



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:36 AM UTC

PDB ID : 8ZJ3 / pdb_00008zj3
Title : Terephthalate 1,2-cis-dihydrodioldehydrogenase/Decarboxylase in complex with 4-Hydroxybenzoate.
Authors : Kumar, K.A.; Pahwa, D.; Kumar, P.
Deposited on : 2024-05-14
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

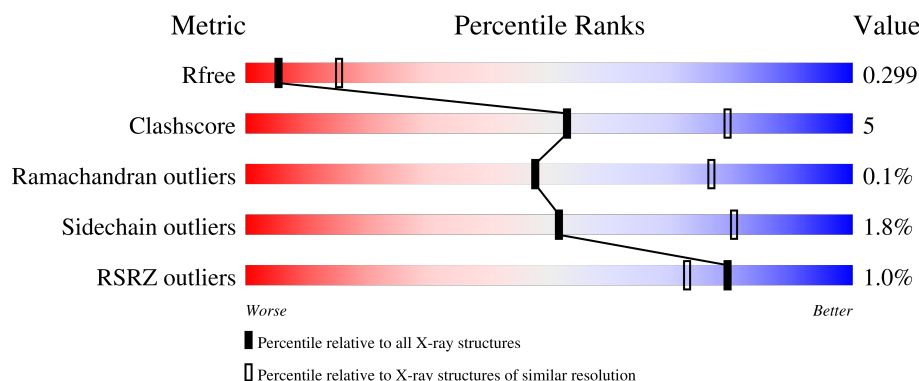
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	316	% 84% 14% ..
1	B	316	% 85% 12% ..
1	C	316	% 84% 14% ..
1	D	316	% 90% 8% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18905 atoms, of which 9475 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 4-hydroxythreonine-4-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total	C	H	N	O	S	68	0	0
			4670	1445	2368	412	432	13			
1	B	313	Total	C	H	N	O	S	68	0	0
			4656	1441	2362	410	431	12			
1	C	312	Total	C	H	N	O	S	68	0	0
			4643	1436	2358	409	427	13			
1	D	314	Total	C	H	N	O	S	68	0	0
			4670	1445	2368	412	432	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP B7WRJ7
B	0	ALA	-	expression tag	UNP B7WRJ7
C	0	ALA	-	expression tag	UNP B7WRJ7
D	0	ALA	-	expression tag	UNP B7WRJ7

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	2	0
			10	2	6	2		

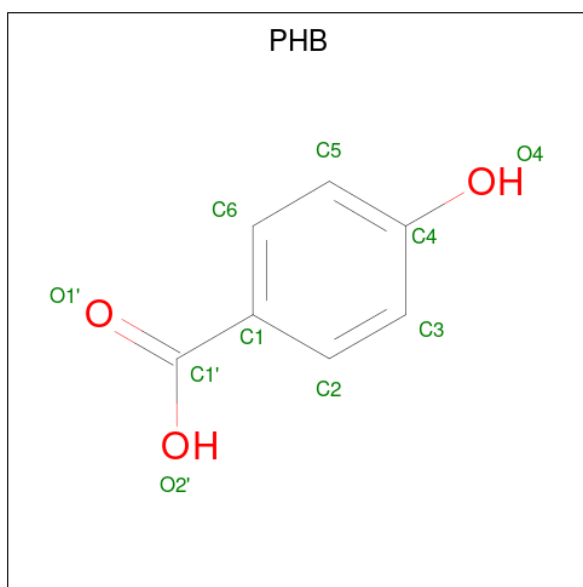
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

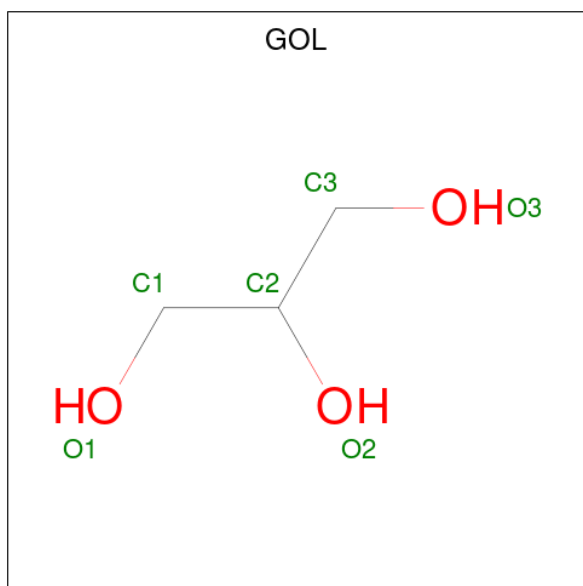
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is P-HYDROXYBENZOIC ACID (CCD ID: PHB) (formula: C₇H₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	1	0
			15	7	5	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	H	O	3	0
			14	3	8	3		

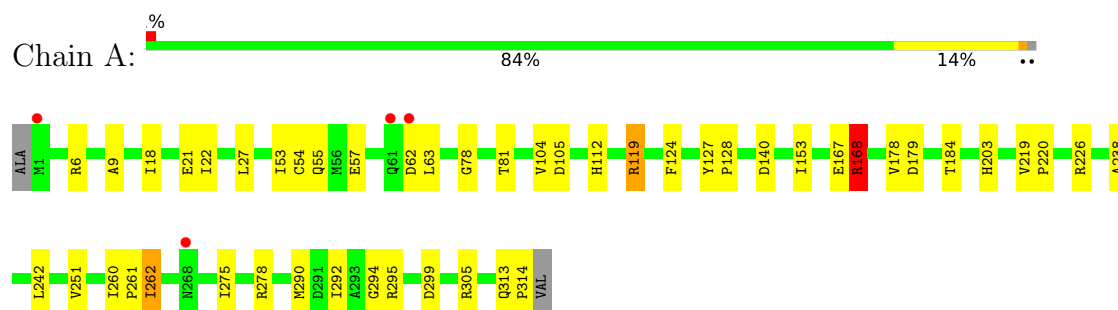
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	66	Total 66	O 66	0	0
7	B	35	Total 35	O 35	0	0
7	C	40	Total 40	O 40	0	0
7	D	79	Total 79	O 79	0	0

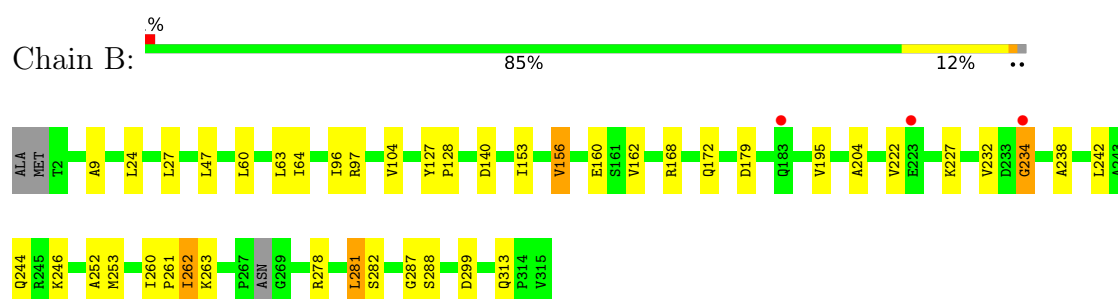
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

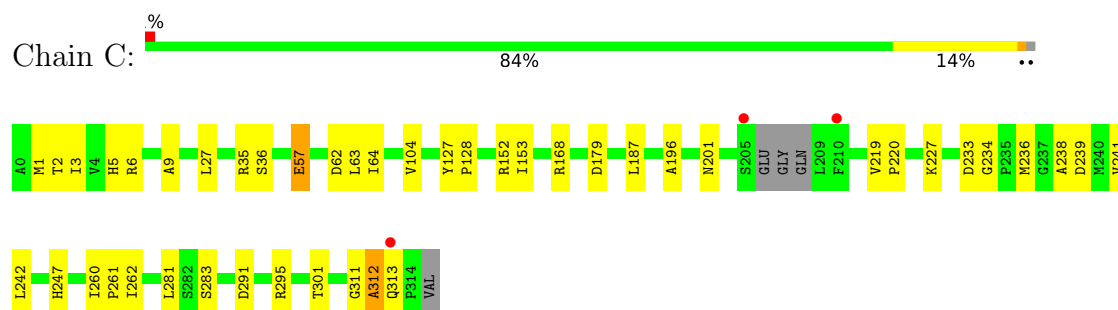
- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase



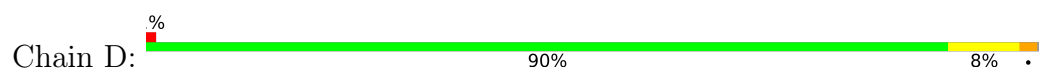
- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase

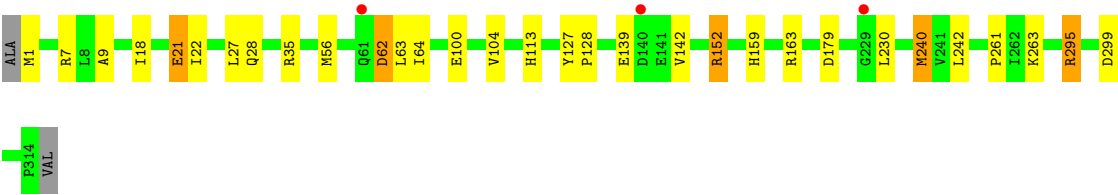


- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase



- Molecule 1: 4-hydroxythreonine-4-phosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.83Å 94.33Å 168.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.90) 98.9 (20.00-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.72 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.238 , 0.279 0.259 , 0.299	Depositor DCC
R_{free} test set	1613 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 5.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	18905	wwPDB-VP
Average B, all atoms (Å ²)	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1117e-03.*

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: ZN, PHB, MG, EDO, GOL

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	0.66	0/2339	1.06	5/3183 (0.2%)
1	B	0.61	0/2330	1.08	10/3169 (0.3%)
1	C	0.59	0/2321	1.05	4/3158 (0.1%)
1	D	0.64	0/2339	1.08	5/3183 (0.2%)
All	All	0.63	0/9329	1.07	24/12693 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	2
1	D	0	4
All	All	0	10

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	THR	CA-CB-OG1	-8.08	97.48	109.60
1	D	299	ASP	CA-CB-CG	6.79	119.39	112.60
1	C	179	ASP	CB-CA-C	6.76	123.64	110.67
1	C	179	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	167	GLU	CB-CG-CD	6.23	123.20	112.60
1	D	62	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	227	LYS	CB-CA-C	-6.14	98.56	110.46
1	D	21	GLU	CB-CA-C	5.99	120.28	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	ASP	CA-CB-CG	5.98	118.58	112.60
1	B	299	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	227	LYS	N-CA-CB	5.84	119.38	110.14
1	C	168	ARG	CA-CB-CG	5.83	125.75	114.10
1	A	299	ASP	CA-CB-CG	5.81	118.41	112.60
1	D	240	MET	CG-SD-CE	5.68	113.40	100.90
1	B	288	SER	N-CA-CB	-5.67	101.57	110.30
1	B	313	GLN	CB-CA-C	5.60	118.88	109.69
1	B	287	GLY	CA-C-N	5.43	129.91	120.68
1	B	287	GLY	C-N-CA	5.43	129.91	120.68
1	A	62	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	179	ASP	CA-CB-CG	5.33	117.94	112.60
1	B	179	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	204	ALA	CA-C-N	-5.25	114.41	122.60
1	B	204	ALA	C-N-CA	-5.25	114.41	122.60
1	A	168	ARG	CG-CD-NE	5.21	123.46	112.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	278	ARG	Sidechain
1	B	234	GLY	Peptide
1	C	152	ARG	Sidechain
1	C	295	ARG	Sidechain
1	D	152	ARG	Sidechain
1	D	163	ARG	Sidechain
1	D	295	ARG	Sidechain
1	D	35	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2302	2368	2357	21	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2294	2362	2347	24	0
1	C	2285	2358	2344	29	0
1	D	2302	2368	2357	22	0
2	A	4	6	6	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	1
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	D	10	5	5	3	0
6	D	6	8	8	1	0
7	A	66	0	0	3	0
7	B	35	0	0	0	0
7	C	40	0	0	6	0
7	D	79	0	0	8	0
All	All	9430	9475	9424	94	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (94) 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:D:28:GLN:OE1	1:D:56:MET:SD	2.27	0.92
1:C:187:LEU:O	1:C:313:GLN:HG3	1.82	0.80
1:C:291:ASP:O	7:C:501:HOH:O	2.04	0.76
1:D:28:GLN:OE1	1:D:56:MET:CE	2.41	0.68
1:A:124:PHE:HA	7:A:545:HOH:O	1.94	0.67
1:C:6:ARG:HH12	1:C:313:GLN:HG2	1.61	0.66
1:C:6:ARG:HH12	1:C:313:GLN:CG	2.11	0.64
1:D:28:GLN:OE1	1:D:56:MET:HE2	1.99	0.64
1:B:27:LEU:HD23	1:B:63:LEU:HD11	1.80	0.63
1:D:7:ARG:NH1	7:D:502:HOH:O	2.32	0.62
1:B:195:VAL:HB	1:B:232:VAL:HG12	1.82	0.61
1:C:311:GLY:O	1:C:313:GLN:NE2	2.32	0.61
1:A:78:GLY:C	1:A:290:MET:HE3	2.26	0.60
1:B:156:VAL:HG12	1:B:252:ALA:O	2.02	0.59
1:B:97:ARG:HH11	1:B:97:ARG:HG2	1.67	0.59
1:D:152:ARG:NH1	7:D:505:HOH:O	2.36	0.59
1:D:242:LEU:HD21	1:D:261:PRO:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:SER:HA	1:C:64:ILE:HD13	1.87	0.56
1:C:153:ILE:HD12	1:C:262:ILE:HD13	1.88	0.56
1:C:234:GLY:HA2	1:C:236:MET:HG3	1.86	0.56
1:C:35:ARG:NH1	7:C:505:HOH:O	2.37	0.56
1:C:238:ALA:O	1:C:242:LEU:HB2	2.06	0.56
1:B:156:VAL:CG1	1:B:253:MET:HA	2.36	0.56
1:B:222:VAL:HG21	1:B:234:GLY:HA2	1.87	0.56
1:A:313:GLN:CG	1:A:314:PRO:HD3	2.37	0.55
1:A:238:ALA:O	1:A:242:LEU:HB2	2.06	0.55
1:B:140:ASP:HB3	1:B:168:ARG:HH22	1.71	0.55
1:D:263:LYS:NZ	5:D:401:PHB:O2'	2.39	0.54
1:C:62:ASP:HB2	7:C:505:HOH:O	2.07	0.54
1:B:153:ILE:HD12	1:B:262:ILE:HD13	1.90	0.54
1:B:238:ALA:O	1:B:242:LEU:HB2	2.08	0.53
1:D:1:MET:HE3	7:D:552:HOH:O	2.10	0.52
1:A:27:LEU:HD13	1:A:63:LEU:HD11	1.91	0.52
1:B:140:ASP:CB	1:B:168:ARG:HH22	2.22	0.52
1:D:159:HIS:CE1	5:D:401:PHB:C5	2.93	0.52
1:C:233:ASP:OD2	1:C:247:HIS:HE1	1.93	0.51
1:B:97:ARG:HG2	1:B:97:ARG:NH1	2.25	0.51
1:B:244:GLN:HB3	1:B:246:LYS:HE3	1.93	0.50
1:A:153:ILE:HD12	1:A:262:ILE:HD13	1.92	0.50
1:C:127:TYR:N	1:C:128:PRO:CD	2.75	0.50
1:D:139:GLU:HB2	7:D:506:HOH:O	2.12	0.50
1:B:9:ALA:HB2	1:B:104:VAL:HG21	1.94	0.49
1:A:6:ARG:HD3	1:A:105:ASP:HB2	1.94	0.49
1:C:5:HIS:CG	1:C:312:ALA:HA	2.47	0.49
1:D:21:GLU:HB3	7:D:542:HOH:O	2.12	0.49
1:C:6:ARG:HH22	1:C:313:GLN:HB2	1.78	0.49
1:B:242:LEU:HD21	1:B:261:PRO:HG3	1.95	0.49
1:B:160:GLU:OE2	1:B:168:ARG:CD	2.61	0.48
1:B:127:TYR:N	1:B:128:PRO:CD	2.76	0.48
1:D:100:GLU:HB3	7:D:545:HOH:O	2.14	0.48
1:D:27:LEU:HD13	1:D:63:LEU:HD11	1.95	0.48
1:D:159:HIS:HE1	5:D:401:PHB:C5	2.27	0.47
1:A:292:ILE:HA	1:A:295:ARG:HD3	1.96	0.47
1:B:160:GLU:OE2	1:B:168:ARG:HD3	2.15	0.47
1:C:57:GLU:HG2	7:C:536:HOH:O	2.14	0.47
1:A:21:GLU:HG3	1:A:54:CYS:SG	2.54	0.47
1:A:127:TYR:N	1:A:128:PRO:CD	2.78	0.46
1:D:113:HIS:HA	6:D:402:GOL:H12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:TYR:N	1:D:128:PRO:CD	2.77	0.46
1:C:311:GLY:O	1:C:312:ALA:HB3	2.16	0.46
1:B:263:LYS:HD2	1:C:239:ASP:HB2	1.98	0.45
1:C:283:SER:HB2	7:C:513:HOH:O	2.16	0.45
1:C:62:ASP:CB	7:C:505:HOH:O	2.64	0.45
1:C:219:VAL:HB	1:C:220:PRO:HD3	1.98	0.45
1:A:260:ILE:N	1:A:261:PRO:HD2	2.33	0.44
1:B:64:ILE:HD12	1:B:64:ILE:N	2.33	0.44
1:B:162:VAL:H	1:C:201:ASN:ND2	2.16	0.44
1:A:305:ARG:O	7:A:502:HOH:O	2.21	0.44
1:D:64:ILE:HD12	1:D:64:ILE:N	2.32	0.44
1:B:260:ILE:N	1:B:261:PRO:HD2	2.33	0.44
1:A:313:GLN:HG2	1:A:314:PRO:HD3	1.99	0.44
1:D:9:ALA:HB2	1:D:104:VAL:HG21	1.99	0.44
1:A:9:ALA:HB2	1:A:104:VAL:HG21	1.99	0.43
1:B:281:LEU:HD12	1:B:282:SER:N	2.34	0.43
1:C:64:ILE:N	1:C:64:ILE:HD12	2.34	0.43
1:A:184:THR:OG1	1:A:275:ILE:HG12	2.19	0.43
1:C:27:LEU:HD13	1:C:63:LEU:CD2	2.49	0.43
1:C:196:ALA:HB1	1:C:241:VAL:HG21	2.00	0.43
1:C:9:ALA:HB2	1:C:104:VAL:HG21	2.00	0.42
1:A:112:HIS:HE1	7:A:515:HOH:O	2.01	0.42
1:A:53:ILE:HD13	1:A:294:GLY:HA2	2.01	0.42
1:C:281:LEU:C	1:C:281:LEU:HD23	2.43	0.42
1:C:260:ILE:N	1:C:261:PRO:HD2	2.35	0.42
1:D:230:LEU:HA	7:D:519:HOH:O	2.19	0.42
1:C:1:MET:HG3	1:C:3:ILE:HG23	2.03	0.41
1:B:96:ILE:HD11	1:B:281:LEU:CD2	2.50	0.41
1:A:140:ASP:HB3	1:A:168:ARG:HH21	1.84	0.41
1:A:219:VAL:HB	1:A:220:PRO:HD3	2.02	0.41
1:D:18:ILE:O	1:D:22:ILE:HG12	2.21	0.41
1:B:47:LEU:HB3	1:B:60:LEU:HD21	2.03	0.40
1:A:18:ILE:O	1:A:22:ILE:HG12	2.21	0.40
1:A:178:VAL:HG22	1:A:251:VAL:HG21	2.03	0.40
1:D:142:VAL:O	7:D:501:HOH:O	2.22	0.40
1:D:295:ARG:HA	1:D:295:ARG:HD2	1.83	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:HIS:HE2	3:D:403:ZN:ZN[4_444]	1.47	0.13

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	312/316 (99%)	303 (97%)	9 (3%)	0	100	100
1	B	309/316 (98%)	301 (97%)	8 (3%)	0	100	100
1	C	308/316 (98%)	303 (98%)	4 (1%)	1 (0%)	36	65
1	D	312/316 (99%)	305 (98%)	7 (2%)	0	100	100
All	All	1241/1264 (98%)	1212 (98%)	28 (2%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	312	ALA

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	243/244 (100%)	237 (98%)	6 (2%)	42	74
1	B	242/244 (99%)	236 (98%)	6 (2%)	42	74
1	C	241/244 (99%)	238 (99%)	3 (1%)	63	86
1	D	243/244 (100%)	241 (99%)	2 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	969/976 (99%)	952 (98%)	17 (2%)	51 80

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	57	GLU
1	A	81	THR
1	A	119	ARG
1	A	168	ARG
1	A	262	ILE
1	B	24	LEU
1	B	156	VAL
1	B	172	GLN
1	B	262	ILE
1	B	278	ARG
1	B	281	LEU
1	C	2	THR
1	C	57	GLU
1	C	227	LYS
1	D	62	ASP
1	D	240	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	112	HIS
1	A	172	GLN
1	A	244	GLN
1	A	268	ASN
1	B	5	HIS
1	B	28	GLN
1	B	52	GLN
1	B	65	HIS
1	B	172	GLN
1	B	194	GLN
1	B	216	GLN
1	B	313	GLN
1	C	49	GLN
1	C	65	HIS

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Mol	Chain	Res	Type
1	C	83	GLN
1	C	112	HIS
1	C	201	ASN
1	C	203	HIS
1	C	216	GLN
1	C	244	GLN
1	C	247	HIS
1	D	65	HIS
1	D	112	HIS
1	D	183	GLN
1	D	203	HIS
1	D	216	GLN
1	D	244	GLN
1	D	268	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 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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
2	EDO	A	401	-	3,3,3	0.33	0	2,2,2	0.31	0
6	GOL	D	402	-	5,5,5	0.29	0	5,5,5	0.46	0
5	PHB	D	401	3	10,10,10	0.78	0	13,13,13	0.76	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
2	EDO	A	401	-	-	0/1/1/1	-
6	GOL	D	402	-	-	4/4/4/4	-
5	PHB	D	401	3	-	4/4/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	402	GOL	O1-C1-C2-C3
5	D	401	PHB	C6-C1-C1'-O1'
5	D	401	PHB	C6-C1-C1'-O2'
6	D	402	GOL	C1-C2-C3-O3
6	D	402	GOL	O1-C1-C2-O2
5	D	401	PHB	C2-C1-C1'-O1'
6	D	402	GOL	O2-C2-C3-O3
5	D	401	PHB	C2-C1-C1'-O2'

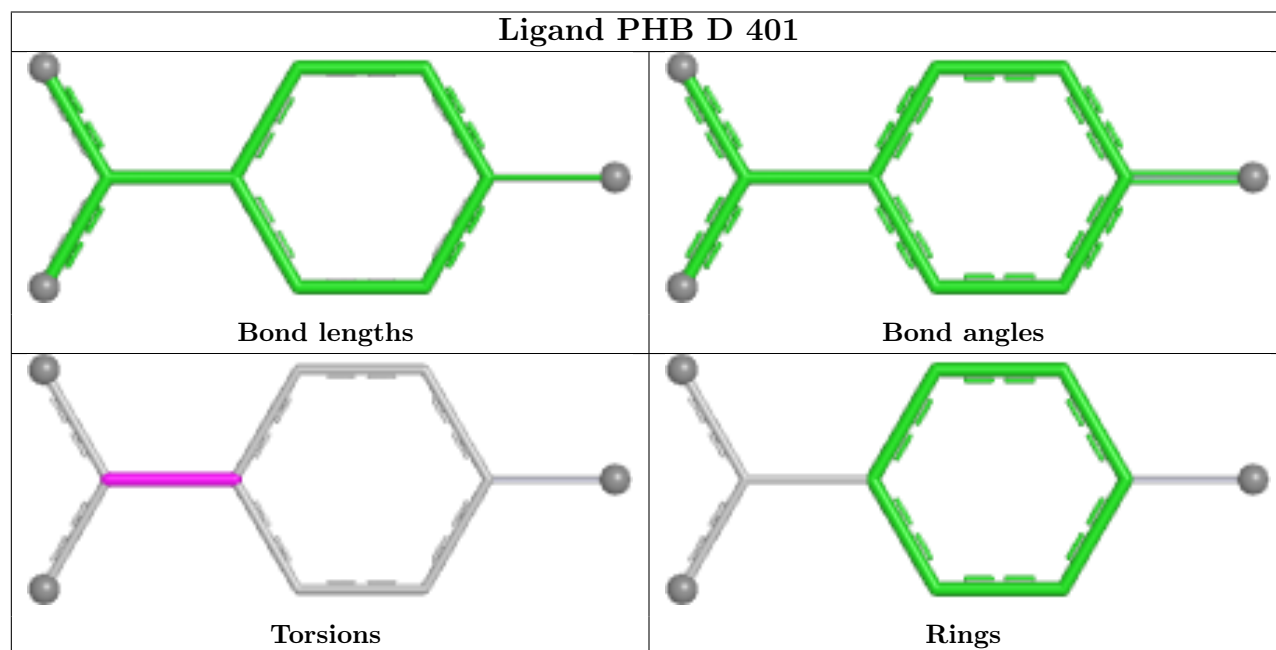
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	402	GOL	1	0
5	D	401	PHB	3	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	314/316 (99%)	0.17	4 (1%) 75 67	0, 0, 0, 1	0
1	B	313/316 (99%)	0.25	3 (0%) 79 73	0, 0, 0, 0	0
1	C	312/316 (98%)	0.21	3 (0%) 79 73	0, 0, 0, 0	0
1	D	314/316 (99%)	0.13	3 (0%) 79 73	0, 0, 0, 1	0
All	All	1253/1264 (99%)	0.19	13 (1%) 79 73	0, 0, 0, 1	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	205	SER	3.2
1	D	229	GLY	2.9
1	A	62	ASP	2.7
1	A	1	MET	2.6
1	C	313	GLN	2.6
1	C	210	PHE	2.5
1	D	61	GLN	2.5
1	B	234	GLY	2.4
1	B	223	GLU	2.3
1	B	183	GLN	2.2
1	A	61	GLN	2.1
1	D	140	ASP	2.1
1	A	268	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

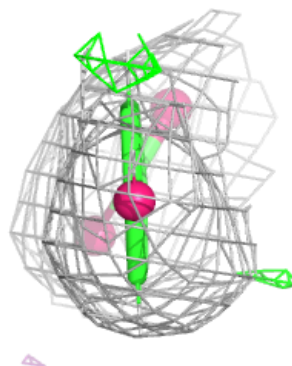
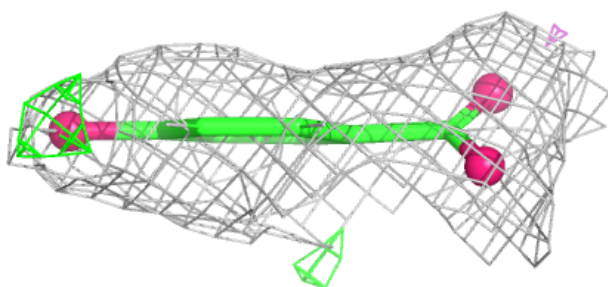
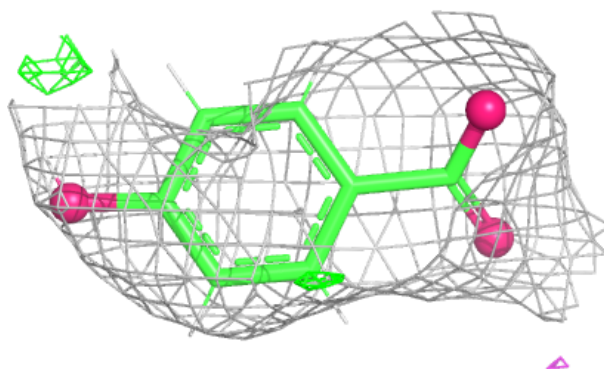
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	MG	A	403	1/1	0.80	0.25	19,19,19,19	0
6	GOL	D	402	6/6	0.84	0.14	0,0,30,30	3
5	PHB	D	401	10/10	0.89	0.10	0,0,0,30	1
4	MG	C	402	1/1	0.89	0.15	22,22,22,22	0
2	EDO	A	401	4/4	0.90	0.12	0,0,30,30	2
4	MG	A	404	1/1	0.92	0.19	21,21,21,21	0
3	ZN	C	401	1/1	0.95	0.17	36,36,36,36	0
3	ZN	B	401	1/1	0.96	0.17	51,51,51,51	0
3	ZN	D	403	1/1	0.98	0.06	29,29,29,29	0
3	ZN	A	402	1/1	0.98	0.15	31,31,31,31	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.

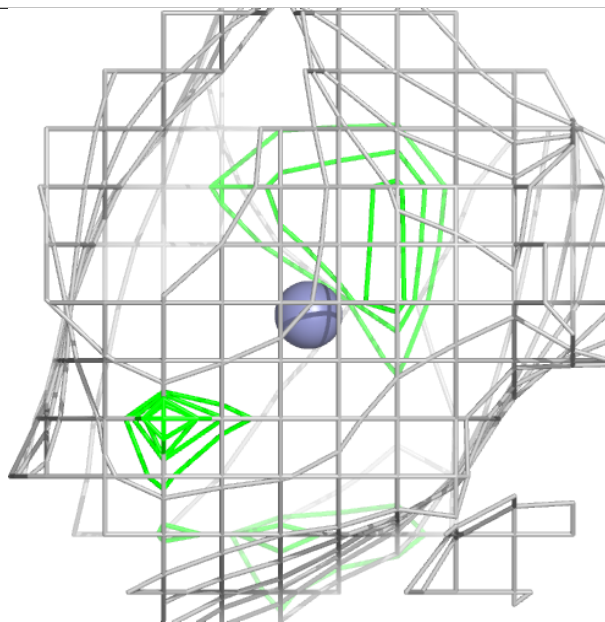
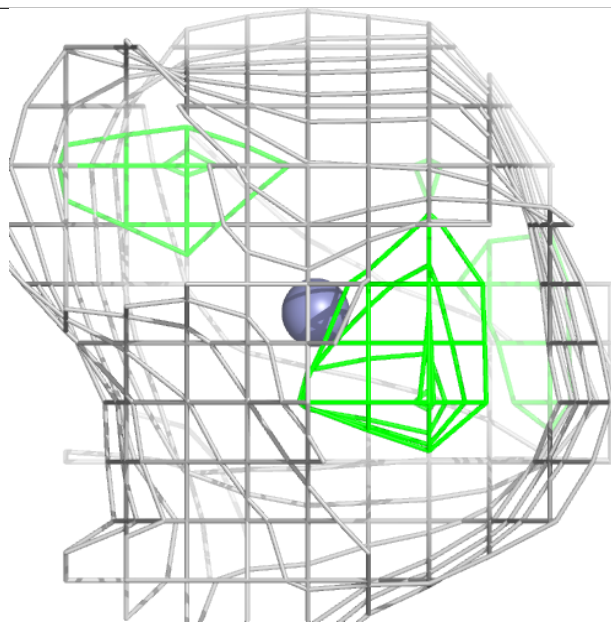
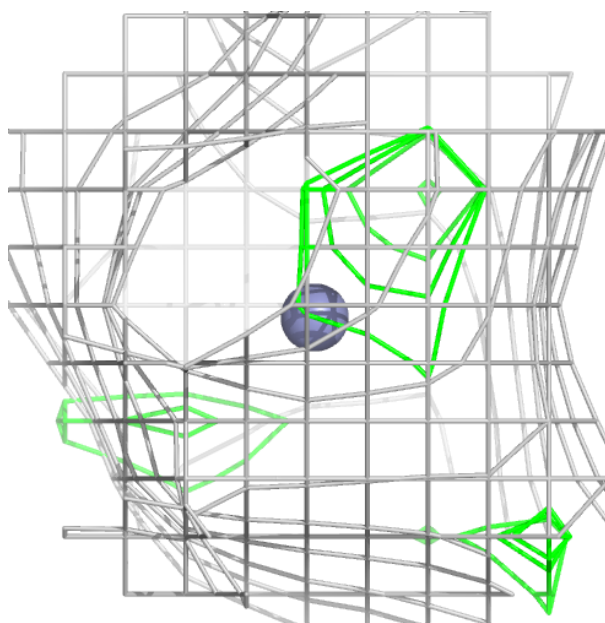
Electron density around PHB D 401:

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



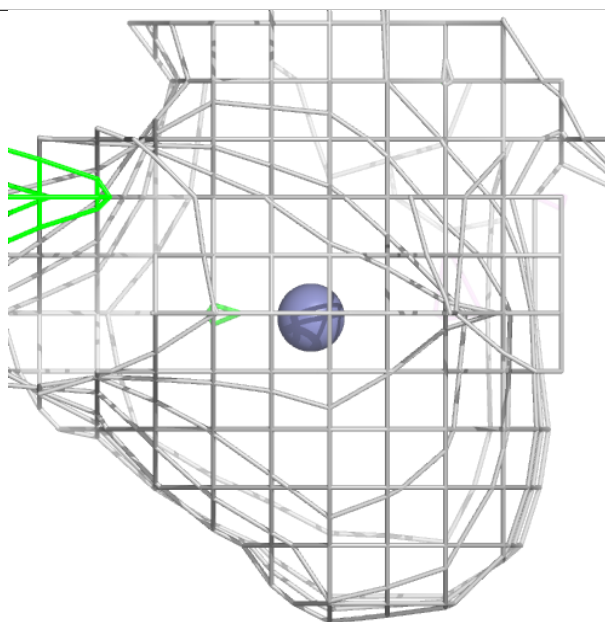
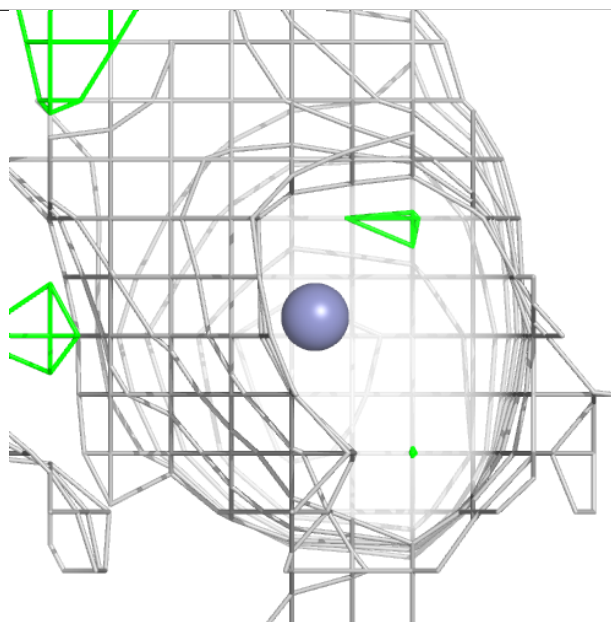
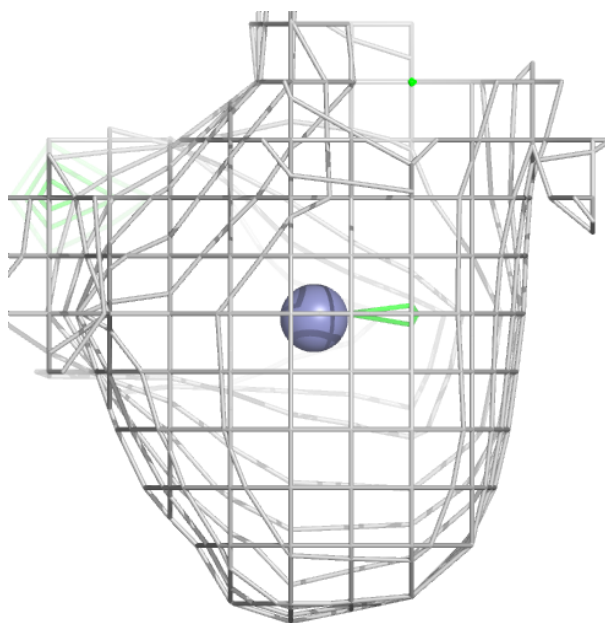
Electron density around ZN C 401:

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



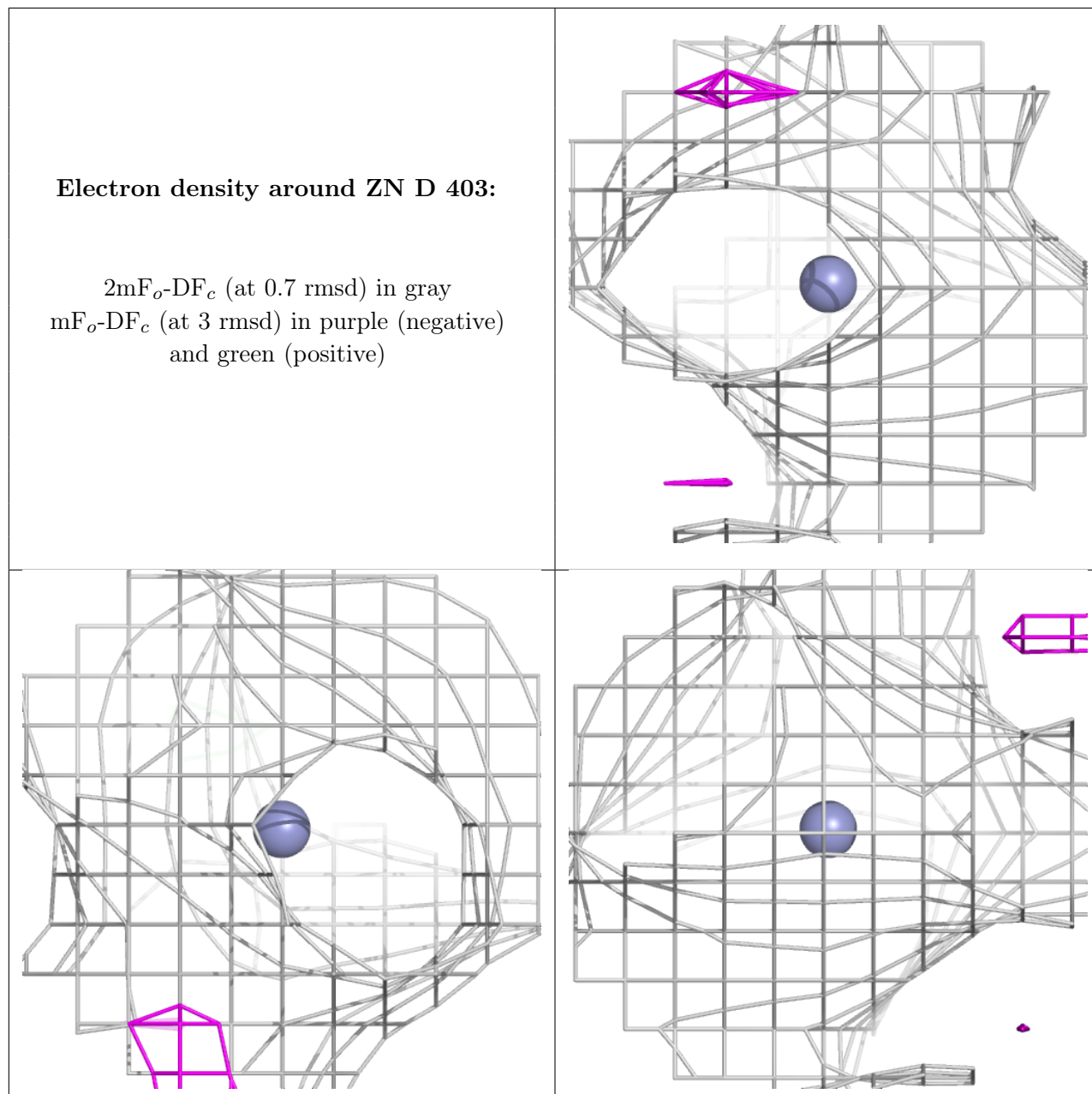
Electron density around ZN B 401:

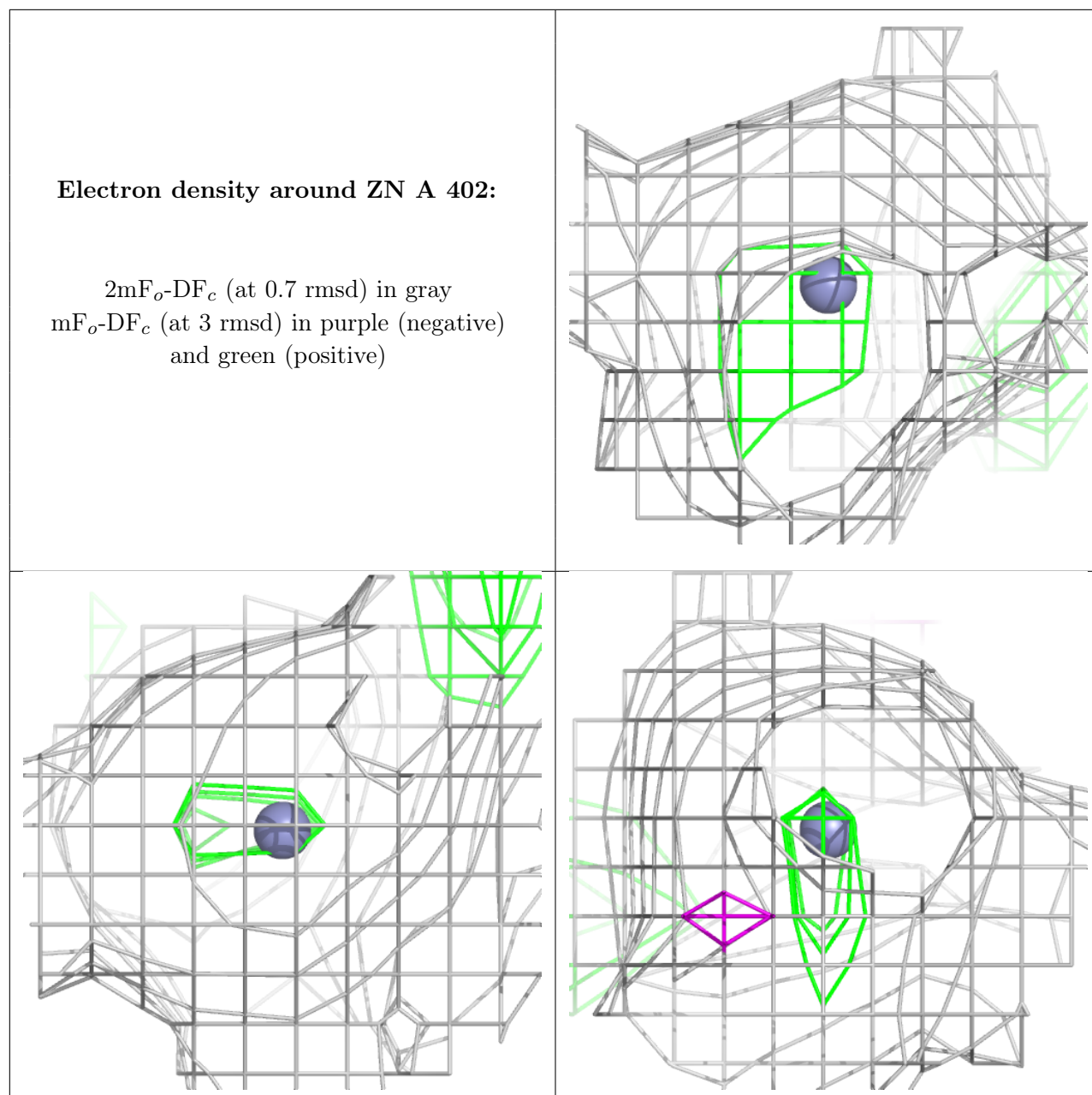
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN D 403:

$2mF_o - DF_c$ (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.