



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:54 PM UTC

PDB ID : 6DK9 / pdb_00006dk9
Title : Yeast Ddi2 Cyanamide Hydratase
Authors : Moore, S.A.; Xiao, W.; Li, J.
Deposited on : 2018-05-29
Resolution : 2.60 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:

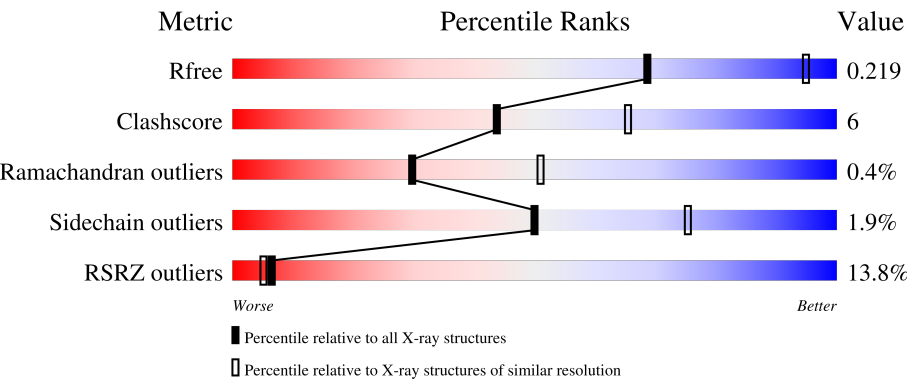
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	234	2% 89%9% .
1	B	234	2% 92%5% ..
1	C	234	2% 89%8% .
1	D	234	3% 88%9% .
1	E	234	3% 90%8% .

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Mol	Chain	Length	Quality of chain
1	F	234	
1	G	234	
1	H	234	
1	I	234	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	E	305	-	-	X	-
3	SO4	F	305	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32460 atoms, of which 15812 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 DNA damage-inducible protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	229	Total	C	H	N	O	S	0	1	0
			3539	1139	1748	305	341	6			
1	B	229	Total	C	H	N	O	S	0	1	0
			3539	1139	1748	305	341	6			
1	C	229	Total	C	H	N	O	S	0	1	0
			3578	1149	1769	309	345	6			
1	D	229	Total	C	H	N	O	S	0	1	0
			3574	1149	1765	309	345	6			
1	E	229	Total	C	H	N	O	S	0	1	0
			3574	1149	1765	309	345	6			
1	F	232	Total	C	H	N	O	S	0	1	0
			3595	1155	1778	311	345	6			
1	G	229	Total	C	H	N	O	S	0	1	0
			3554	1142	1757	308	341	6			
1	H	227	Total	C	H	N	O	S	0	0	0
			3505	1127	1734	303	336	5			
1	I	226	Total	C	H	N	O	S	0	0	0
			3527	1131	1748	306	336	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP A7A1Y4
A	-6	PRO	-	expression tag	UNP A7A1Y4
A	-5	LEU	-	expression tag	UNP A7A1Y4
A	-4	GLY	-	expression tag	UNP A7A1Y4
A	-3	SER	-	expression tag	UNP A7A1Y4
A	-2	PRO	-	expression tag	UNP A7A1Y4
A	-1	GLU	-	expression tag	UNP A7A1Y4
A	0	PHE	-	expression tag	UNP A7A1Y4
B	-7	GLY	-	expression tag	UNP A7A1Y4
B	-6	PRO	-	expression tag	UNP A7A1Y4
B	-5	LEU	-	expression tag	UNP A7A1Y4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP A7A1Y4
B	-3	SER	-	expression tag	UNP A7A1Y4
B	-2	PRO	-	expression tag	UNP A7A1Y4
B	-1	GLU	-	expression tag	UNP A7A1Y4
B	0	PHE	-	expression tag	UNP A7A1Y4
C	-7	GLY	-	expression tag	UNP A7A1Y4
C	-6	PRO	-	expression tag	UNP A7A1Y4
C	-5	LEU	-	expression tag	UNP A7A1Y4
C	-4	GLY	-	expression tag	UNP A7A1Y4
C	-3	SER	-	expression tag	UNP A7A1Y4
C	-2	PRO	-	expression tag	UNP A7A1Y4
C	-1	GLU	-	expression tag	UNP A7A1Y4
C	0	PHE	-	expression tag	UNP A7A1Y4
D	-7	GLY	-	expression tag	UNP A7A1Y4
D	-6	PRO	-	expression tag	UNP A7A1Y4
D	-5	LEU	-	expression tag	UNP A7A1Y4
D	-4	GLY	-	expression tag	UNP A7A1Y4
D	-3	SER	-	expression tag	UNP A7A1Y4
D	-2	PRO	-	expression tag	UNP A7A1Y4
D	-1	GLU	-	expression tag	UNP A7A1Y4
D	0	PHE	-	expression tag	UNP A7A1Y4
E	-7	GLY	-	expression tag	UNP A7A1Y4
E	-6	PRO	-	expression tag	UNP A7A1Y4
E	-5	LEU	-	expression tag	UNP A7A1Y4
E	-4	GLY	-	expression tag	UNP A7A1Y4
E	-3	SER	-	expression tag	UNP A7A1Y4
E	-2	PRO	-	expression tag	UNP A7A1Y4
E	-1	GLU	-	expression tag	UNP A7A1Y4
E	0	PHE	-	expression tag	UNP A7A1Y4
F	-7	GLY	-	expression tag	UNP A7A1Y4
F	-6	PRO	-	expression tag	UNP A7A1Y4
F	-5	LEU	-	expression tag	UNP A7A1Y4
F	-4	GLY	-	expression tag	UNP A7A1Y4
F	-3	SER	-	expression tag	UNP A7A1Y4
F	-2	PRO	-	expression tag	UNP A7A1Y4
F	-1	GLU	-	expression tag	UNP A7A1Y4
F	0	PHE	-	expression tag	UNP A7A1Y4
G	-7	GLY	-	expression tag	UNP A7A1Y4
G	-6	PRO	-	expression tag	UNP A7A1Y4
G	-5	LEU	-	expression tag	UNP A7A1Y4
G	-4	GLY	-	expression tag	UNP A7A1Y4
G	-3	SER	-	expression tag	UNP A7A1Y4

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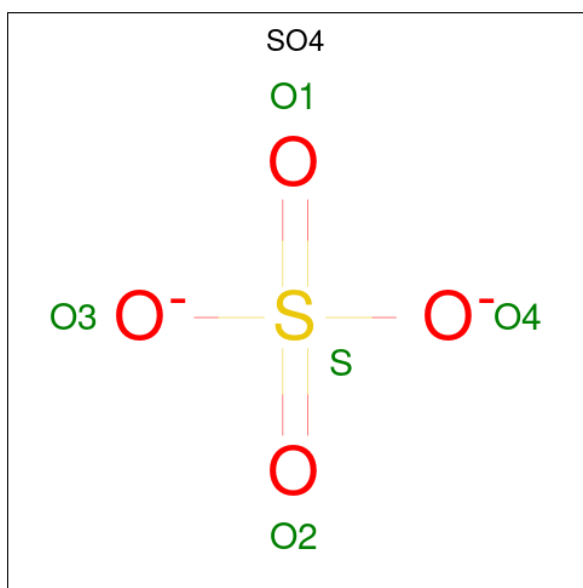
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	PRO	-	expression tag	UNP A7A1Y4
G	-1	GLU	-	expression tag	UNP A7A1Y4
G	0	PHE	-	expression tag	UNP A7A1Y4
H	-7	GLY	-	expression tag	UNP A7A1Y4
H	-6	PRO	-	expression tag	UNP A7A1Y4
H	-5	LEU	-	expression tag	UNP A7A1Y4
H	-4	GLY	-	expression tag	UNP A7A1Y4
H	-3	SER	-	expression tag	UNP A7A1Y4
H	-2	PRO	-	expression tag	UNP A7A1Y4
H	-1	GLU	-	expression tag	UNP A7A1Y4
H	0	PHE	-	expression tag	UNP A7A1Y4
I	-7	GLY	-	expression tag	UNP A7A1Y4
I	-6	PRO	-	expression tag	UNP A7A1Y4
I	-5	LEU	-	expression tag	UNP A7A1Y4
I	-4	GLY	-	expression tag	UNP A7A1Y4
I	-3	SER	-	expression tag	UNP A7A1Y4
I	-2	PRO	-	expression tag	UNP A7A1Y4
I	-1	GLU	-	expression tag	UNP A7A1Y4
I	0	PHE	-	expression tag	UNP A7A1Y4

- 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	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	I	1	Total Zn 1 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	48	Total	O	0	0
			48	48		
4	C	62	Total	O	0	0
			62	62		
4	D	53	Total	O	0	0
			53	53		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	68	Total 68	O 68	0	0
4	F	38	Total 38	O 38	0	0
4	G	23	Total 23	O 23	0	0

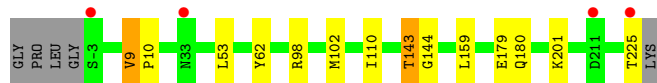
3 Residue-property plots [i](#)

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.

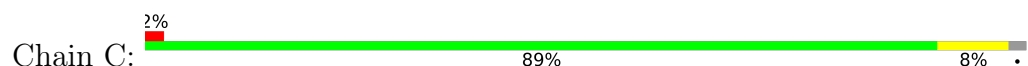
- Molecule 1: DNA damage-inducible protein



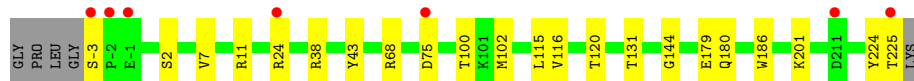
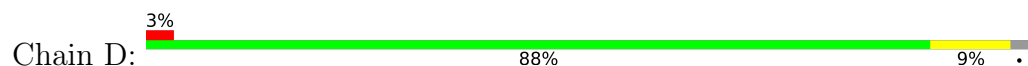
- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein



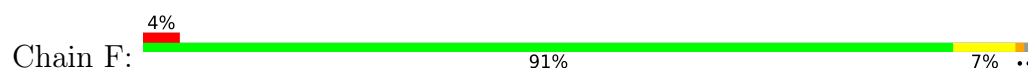
- Molecule 1: DNA damage-inducible protein



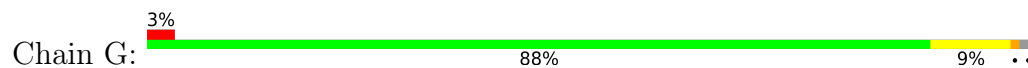
- Molecule 1: DNA damage-inducible protein



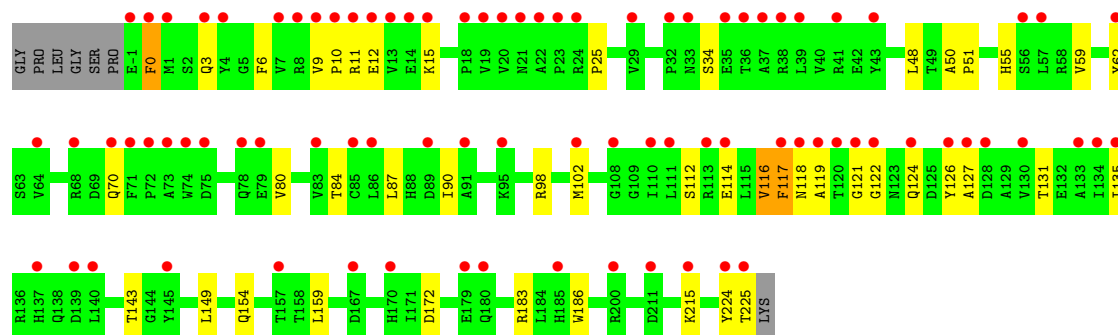
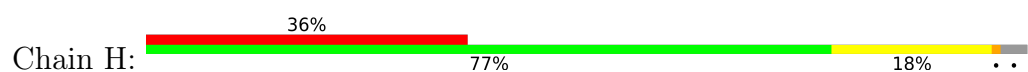
- Molecule 1: DNA damage-inducible protein



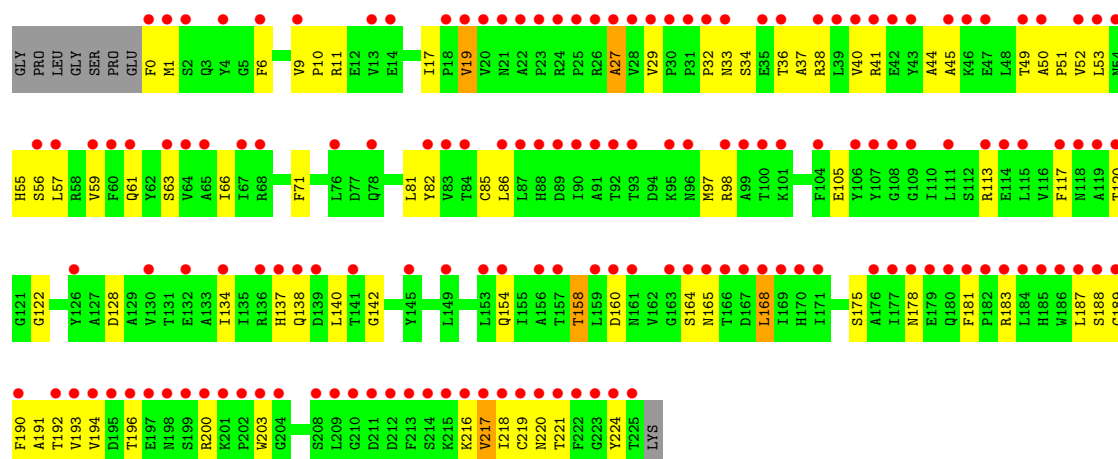
- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.46Å 264.46Å 119.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.70 – 2.60 39.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.70-2.60) 98.8 (39.70-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.201 , 0.217 0.202 , 0.219	Depositor DCC
R_{free} test set	7194 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32460	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: SO4, ZN

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	0.19	0/1836	0.45	0/2510
1	B	0.18	0/1836	0.44	0/2510
1	C	0.21	0/1854	0.49	0/2531
1	D	0.21	0/1854	0.45	0/2531
1	E	0.18	0/1854	0.46	0/2531
1	F	0.20	0/1863	0.43	0/2545
1	G	0.19	0/1842	0.47	0/2517
1	H	0.21	0/1812	0.48	0/2476
1	I	0.25	0/1820	0.55	0/2484
All	All	0.20	0/16571	0.47	0/22635

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	SER	Peptide
1	D	-3	SER	Peptide

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	1791	1748	1746	10	1
1	B	1791	1748	1746	8	0
1	C	1809	1769	1776	12	0
1	D	1809	1765	1776	11	0
1	E	1809	1765	1776	15	0
1	F	1817	1778	1781	16	0
1	G	1797	1757	1757	23	0
1	H	1771	1734	1731	36	1
1	I	1779	1748	1753	76	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
2	I	1	0	0	0	0
3	A	15	0	0	1	0
3	B	15	0	0	0	0
3	C	25	0	0	1	0
3	D	35	0	0	3	0
3	E	25	0	0	3	0
3	F	20	0	0	6	0
3	G	5	0	0	0	0
4	A	34	0	0	0	0
4	B	48	0	0	1	0
4	C	62	0	0	1	0
4	D	53	0	0	0	0
4	E	68	0	0	5	0
4	F	38	0	0	1	0
4	G	23	0	0	1	0
All	All	16648	15812	15842	196	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 6.

All (196) 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:2:SER:OG	1:D:75:ASP:OD2	1.66	1.14
1:E:118:ASN:OD1	4:E:401:HOH:O	1.82	0.97
1:I:190:PHE:CD1	1:I:217:VAL:HG21	2.00	0.96
1:F:1:MET:HE2	1:G:101:LYS:HE2	1.47	0.95
1:I:32:PRO:HB2	1:I:37:ALA:HB1	1.53	0.91
1:A:2:SER:OG	1:A:75:ASP:OD2	1.94	0.86
1:C:35:GLU:OE1	4:C:401:HOH:O	1.95	0.85
1:E:2:SER:OG	1:E:75:ASP:OD2	1.94	0.84
1:I:36:THR:HG21	1:I:120:THR:HG22	1.59	0.84
1:D:2:SER:CB	1:D:75:ASP:OD2	2.30	0.79
1:G:178:ASN:OD1	1:G:183:ARG:NH1	2.17	0.77
1:I:66:ILE:HD13	1:I:168:LEU:HD21	1.66	0.76
1:I:154:GLN:O	1:I:158:THR:OG1	2.02	0.75
1:I:34:SER:O	1:I:38:ARG:HB2	1.87	0.75
3:E:305:SO4:O3	4:E:402:HOH:O	2.04	0.75
1:I:190:PHE:CE1	1:I:217:VAL:HG21	2.23	0.73
1:I:165:ASN:O	1:I:168:LEU:HD22	1.90	0.70
3:E:305:SO4:O4	4:E:403:HOH:O	2.10	0.70
1:C:183:ARG:NH1	3:C:302:SO4:O4	2.24	0.69
1:D:131:THR:HB	1:E:102:MET:HE2	1.73	0.69
1:G:12:GLU:OE1	4:G:401:HOH:O	2.13	0.67
1:I:29:VAL:HG22	1:I:61:GLN:NE2	2.11	0.65
1:F:1:MET:HE2	1:G:101:LYS:CE	2.25	0.64
1:I:34:SER:OG	1:I:37:ALA:HB3	1.98	0.64
1:I:34:SER:O	1:I:38:ARG:N	2.31	0.64
1:F:32:PRO:O	1:F:41:ARG:NH2	2.30	0.63
1:E:114:GLU:OE2	1:E:118:ASN:ND2	2.31	0.63
1:I:32:PRO:HG2	1:I:82:TYR:CG	2.34	0.63
1:B:102:MET:HE1	1:B:110:ILE:HD12	1.80	0.63
1:I:63:SER:CB	1:I:81:LEU:HD21	2.30	0.62
1:I:32:PRO:HG2	1:I:82:TYR:CD2	2.35	0.61
1:I:134:ILE:O	1:I:137:HIS:ND1	2.32	0.61
1:I:189:CYS:O	1:I:193:VAL:HG23	2.01	0.61
1:H:112:SER:O	1:H:116:VAL:HG23	1.99	0.61
1:I:66:ILE:CD1	1:I:168:LEU:HD21	2.30	0.61
1:I:41:ARG:HB2	1:I:82:TYR:OH	2.00	0.61
1:B:143:THR:HG23	1:B:144:GLY:N	2.16	0.60
1:D:43:TYR:CE2	1:D:115:LEU:HD11	2.37	0.59
1:E:43:TYR:CE2	1:E:115:LEU:HD11	2.37	0.59
1:I:1:MET:HE3	1:I:6:PHE:O	2.03	0.58
1:H:80:VAL:HG22	1:H:126:TYR:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:PHE:CE1	1:I:194:VAL:CG2	2.87	0.58
1:F:211:ASP:OD1	1:F:211:ASP:N	2.36	0.58
1:I:98:ARG:HA	1:I:200:ARG:NH2	2.19	0.57
1:I:36:THR:O	1:I:40:VAL:HG23	2.04	0.57
1:I:63:SER:HB2	1:I:81:LEU:HD21	1.87	0.57
1:H:114:GLU:O	1:H:118:ASN:HB2	2.04	0.57
1:A:186:TRP:N	3:A:303:SO4:O1	2.39	0.56
1:D:186:TRP:N	3:D:304:SO4:O2	2.39	0.56
1:H:183:ARG:NH1	1:H:224:TYR:CG	2.74	0.56
1:I:33:ASN:OD1	1:I:33:ASN:O	2.23	0.56
1:H:102:MET:HE1	1:I:113:ARG:HD2	1.88	0.56
1:E:97:MET:HE2	1:E:196:THR:HG22	1.87	0.55
1:C:143:THR:HG23	1:C:144:GLY:N	2.20	0.55
1:H:25:PRO:HB3	1:H:172:ASP:HB2	1.88	0.55
1:I:168:LEU:C	1:I:168:LEU:HD23	2.32	0.55
1:I:188:SER:HA	1:I:218:ILE:CD1	2.37	0.54
1:B:9:VAL:HG23	1:B:10:PRO:HD2	1.89	0.54
1:C:143:THR:CG2	1:C:144:GLY:N	2.70	0.54
1:A:102:MET:HE1	1:A:110:ILE:HD12	1.90	0.54
1:H:114:GLU:OE2	1:H:118:ASN:ND2	2.41	0.53
1:H:84:THR:OG1	1:H:149:LEU:HD21	2.09	0.53
1:I:40:VAL:HG12	1:I:86:LEU:HD12	1.91	0.53
1:C:200:ARG:HG2	1:E:1:MET:HE2	1.91	0.53
1:G:98:ARG:CZ	1:I:0:PHE:CE1	2.91	0.53
1:F:1:MET:N	3:F:305:SO4:O3	2.40	0.53
1:G:97:MET:HE1	1:G:197:GLU:OE1	2.09	0.53
1:F:1:MET:HG2	3:F:305:SO4:O3	2.09	0.52
1:I:63:SER:HB3	1:I:81:LEU:HD21	1.91	0.52
1:I:1:MET:HG2	1:I:6:PHE:HB2	1.92	0.52
1:B:201:LYS:NZ	4:B:403:HOH:O	2.42	0.52
1:H:12:GLU:OE1	1:H:15:LYS:HE3	2.10	0.51
1:I:32:PRO:HB2	1:I:37:ALA:CB	2.33	0.51
1:G:98:ARG:HA	1:G:200:ARG:NH2	2.26	0.51
1:H:117:PHE:HB2	1:H:127:ALA:HB2	1.93	0.51
1:F:186:TRP:N	3:F:304:SO4:O2	2.43	0.51
1:I:216:LYS:HA	1:I:219:CYS:HB2	1.93	0.51
1:H:12:GLU:CD	1:H:15:LYS:HE3	2.36	0.51
1:I:160:ASP:O	1:I:224:TYR:OH	2.25	0.50
1:F:34:SER:OG	1:F:79:GLU:OE1	2.28	0.50
1:G:166:THR:HG21	1:G:222:PHE:CE1	2.47	0.50
1:C:2:SER:OG	1:C:75:ASP:OD2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:THR:CG2	1:B:144:GLY:N	2.74	0.50
1:H:12:GLU:OE2	1:H:15:LYS:NZ	2.43	0.50
1:G:12:GLU:O	1:G:13:VAL:HB	2.11	0.49
1:D:43:TYR:CZ	1:D:115:LEU:HD11	2.47	0.49
1:E:97:MET:HE1	1:E:197:GLU:HA	1.94	0.49
1:I:57:LEU:HD13	1:I:181:PHE:CD1	2.48	0.49
1:E:101:LYS:N	4:E:404:HOH:O	2.35	0.49
1:D:100:THR:OG1	1:D:102:MET:HG2	2.12	0.49
1:H:117:PHE:CE1	1:H:124:GLN:NE2	2.81	0.48
1:H:11:ARG:NH1	1:H:154:GLN:OE1	2.46	0.48
1:I:190:PHE:O	1:I:194:VAL:HG23	2.12	0.48
1:G:222:PHE:HD2	1:G:224:TYR:CE1	2.32	0.48
1:I:11:ARG:HH21	1:I:142:GLY:C	2.21	0.48
1:I:190:PHE:CE1	1:I:194:VAL:HG21	2.49	0.48
1:A:-1:GLU:HG2	1:B:98:ARG:HH12	1.79	0.48
1:G:62:TYR:CD2	1:G:159:LEU:HD23	2.49	0.48
1:G:200:ARG:HD3	1:I:1:MET:CE	2.43	0.48
1:G:222:PHE:HD2	1:G:224:TYR:CZ	2.32	0.48
1:C:-2:PRO:HA	1:C:4:TYR:OH	2.14	0.48
1:G:35:GLU:O	1:G:39:LEU:HB2	2.14	0.48
1:H:55:HIS:O	1:H:59:VAL:HG23	2.12	0.47
1:G:59:VAL:HG13	1:G:156:ALA:HB3	1.97	0.47
1:I:66:ILE:HG23	1:I:168:LEU:HG	1.94	0.47
1:I:117:PHE:CD1	1:I:122:GLY:HA2	2.50	0.47
1:H:50:ALA:HB3	1:H:51:PRO:HD3	1.96	0.47
1:H:6:PHE:HB3	1:I:203:TRP:CH2	2.50	0.47
1:I:9:VAL:HG22	1:I:10:PRO:HD2	1.97	0.47
1:H:131:THR:HG22	1:H:135:ILE:HD12	1.95	0.47
1:A:40:VAL:HG11	1:A:83:VAL:HG13	1.97	0.47
1:D:68:ARG:NH2	3:D:307:SO4:O2	2.43	0.46
1:H:117:PHE:CE1	1:H:122:GLY:HA2	2.50	0.46
1:F:1:MET:HE1	1:F:125:ASP:OD2	2.15	0.46
1:G:224:TYR:N	1:G:224:TYR:CD1	2.83	0.46
1:H:12:GLU:HB2	1:H:15:LYS:HD2	1.96	0.46
1:I:40:VAL:HG12	1:I:86:LEU:CD1	2.45	0.46
1:E:43:TYR:CZ	1:E:115:LEU:HD11	2.50	0.46
1:E:75:ASP:OD1	1:E:75:ASP:N	2.44	0.46
1:I:105:GLU:OE1	1:I:138:GLN:NE2	2.44	0.46
1:B:225:THR:HG22	1:B:225:THR:O	2.15	0.46
1:H:12:GLU:OE2	1:H:143:THR:HG22	2.15	0.46
1:C:62:TYR:CD2	1:C:159:LEU:HD23	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:ILE:HD11	1:I:71:PHE:CZ	2.51	0.46
1:F:18:PRO:HG3	1:H:215:LYS:HG3	1.97	0.46
1:H:48:LEU:HD21	1:H:90:ILE:HA	1.98	0.46
1:H:62:TYR:CD2	1:H:159:LEU:HD23	2.51	0.46
1:H:183:ARG:NH1	1:H:224:TYR:CD1	2.84	0.46
1:B:62:TYR:CG	1:B:159:LEU:HD23	2.50	0.46
1:I:32:PRO:HD2	1:I:82:TYR:CE1	2.51	0.46
1:A:9:VAL:HG23	1:A:10:PRO:HD2	1.98	0.45
1:I:178:ASN:OD1	1:I:183:ARG:HG2	2.17	0.45
1:A:62:TYR:CD2	1:A:159:LEU:HD23	2.51	0.45
1:I:19:VAL:O	1:I:19:VAL:CG1	2.64	0.45
1:H:117:PHE:HB2	1:H:127:ALA:CB	2.47	0.44
1:G:224:TYR:O	1:G:225:THR:C	2.59	0.44
1:I:44:ALA:HB1	1:I:86:LEU:HD22	1.99	0.44
1:I:45:ALA:HA	1:I:53:LEU:HD22	1.99	0.44
3:F:305:SO4:O4	1:H:98:ARG:HB2	2.17	0.44
1:H:0:PHE:HB2	1:H:3:GLN:HG3	2.00	0.44
1:H:183:ARG:HH21	1:H:186:TRP:HD1	1.64	0.44
1:I:11:ARG:NH2	1:I:142:GLY:O	2.48	0.44
1:I:50:ALA:HB3	1:I:51:PRO:HD3	2.00	0.44
1:C:143:THR:HG23	1:C:144:GLY:H	1.81	0.44
1:G:12:GLU:O	1:G:13:VAL:CB	2.64	0.44
1:I:190:PHE:HB3	1:I:217:VAL:HG11	2.00	0.44
1:A:24:ARG:O	1:A:26:ARG:HG3	2.16	0.44
1:G:9:VAL:CG2	1:G:10:PRO:HD2	2.48	0.44
1:H:102:MET:HE3	1:I:128:ASP:OD1	2.18	0.44
1:A:211:ASP:N	1:A:211:ASP:OD1	2.50	0.43
1:I:34:SER:OG	1:I:37:ALA:CB	2.65	0.43
3:F:305:SO4:O4	1:H:98:ARG:HD3	2.18	0.43
1:I:219:CYS:O	1:I:221:THR:HG23	2.19	0.43
1:I:59:VAL:HG12	1:I:85:CYS:SG	2.59	0.43
1:E:41:ARG:NE	4:E:402:HOH:O	2.46	0.43
1:I:27:ALA:O	1:I:29:VAL:HG13	2.19	0.43
1:I:117:PHE:O	1:I:117:PHE:HD1	2.02	0.43
1:G:98:ARG:HA	1:G:200:ARG:HH21	1.84	0.43
1:E:186:TRP:N	3:E:303:SO4:O4	2.52	0.42
1:I:220:ASN:HD21	1:I:224:TYR:HE1	1.67	0.42
1:C:62:TYR:CG	1:C:159:LEU:HD23	2.54	0.42
1:G:9:VAL:HG22	1:G:10:PRO:HD2	2.01	0.42
1:H:12:GLU:OE2	1:H:15:LYS:CE	2.67	0.42
1:I:158:THR:HG22	1:I:164:SER:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:GLU:O	1:E:136:ARG:HG2	2.20	0.42
1:D:116:VAL:O	1:D:120:THR:HG23	2.20	0.42
1:F:50:ALA:HB3	1:F:51:PRO:HD3	2.02	0.42
1:C:50:ALA:HB3	1:C:51:PRO:HD3	2.02	0.42
1:I:175:SER:HA	1:I:224:TYR:O	2.19	0.42
1:I:191:ALA:CB	1:I:218:ILE:HD11	2.49	0.42
1:F:1:MET:HE1	1:F:125:ASP:CG	2.45	0.42
1:I:117:PHE:CD1	1:I:117:PHE:C	2.98	0.42
1:F:-2:PRO:HG2	1:F:4:TYR:CE1	2.54	0.41
1:D:144:GLY:N	3:D:305:SO4:O4	2.43	0.41
1:E:211:ASP:OD1	1:E:211:ASP:N	2.52	0.41
1:H:102:MET:HE2	1:I:128:ASP:HA	2.01	0.41
1:G:200:ARG:HD3	1:I:1:MET:HE1	2.03	0.41
1:I:49:THR:OG1	1:I:52:VAL:HG23	2.21	0.41
1:I:196:THR:O	1:I:200:ARG:HG3	2.20	0.41
1:F:0:PHE:HD1	3:F:305:SO4:O4	2.03	0.41
1:I:158:THR:HG22	1:I:164:SER:HB2	2.02	0.41
1:I:187:LEU:O	1:I:218:ILE:HD13	2.20	0.41
1:H:87:LEU:O	1:H:90:ILE:HG22	2.20	0.41
1:I:158:THR:HG22	1:I:164:SER:OG	2.21	0.41
1:H:9:VAL:HG23	1:H:10:PRO:HD2	2.03	0.41
1:I:56:SER:HB3	1:I:86:LEU:HA	2.03	0.41
1:D:224:TYR:O	1:D:225:THR:C	2.64	0.41
1:A:166:THR:HG21	1:A:222:PHE:CE1	2.56	0.40
1:F:97:MET:HE3	1:F:196:THR:HG22	2.03	0.40
1:I:55:HIS:O	1:I:59:VAL:HG23	2.21	0.40
1:I:117:PHE:HD1	1:I:117:PHE:C	2.30	0.40
1:G:33:ASN:O	1:G:33:ASN:OD1	2.40	0.40
1:H:183:ARG:HH21	1:H:186:TRP:CD1	2.39	0.40
1:I:138:GLN:HA	1:I:140:LEU:HG	2.03	0.40
1:C:97:MET:HE3	1:C:196:THR:HG22	2.02	0.40
1:F:225:THR:HG22	4:F:430:HOH:O	2.21	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:82:TYR:OH	1:H:121:GLY:O[3_566]	2.15	0.05

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	228/234 (97%)	222 (97%)	6 (3%)	0	100	100
1	B	228/234 (97%)	222 (97%)	6 (3%)	0	100	100
1	C	228/234 (97%)	222 (97%)	5 (2%)	1 (0%)	30	51
1	D	228/234 (97%)	224 (98%)	4 (2%)	0	100	100
1	E	228/234 (97%)	225 (99%)	3 (1%)	0	100	100
1	F	231/234 (99%)	224 (97%)	6 (3%)	1 (0%)	30	51
1	G	228/234 (97%)	225 (99%)	2 (1%)	1 (0%)	30	51
1	H	225/234 (96%)	213 (95%)	7 (3%)	5 (2%)	5	10
1	I	224/234 (96%)	213 (95%)	10 (4%)	1 (0%)	30	51
All	All	2048/2106 (97%)	1990 (97%)	49 (2%)	9 (0%)	30	51

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-1	GLU
1	H	34	SER
1	H	116	VAL
1	H	119	ALA
1	F	-3	SER
1	H	0	PHE
1	H	117	PHE
1	I	27	ALA
1	G	13	VAL

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	195/202 (96%)	193 (99%)	2 (1%)	68	86
1	B	195/202 (96%)	190 (97%)	5 (3%)	40	68
1	C	199/202 (98%)	194 (98%)	5 (2%)	42	69
1	D	199/202 (98%)	192 (96%)	7 (4%)	32	59
1	E	199/202 (98%)	196 (98%)	3 (2%)	57	80
1	F	199/202 (98%)	196 (98%)	3 (2%)	57	80
1	G	196/202 (97%)	195 (100%)	1 (0%)	81	92
1	H	192/202 (95%)	190 (99%)	2 (1%)	68	86
1	I	195/202 (96%)	189 (97%)	6 (3%)	35	63
All	All	1769/1818 (97%)	1735 (98%)	34 (2%)	50	75

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	225	THR
1	B	9	VAL
1	B	53	LEU
1	B	143	THR
1	B	179	GLU
1	B	180	GLN
1	C	143	THR
1	C	180	GLN
1	C	201	LYS
1	C	211	ASP
1	C	225	THR
1	D	7	VAL
1	D	11	ARG
1	D	24	ARG
1	D	38	ARG
1	D	179	GLU
1	D	180	GLN
1	D	201	LYS
1	E	117	PHE
1	E	136	ARG
1	E	201	LYS
1	F	1	MET

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Mol	Chain	Res	Type
1	F	201	LYS
1	F	211	ASP
1	G	12	GLU
1	H	70	GLN
1	H	225	THR
1	I	19	VAL
1	I	97	MET
1	I	158	THR
1	I	168	LEU
1	I	192	THR
1	I	217	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	B	185	HIS
1	B	198	ASN
1	C	185	HIS
1	C	198	ASN
1	E	3	GLN
1	E	185	HIS
1	G	78	GLN
1	G	220	ASN
1	H	124	GLN
1	H	165	ASN
1	I	33	ASN
1	I	61	GLN
1	I	198	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 37 ligands modelled in this entry, 9 are monoatomic - leaving 28 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	$\# Z > 2$
3	SO4	B	304	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	F	301	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	C	306	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	F	304	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	G	302	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	C	304	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	D	303	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	D	304	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	E	303	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	D	308	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	B	303	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	D	307	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	C	303	-	4,4,4	0.22	0	6,6,6	0.09	0
3	SO4	F	303	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	C	305	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	F	305	-	4,4,4	0.31	0	6,6,6	0.28	0
3	SO4	B	301	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	E	305	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.19	0
3	SO4	D	301	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	D	306	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	E	306	-	4,4,4	0.23	0	6,6,6	0.31	0
3	SO4	A	304	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	D	305	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	E	304	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	E	302	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	303	-	4,4,4	0.26	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	304	SO4	1	0
3	D	304	SO4	1	0
3	E	303	SO4	1	0
3	D	307	SO4	1	0
3	F	305	SO4	5	0
3	E	305	SO4	2	0
3	C	302	SO4	1	0
3	D	305	SO4	1	0
3	A	303	SO4	1	0

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	229/234 (97%)	-0.17	4 (1%) 69 64	35, 59, 85, 130	1 (0%)
1	B	229/234 (97%)	-0.27	4 (1%) 69 64	31, 56, 77, 115	1 (0%)
1	C	229/234 (97%)	-0.39	5 (2%) 62 57	32, 45, 71, 117	1 (0%)
1	D	229/234 (97%)	-0.38	7 (3%) 51 45	30, 49, 68, 137	1 (0%)
1	E	229/234 (97%)	-0.35	7 (3%) 51 45	33, 45, 70, 160	1 (0%)
1	F	232/234 (99%)	-0.17	10 (4%) 40 34	40, 54, 81, 150	1 (0%)
1	G	229/234 (97%)	0.06	7 (3%) 51 45	40, 69, 96, 114	1 (0%)
1	H	227/234 (97%)	1.73	85 (37%) 1 0	74, 115, 151, 187	0
1	I	226/234 (96%)	2.95	155 (68%) 0 0	87, 155, 199, 274	0
All	All	2059/2106 (97%)	0.33	284 (13%) 6 5	30, 58, 159, 274	7 (0%)

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-3	SER	12.0
1	I	28	VAL	10.3
1	D	-3	SER	10.0
1	F	-6	PRO	9.5
1	I	187	LEU	9.1
1	I	90	ILE	9.0
1	H	225	THR	8.6
1	I	192	THR	8.6
1	H	0	PHE	8.4
1	B	-3	SER	7.9
1	I	39	LEU	7.3
1	I	225	THR	7.2
1	I	176	ALA	7.1
1	I	96	ASN	6.9
1	I	213	PHE	6.7

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Mol	Chain	Res	Type	RSRZ
1	I	57	LEU	6.4
1	I	190	PHE	6.3
1	I	82	TYR	6.2
1	F	225	THR	6.2
1	C	-3	SER	6.1
1	I	193	VAL	5.9
1	B	225	THR	5.9
1	I	185	HIS	5.8
1	I	91	ALA	5.8
1	F	-4	GLY	5.6
1	I	117	PHE	5.6
1	I	217	VAL	5.6
1	I	181	PHE	5.6
1	I	220	ASN	5.5
1	H	120	THR	5.5
1	C	-2	PRO	5.3
1	H	-1	GLU	5.3
1	I	170	HIS	5.2
1	I	99	ALA	5.1
1	I	204	GLY	5.0
1	I	19	VAL	4.9
1	H	14	GLU	4.9
1	A	225	THR	4.8
1	I	86	LEU	4.7
1	E	225	THR	4.7
1	I	84	THR	4.7
1	H	19	VAL	4.7
1	G	225	THR	4.7
1	H	35	GLU	4.6
1	I	139	ASP	4.6
1	I	196	THR	4.6
1	I	218	ILE	4.6
1	H	121	GLY	4.6
1	G	-3	SER	4.6
1	I	169	ILE	4.5
1	H	24	ARG	4.5
1	I	33	ASN	4.5
1	I	188	SER	4.4
1	H	73	ALA	4.3
1	I	216	LYS	4.3
1	I	43	TYR	4.3
1	I	211	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	83	VAL	4.3
1	I	111	LEU	4.3
1	I	61	GLN	4.3
1	I	27	ALA	4.2
1	H	114	GLU	4.2
1	I	29	VAL	4.2
1	I	107	TYR	4.2
1	H	72	PRO	4.2
1	I	114	GLU	4.2
1	I	1	MET	4.2
1	I	13	VAL	4.2
1	I	41	ARG	4.2
1	I	88	HIS	4.2
1	I	203	TRP	4.1
1	I	22	ALA	4.1
1	I	212	ASP	4.1
1	F	-5	LEU	4.1
1	A	-3	SER	4.1
1	H	7	VAL	4.1
1	I	168	LEU	4.1
1	I	215	LYS	4.0
1	I	20	VAL	4.0
1	I	46	LYS	4.0
1	I	106	TYR	4.0
1	D	225	THR	3.9
1	I	221	THR	3.9
1	I	157	THR	3.9
1	H	127	ALA	3.9
1	I	171	ILE	3.9
1	A	24	ARG	3.9
1	I	50	ALA	3.9
1	I	95	LYS	3.9
1	H	180	GLN	3.9
1	I	60	PHE	3.9
1	I	21	ASN	3.8
1	I	2	SER	3.8
1	H	119	ALA	3.8
1	H	4	TYR	3.7
1	I	200	ARG	3.7
1	I	35	GLU	3.7
1	H	133	ALA	3.7
1	H	1	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	24	ARG	3.6
1	H	145	TYR	3.6
1	H	22	ALA	3.6
1	I	65	ALA	3.6
1	I	47	GLU	3.6
1	I	53	LEU	3.6
1	I	184	LEU	3.6
1	I	156	ALA	3.6
1	H	43	TYR	3.6
1	I	0	PHE	3.6
1	I	209	LEU	3.5
1	I	119	ALA	3.5
1	I	14	GLU	3.5
1	H	32	PRO	3.5
1	I	115	LEU	3.4
1	I	194	VAL	3.4
1	I	98	ARG	3.4
1	I	183	ARG	3.4
1	I	177	ILE	3.4
1	I	45	ALA	3.3
1	I	210	GLY	3.3
1	I	165	ASN	3.3
1	I	167	ASP	3.3
1	H	91	ALA	3.3
1	I	164	SER	3.3
1	I	179	GLU	3.3
1	H	85	CYS	3.2
1	F	141	THR	3.2
1	I	49	THR	3.2
1	I	92	THR	3.2
1	H	20	VAL	3.2
1	H	118	ASN	3.2
1	D	24	ARG	3.2
1	H	36	THR	3.2
1	I	224	TYR	3.2
1	I	104	PHE	3.2
1	F	-3	SER	3.2
1	C	-1	GLU	3.2
1	H	18	PRO	3.1
1	I	186	TRP	3.1
1	I	178	ASN	3.1
1	D	75	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	13	VAL	3.1
1	I	219	CYS	3.1
1	I	199	SER	3.1
1	H	111	LEU	3.1
1	H	139	ASP	3.1
1	I	25	PRO	3.1
1	I	30	PRO	3.1
1	H	117	PHE	3.1
1	H	39	LEU	3.0
1	H	224	TYR	3.0
1	I	153	LEU	3.0
1	I	101	LYS	3.0
1	H	79	GLU	3.0
1	H	71	PHE	3.0
1	H	21	ASN	2.9
1	B	211	ASP	2.9
1	G	211	ASP	2.9
1	F	-1	GLU	2.9
1	I	23	PRO	2.9
1	D	211	ASP	2.9
1	I	118	ASN	2.9
1	I	222	PHE	2.9
1	H	74	TRP	2.8
1	I	67	ILE	2.8
1	I	36	THR	2.8
1	C	35	GLU	2.8
1	D	-2	PRO	2.8
1	H	75	ASP	2.8
1	I	132	GLU	2.8
1	I	32	PRO	2.8
1	G	139[A]	ASP	2.8
1	I	93	THR	2.8
1	H	185	HIS	2.8
1	H	64	VAL	2.8
1	I	134	ILE	2.7
1	I	42	GLU	2.7
1	I	141	THR	2.7
1	G	98	ARG	2.7
1	E	-2	PRO	2.7
1	I	87	LEU	2.7
1	E	33	ASN	2.7
1	H	37	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	89	ASP	2.7
1	I	136	ARG	2.7
1	I	208	SER	2.7
1	I	100	THR	2.7
1	H	89	ASP	2.7
1	H	126	TYR	2.6
1	H	38	ARG	2.6
1	I	113	ARG	2.6
1	I	56	SER	2.6
1	I	198	ASN	2.6
1	I	214	SER	2.6
1	I	138	GLN	2.6
1	I	180	GLN	2.6
1	I	145	TYR	2.6
1	H	15	LYS	2.6
1	H	83	VAL	2.6
1	I	68	ARG	2.6
1	B	33	ASN	2.6
1	I	154	GLN	2.6
1	H	86	LEU	2.5
1	I	197	GLU	2.5
1	I	63	SER	2.5
1	I	108	GLY	2.5
1	H	12	GLU	2.5
1	I	109	GLY	2.5
1	I	31	PRO	2.5
1	I	59	VAL	2.5
1	E	118	ASN	2.5
1	H	124	GLN	2.5
1	A	33	ASN	2.4
1	F	24	ARG	2.4
1	C	34	SER	2.4
1	H	122	GLY	2.4
1	I	182	PRO	2.4
1	H	68	ARG	2.4
1	H	57	LEU	2.4
1	I	76	LEU	2.4
1	F	75	ASP	2.4
1	H	10	PRO	2.4
1	I	26	ARG	2.4
1	D	-1	GLU	2.4
1	H	167	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	223	GLY	2.4
1	I	78	GLN	2.4
1	H	130	VAL	2.4
1	H	41	ARG	2.4
1	I	54	ASN	2.4
1	H	179	GLU	2.4
1	F	211	ASP	2.4
1	H	108	GLY	2.4
1	I	64	VAL	2.4
1	I	126	TYR	2.3
1	H	135	ILE	2.3
1	H	102	MET	2.3
1	H	211	ASP	2.3
1	G	163	GLY	2.3
1	H	9	VAL	2.3
1	I	38	ARG	2.3
1	I	40	VAL	2.3
1	I	159	LEU	2.3
1	I	201	LYS	2.3
1	I	161	ASN	2.3
1	H	113	ARG	2.3
1	I	130	VAL	2.3
1	H	95	LYS	2.3
1	I	166	THR	2.3
1	H	128	ASP	2.3
1	H	200	ARG	2.3
1	H	3	GLN	2.3
1	E	-1	GLU	2.2
1	H	33	ASN	2.2
1	H	56	SER	2.2
1	H	157	THR	2.2
1	H	8	ARG	2.2
1	I	4	TYR	2.2
1	I	160	ASP	2.2
1	I	195	ASP	2.2
1	H	29	VAL	2.2
1	H	170	HIS	2.2
1	I	137	HIS	2.2
1	I	163	GLY	2.2
1	H	134	ILE	2.2
1	I	9	VAL	2.2
1	G	12	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	78	GLN	2.1
1	H	140	LEU	2.1
1	H	137	HIS	2.1
1	H	11	ARG	2.1
1	I	18	PRO	2.1
1	H	110	ILE	2.1
1	I	52	VAL	2.1
1	H	215	LYS	2.1
1	H	23	PRO	2.1
1	I	202	PRO	2.1
1	I	189	CYS	2.1
1	H	62	TYR	2.1
1	I	6	PHE	2.1
1	I	120	THR	2.0
1	H	70	GLN	2.0
1	E	136	ARG	2.0
1	I	149	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	H	500	1/1	0.79	0.18	94,94,94,94	1
3	SO4	F	305	5/5	0.80	0.24	148,149,151,151	5
2	ZN	I	500	1/1	0.82	0.16	132,132,132,132	1
3	SO4	D	303	5/5	0.83	0.16	98,102,103,105	0
3	SO4	D	306	5/5	0.84	0.17	57,59,61,66	5
3	SO4	G	302	5/5	0.85	0.18	84,85,86,86	5

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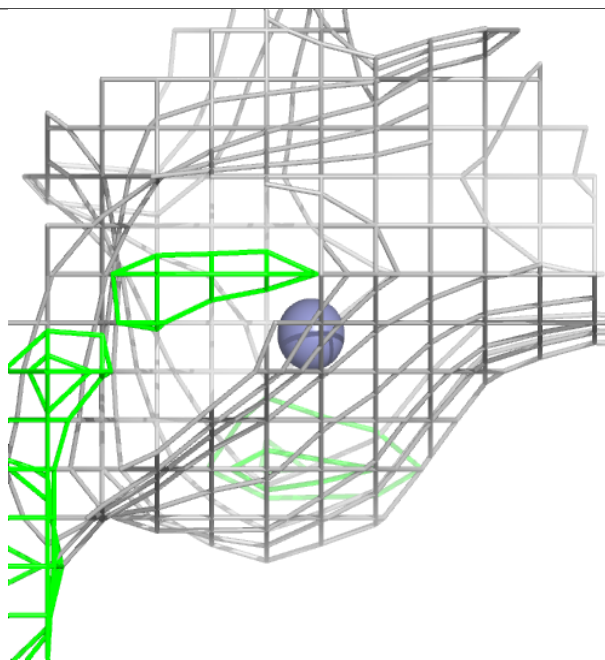
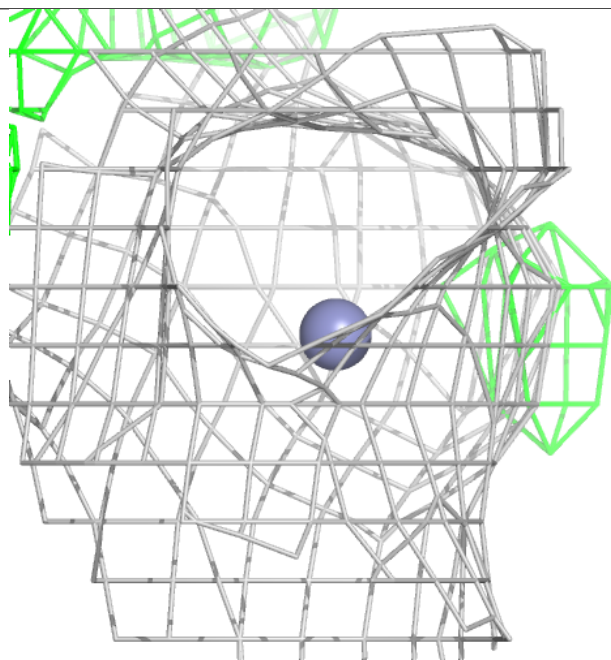
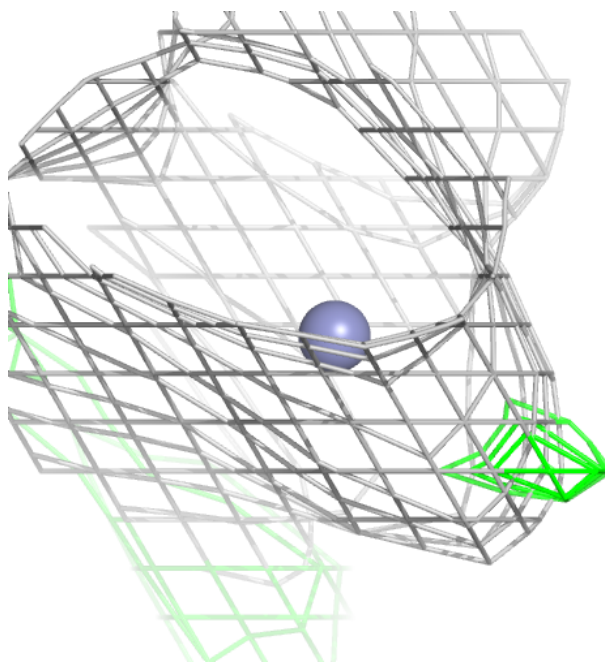
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	306	5/5	0.86	0.19	69,70,71,73	5
2	ZN	G	301	1/1	0.87	0.15	96,96,96,96	1
3	SO4	D	307	5/5	0.87	0.18	70,71,73,76	5
3	SO4	D	308	5/5	0.87	0.16	69,71,72,77	5
3	SO4	D	301	5/5	0.87	0.20	75,87,92,95	0
3	SO4	B	301	5/5	0.87	0.18	90,95,99,104	0
3	SO4	E	305	5/5	0.88	0.21	41,42,44,46	5
3	SO4	D	305	5/5	0.88	0.21	82,86,88,88	5
3	SO4	B	303	5/5	0.88	0.20	86,90,93,93	5
3	SO4	C	305	5/5	0.89	0.19	83,84,84,87	5
3	SO4	E	302	5/5	0.91	0.24	69,73,73,77	5
3	SO4	B	304	5/5	0.91	0.16	42,50,56,59	5
3	SO4	F	301	5/5	0.91	0.17	48,61,64,71	5
3	SO4	F	304	5/5	0.91	0.19	42,42,47,50	5
3	SO4	D	304	5/5	0.91	0.16	68,71,78,84	0
3	SO4	A	303	5/5	0.91	0.17	46,47,54,56	5
3	SO4	C	304	5/5	0.92	0.16	42,55,59,61	5
3	SO4	A	302	5/5	0.92	0.16	69,72,75,77	5
3	SO4	F	303	5/5	0.93	0.19	71,72,74,75	5
3	SO4	E	304	5/5	0.93	0.15	52,61,63,66	5
3	SO4	E	303	5/5	0.94	0.20	46,49,54,57	5
3	SO4	C	302	5/5	0.94	0.14	33,33,40,42	5
3	SO4	A	304	5/5	0.94	0.13	41,52,56,57	5
2	ZN	A	301	1/1	0.94	0.12	68,68,68,68	1
3	SO4	C	303	5/5	0.95	0.13	69,76,78,80	5
2	ZN	C	301	1/1	0.95	0.10	64,64,64,64	1
2	ZN	B	302	1/1	0.96	0.08	71,71,71,71	1
2	ZN	E	301	1/1	0.96	0.08	66,66,66,66	1
2	ZN	F	302	1/1	0.96	0.08	64,64,64,64	1
3	SO4	E	306	5/5	0.97	0.07	37,45,50,51	0
2	ZN	D	302	1/1	0.98	0.05	62,62,62,62	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.

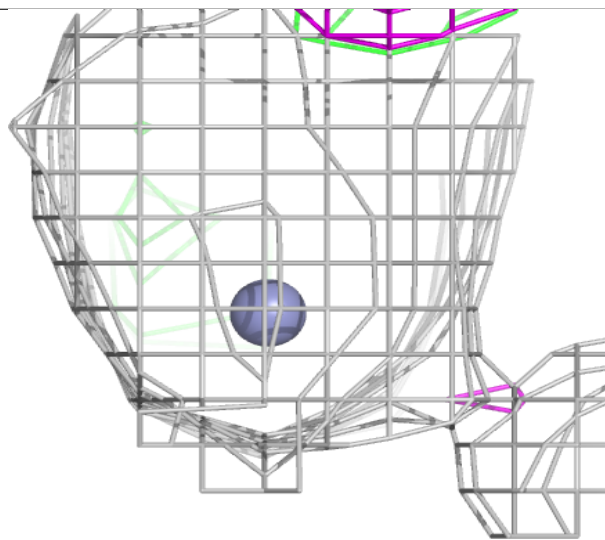
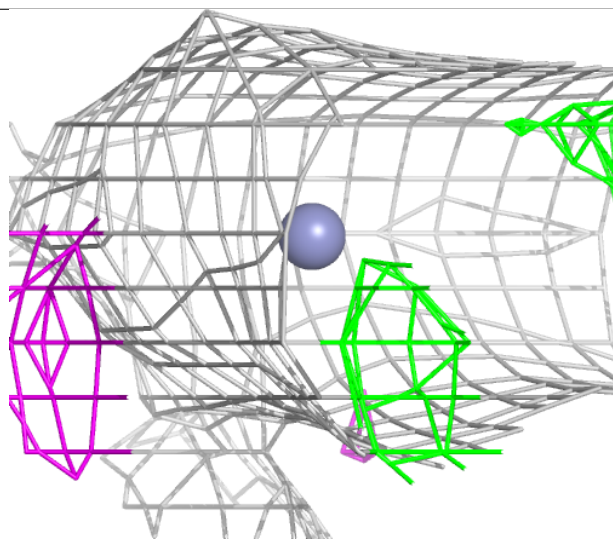
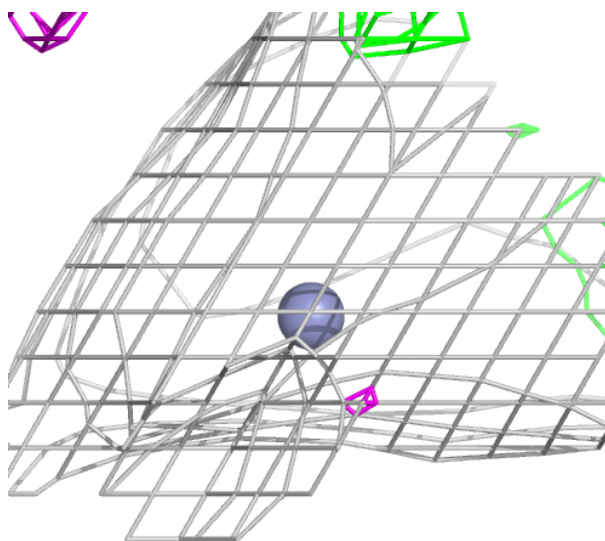
Electron density around ZN H 500:

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



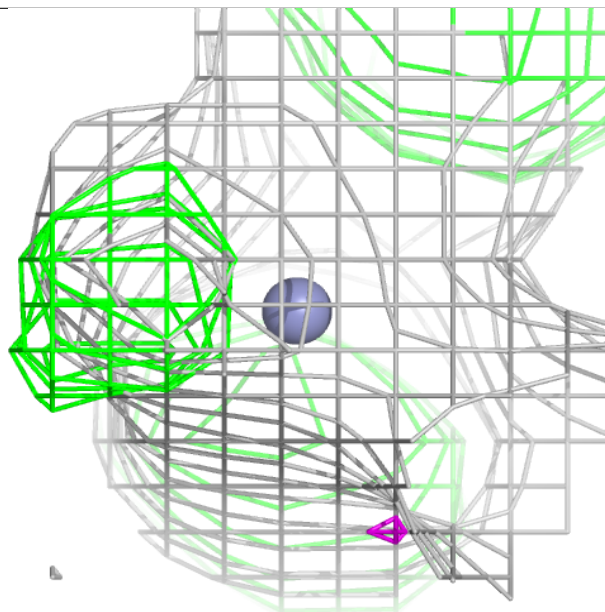
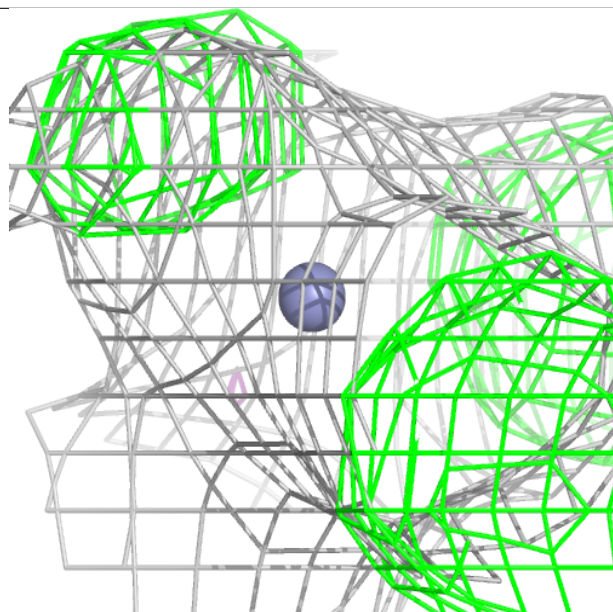
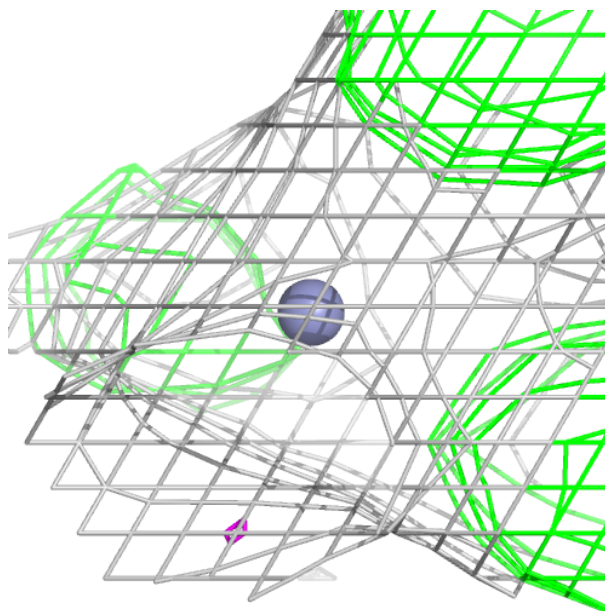
Electron density around ZN I 500:

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



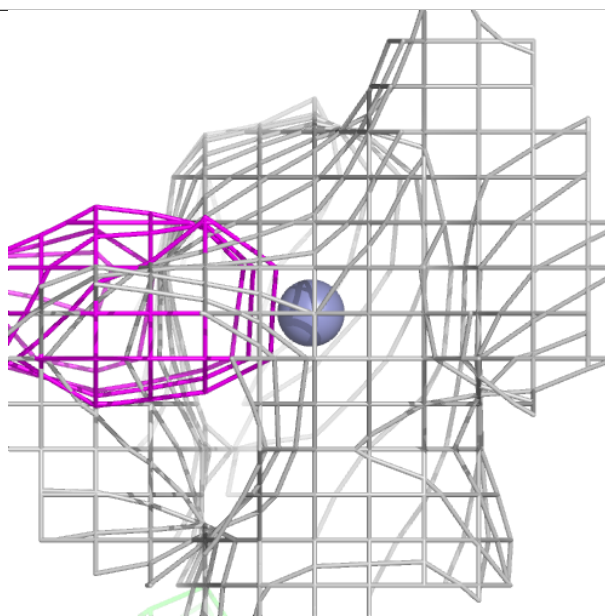
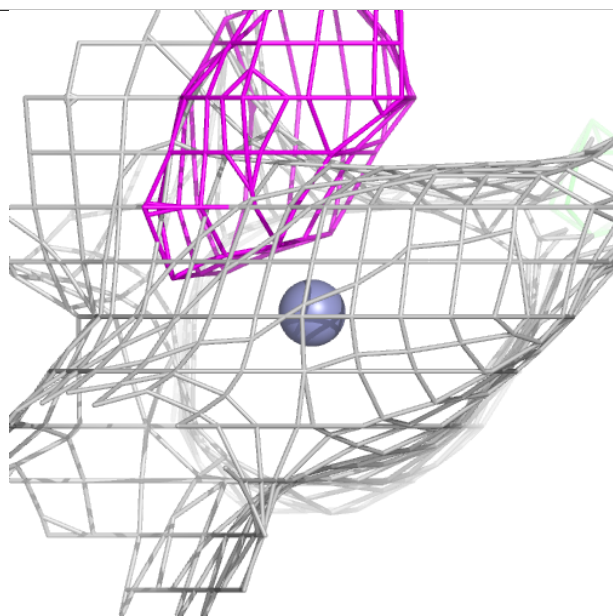
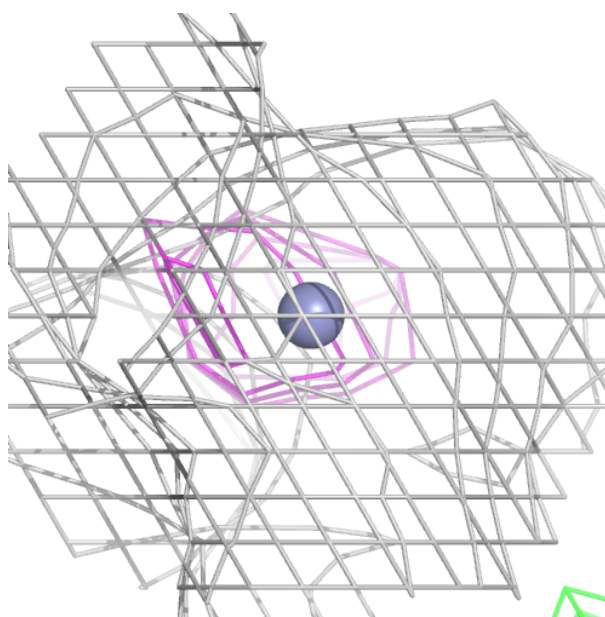
Electron density around ZN G 301:

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



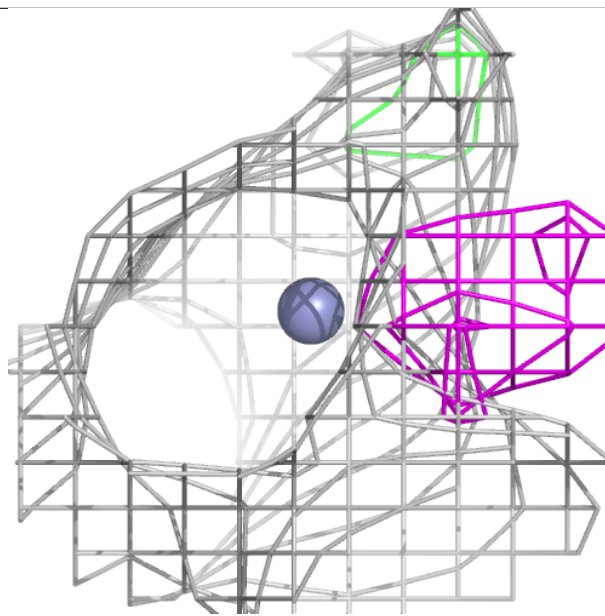
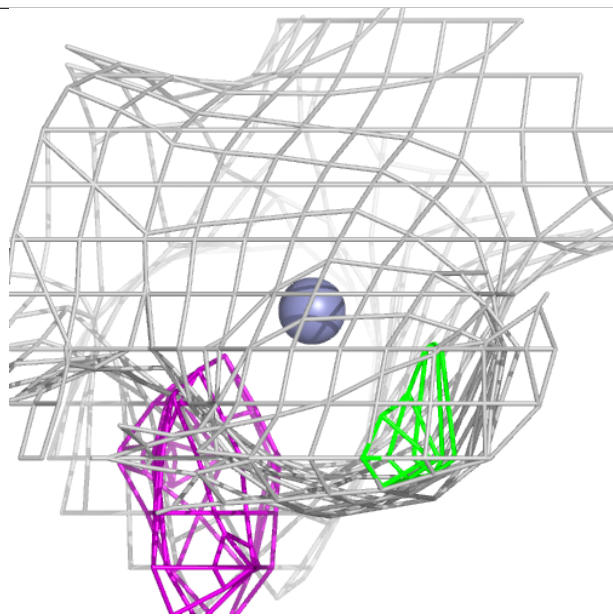
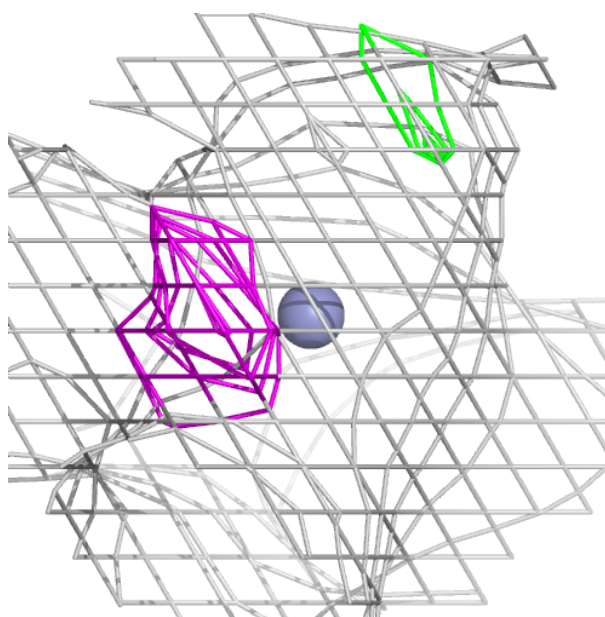
Electron density around ZN A 301:

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



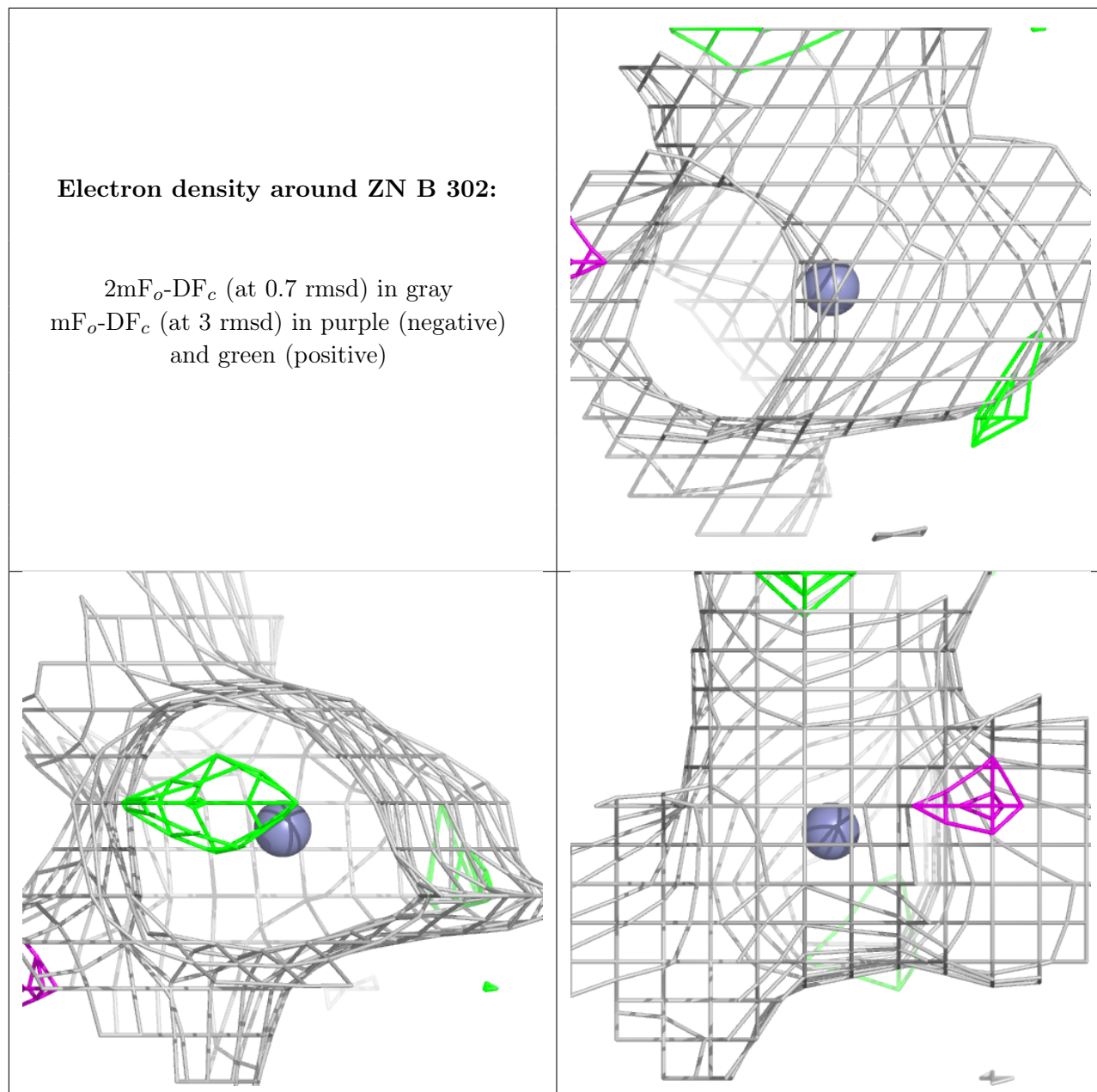
Electron density around ZN C 301:

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



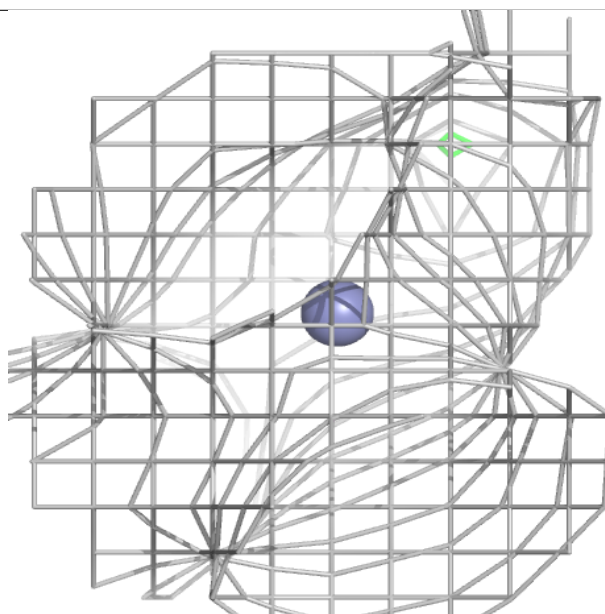
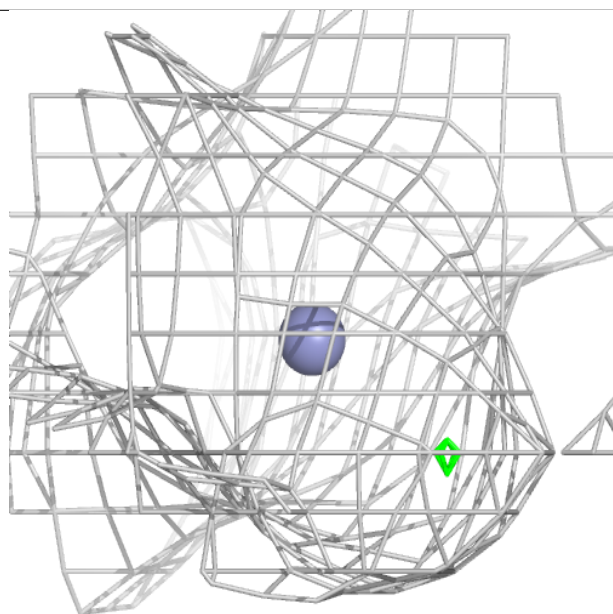
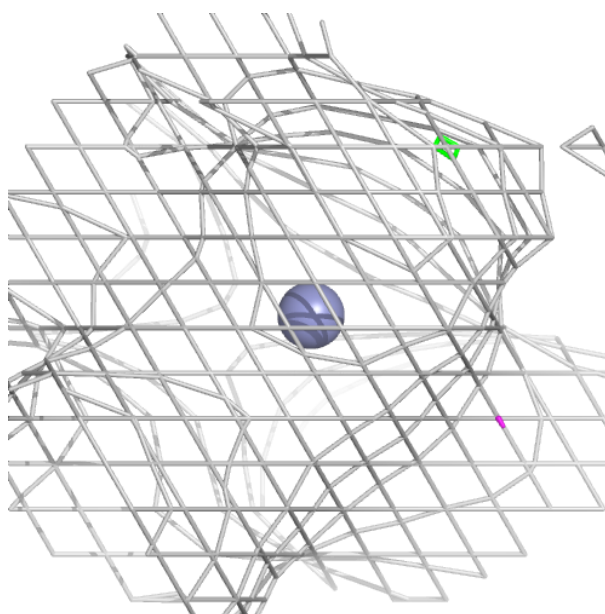
Electron density around ZN B 302:

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



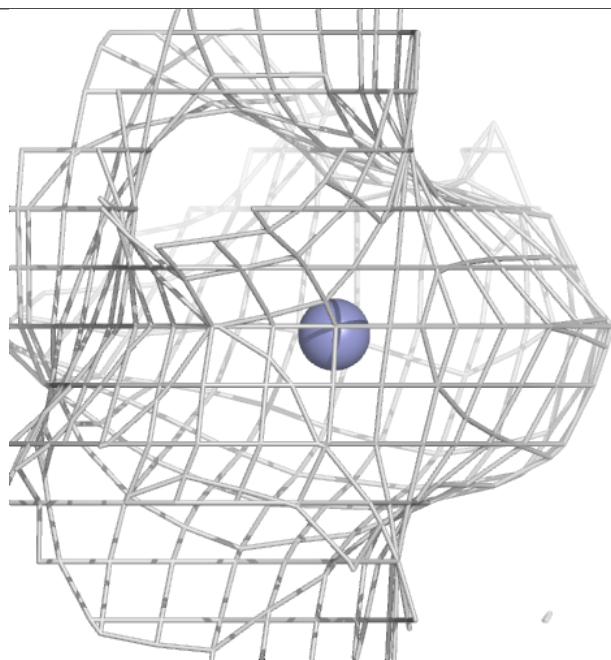
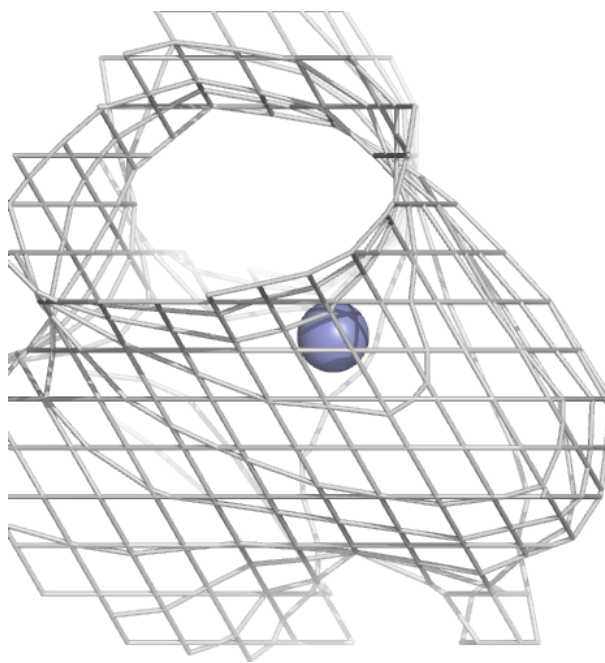
Electron density around ZN E 301:

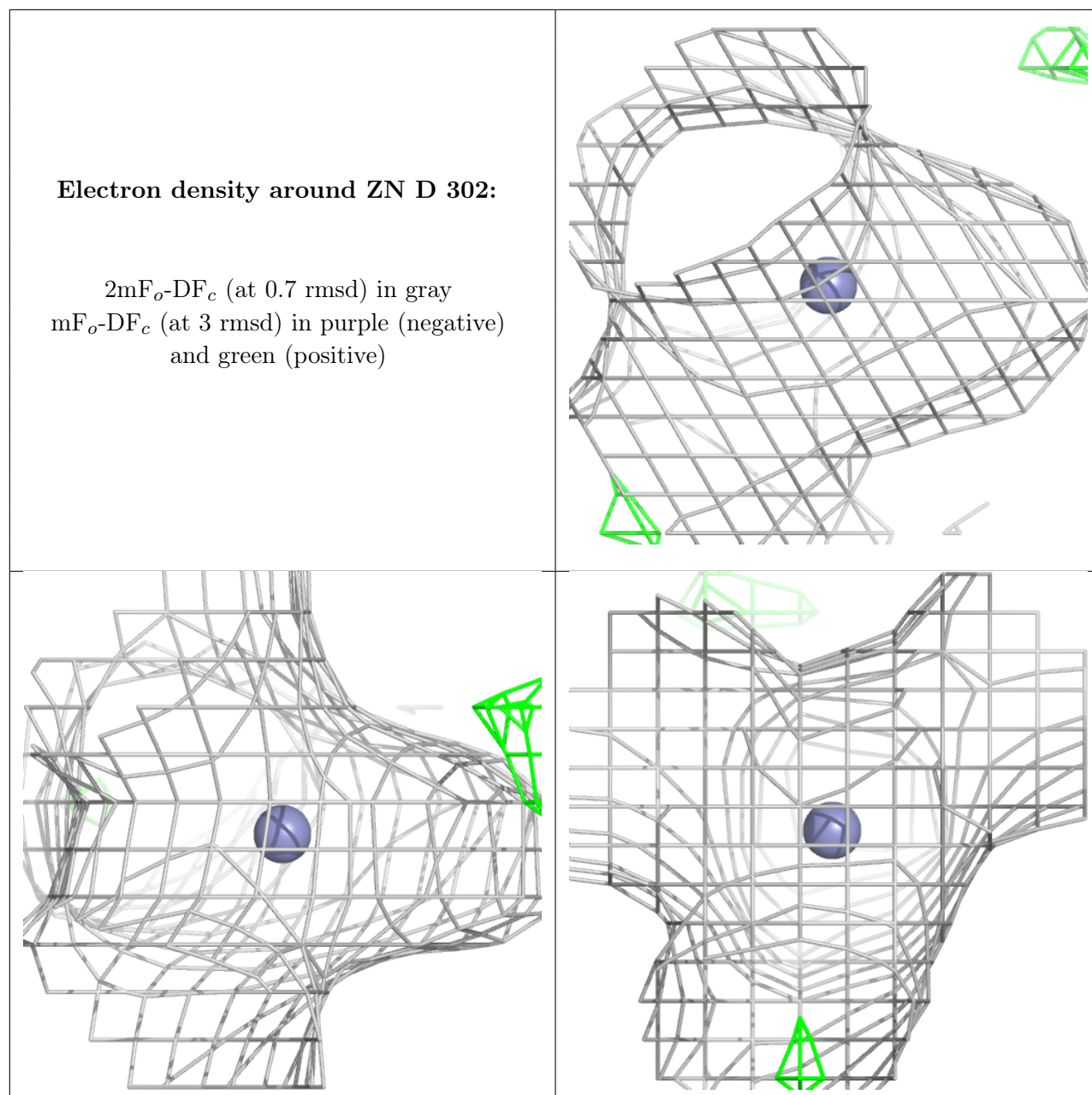
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN F 302:

$2mF_o-DF_c$ (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.