	410	-	3,3,3	0.53	0	2,2,2	0.13	0
6	PRO	A	406	-	8,8,8	0.88	0	10,10,10	1.06	0
8	EDO	B	408	-	3,3,3	0.69	0	2,2,2	0.17	0
8	EDO	A	409	-	3,3,3	0.51	0	2,2,2	0.37	0
8	EDO	B	410	-	3,3,3	0.51	0	2,2,2	0.34	0
5	DMS	A	405	-	3,3,3	0.35	0	3,3,3	0.35	0
8	EDO	B	411	-	3,3,3	0.60	0	2,2,2	0.27	0
3	7WK	B	402	-	22,23,23	0.52	0	27,34,34	0.72	1 (3%)
7	PEG	A	408	-	6,6,6	0.15	0	5,5,5	0.14	0
5	DMS	B	405	-	3,3,3	0.15	0	3,3,3	0.86	0
5	DMS	B	404	-	3,3,3	0.24	0	3,3,3	0.37	0
3	7WK	A	402	-	22,23,23	0.61	0	27,34,34	0.64	1 (3%)
8	EDO	B	409	-	3,3,3	0.48	0	2,2,2	0.40	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
9	PGE	B	407	-	-	3/7/7/7	-
6	PRO	A	407	-	-	0/4/11/11	0/1/1/1
8	EDO	A	410	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PRO	A	406	-	-	0/4/11/11	0/1/1/1
3	7WK	A	402	-	-	3/13/13/13	0/2/2/2
8	EDO	B	408	-	-	1/1/1/1	-
8	EDO	A	409	-	-	0/1/1/1	-
8	EDO	B	410	-	-	0/1/1/1	-
8	EDO	B	411	-	-	1/1/1/1	-
3	7WK	B	402	-	-	3/13/13/13	0/2/2/2
8	EDO	B	409	-	-	0/1/1/1	-
7	PEG	A	408	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	7WK	O-C1-C2	2.41	127.13	124.36
3	A	402	7WK	O-C1-C2	2.04	126.70	124.36
6	A	407	PRO	OXT-C-CA	2.02	120.34	113.51

There are no chirality outliers.

All (13) torsion outliers are listed below:

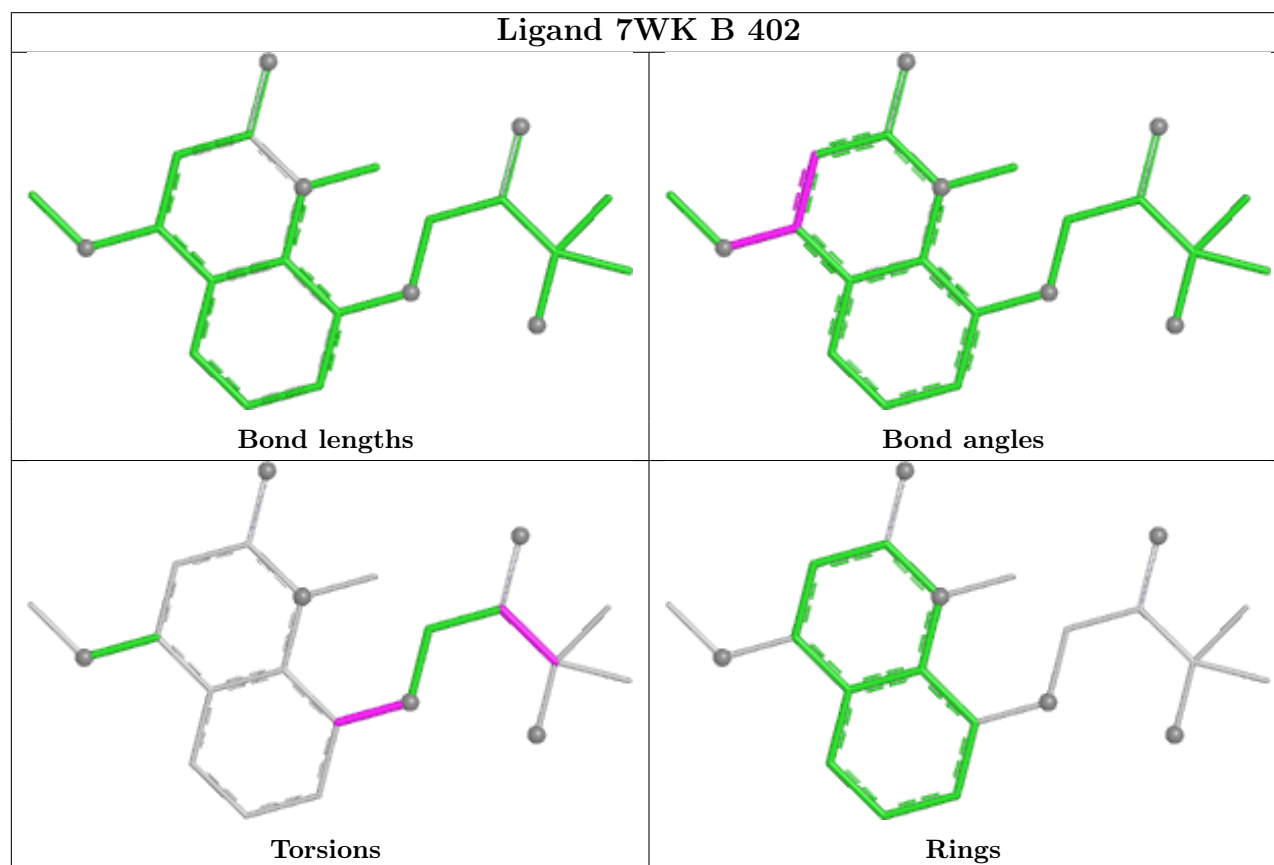
Mol	Chain	Res	Type	Atoms
7	A	408	PEG	O2-C3-C4-O4
8	B	408	EDO	O1-C1-C2-O2
8	B	411	EDO	O1-C1-C2-O2
3	B	402	7WK	C5-C10-O2-C11
3	A	402	7WK	C12-C11-O2-C10
9	B	407	PGE	C1-C2-O2-C3
7	A	408	PEG	C1-C2-O2-C3
9	B	407	PGE	C4-C3-O2-C2
3	A	402	7WK	C5-C10-O2-C11
3	B	402	7WK	C9-C10-O2-C11
3	A	402	7WK	C9-C10-O2-C11
3	B	402	7WK	C11-C12-C13-C15
9	B	407	PGE	C3-C4-O3-C5

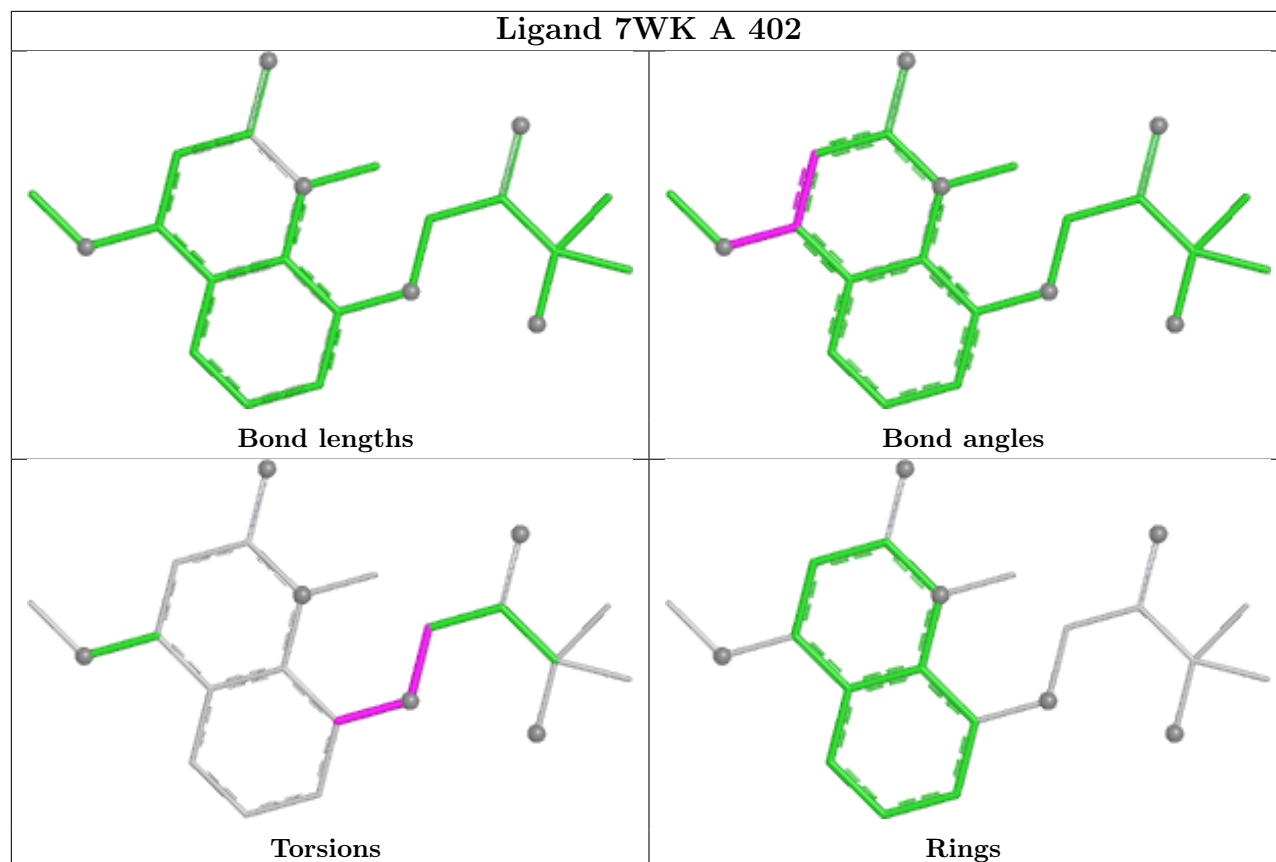
There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	407	PGE	1	0
8	B	408	EDO	1	0
8	B	411	EDO	1	0
3	B	402	7WK	1	0
7	A	408	PEG	1	0
3	A	402	7WK	1	0
8	B	409	EDO	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.





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	344/402 (85%)	0.34	34 (9%) 13 12	14, 33, 69, 90	8 (2%)
1	B	348/402 (86%)	0.29	38 (10%) 10 10	15, 34, 65, 82	10 (2%)
All	All	692/804 (86%)	0.31	72 (10%) 11 11	14, 33, 66, 90	18 (2%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	ILE	6.9
1	A	192	ILE	6.7
1	A	213	VAL	6.5
1	B	192	ILE	6.3
1	A	189	CYS	6.1
1	A	187	PRO	5.3
1	B	198	THR	5.3
1	B	167	GLY	5.1
1	B	214	PRO	5.1
1	A	191	TYR	4.9
1	A	214	PRO	4.9
1	A	190	ASP	4.9
1	A	198	THR	4.6
1	B	191	TYR	4.6
1	B	213	VAL	4.6
1	B	149	ILE	4.6
1	A	186	LEU	4.6
1	B	163	THR	4.5
1	B	33	PRO	4.5
1	A	146	THR	4.3
1	A	150	ASN	4.1
1	A	34	VAL	4.0
1	B	146	THR	3.9
1	B	311	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	161	SER	3.6
1	B	148	ALA	3.5
1	A	100	SER	3.5
1	B	186	LEU	3.3
1	B	190	ASP	3.3
1	A	147	ARG	3.3
1	B	195	TYR	3.1
1	A	117	ASN	3.1
1	A	161	SER	3.1
1	B	169	TYR	3.1
1	A	184	LEU	3.1
1	A	148	ALA	3.1
1	A	196	ILE	3.0
1	B	145	LYS	3.0
1	A	215	SER	3.0
1	B	215	SER	2.9
1	B	144	LYS	2.8
1	B	183	ILE	2.8
1	B	150	ASN	2.7
1	B	162	ARG	2.7
1	B	34	VAL	2.7
1	B	189	CYS	2.7
1	A	57	ASP	2.7
1	A	35	THR	2.6
1	B	160	ASP	2.6
1	B	193	ASN	2.6
1	A	195	TYR	2.5
1	A	58	PHE	2.5
1	B	196	ILE	2.5
1	B	229	GLY	2.5
1	B	312	ASN	2.5
1	A	153	GLU	2.4
1	A	145	LYS	2.4
1	B	197	LYS	2.4
1	B	184	LEU	2.3
1	B	115[A]	TYR	2.3
1	A	183	ILE	2.3
1	A	168	LYS	2.3
1	A	169	TYR	2.2
1	B	168	LYS	2.2
1	B	58	PHE	2.1
1	A	197	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	LYS	2.1
1	A	312	ASN	2.1
1	B	142	PRO	2.1
1	A	394	ALA	2.1
1	B	147	ARG	2.1
1	B	187	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

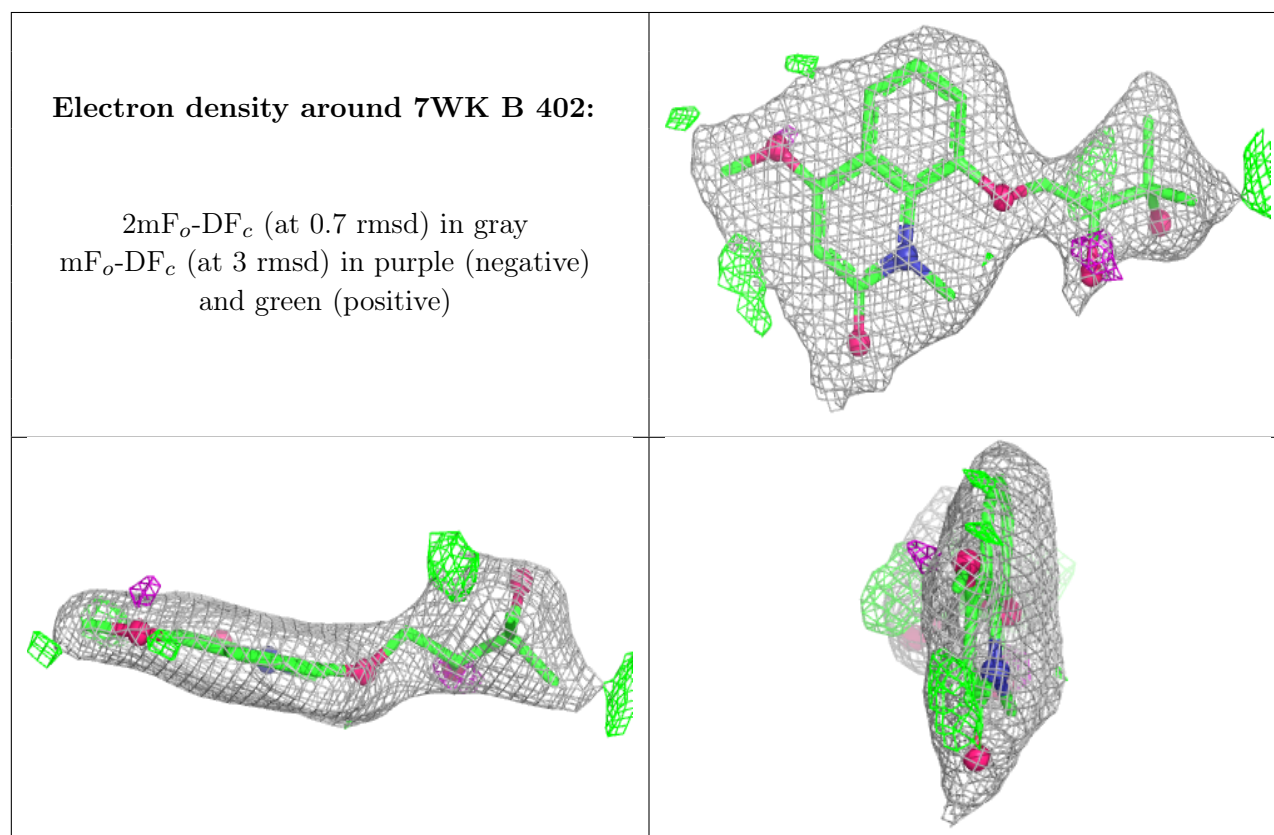
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PGE	B	407	10/10	0.61	0.33	76,76,77,77	0
7	PEG	A	408	7/7	0.63	0.25	72,72,73,73	0
8	EDO	A	409	4/4	0.68	0.24	74,74,74,74	0
8	EDO	B	410	4/4	0.69	0.27	76,76,77,77	0
8	EDO	B	411	4/4	0.75	0.23	54,55,55,56	0
8	EDO	A	410	4/4	0.77	0.22	58,58,59,59	0
8	EDO	B	409	4/4	0.81	0.22	59,59,59,60	0
5	DMS	B	404	4/4	0.81	0.25	73,73,74,74	0
6	PRO	A	406	8/8	0.83	0.18	60,62,63,66	0
8	EDO	B	408	4/4	0.84	0.18	42,44,45,45	0
3	7WK	B	402	22/22	0.85	0.15	47,47,55,56	0
6	PRO	A	407	8/8	0.88	0.14	42,44,45,50	0
3	7WK	A	402	22/22	0.89	0.13	43,45,51,52	0
4	CL	A	404	1/1	0.90	0.15	69,69,69,69	1
5	DMS	B	406	4/4	0.91	0.22	87,87,87,88	0
4	CL	B	403	1/1	0.93	0.10	43,43,43,43	1
5	DMS	A	405	4/4	0.94	0.17	37,38,39,39	0

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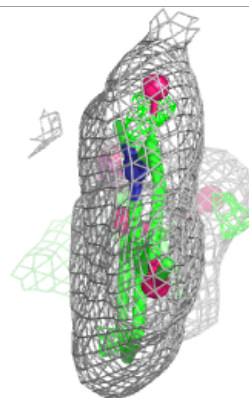
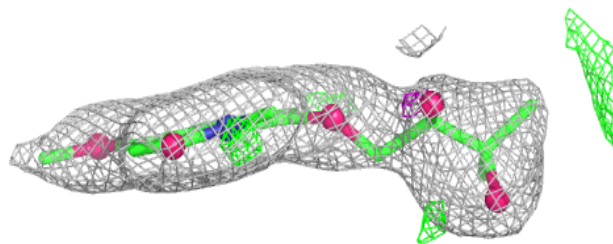
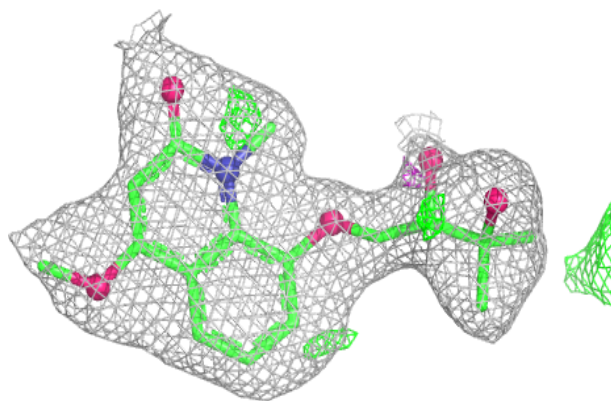
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	405	4/4	0.95	0.11	38,39,40,40	0
4	CL	A	403	1/1	0.98	0.07	40,40,40,40	1
2	ZN	B	401	1/1	1.00	0.01	31,31,31,31	1
2	ZN	A	401	1/1	1.00	0.02	30,30,30,30	1

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.



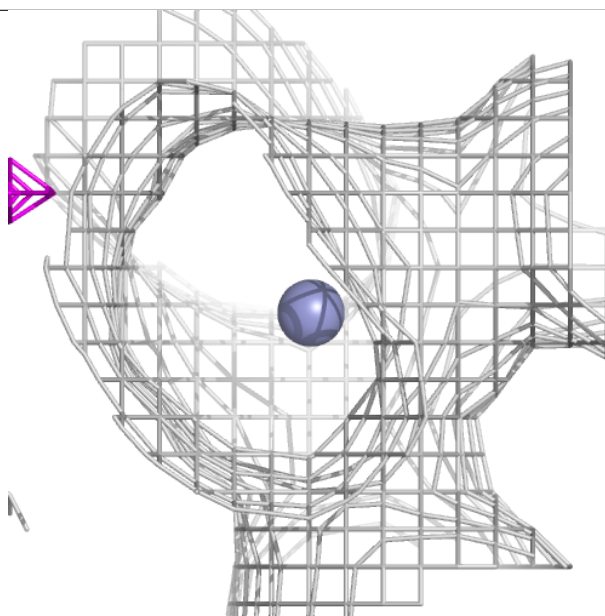
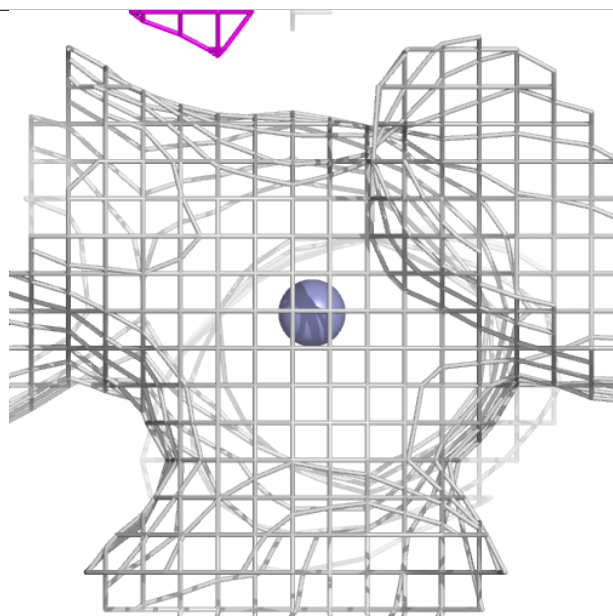
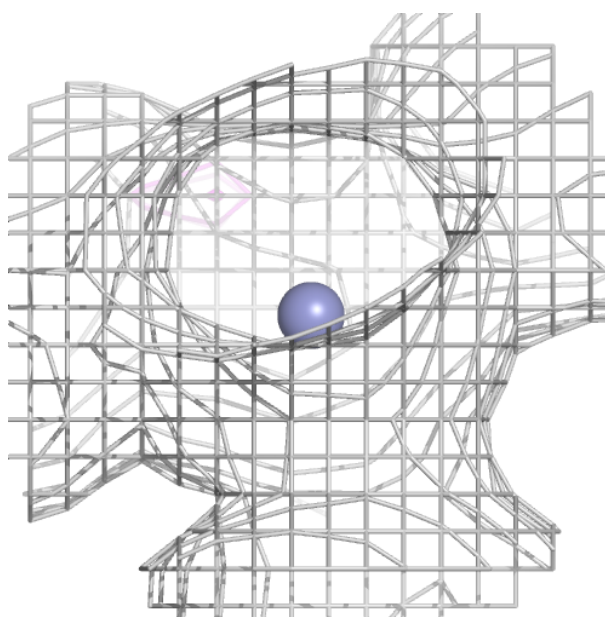
Electron density around 7WK A 402:

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



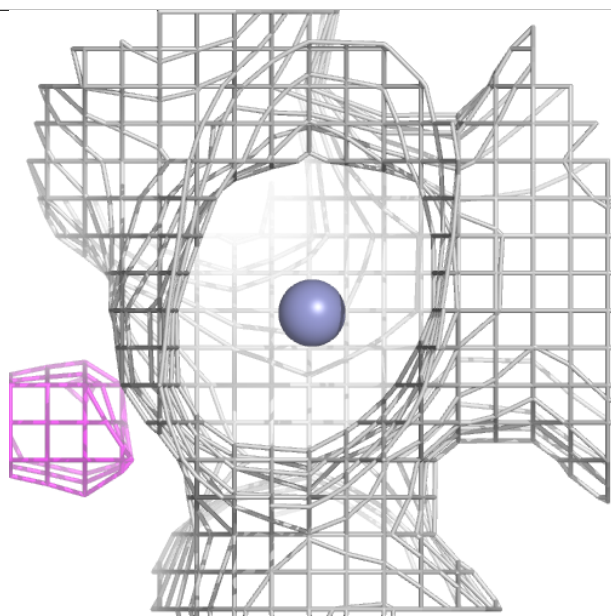
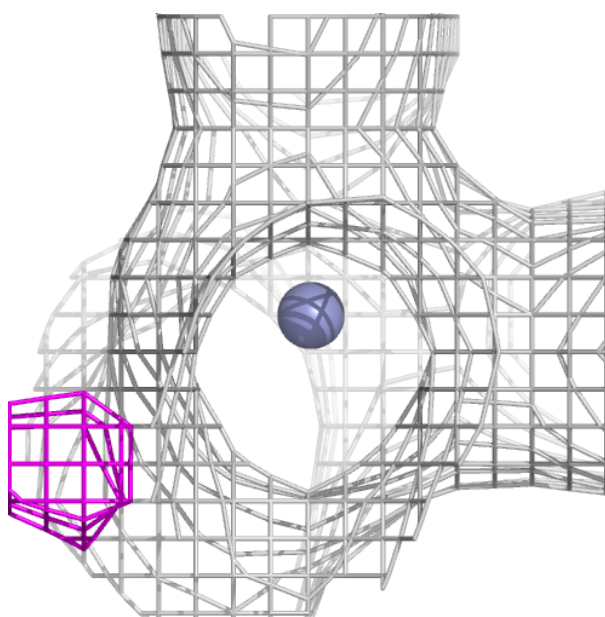
Electron density around ZN B 401:

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



Electron density around ZN 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.