



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:13 AM UTC

PDB ID : 9DR5 / pdb_00009dr5
Title : Crystal structure of Catechol 1,2-dioxygenase from Burkholderia multivorans (Zinc bound, P1 form)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-09-25
Resolution : 1.71 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:

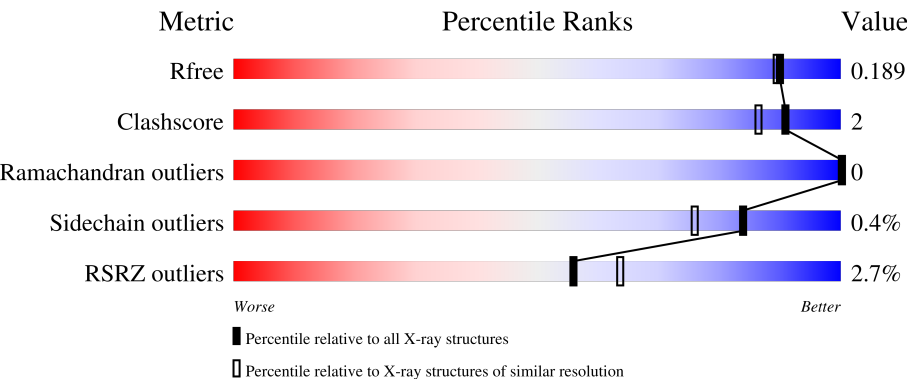
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	319	3% 93% • •
1	B	319	2% 95% • •
1	C	319	3% 93% • •
1	D	319	2% 92% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	319	2% 91% 6%
1	F	319	4% 94%
1	G	319	3% 92% 5%
1	H	319	3% 93%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22348 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 Catechol 1,2-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	7	0
			2401	1507	427	462	5			
1	B	310	Total	C	N	O	S	0	8	0
			2402	1508	429	460	5			
1	C	310	Total	C	N	O	S	0	9	0
			2408	1513	429	460	6			
1	D	310	Total	C	N	O	S	0	7	0
			2395	1504	427	459	5			
1	E	308	Total	C	N	O	S	0	8	0
			2383	1501	422	455	5			
1	F	310	Total	C	N	O	S	0	10	0
			2417	1519	432	461	5			
1	G	310	Total	C	N	O	S	0	16	0
			2457	1541	439	472	5			
1	H	309	Total	C	N	O	S	0	9	0
			2399	1509	425	460	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A0A0H3KXJ8
A	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
A	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
A	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
A	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
A	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
A	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
A	0	HIS	-	expression tag	UNP A0A0H3KXJ8
B	-7	MET	-	expression tag	UNP A0A0H3KXJ8
B	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
B	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
B	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
B	-3	HIS	-	expression tag	UNP A0A0H3KXJ8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
B	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
B	0	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-7	MET	-	expression tag	UNP A0A0H3KXJ8
C	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
C	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
C	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
C	0	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-7	MET	-	expression tag	UNP A0A0H3KXJ8
D	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
D	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
D	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
D	0	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-7	MET	-	expression tag	UNP A0A0H3KXJ8
E	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
E	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
E	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
E	0	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-7	MET	-	expression tag	UNP A0A0H3KXJ8
F	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
F	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
F	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
F	0	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-7	MET	-	expression tag	UNP A0A0H3KXJ8
G	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
G	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
G	-1	HIS	-	expression tag	UNP A0A0H3KXJ8

Continued on next page...

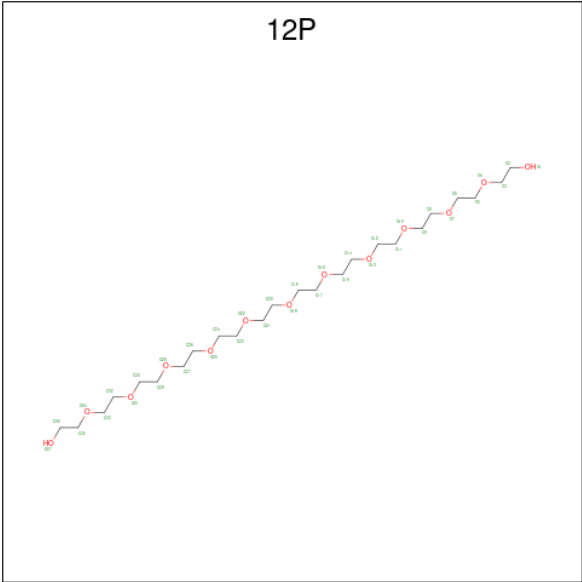
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-7	MET	-	expression tag	UNP A0A0H3KXJ8
H	-6	ALA	-	expression tag	UNP A0A0H3KXJ8
H	-5	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-4	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-3	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-2	HIS	-	expression tag	UNP A0A0H3KXJ8
H	-1	HIS	-	expression tag	UNP A0A0H3KXJ8
H	0	HIS	-	expression tag	UNP A0A0H3KXJ8

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

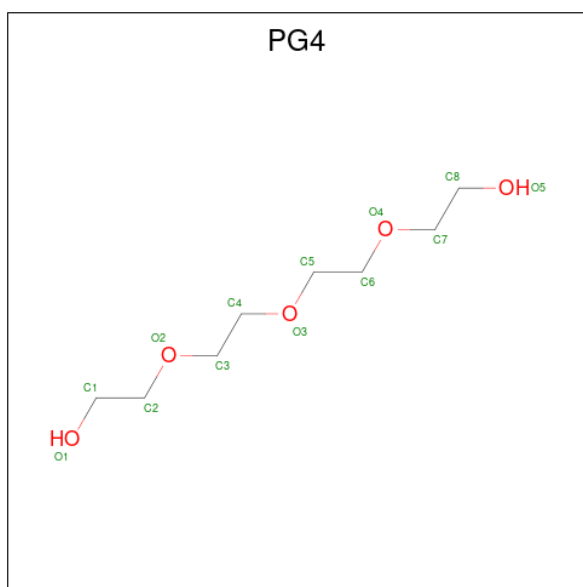
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	1
2	B	1	Total Zn 1 1	0	1
2	C	1	Total Zn 1 1	0	1
2	D	1	Total Zn 1 1	0	1
2	E	1	Total Zn 1 1	0	1
2	F	1	Total Zn 1 1	0	1
2	G	1	Total Zn 1 1	0	1
2	H	1	Total Zn 1 1	0	1

- Molecule 3 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



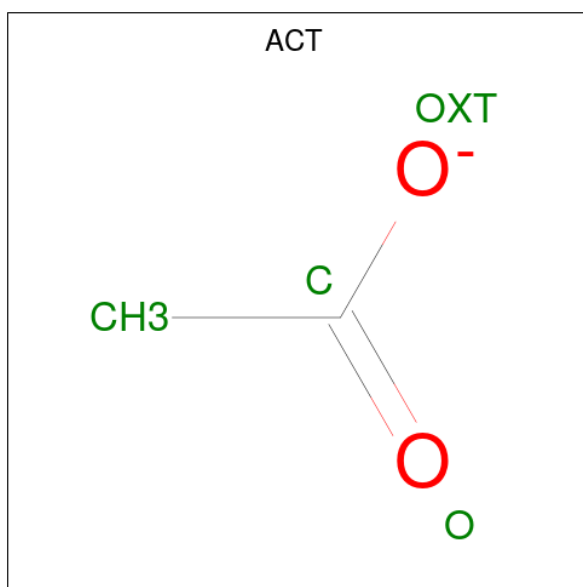
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			37	24	13		
3	A	1	Total	C	O	0	0
			37	24	13		
3	C	1	Total	C	O	0	0
			37	24	13		
3	C	1	Total	C	O	0	0
			37	24	13		
3	F	1	Total	C	O	0	0
			37	24	13		
3	F	1	Total	C	O	0	0
			37	24	13		
3	G	1	Total	C	O	0	0
			37	24	13		
3	H	1	Total	C	O	0	0
			37	24	13		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		
4	G	1	Total	C	O	0	0
			13	8	5		
4	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



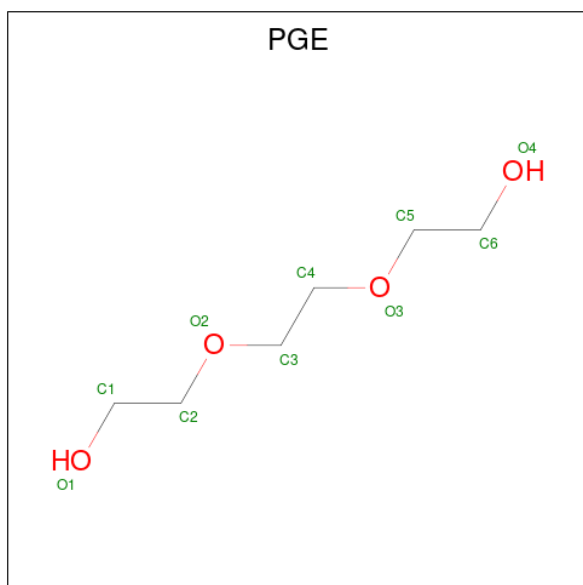
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	1
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	1
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	1
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	1
			4	2	2		
5	E	1	Total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

Continued on next page...

Continued from previous page...

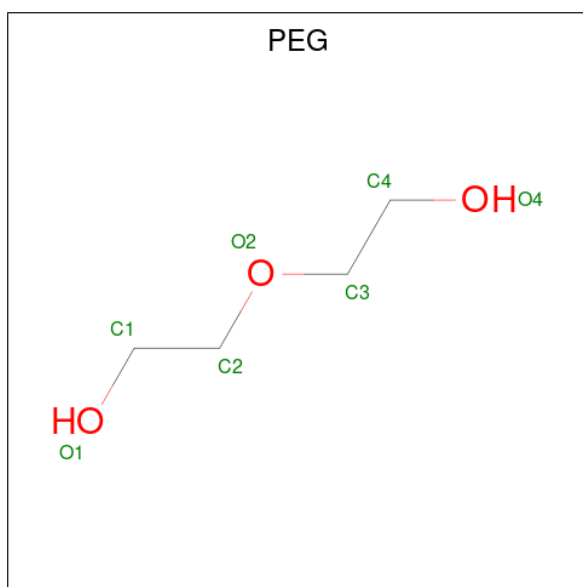
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	1
			4	2	2		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		
6	H	1	Total	C	O	0	0
			10	6	4		

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



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	333	Total	O	0	0
			333	333		
8	B	298	Total	O	0	0
			298	298		
8	C	282	Total	O	0	0
			282	282		
8	D	304	Total	O	0	0
			304	304		
8	E	353	Total	O	0	0
			353	353		
8	F	293	Total	O	0	0
			293	293		
8	G	337	Total	O	0	0
			337	337		
8	H	320	Total	O	0	0
			320	320		

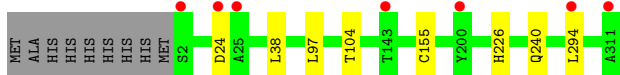
3 Residue-property plots [i](#)

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: Catechol 1,2-dioxygenase



- Molecule 1: Catechol 1,2-dioxygenase



- Molecule 1: Catechol 1,2-dioxygenase



- Molecule 1: Catechol 1,2-dioxygenase



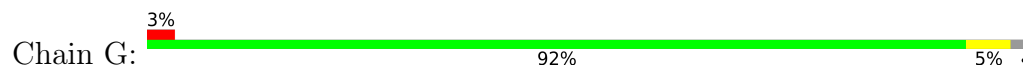
- Molecule 1: Catechol 1,2-dioxygenase



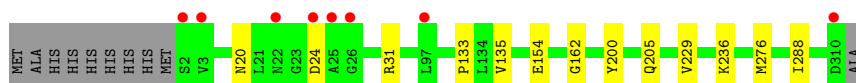
- Molecule 1: Catechol 1,2-dioxygenase



- Molecule 1: Catechol 1,2-dioxygenase



- Molecule 1: Catechol 1,2-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.97Å 86.27Å 110.16Å 106.04° 96.74° 113.15°	Depositor
Resolution (Å)	51.99 – 1.71 51.99 – 1.71	Depositor EDS
% Data completeness (in resolution range)	96.4 (51.99-1.71) 96.4 (51.99-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.71Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5156: ???)	Depositor
R, R_{free}	0.151 , 0.183 0.159 , 0.189	Depositor DCC
R_{free} test set	14082 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22348	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.87% 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: PEG, PGE, 12P, ZN, PG4, ACT

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	0.32	0/2458	0.52	0/3336
1	B	0.32	0/2461	0.50	0/3342
1	C	0.29	0/2474	0.49	0/3356
1	D	0.33	0/2454	0.52	0/3331
1	E	0.34	0/2445	0.55	0/3320
1	F	0.30	0/2480	0.49	0/3365
1	G	0.34	0/2523	0.53	0/3424
1	H	0.34	0/2462	0.53	0/3342
All	All	0.32	0/19757	0.52	0/26816

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2401	0	2331	9	0
1	B	2402	0	2345	4	0
1	C	2408	0	2353	9	0
1	D	2395	0	2337	9	0
1	E	2383	0	2335	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2417	0	2363	6	0
1	G	2457	0	2396	9	0
1	H	2399	0	2345	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	74	0	100	0	0
3	C	74	0	100	0	0
3	F	74	0	100	0	0
3	G	37	0	50	0	0
3	H	37	0	50	0	0
4	A	13	0	18	1	0
4	B	13	0	18	0	0
4	C	13	0	18	1	0
4	D	13	0	18	0	0
4	E	13	0	18	0	0
4	F	13	0	18	0	0
4	G	13	0	18	0	0
4	H	13	0	18	2	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
5	C	8	0	6	1	0
5	D	8	0	6	0	0
5	E	8	0	6	0	0
5	F	8	0	6	0	0
5	G	8	0	6	0	0
5	H	8	0	6	0	0
6	A	10	0	14	0	0
6	B	10	0	14	0	0
6	C	10	0	14	0	0
6	D	10	0	14	0	0
6	E	10	0	14	0	0
6	F	10	0	14	0	0
6	G	10	0	14	0	0
6	H	10	0	14	0	0
7	E	7	0	10	0	0
7	H	7	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	333	0	0	2	0
8	B	298	0	0	0	0
8	C	282	0	0	2	0
8	D	304	0	0	0	0
8	E	353	0	0	1	0
8	F	293	0	0	1	0
8	G	337	0	0	1	0
8	H	320	0	0	1	0
All	All	22348	0	19529	67	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 (67) 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:78:ILE:HD13	1:D:38:LEU:HD11	1.58	0.83
4:C:404:PG4:O5	5:C:405:ACT:H2	1.87	0.74
1:B:104:THR:HG21	1:B:240:GLN:HG2	1.80	0.62
1:F:303[B]:HIS:ND1	8:F:501:HOH:O	2.32	0.60
1:E:104:THR:HG21	1:E:240:GLN:HG2	1.84	0.59
1:D:104:THR:HG21	1:D:240:GLN:HG2	1.83	0.59
1:E:135:VAL:HG23	1:E:276:MET:HE2	1.87	0.56
1:A:104:THR:HG21	1:A:240:GLN:HG2	1.87	0.56
1:A:200[B]:TYR:HB2	8:A:615:HOH:O	2.09	0.53
1:F:162:GLY:HA3	1:F:200[B]:TYR:HB3	1.90	0.53
1:G:229:VAL:HG21	1:G:288:ILE:HD13	1.91	0.53
1:E:133:PRO:HB2	1:E:276:MET:HE3	1.92	0.51
1:E:162:GLY:HA3	1:E:200[B]:TYR:HB3	1.91	0.51
1:E:104:THR:HG22	1:E:239:THR:HA	1.93	0.51
1:C:162:GLY:HA3	1:C:200[B]:TYR:HB3	1.93	0.50
1:C:74:LEU:O	1:C:78:ILE:HG13	2.12	0.50
1:H:133:PRO:HB2	1:H:276:MET:HE3	1.94	0.49
1:C:93:ARG:NH2	8:C:505:HOH:O	2.45	0.49
1:B:97:LEU:HD11	1:B:294:LEU:HB2	1.95	0.49
1:H:135:VAL:HG23	1:H:276:MET:HE2	1.94	0.48
1:C:118:ASP:OD1	1:C:183:ARG:NH1	2.41	0.48
1:G:133:PRO:HB2	1:G:276:MET:HE3	1.95	0.48
1:H:20:ASN:O	1:H:31:ARG:HD2	2.14	0.47
1:C:133:PRO:HB2	1:C:276[A]:MET:HE3	1.97	0.47
1:H:162:GLY:HA3	1:H:200[B]:TYR:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200[B]:TYR:HB2	8:C:657:HOH:O	2.15	0.47
1:A:162:GLY:HA3	1:A:200[B]:TYR:HB3	1.97	0.46
1:C:310:ASP:O	1:C:311:ALA:HB2	2.16	0.46
1:G:311:ALA:HB3	8:G:545:HOH:O	2.15	0.46
1:D:229:VAL:HG21	1:D:288:ILE:HD13	1.98	0.45
1:B:155:CYS:HA	1:B:226:HIS:O	2.17	0.45
1:H:154[B]:GLU:OE2	4:H:403:PG4:H62	2.16	0.45
1:E:200[B]:TYR:N	8:E:509:HOH:O	2.49	0.45
1:E:162:GLY:CA	1:E:200[B]:TYR:HB3	2.47	0.45
1:H:236:LYS:NZ	4:H:403:PG4:O5	2.50	0.44
1:E:117:ARG:HD2	1:E:121:ALA:HA	2.00	0.44
1:G:174[A]:THR:HG22	1:G:175:ALA:N	2.31	0.44
1:F:133:PRO:HB2	1:F:276:MET:HE3	2.00	0.43
1:H:229:VAL:HG21	1:H:288:ILE:HD13	2.00	0.43
1:D:155:CYS:HA	1:D:226:HIS:O	2.17	0.43
1:A:78:ILE:HD13	1:B:38:LEU:HD11	1.99	0.43
1:G:162:GLY:HA3	1:G:200[B]:TYR:HB3	2.00	0.43
1:D:48:LEU:N	1:D:48:LEU:HD12	2.33	0.43
1:A:154[B]:GLU:OE2	4:A:404:PG4:H62	2.18	0.43
1:D:74:LEU:O	1:D:78:ILE:HG13	2.18	0.42
1:A:48:LEU:HD12	1:A:48:LEU:N	2.34	0.42
1:E:229:VAL:HG21	1:E:288:ILE:HD13	2.02	0.42
1:G:203:PRO:HA	1:G:204:PRO:HD3	1.94	0.42
1:D:198[A]:VAL:HG12	1:D:199[A]:GLY:N	2.34	0.42
1:G:104:THR:HG21	1:G:240:GLN:HG2	2.02	0.42
1:G:16:LYS:HD3	1:G:22:ASN:OD1	2.20	0.42
1:H:24:ASP:OD1	1:H:24:ASP:N	2.52	0.41
1:A:222:PRO:HB2	8:A:648:HOH:O	2.20	0.41
1:F:6:PHE:CD2	1:F:43[A]:LYS:HD3	2.55	0.41
1:H:200[B]:TYR:HB2	8:H:587:HOH:O	2.20	0.41
1:A:98:ASP:OD1	1:A:98:ASP:N	2.53	0.41
1:F:104:THR:CG2	1:F:261:LEU:CD1	2.99	0.41
1:F:154:GLU:O	1:F:227:PHE:HA	2.20	0.41
1:A:174:THR:HG22	1:A:175:ALA:N	2.36	0.41
1:D:203:PRO:HA	1:D:204:PRO:HD3	1.98	0.41
1:D:162:GLY:HA3	1:D:200[B]:TYR:HB3	2.02	0.41
1:G:155:CYS:HA	1:G:226:HIS:O	2.21	0.41
1:E:155:CYS:HA	1:E:226:HIS:O	2.20	0.40
1:C:78:ILE:HD12	1:C:80:LEU:H	1.87	0.40
1:E:74:LEU:O	1:E:78:ILE:HG13	2.21	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	315/319 (99%)	308 (98%)	7 (2%)	0	100	100
1	B	316/319 (99%)	312 (99%)	4 (1%)	0	100	100
1	C	317/319 (99%)	311 (98%)	6 (2%)	0	100	100
1	D	315/319 (99%)	309 (98%)	6 (2%)	0	100	100
1	E	314/319 (98%)	307 (98%)	7 (2%)	0	100	100
1	F	318/319 (100%)	312 (98%)	6 (2%)	0	100	100
1	G	324/319 (102%)	316 (98%)	8 (2%)	0	100	100
1	H	316/319 (99%)	310 (98%)	6 (2%)	0	100	100
All	All	2535/2552 (99%)	2485 (98%)	50 (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	243/246 (99%)	239 (98%)	4 (2%)	55	34
1	B	244/246 (99%)	243 (100%)	1 (0%)	84	76
1	C	245/246 (100%)	244 (100%)	1 (0%)	84	76
1	D	243/246 (99%)	242 (100%)	1 (0%)	84	76
1	E	243/246 (99%)	242 (100%)	1 (0%)	84	76
1	F	246/246 (100%)	246 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	250/246 (102%)	250 (100%)	0	100	100
1	H	245/246 (100%)	244 (100%)	1 (0%)	84	76
All	All	1959/1968 (100%)	1950 (100%)	9 (0%)	84	71

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10[A]	GLU
1	A	10[B]	GLU
1	A	127	ASP
1	A	146	LYS
1	B	24	ASP
1	C	4	LYS
1	D	16	LYS
1	E	205	GLN
1	H	205	GLN

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

Mol	Chain	Res	Type
1	A	32	GLN
1	D	264	HIS
1	E	210	GLN
1	F	210	GLN
1	G	210	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 50 ligands modelled in this entry, 8 are monoatomic - leaving 42 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	$\# Z > 2$
6	PGE	B	405	-	9,9,9	0.34	0	8,8,8	0.46	0
5	ACT	C	405	-	3,3,3	1.21	0	3,3,3	1.06	0
3	12P	A	402	-	36,36,36	0.30	0	35,35,35	0.34	0
7	PEG	E	405	-	6,6,6	0.28	0	5,5,5	0.24	0
6	PGE	G	406	-	9,9,9	0.36	0	8,8,8	0.57	0
4	PG4	G	403	-	12,12,12	0.32	0	11,11,11	0.22	0
5	ACT	H	404	-	3,3,3	0.98	0	3,3,3	1.57	1 (33%)
3	12P	G	402	-	36,36,36	0.29	0	35,35,35	0.43	0
4	PG4	B	402	-	12,12,12	0.32	0	11,11,11	0.15	0
5	ACT	C	406[A]	2	3,3,3	1.30	0	3,3,3	0.93	0
3	12P	H	402	-	36,36,36	0.29	0	35,35,35	0.40	0
4	PG4	D	402	-	12,12,12	0.29	0	11,11,11	0.22	0
5	ACT	F	406[A]	2	3,3,3	1.16	0	3,3,3	1.15	0
5	ACT	F	405	-	3,3,3	1.06	0	3,3,3	1.45	0
4	PG4	H	403	-	12,12,12	0.34	0	11,11,11	0.27	0
5	ACT	D	403	-	3,3,3	1.03	0	3,3,3	1.57	1 (33%)
6	PGE	E	406	-	9,9,9	0.39	0	8,8,8	0.54	0
3	12P	C	402	-	36,36,36	0.30	0	35,35,35	0.52	0
6	PGE	D	405	-	9,9,9	0.36	0	8,8,8	0.57	0
4	PG4	F	404	-	12,12,12	0.31	0	11,11,11	0.18	0
5	ACT	E	403	-	3,3,3	1.05	0	3,3,3	1.62	1 (33%)
3	12P	C	403	-	36,36,36	0.30	0	35,35,35	0.38	0
5	ACT	G	404	-	3,3,3	1.01	0	3,3,3	1.67	1 (33%)
5	ACT	E	404[A]	2	3,3,3	1.20	0	3,3,3	0.93	0
6	PGE	C	407	-	9,9,9	0.33	0	8,8,8	0.49	0
3	12P	A	403	-	36,36,36	0.30	0	35,35,35	0.33	0
3	12P	F	403	-	36,36,36	0.31	0	35,35,35	0.31	0
6	PGE	A	407	-	9,9,9	0.33	0	8,8,8	0.49	0
3	12P	F	402	-	36,36,36	0.30	0	35,35,35	0.35	0
4	PG4	C	404	-	12,12,12	0.33	0	11,11,11	0.26	0
5	ACT	G	405[A]	2	3,3,3	1.32	0	3,3,3	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PEG	H	406	-	6,6,6	0.25	0	5,5,5	0.26	0
6	PGE	H	407	-	9,9,9	0.36	0	8,8,8	0.42	0
5	ACT	H	405[A]	2	3,3,3	1.23	0	3,3,3	0.98	0
4	PG4	A	404	-	12,12,12	0.33	0	11,11,11	0.29	0
5	ACT	A	405	-	3,3,3	0.98	0	3,3,3	1.61	1 (33%)
5	ACT	D	404[A]	2	3,3,3	1.20	0	3,3,3	0.93	0
5	ACT	A	406[A]	2	3,3,3	1.27	0	3,3,3	0.86	0
5	ACT	B	403	-	3,3,3	1.00	0	3,3,3	1.53	1 (33%)
6	PGE	F	407	-	9,9,9	0.32	0	8,8,8	0.45	0
4	PG4	E	402	-	12,12,12	0.35	0	11,11,11	0.27	0
5	ACT	B	404[A]	2	3,3,3	1.16	0	3,3,3	0.94	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
6	PGE	B	405	-	-	2/7/7/7	-
3	12P	A	402	-	-	16/34/34/34	-
7	PEG	E	405	-	-	2/4/4/4	-
6	PGE	G	406	-	-	3/7/7/7	-
4	PG4	G	403	-	-	1/10/10/10	-
3	12P	G	402	-	-	14/34/34/34	-
4	PG4	B	402	-	-	2/10/10/10	-
3	12P	H	402	-	-	18/34/34/34	-
4	PG4	D	402	-	-	1/10/10/10	-
4	PG4	H	403	-	-	3/10/10/10	-
6	PGE	E	406	-	-	2/7/7/7	-
3	12P	C	402	-	-	16/34/34/34	-
6	PGE	D	405	-	-	0/7/7/7	-
4	PG4	F	404	-	-	1/10/10/10	-
3	12P	C	403	-	-	16/34/34/34	-
3	12P	A	403	-	-	21/34/34/34	-
3	12P	F	403	-	-	18/34/34/34	-
6	PGE	A	407	-	-	4/7/7/7	-
3	12P	F	402	-	-	17/34/34/34	-
4	PG4	C	404	-	-	2/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	H	406	-	-	2/4/4/4	-
6	PGE	H	407	-	-	0/7/7/7	-
4	PG4	A	404	-	-	2/10/10/10	-
6	PGE	F	407	-	-	1/7/7/7	-
4	PG4	E	402	-	-	2/10/10/10	-
6	PGE	C	407	-	-	2/7/7/7	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	404	ACT	O-C-CH3	-2.28	113.19	122.53
5	E	403	ACT	O-C-CH3	-2.20	113.50	122.53
5	A	405	ACT	O-C-CH3	-2.17	113.61	122.53
5	H	404	ACT	O-C-CH3	-2.14	113.77	122.53
5	D	403	ACT	O-C-CH3	-2.12	113.83	122.53
5	B	403	ACT	O-C-CH3	-2.04	114.17	122.53

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	12P	C24-C23-O22-C21
3	C	403	12P	O19-C20-C21-O22
3	C	403	12P	O31-C32-C33-O34
3	C	403	12P	O22-C23-C24-O25
3	G	402	12P	O19-C20-C21-O22
3	H	402	12P	O19-C20-C21-O22
3	A	402	12P	O19-C20-C21-O22
3	C	402	12P	O31-C32-C33-O34
3	G	402	12P	O22-C23-C24-O25
3	H	402	12P	O22-C23-C24-O25
3	A	402	12P	O16-C17-C18-O19
3	F	403	12P	O4-C5-C6-O7
3	H	402	12P	O31-C32-C33-O34
3	A	402	12P	O34-C35-C36-O37
3	A	403	12P	O34-C35-C36-O37
3	A	402	12P	O22-C23-C24-O25
3	F	402	12P	O31-C32-C33-O34
3	F	403	12P	O31-C32-C33-O34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	403	12P	O19-C20-C21-O22
3	F	402	12P	O19-C20-C21-O22
3	A	402	12P	O31-C32-C33-O34
3	F	403	12P	O22-C23-C24-O25
3	C	403	12P	O4-C5-C6-O7
3	F	402	12P	O22-C23-C24-O25
3	A	402	12P	O4-C5-C6-O7
3	F	403	12P	O16-C17-C18-O19
3	A	403	12P	O1-C2-C3-O4
3	C	402	12P	O34-C35-C36-O37
3	H	402	12P	O1-C2-C3-O4
6	G	406	PGE	O1-C1-C2-O2
7	E	405	PEG	O1-C1-C2-O2
3	A	403	12P	O22-C23-C24-O25
3	A	403	12P	O31-C32-C33-O34
3	G	402	12P	O16-C17-C18-O19
3	G	402	12P	O31-C32-C33-O34
3	F	403	12P	O34-C35-C36-O37
3	H	402	12P	O4-C5-C6-O7
3	F	402	12P	O16-C17-C18-O19
3	A	403	12P	O4-C5-C6-O7
3	A	402	12P	O1-C2-C3-O4
3	H	402	12P	O34-C35-C36-O37
3	A	403	12P	O19-C20-C21-O22
3	F	402	12P	O4-C5-C6-O7
3	A	403	12P	O16-C17-C18-O19
3	C	402	12P	C21-C20-O19-C18
3	C	403	12P	O16-C17-C18-O19
3	H	402	12P	O16-C17-C18-O19
3	C	403	12P	O34-C35-C36-O37
3	F	402	12P	O34-C35-C36-O37
4	H	403	PG4	O1-C1-C2-O2
3	C	402	12P	O16-C17-C18-O19
7	H	406	PEG	O2-C3-C4-O4
3	C	402	12P	O4-C5-C6-O7
3	F	403	12P	C24-C23-O22-C21
4	C	404	PG4	O2-C3-C4-O3
4	A	404	PG4	O2-C3-C4-O3
3	H	402	12P	O7-C8-C9-O10
3	H	402	12P	O10-C11-C12-O13
3	F	402	12P	O1-C2-C3-O4
3	F	403	12P	C33-C32-O31-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	402	PG4	C3-C4-O3-C5
3	A	403	12P	O7-C8-C9-O10
3	A	402	12P	C14-C15-O16-C17
6	E	406	PGE	C1-C2-O2-C3
3	C	403	12P	C20-C21-O22-C23
3	A	403	12P	C20-C21-O22-C23
3	H	402	12P	C12-C11-O10-C9
3	H	402	12P	C20-C21-O22-C23
3	G	402	12P	C14-C15-O16-C17
6	C	407	PGE	C1-C2-O2-C3
6	A	407	PGE	C1-C2-O2-C3
3	A	402	12P	C36-C35-O34-C33
4	H	403	PG4	C3-C4-O3-C5
3	F	403	12P	C36-C35-O34-C33
3	F	403	12P	C29-C30-O31-C32
3	F	402	12P	C36-C35-O34-C33
3	C	402	12P	O1-C2-C3-O4
3	C	403	12P	O1-C2-C3-O4
6	F	407	PGE	O3-C5-C6-O4
7	E	405	PEG	O2-C3-C4-O4
3	A	402	12P	C20-C21-O22-C23
3	H	402	12P	C36-C35-O34-C33
6	E	406	PGE	C4-C3-O2-C2
3	A	402	12P	C33-C32-O31-C30
3	G	402	12P	C20-C21-O22-C23
3	F	403	12P	C14-C15-O16-C17
3	A	403	12P	C14-C15-O16-C17
3	C	402	12P	C36-C35-O34-C33
6	G	406	PGE	C4-C3-O2-C2
3	C	402	12P	C14-C15-O16-C17
3	F	402	12P	C12-C11-O10-C9
3	G	402	12P	C12-C11-O10-C9
3	C	403	12P	C12-C11-O10-C9
3	F	402	12P	C20-C21-O22-C23
3	G	402	12P	C33-C32-O31-C30
4	D	402	PG4	O2-C3-C4-O3
3	A	402	12P	C12-C11-O10-C9
3	A	402	12P	O10-C11-C12-O13
3	F	403	12P	O1-C2-C3-O4
3	G	402	12P	O1-C2-C3-O4
6	A	407	PGE	O3-C5-C6-O4
4	H	403	PG4	O2-C3-C4-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	402	12P	C36-C35-O34-C33
3	H	402	12P	C33-C32-O31-C30
3	H	402	12P	C14-C15-O16-C17
3	C	402	12P	C12-C11-O10-C9
3	A	403	12P	C33-C32-O31-C30
4	B	402	PG4	O2-C3-C4-O3
3	F	402	12P	C14-C15-O16-C17
3	C	403	12P	C14-C15-O16-C17
7	H	406	PEG	O1-C1-C2-O2
3	A	403	12P	C36-C35-O34-C33
4	C	404	PG4	C6-C5-O3-C4
3	A	402	12P	O13-C14-C15-O16
3	A	402	12P	C24-C23-O22-C21
3	F	403	12P	C20-C21-O22-C23
3	A	403	12P	C12-C11-O10-C9
4	A	404	PG4	C3-C4-O3-C5
4	G	403	PG4	C3-C4-O3-C5
3	A	403	12P	C29-C30-O31-C32
4	E	402	PG4	C3-C4-O3-C5
3	A	403	12P	C5-C6-O7-C8
3	F	402	12P	C29-C30-O31-C32
6	G	406	PGE	C1-C2-O2-C3
4	F	404	PG4	C3-C4-O3-C5
6	B	405	PGE	C1-C2-O2-C3
4	E	402	PG4	O2-C3-C4-O3
3	A	403	12P	O28-C29-C30-O31
3	C	402	12P	O10-C11-C12-O13
6	C	407	PGE	C4-C3-O2-C2
3	C	402	12P	C33-C32-O31-C30
3	C	403	12P	O10-C11-C12-O13
6	A	407	PGE	O2-C3-C4-O3
3	C	403	12P	C23-C24-O25-C26
3	G	402	12P	O4-C5-C6-O7
3	A	403	12P	C24-C23-O22-C21
3	H	402	12P	C32-C33-O34-C35
3	F	402	12P	O10-C11-C12-O13
3	C	403	12P	C33-C32-O31-C30
3	C	403	12P	O13-C14-C15-O16
3	F	403	12P	O10-C11-C12-O13
3	C	402	12P	C29-C30-O31-C32
3	F	403	12P	O13-C14-C15-O16
3	F	402	12P	C33-C32-O31-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	402	12P	C29-C30-O31-C32
3	G	402	12P	O7-C8-C9-O10
3	F	403	12P	C30-C29-O28-C27
3	A	403	12P	C26-C27-O28-C29
3	A	403	12P	O25-C26-C27-O28
3	H	402	12P	C29-C30-O31-C32
3	F	402	12P	O25-C26-C27-O28
3	C	402	12P	O13-C14-C15-O16
3	F	403	12P	O7-C8-C9-O10
3	F	402	12P	C30-C29-O28-C27
6	A	407	PGE	C4-C3-O2-C2
3	F	403	12P	O25-C26-C27-O28
3	H	402	12P	O13-C14-C15-O16
3	C	403	12P	O7-C8-C9-O10
6	B	405	PGE	O3-C5-C6-O4
3	A	403	12P	O10-C11-C12-O13
3	C	402	12P	C30-C29-O28-C27
3	A	403	12P	O13-C14-C15-O16
3	G	402	12P	O13-C14-C15-O16
3	H	402	12P	O25-C26-C27-O28
3	F	402	12P	O13-C14-C15-O16
3	C	402	12P	O25-C26-C27-O28
3	C	403	12P	O25-C26-C27-O28
3	G	402	12P	O25-C26-C27-O28

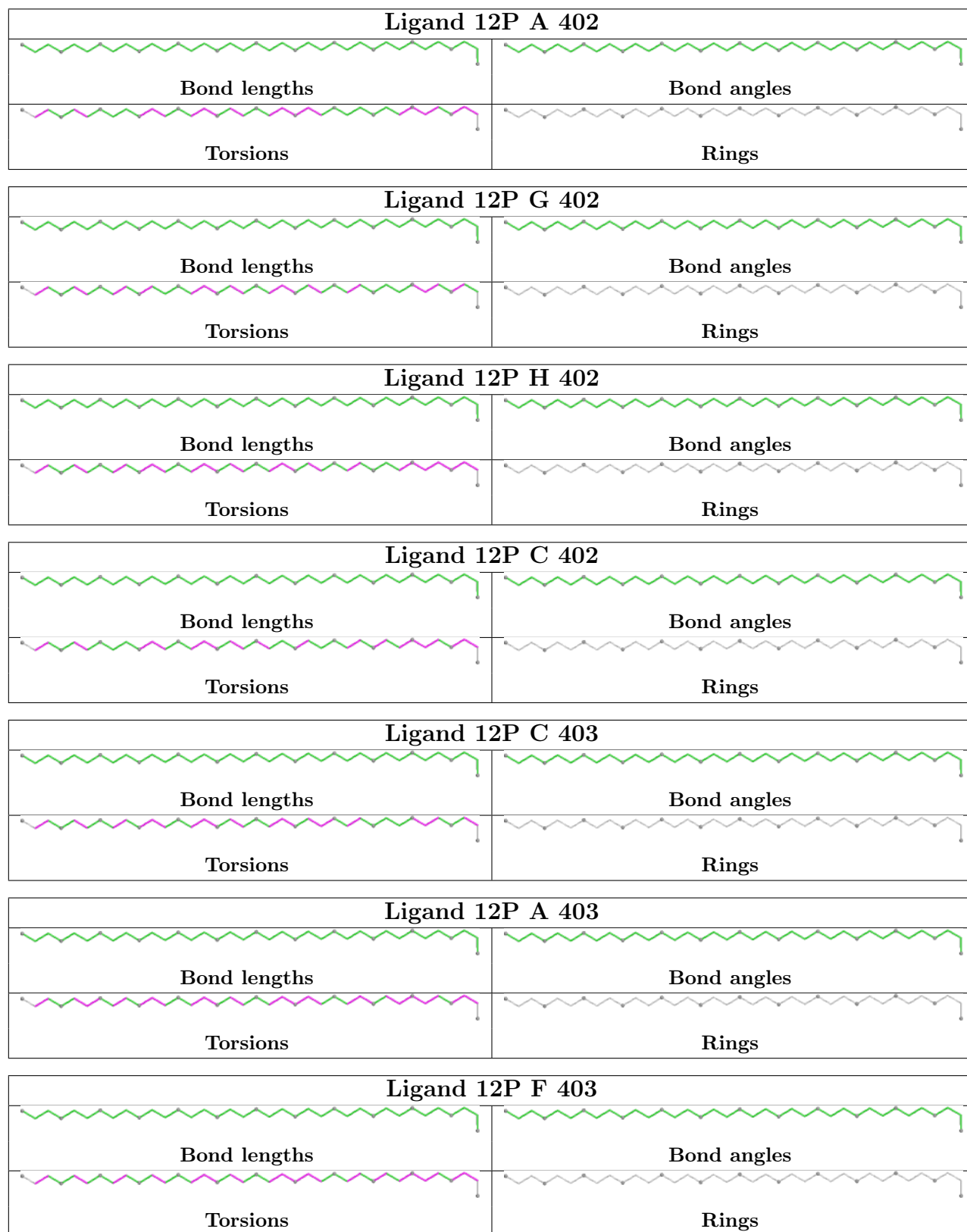
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	405	ACT	1	0
4	H	403	PG4	2	0
4	C	404	PG4	1	0
4	A	404	PG4	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 12P F 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	310/319 (97%)	-0.12	9 (2%)	53	62	10, 24, 46, 85	7 (2%)
1	B	310/319 (97%)	-0.17	7 (2%)	61	69	10, 24, 41, 75	8 (2%)
1	C	310/319 (97%)	-0.04	9 (2%)	53	62	11, 25, 49, 84	9 (2%)
1	D	310/319 (97%)	-0.17	6 (1%)	66	73	9, 23, 46, 97	7 (2%)
1	E	308/319 (96%)	-0.24	6 (1%)	66	73	9, 22, 40, 89	8 (2%)
1	F	310/319 (97%)	0.05	12 (3%)	43	51	11, 26, 54, 102	10 (3%)
1	G	310/319 (97%)	-0.17	9 (2%)	53	62	10, 22, 46, 87	16 (5%)
1	H	309/319 (96%)	-0.17	8 (2%)	57	65	10, 23, 45, 130	9 (2%)
All	All	2477/2552 (97%)	-0.13	66 (2%)	56	64	9, 23, 47, 130	74 (2%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	172[A]	ALA	9.8
1	C	311	ALA	5.5
1	G	311	ALA	5.1
1	H	25	ALA	4.9
1	F	294	LEU	4.3
1	G	97	LEU	4.1
1	F	311	ALA	4.0
1	A	311	ALA	3.9
1	H	24	ASP	3.8
1	F	25	ALA	3.7
1	B	294	LEU	3.6
1	F	24	ASP	3.6
1	E	2	SER	3.5
1	D	311	ALA	3.4
1	A	294	LEU	3.4
1	C	22	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	294	LEU	3.3
1	E	98	ASP	3.2
1	C	21	LEU	3.2
1	D	24	ASP	3.2
1	E	97	LEU	3.1
1	F	97	LEU	3.1
1	D	3	VAL	3.0
1	B	2	SER	2.9
1	F	95	ALA	2.9
1	H	26	GLY	2.9
1	E	143	THR	2.9
1	C	27	ASN	2.9
1	H	97	LEU	2.8
1	H	310	ASP	2.8
1	D	22	ASN	2.7
1	H	3	VAL	2.7
1	A	94	ALA	2.7
1	D	2	SER	2.6
1	H	22	ASN	2.6
1	G	2	SER	2.6
1	G	294	LEU	2.5
1	C	2	SER	2.5
1	F	26	GLY	2.4
1	B	311	ALA	2.4
1	H	2	SER	2.4
1	C	23	GLY	2.4
1	E	309	ALA	2.4
1	F	272	ALA	2.4
1	G	96	GLY	2.3
1	G	93	ARG	2.3
1	A	98	ASP	2.3
1	C	96	GLY	2.3
1	F	3	VAL	2.3
1	B	25	ALA	2.2
1	B	143	THR	2.2
1	B	24	ASP	2.2
1	A	97	LEU	2.2
1	D	21	LEU	2.2
1	G	295	ASP	2.1
1	B	200[A]	TYR	2.1
1	C	95	ALA	2.1
1	F	295	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	2.0
1	A	25	ALA	2.0
1	E	3	VAL	2.0
1	G	98	ASP	2.0
1	A	115	PRO	2.0
1	F	296	GLY	2.0
1	A	95	ALA	2.0
1	F	116	VAL	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
6	PGE	A	407	10/10	0.80	0.15	34,44,46,55	0
6	PGE	C	407	10/10	0.80	0.15	30,44,52,53	0
4	PG4	C	404	13/13	0.81	0.15	36,51,59,61	0
5	ACT	C	405	4/4	0.81	0.18	35,46,51,60	0
6	PGE	H	407	10/10	0.81	0.14	31,34,47,52	0
4	PG4	B	402	13/13	0.82	0.15	34,54,67,69	0
3	12P	F	403	37/37	0.83	0.14	34,48,63,69	0
5	ACT	D	403	4/4	0.83	0.17	27,32,39,39	0
5	ACT	G	404	4/4	0.83	0.16	31,37,39,41	0
3	12P	H	402	37/37	0.83	0.15	31,49,62,76	0
3	12P	C	402	37/37	0.83	0.14	31,51,60,65	0
6	PGE	E	406	10/10	0.83	0.14	29,46,50,60	0
6	PGE	G	406	10/10	0.83	0.15	30,40,54,57	0
3	12P	F	402	37/37	0.83	0.15	29,48,69,73	0
7	PEG	E	405	7/7	0.83	0.15	37,44,56,61	0

Continued on next page...

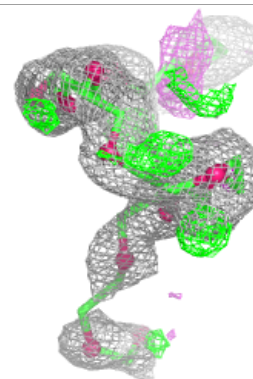
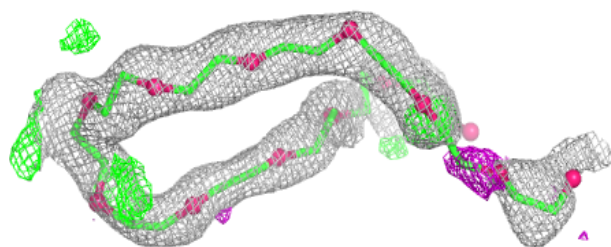
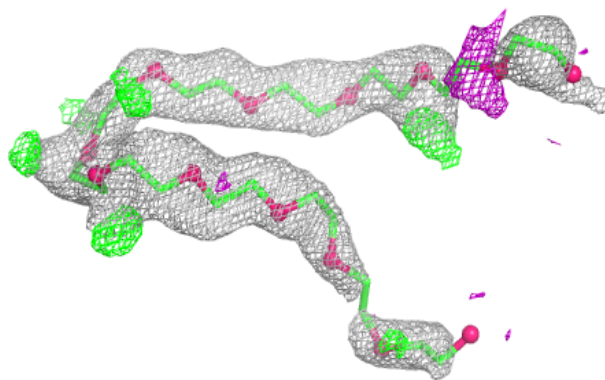
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PEG	H	406	7/7	0.83	0.17	45,49,56,66	0
5	ACT	A	406[A]	4/4	0.84	0.14	22,23,23,24	4
6	PGE	B	405	10/10	0.84	0.13	30,43,46,57	0
5	ACT	B	403	4/4	0.84	0.17	29,33,43,44	0
3	12P	A	403	37/37	0.84	0.15	34,51,62,76	0
3	12P	C	403	37/37	0.84	0.15	34,48,65,76	0
5	ACT	F	405	4/4	0.84	0.16	39,47,48,51	0
3	12P	G	402	37/37	0.84	0.15	28,49,63,70	0
5	ACT	G	405[A]	4/4	0.84	0.20	16,18,20,23	4
3	12P	A	402	37/37	0.85	0.14	29,48,60,74	0
5	ACT	H	404	4/4	0.85	0.16	29,31,42,43	0
4	PG4	A	404	13/13	0.85	0.15	33,53,70,71	0
5	ACT	F	406[A]	4/4	0.85	0.17	22,24,26,28	4
4	PG4	H	403	13/13	0.85	0.13	37,50,62,65	0
5	ACT	A	405	4/4	0.86	0.16	31,41,47,50	0
4	PG4	F	404	13/13	0.86	0.13	37,49,58,63	0
6	PGE	F	407	10/10	0.87	0.12	29,32,42,53	0
5	ACT	E	403	4/4	0.88	0.14	37,42,46,50	0
4	PG4	E	402	13/13	0.88	0.14	28,41,59,69	0
5	ACT	B	404[A]	4/4	0.88	0.25	17,21,22,24	4
4	PG4	D	402	13/13	0.89	0.12	34,41,54,57	0
4	PG4	G	403	13/13	0.89	0.13	29,42,63,65	0
6	PGE	D	405	10/10	0.89	0.11	25,35,39,47	0
5	ACT	C	406[A]	4/4	0.91	0.14	21,22,22,22	4
5	ACT	H	405[A]	4/4	0.91	0.15	17,20,24,24	4
5	ACT	E	404[A]	4/4	0.91	0.14	17,19,23,23	4
5	ACT	D	404[A]	4/4	0.91	0.18	15,18,21,24	4
2	ZN	B	401[A]	1/1	0.98	0.03	23,23,23,23	1
2	ZN	F	401[A]	1/1	0.98	0.06	28,28,28,28	1
2	ZN	A	401[A]	1/1	0.99	0.07	27,27,27,27	1
2	ZN	G	401[A]	1/1	0.99	0.05	23,23,23,23	1
2	ZN	H	401[A]	1/1	0.99	0.04	24,24,24,24	1
2	ZN	C	401[A]	1/1	0.99	0.09	29,29,29,29	1
2	ZN	D	401[A]	1/1	0.99	0.03	23,23,23,23	1
2	ZN	E	401[A]	1/1	1.00	0.09	24,24,24,24	1

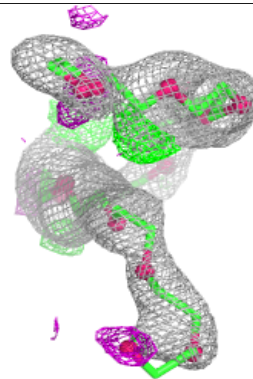
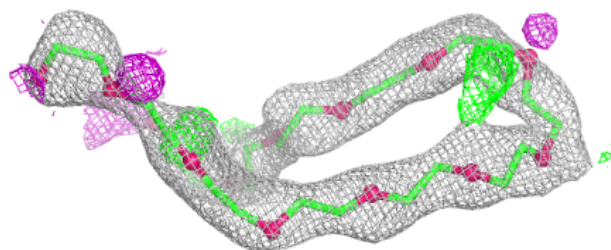
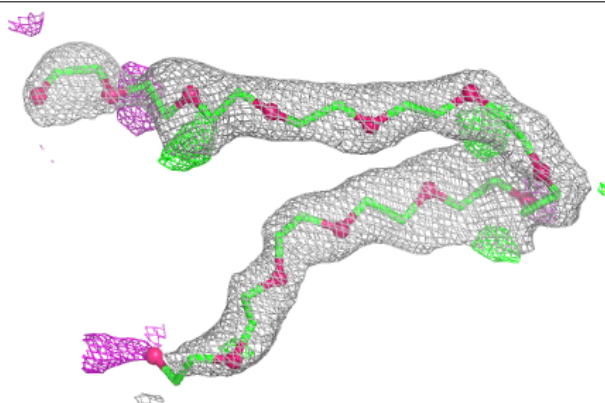
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 12P F 403:

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

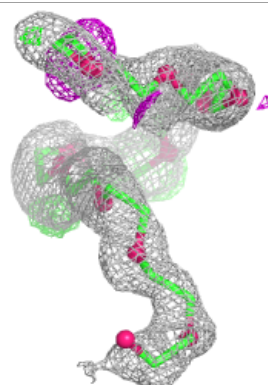
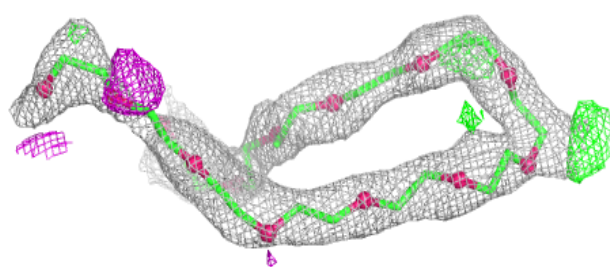
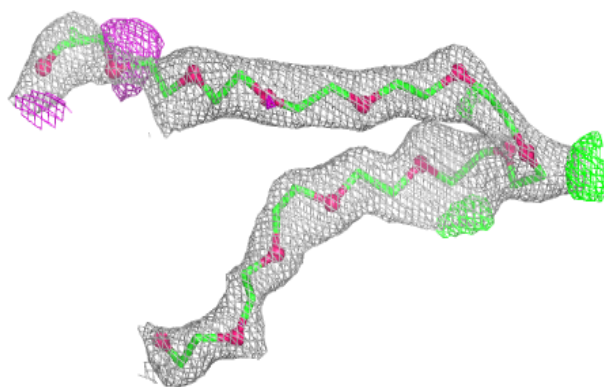
**Electron density around 12P H 402:**

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

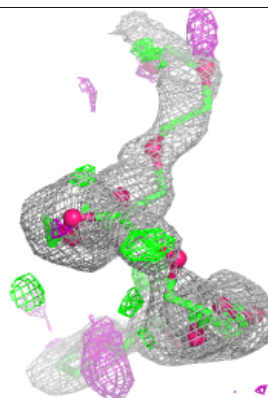
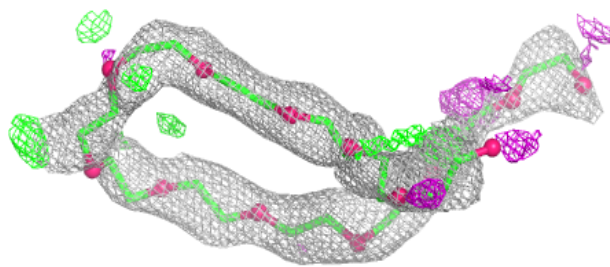
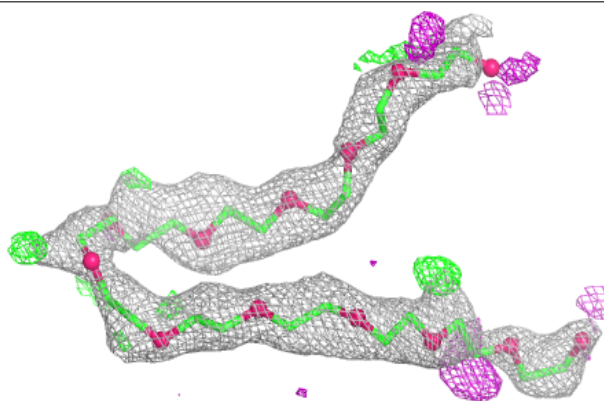


Electron density around 12P C 402:

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

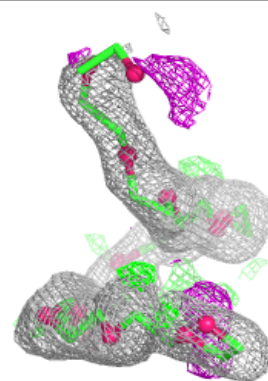
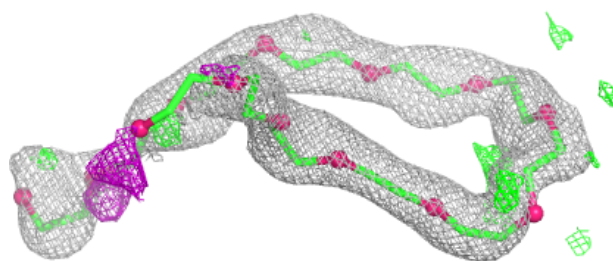
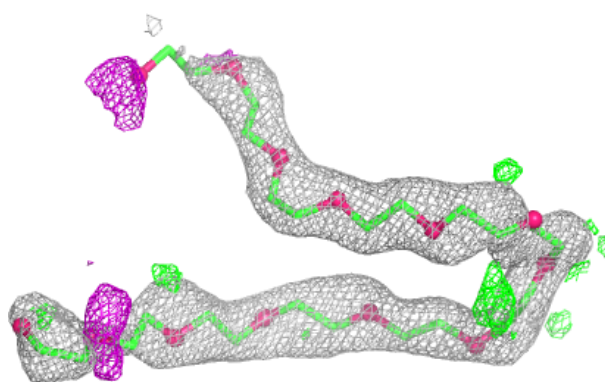
**Electron density around 12P F 402:**

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

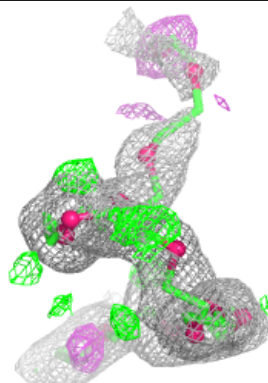
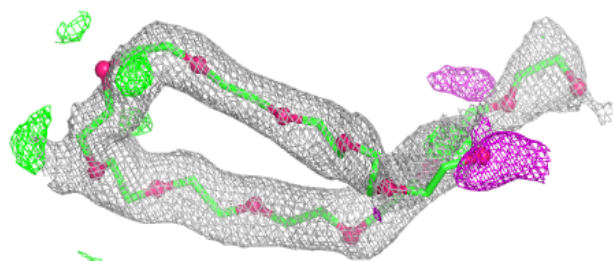
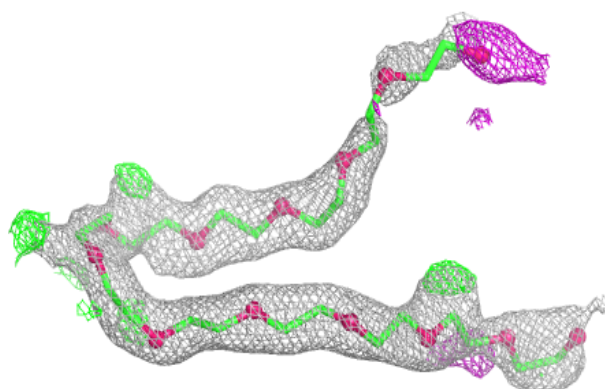


Electron density around 12P A 403:

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

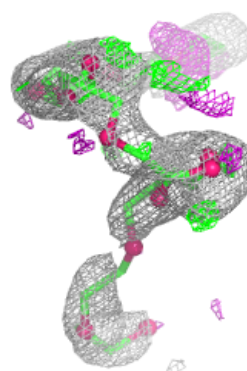
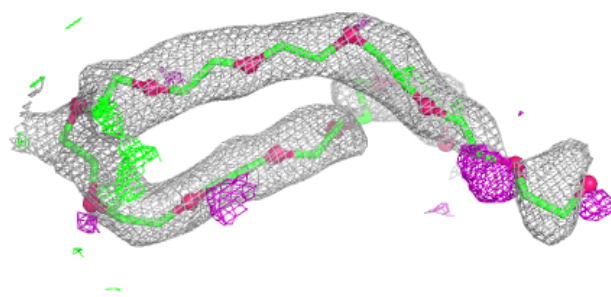
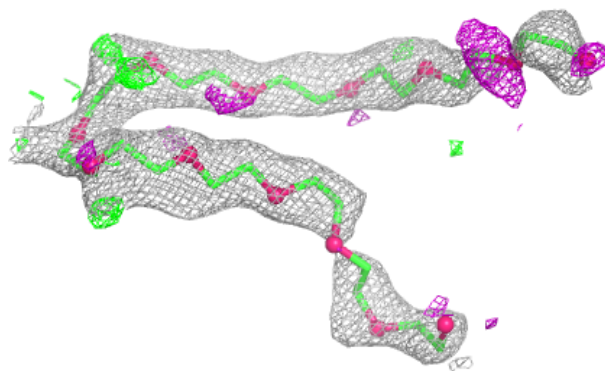
**Electron density around 12P C 403:**

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

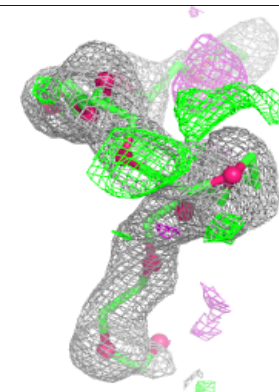
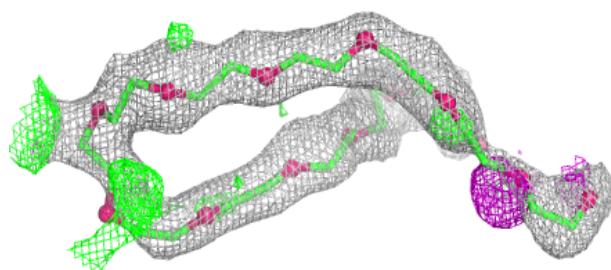
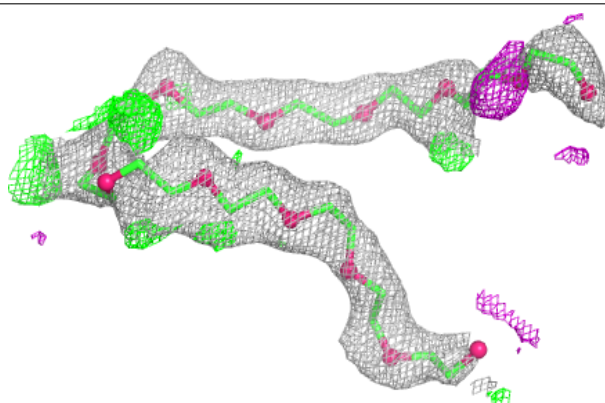


Electron density around 12P G 402:

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

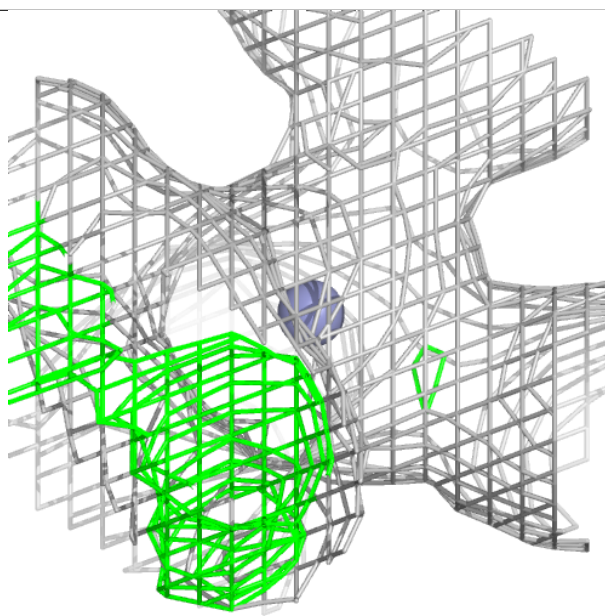
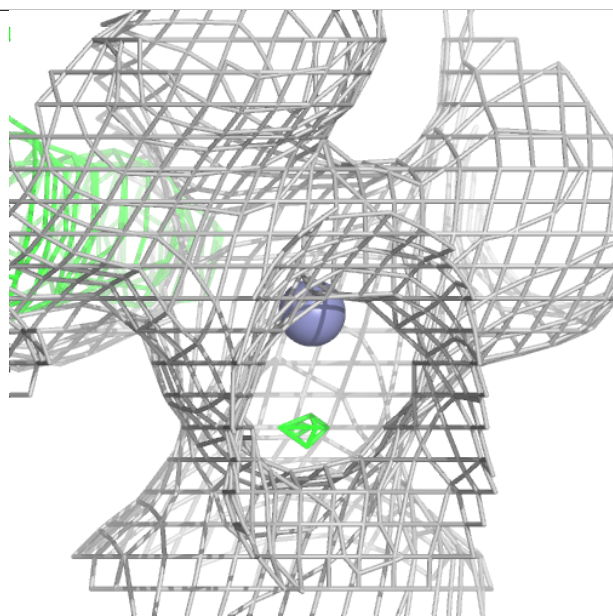
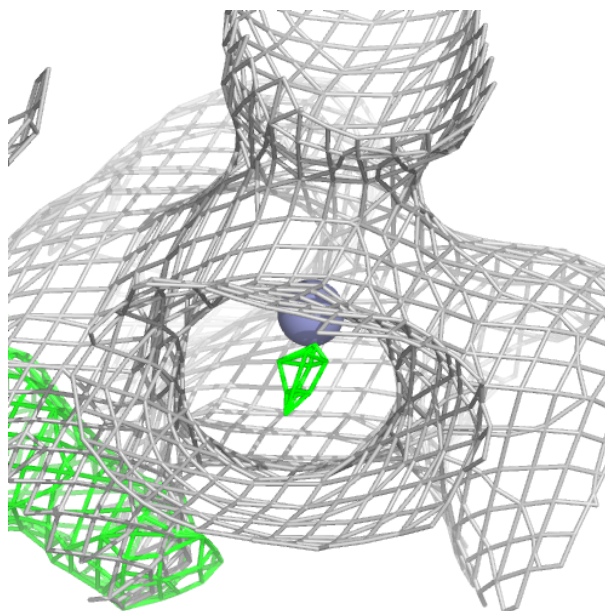
**Electron density around 12P A 402:**

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



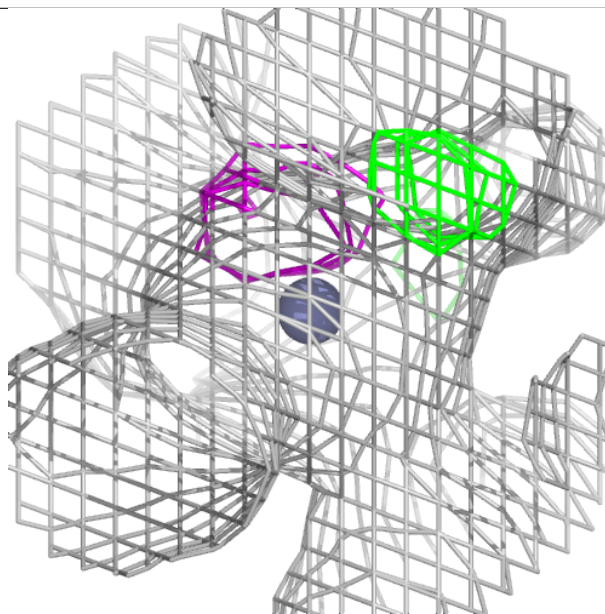
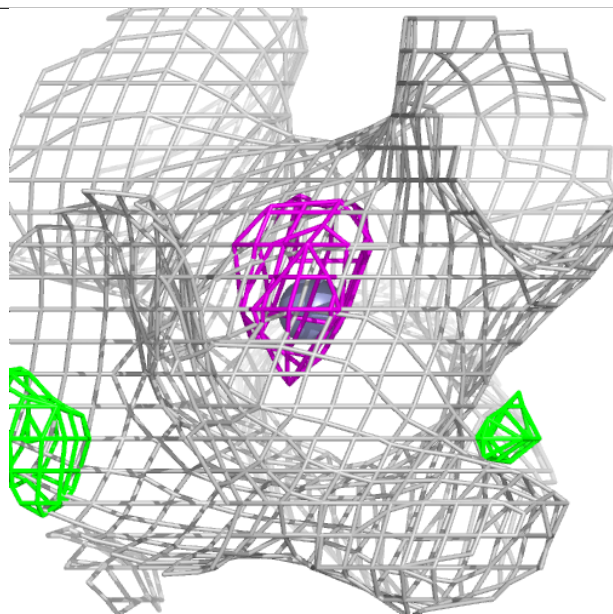
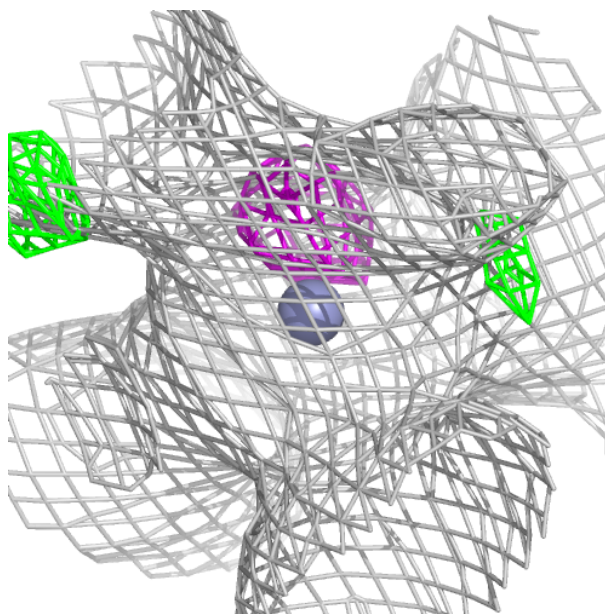
Electron density around ZN B 401 (A):

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



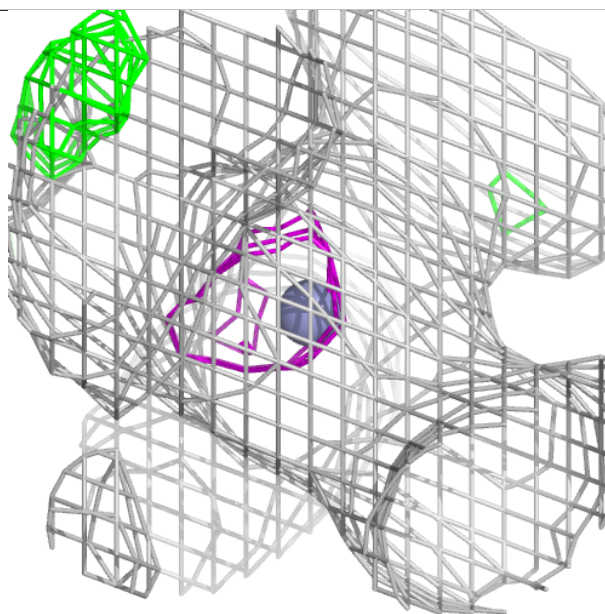
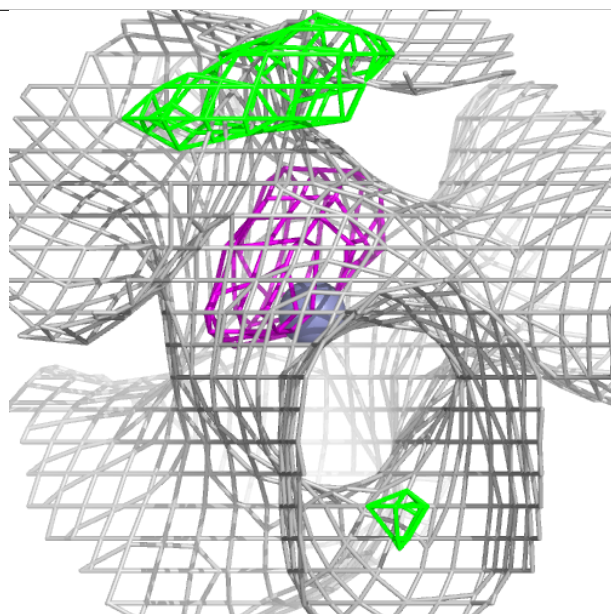
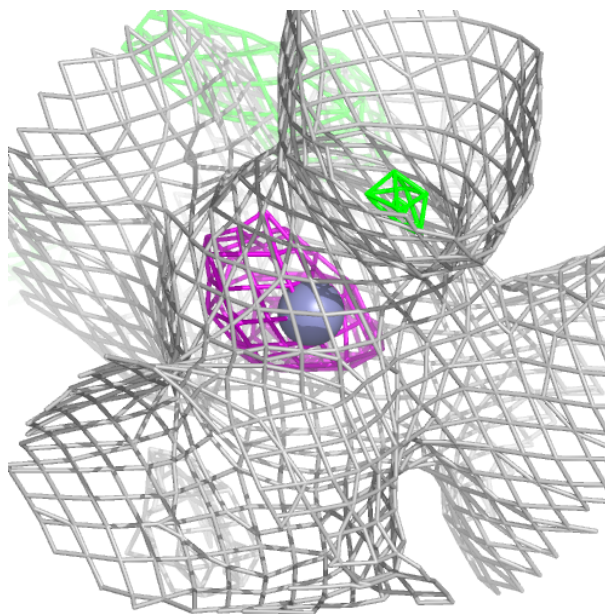
Electron density around ZN F 401 (A):

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



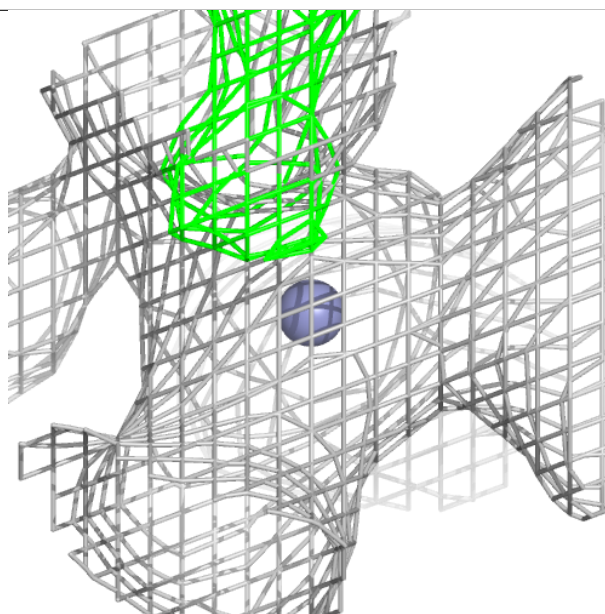
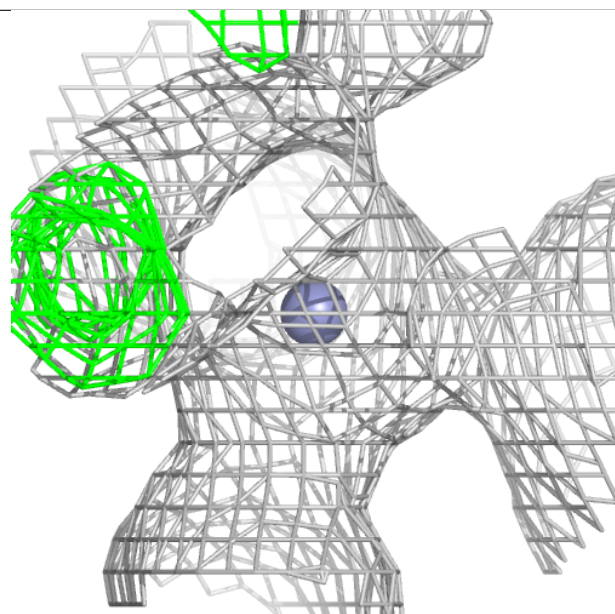
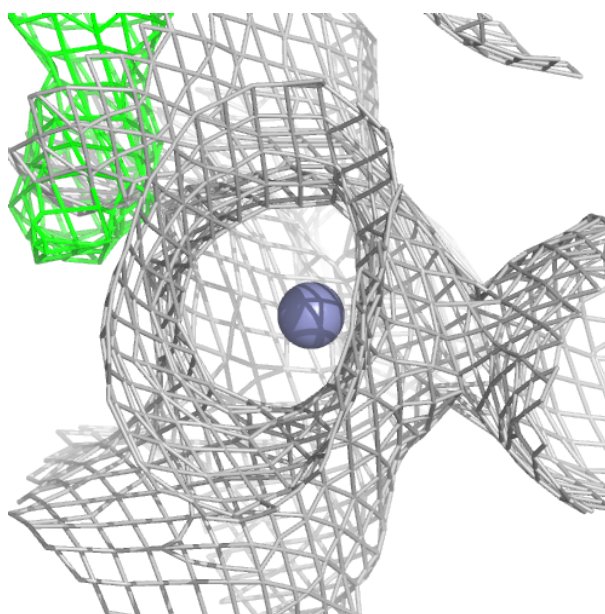
Electron density around ZN A 401 (A):

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



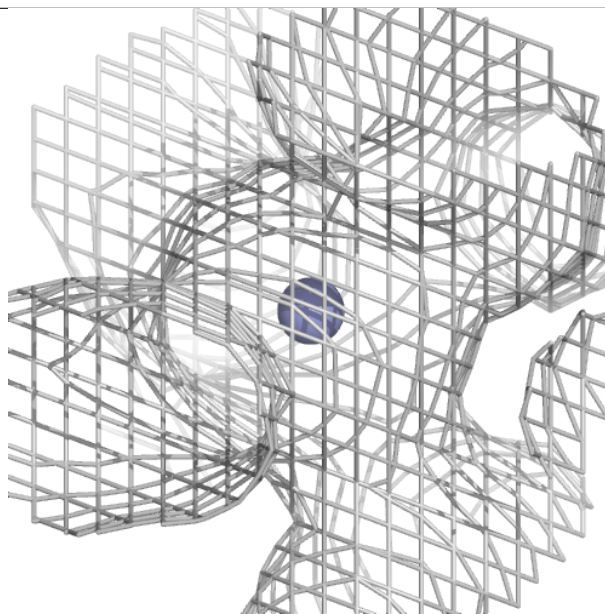
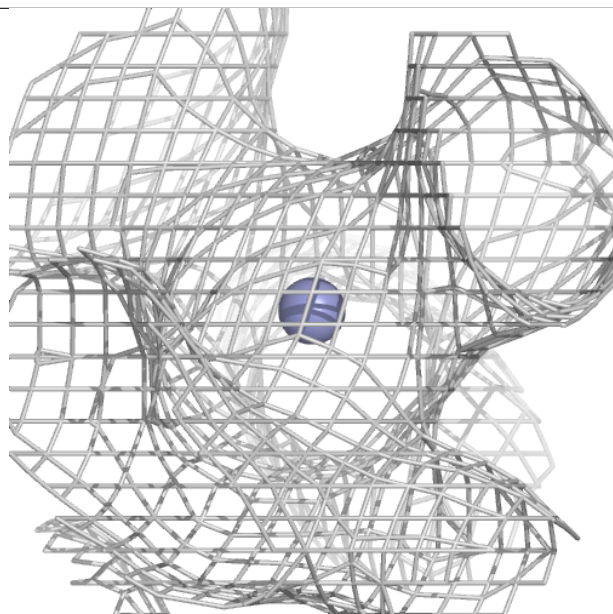
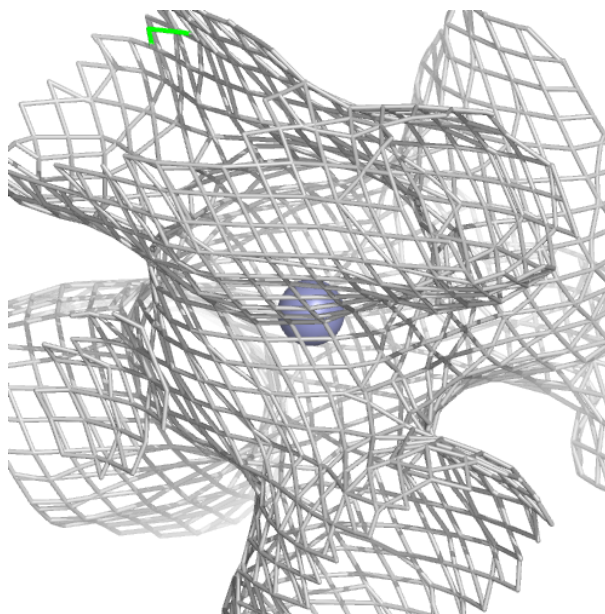
Electron density around ZN G 401 (A):

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



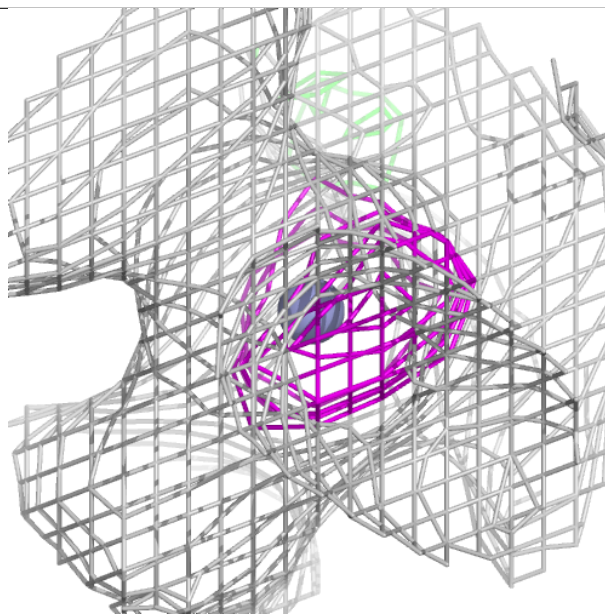
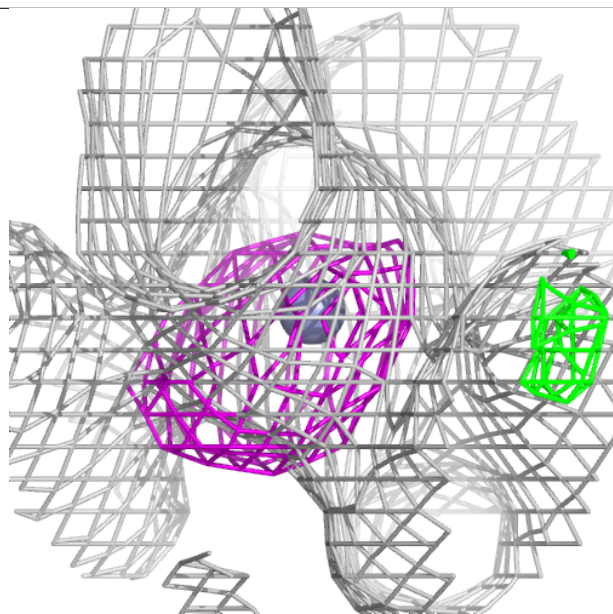
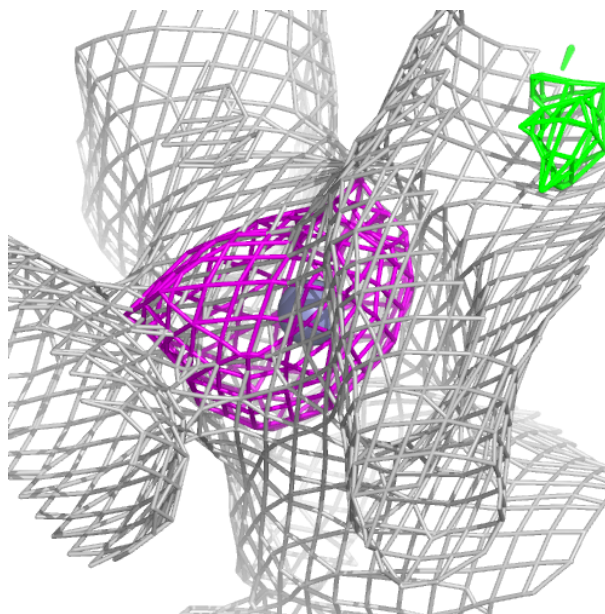
Electron density around ZN H 401 (A):

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



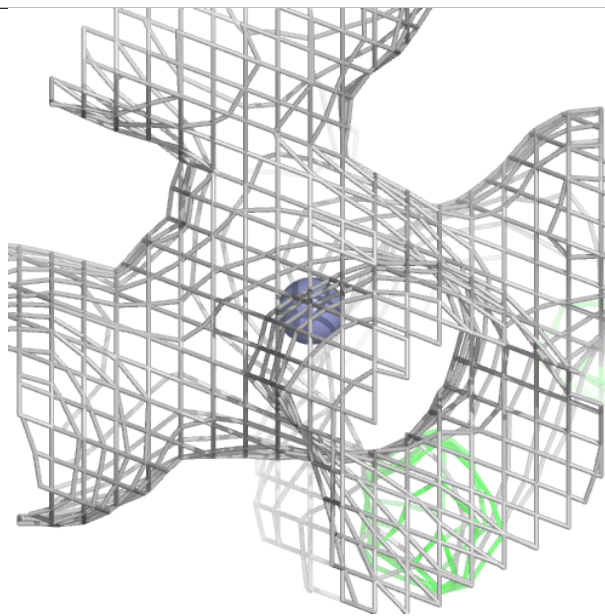
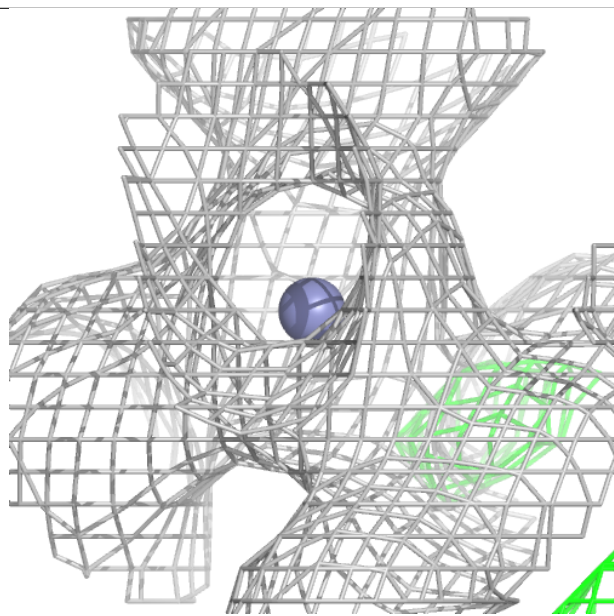
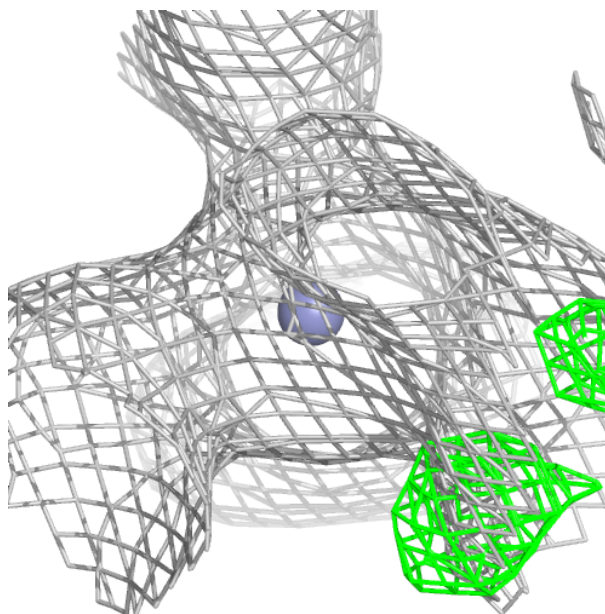
Electron density around ZN C 401 (A):

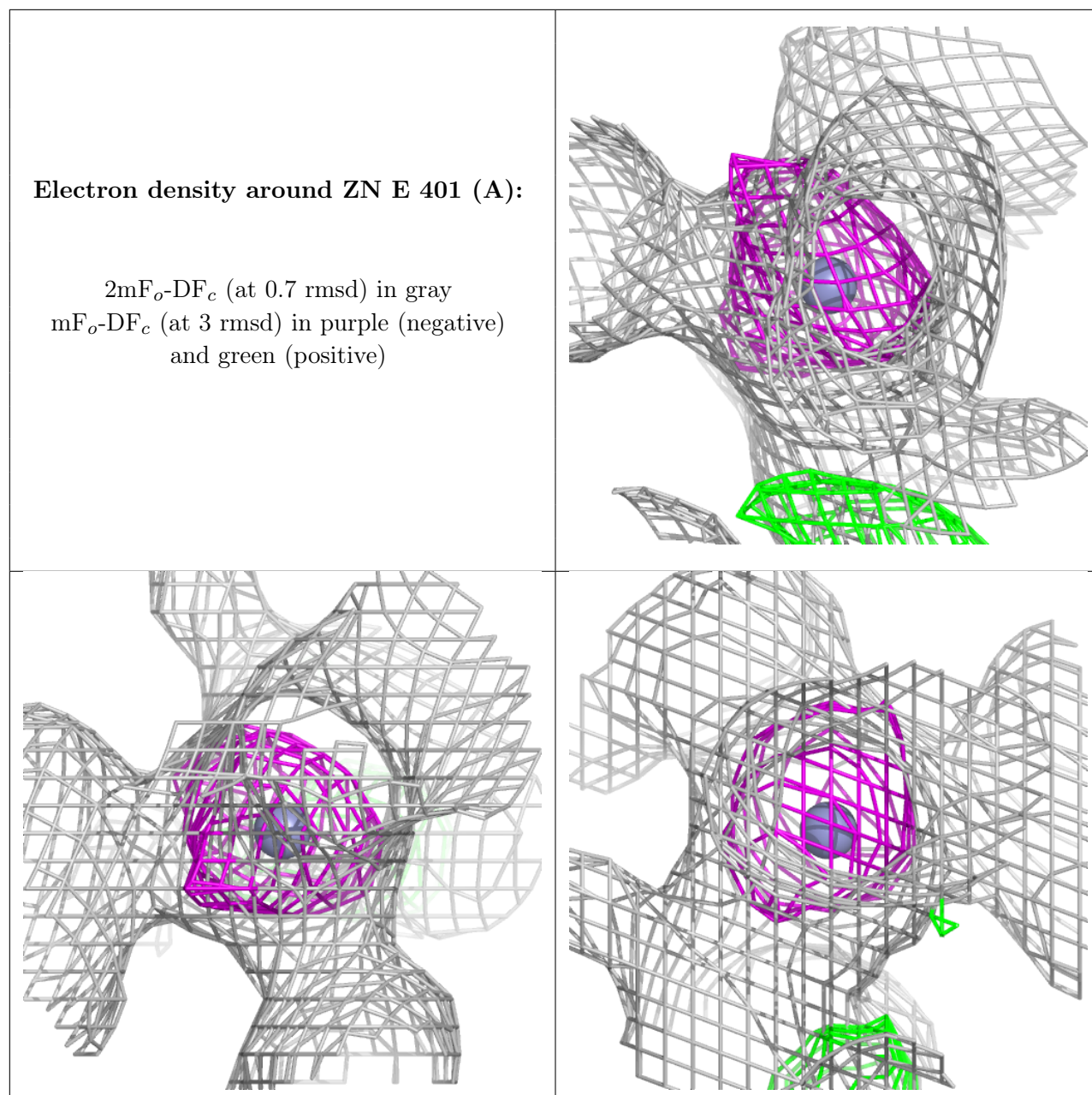
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN D 401 (A):

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





6.5 Other polymers ⓘ

There are no such residues in this entry.