Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 06:40 PM EST

PDB ID	:	6DK9
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 (i) 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 (i)) were used in the production of this report:

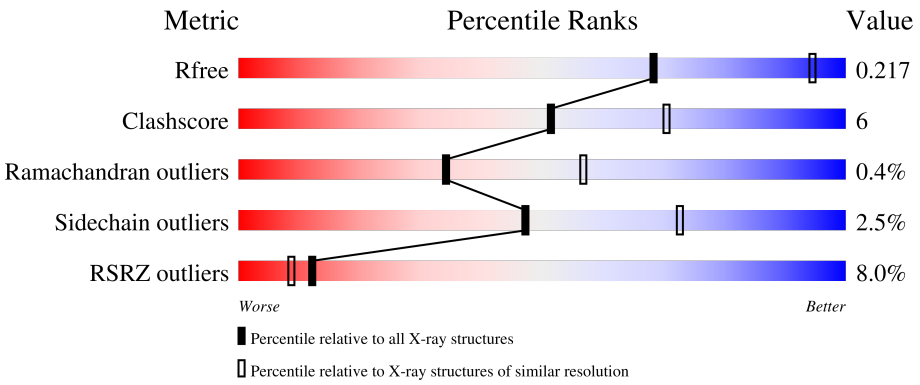
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	% 89% 9% •
1	B	234	92% 5% •
1	C	234	90% 7% •
1	D	234	88% 9% •
1	E	234	91% 6% • •

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Mol	Chain	Length	Quality of chain
1	F	234	% 92% 6%
1	G	234	88% 9%
1	H	234	23% 78% 18%
1	I	234	44% 63% 31%

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	X

2 Entry composition (i)

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

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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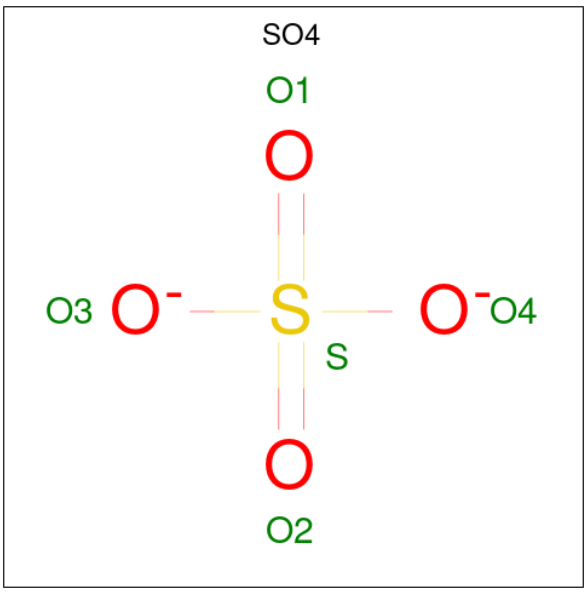
Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	PRO	-	expression tag	UNP A7A1Y4
G	-1	GLU	-	expression tag	UNP A7A1Y4
G	0	PHE	-	expression tag	UNP A7A1Y4
H	-7	GLY	-	expression tag	UNP A7A1Y4
H	-6	PRO	-	expression tag	UNP A7A1Y4
H	-5	LEU	-	expression tag	UNP A7A1Y4
H	-4	GLY	-	expression tag	UNP A7A1Y4
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 (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 4 is water.

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

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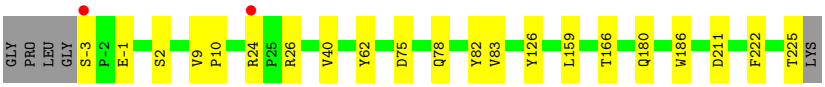
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	68	68	68	0	0
			Total	O		
4	F	38	38	38	0	0
			Total	O		
4	G	23	23	23	0	0

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.

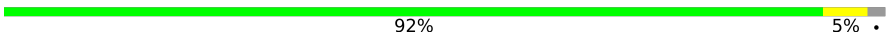
• Molecule 1: DNA damage-inducible protein

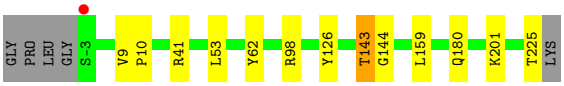
Chain A:



• Molecule 1: DNA damage-inducible protein

Chain B:



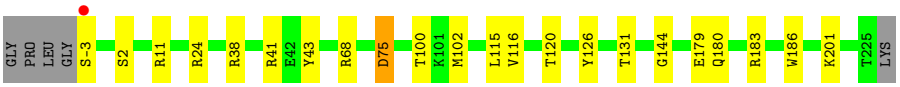


• Molecule 1: DNA damage-inducible protein

Chain C:

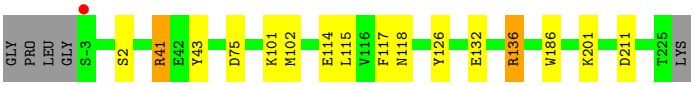
• Molecule 1: DNA damage-inducible protein

Chain D:



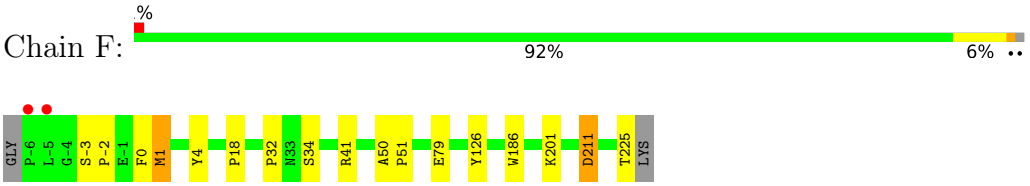
• Molecule 1: DNA damage-inducible protein

Chain E:



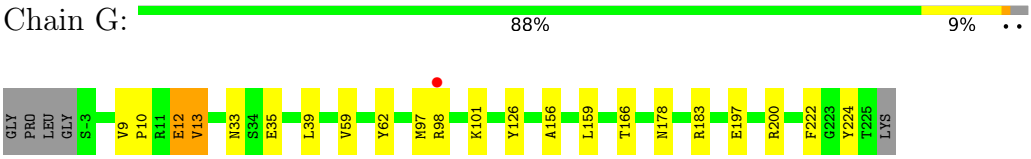
• Molecule 1: DNA damage-inducible protein

Chain F:



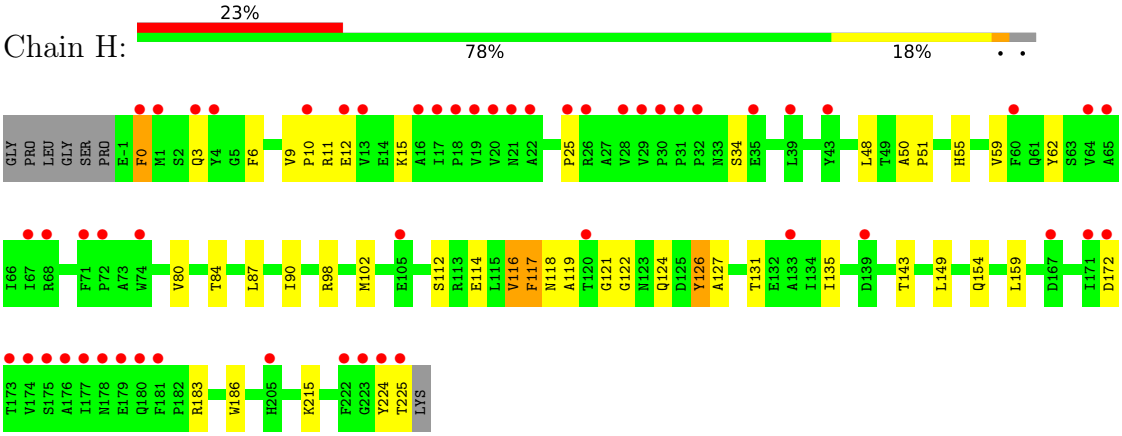
• Molecule 1: DNA damage-inducible protein

Chain G:



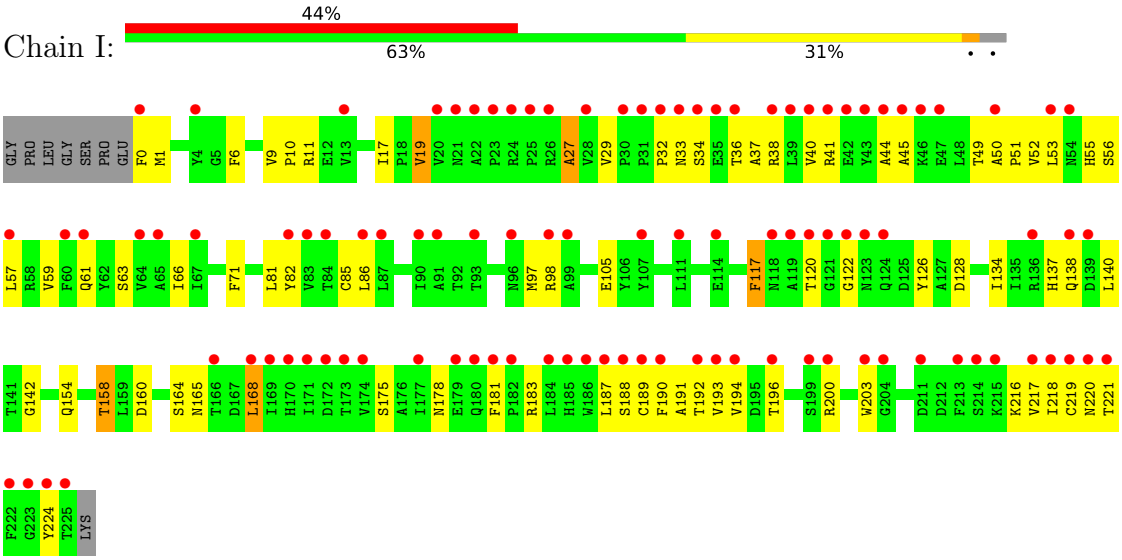
• Molecule 1: DNA damage-inducible protein

Chain H:



• Molecule 1: DNA damage-inducible protein

Chain I:



4 Data and refinement statistics (i)

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 39.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.70-2.60) 98.8 (39.72-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.201 , 0.217 0.201 , 0.217	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 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.29	0/1836	0.51	0/2510
1	B	0.28	0/1836	0.51	0/2510
1	C	0.29	0/1854	0.54	0/2531
1	D	0.30	0/1854	0.53	1/2531 (0.0%)
1	E	0.28	0/1854	0.53	0/2531
1	F	0.28	0/1863	0.49	0/2545
1	G	0.29	0/1842	0.53	0/2517
1	H	0.29	0/1812	0.51	0/2476
1	I	0.30	0/1820	0.57	0/2484
All	All	0.29	0/16571	0.53	1/22635 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	75	ASP	CB-CG-OD2	-5.63	113.23	118.30

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 (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	1791	1748	1746	9	1
1	B	1791	1748	1746	7	0
1	C	1809	1769	1776	10	0
1	D	1809	1765	1776	10	0
1	E	1809	1765	1776	12	0
1	F	1817	1778	1781	14	0
1	G	1797	1757	1757	23	0
1	H	1771	1734	1731	33	1
1	I	1779	1748	1753	71	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16648	15812	15842	180	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 (180) 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: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: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:H:102:MET:HE2	1:I:128:ASP:HA	1.80	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:F:1:MET:HE1	1:G:101:LYS:HE2	1.80	0.62
1:D:131:THR:HB	1:E:102:MET:HE2	1.80	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:80:VAL:HG22	1:H:126:TYR:CE1	2.38	0.58
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:G:200:ARG:HD3	1:I:1:MET:HE2	1.86	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: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:C:2:SER:OG	1:C:75:ASP:OD2	2.25	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: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:I:160:ASP:O	1:I:224:TYR:OH	2.25	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:F:1:MET:HG2	3:F:305:SO4:O3	2.09	0.52
1:F:1:MET:CE	1:G:101:LYS:HE2	2.40	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: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:F:34:SER:OG	1:F:79:GLU:OE1	2.28	0.50
1:G:97:MET:HE1	1:G:197:GLU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:THR:HG21	1:G:222:PHE:CE1	2.47	0.50
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:I:168:LEU:C	1:I:168:LEU:HD23	2.32	0.49
1:D:43:TYR:CZ	1:D:115:LEU:HD11	2.47	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: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:B:201:LYS:NZ	4:B:403:HOH:O	2.42	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:H:12:GLU:CD	1:H:15:LYS:HE3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:TYR:CD2	1:C:159:LEU:HD23	2.49	0.46
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: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:A:211:ASP:N	1:A:211:ASP:OD1	2.50	0.43
1:I:11:ARG:HH21	1:I:142:GLY:C	2.21	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:F:1:MET:HE2	1:G:101:LYS:CD	2.50	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:-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: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:A:166:THR:HG21	1:A:222:PHE:CE1	2.56	0.40
1:I:55:HIS:O	1:I:59:VAL:HG23	2.21	0.40
1:G:33:ASN:O	1:G:33:ASN:OD1	2.40	0.40
1:I:138:GLN:HA	1:I:140:LEU:HG	2.03	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%)	34	57
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%)	34	57
1	G	228/234 (97%)	225 (99%)	2 (1%)	1 (0%)	34	57
1	H	225/234 (96%)	213 (95%)	7 (3%)	5 (2%)	6	12
1	I	224/234 (96%)	213 (95%)	10 (4%)	1 (0%)	34	57
All	All	2048/2106 (97%)	1990 (97%)	49 (2%)	9 (0%)	34	57

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%)	191 (98%)	4 (2%)	53	77
1	B	195/202 (96%)	190 (97%)	5 (3%)	46	72
1	C	199/202 (98%)	193 (97%)	6 (3%)	41	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	199/202 (98%)	190 (96%)	9 (4%)	27	52
1	E	199/202 (98%)	194 (98%)	5 (2%)	47	73
1	F	199/202 (98%)	195 (98%)	4 (2%)	55	78
1	G	196/202 (97%)	194 (99%)	2 (1%)	76	90
1	H	192/202 (95%)	190 (99%)	2 (1%)	76	90
1	I	195/202 (96%)	188 (96%)	7 (4%)	35	61
All	All	1769/1818 (97%)	1725 (98%)	44 (2%)	47	73

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	126	TYR
1	A	180	GLN
1	A	225	THR
1	B	41	ARG
1	B	53	LEU
1	B	126	TYR
1	B	143	THR
1	B	180	GLN
1	C	126	TYR
1	C	143	THR
1	C	180	GLN
1	C	201	LYS
1	C	211	ASP
1	C	225	THR
1	D	11	ARG
1	D	24	ARG
1	D	38	ARG
1	D	41	ARG
1	D	126	TYR
1	D	179	GLU
1	D	180	GLN
1	D	183	ARG
1	D	201	LYS
1	E	41	ARG
1	E	117	PHE
1	E	126	TYR
1	E	136	ARG
1	E	201	LYS

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Mol	Chain	Res	Type
1	F	1	MET
1	F	126	TYR
1	F	201	LYS
1	F	211	ASP
1	G	12	GLU
1	G	126	TYR
1	H	126	TYR
1	H	225	THR
1	I	19	VAL
1	I	97	MET
1	I	117	PHE
1	I	126	TYR
1	I	158	THR
1	I	168	LEU
1	I	192	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	H	124	GLN
1	H	165	ASN
1	I	33	ASN
1	I	61	GLN
1	I	198	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 monosaccharides 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	303	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	F	301	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	G	302	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	F	304	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	D	303	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	306	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	D	308	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	E	305	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	E	302	-	4,4,4	0.14	0	6,6,6	0.11	0
3	SO4	A	304	-	4,4,4	0.16	0	6,6,6	0.21	0
3	SO4	A	303	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	E	303	-	4,4,4	0.13	0	6,6,6	0.16	0
3	SO4	D	304	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	D	301	-	4,4,4	0.15	0	6,6,6	0.12	0
3	SO4	D	305	-	4,4,4	0.15	0	6,6,6	0.04	0
3	SO4	E	306	-	4,4,4	0.13	0	6,6,6	0.30	0
3	SO4	C	303	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	F	303	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	C	306	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	F	305	-	4,4,4	0.23	0	6,6,6	0.39	0
3	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	C	304	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	D	307	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	E	304	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.17	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	E	305	SO4	2	0
3	A	303	SO4	1	0
3	E	303	SO4	1	0
3	D	304	SO4	1	0
3	D	305	SO4	1	0
3	F	305	SO4	5	0
3	D	307	SO4	1	0
3	C	302	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.23	2 (0%)	84	82	39, 54, 76, 114	0
1	B	229/234 (97%)	-0.29	1 (0%)	92	91	37, 51, 70, 104	0
1	C	229/234 (97%)	-0.45	1 (0%)	92	91	32, 41, 64, 106	0
1	D	229/234 (97%)	-0.35	1 (0%)	92	91	34, 44, 61, 127	0
1	E	229/234 (97%)	-0.37	1 (0%)	92	91	33, 41, 63, 146	0
1	F	232/234 (99%)	-0.21	2 (0%)	84	82	38, 49, 72, 136	0
1	G	229/234 (97%)	-0.10	1 (0%)	92	91	44, 63, 87, 107	0
1	H	227/234 (97%)	1.03	53 (23%)	0	0	69, 104, 140, 171	0
1	I	226/234 (96%)	1.97	102 (45%)	0	0	82, 140, 182, 247	0
All	All	2059/2106 (97%)	0.11	164 (7%)	12	9	32, 53, 146, 247	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	192	THR	7.5
1	I	90	ILE	7.5
1	I	177	ILE	6.8
1	I	225	THR	6.4
1	I	173	THR	6.3
1	I	169	ILE	6.1
1	H	0	PHE	6.1
1	I	82	TYR	6.1
1	I	39	LEU	6.0
1	I	218	ILE	5.8
1	I	217	VAL	5.7
1	I	188	SER	5.6
1	I	42	GLU	5.6
1	I	213	PHE	5.6
1	I	139	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	I	193	VAL	5.3
1	I	98	ARG	5.3
1	I	46	LYS	5.3
1	I	86	LEU	5.3
1	I	220	ASN	5.2
1	H	19	VAL	5.1
1	H	181	PHE	5.0
1	I	196	THR	5.0
1	I	190	PHE	4.9
1	I	200	ARG	4.9
1	I	211	ASP	4.9
1	I	96	ASN	4.9
1	I	61	GLN	4.7
1	H	64	VAL	4.6
1	I	184	LEU	4.6
1	I	194	VAL	4.6
1	I	25	PRO	4.6
1	H	28	VAL	4.5
1	I	222	PHE	4.3
1	I	168	LEU	4.2
1	I	185	HIS	4.2
1	H	29	VAL	4.1
1	I	166	THR	4.1
1	I	40	VAL	4.1
1	I	224	TYR	4.0
1	I	83	VAL	4.0
1	H	30	PRO	4.0
1	I	43	TYR	3.9
1	F	-6	PRO	3.9
1	H	32	PRO	3.9
1	I	99	ALA	3.9
1	I	84	THR	3.8
1	I	214	SER	3.8
1	H	225	THR	3.8
1	I	35	GLU	3.8
1	D	-3	SER	3.7
1	I	33	ASN	3.7
1	I	65	ALA	3.7
1	I	20	VAL	3.6
1	I	28	VAL	3.6
1	I	57	LEU	3.6
1	I	38	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	172	ASP	3.6
1	E	-3	SER	3.6
1	I	107	TYR	3.6
1	H	74	TRP	3.5
1	I	24	ARG	3.5
1	I	215	LYS	3.5
1	I	119	ALA	3.5
1	H	139	ASP	3.4
1	H	1	MET	3.4
1	I	21	ASN	3.4
1	H	25	PRO	3.4
1	H	71	PHE	3.4
1	C	-3	SER	3.3
1	I	22	ALA	3.3
1	I	34	SER	3.3
1	H	20	VAL	3.2
1	I	120	THR	3.2
1	I	122	GLY	3.2
1	I	30	PRO	3.2
1	I	187	LEU	3.2
1	I	181	PHE	3.1
1	I	121	GLY	3.1
1	H	177	ILE	3.1
1	I	199	SER	3.0
1	I	50	ALA	3.0
1	I	189	CYS	3.0
1	I	47	GLU	3.0
1	I	170	HIS	3.0
1	H	3	GLN	2.9
1	I	31	PRO	2.9
1	I	93	THR	2.9
1	I	118	ASN	2.9
1	I	114	GLU	2.8
1	I	23	PRO	2.8
1	I	26	ARG	2.8
1	I	204	GLY	2.8
1	A	24	ARG	2.8
1	H	68	ARG	2.7
1	I	60	PHE	2.7
1	H	180	GLN	2.7
1	H	179	GLU	2.7
1	I	67	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	173	THR	2.7
1	I	36	THR	2.7
1	F	-5	LEU	2.7
1	I	123	ASN	2.7
1	B	-3	SER	2.7
1	H	60	PHE	2.6
1	H	22	ALA	2.6
1	I	53	LEU	2.6
1	H	65	ALA	2.6
1	H	176	ALA	2.6
1	H	17	ILE	2.5
1	H	31	PRO	2.5
1	H	167	ASP	2.5
1	H	16	ALA	2.5
1	I	171	ILE	2.5
1	H	223	GLY	2.5
1	H	72	PRO	2.5
1	H	172	ASP	2.5
1	I	186	TRP	2.5
1	H	133	ALA	2.5
1	I	174	VAL	2.5
1	I	87	LEU	2.5
1	H	21	ASN	2.5
1	I	180	GLN	2.4
1	H	224	TYR	2.4
1	I	179	GLU	2.4
1	I	91	ALA	2.4
1	H	67	ILE	2.4
1	I	219	CYS	2.4
1	I	138	GLN	2.4
1	H	13	VAL	2.4
1	H	174	VAL	2.4
1	H	222	PHE	2.4
1	I	13	VAL	2.4
1	I	32	PRO	2.3
1	I	203	TRP	2.3
1	I	111	LEU	2.3
1	H	35	GLU	2.3
1	I	45	ALA	2.3
1	I	54	ASN	2.3
1	H	43	TYR	2.3
1	I	223	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	105	GLU	2.2
1	H	4	TYR	2.2
1	H	18	PRO	2.2
1	H	39	LEU	2.2
1	H	26	ARG	2.2
1	H	205	HIS	2.2
1	I	182	PRO	2.2
1	I	4	TYR	2.2
1	G	98	ARG	2.2
1	H	171	ILE	2.2
1	H	120	THR	2.2
1	I	124	GLN	2.1
1	I	136	ARG	2.1
1	A	-3	SER	2.1
1	H	12	GLU	2.1
1	H	178	ASN	2.1
1	I	41	ARG	2.1
1	H	175	SER	2.1
1	I	0	PHE	2.1
1	H	10	PRO	2.1
1	I	64	VAL	2.0
1	I	44	ALA	2.0
1	I	221	THR	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 monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

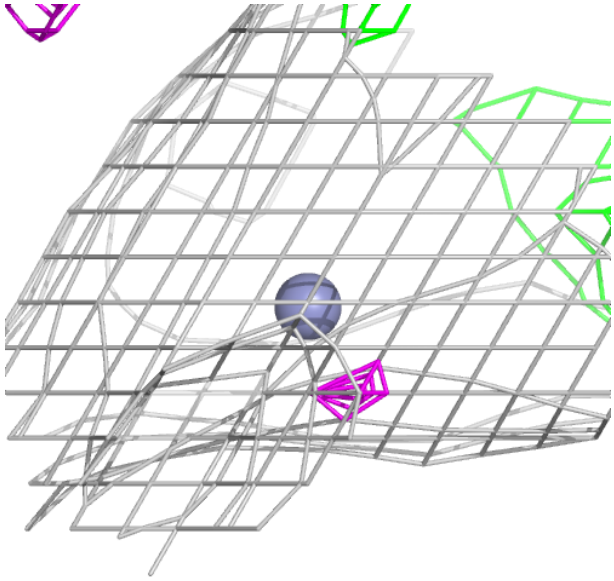
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	I	500	1/1	0.03	0.18	132,132,132,132	1
3	SO4	F	305	5/5	0.56	0.42	148,149,151,151	5
2	ZN	G	301	1/1	0.72	0.18	96,96,96,96	1
2	ZN	H	500	1/1	0.79	0.19	94,94,94,94	1
3	SO4	D	305	5/5	0.84	0.26	82,86,88,88	5
3	SO4	B	303	5/5	0.86	0.21	86,90,93,93	5
2	ZN	E	301	1/1	0.87	0.08	66,66,66,66	1
3	SO4	D	308	5/5	0.88	0.21	69,71,72,77	5
3	SO4	E	305	5/5	0.88	0.37	41,42,44,46	5
3	SO4	D	306	5/5	0.88	0.32	57,59,61,66	5
3	SO4	D	307	5/5	0.89	0.20	70,71,73,76	5
3	SO4	D	301	5/5	0.89	0.16	75,87,92,95	0
3	SO4	C	306	5/5	0.90	0.26	69,70,71,73	5
3	SO4	C	305	5/5	0.90	0.26	83,84,84,87	5
3	SO4	C	302	5/5	0.91	0.29	33,33,40,42	5
3	SO4	A	302	5/5	0.91	0.18	69,72,75,77	5
3	SO4	F	301	5/5	0.91	0.21	48,61,64,71	5
3	SO4	D	303	5/5	0.91	0.22	98,102,103,105	0
3	SO4	G	302	5/5	0.91	0.28	84,85,86,86	5
3	SO4	A	303	5/5	0.92	0.21	46,47,54,56	5
2	ZN	C	301	1/1	0.92	0.09	64,64,64,64	1
3	SO4	B	304	5/5	0.92	0.27	42,50,56,59	5
3	SO4	E	303	5/5	0.92	0.28	46,49,54,57	5
3	SO4	B	301	5/5	0.93	0.14	90,95,99,104	0
3	SO4	F	304	5/5	0.93	0.22	42,42,47,50	5
3	SO4	E	304	5/5	0.93	0.21	52,61,63,66	5
3	SO4	E	302	5/5	0.93	0.21	69,73,73,77	5
3	SO4	A	304	5/5	0.94	0.18	41,52,56,57	5
3	SO4	C	304	5/5	0.94	0.16	42,55,59,61	5
2	ZN	A	301	1/1	0.94	0.08	68,68,68,68	1
3	SO4	C	303	5/5	0.95	0.22	69,76,78,80	5
3	SO4	D	304	5/5	0.96	0.20	68,71,78,84	0
2	ZN	D	302	1/1	0.96	0.09	62,62,62,62	1
3	SO4	F	303	5/5	0.96	0.18	71,72,74,75	5
2	ZN	B	302	1/1	0.97	0.06	71,71,71,71	1
2	ZN	F	302	1/1	0.97	0.06	64,64,64,64	1
3	SO4	E	306	5/5	0.98	0.15	37,45,50,51	0

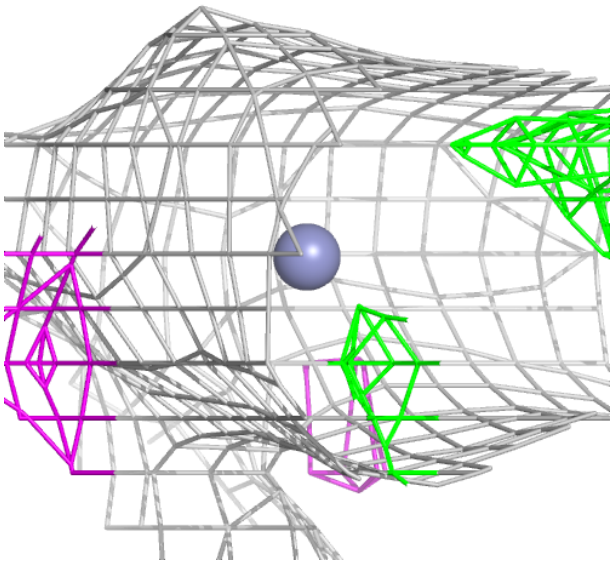
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

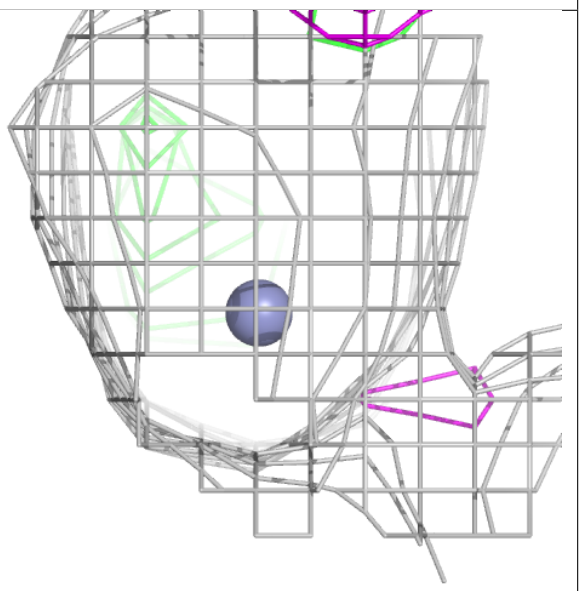
orientation to approximate a three-dimensional view.

Electron density around 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)

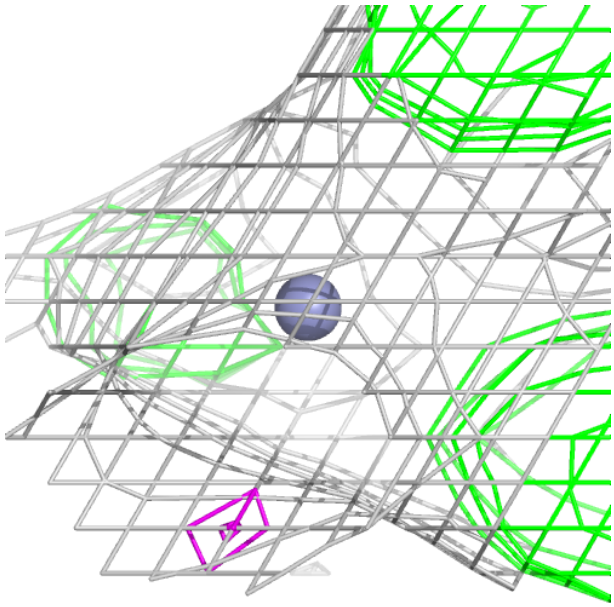


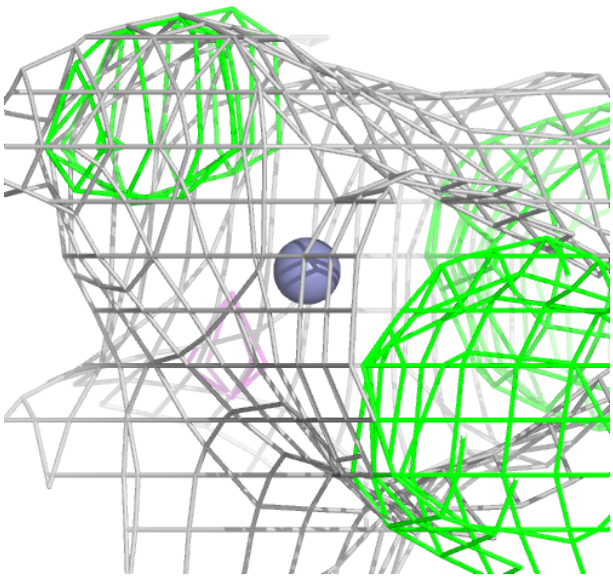


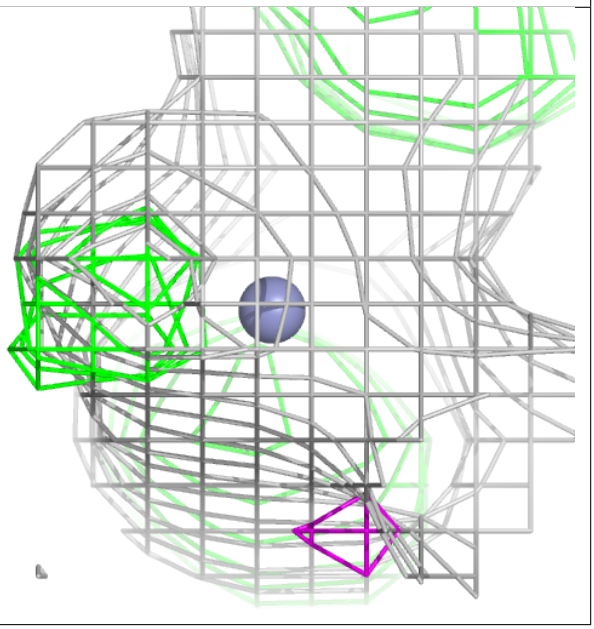


Electron density around ZN G 301:

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

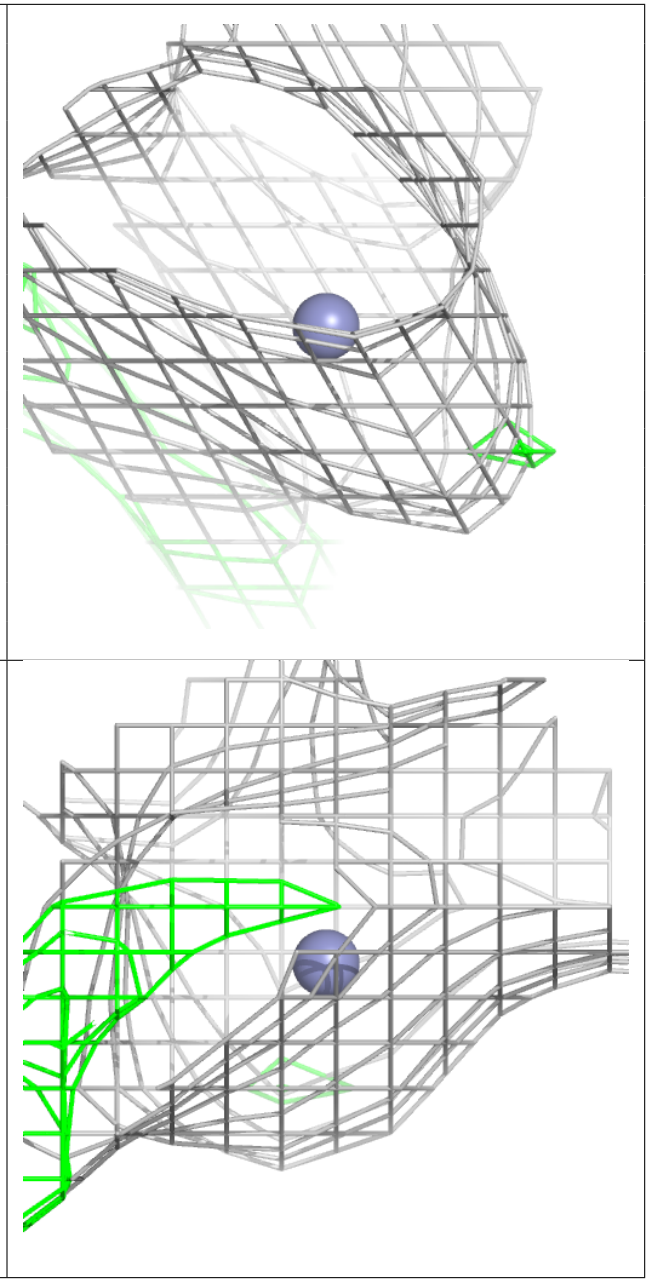






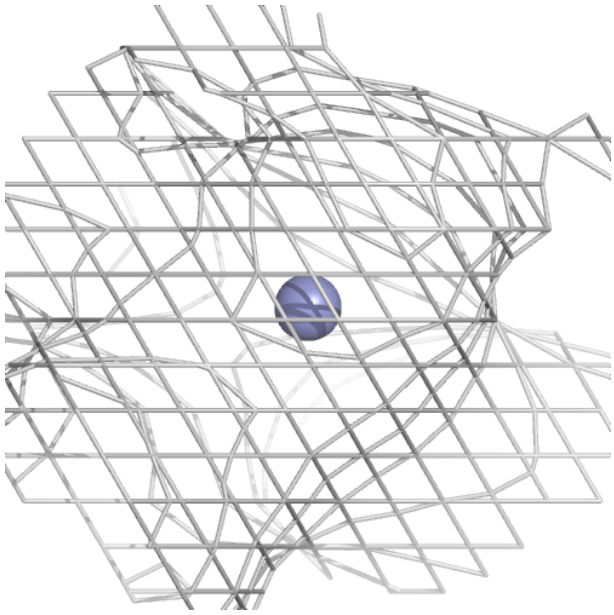
Electron density around ZN H 500:

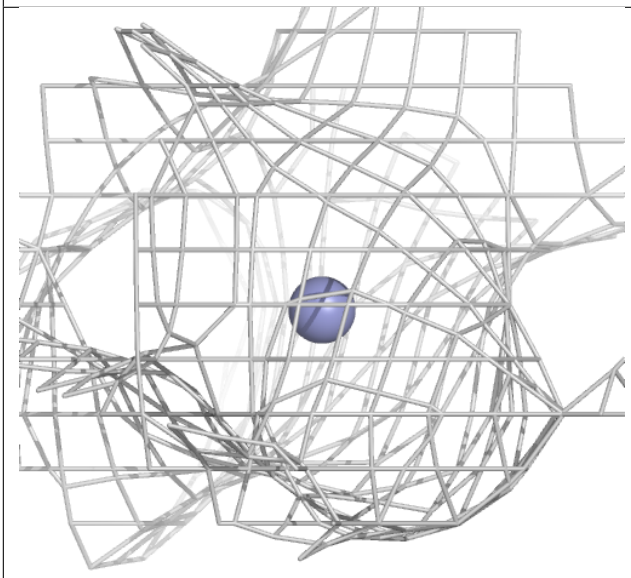
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

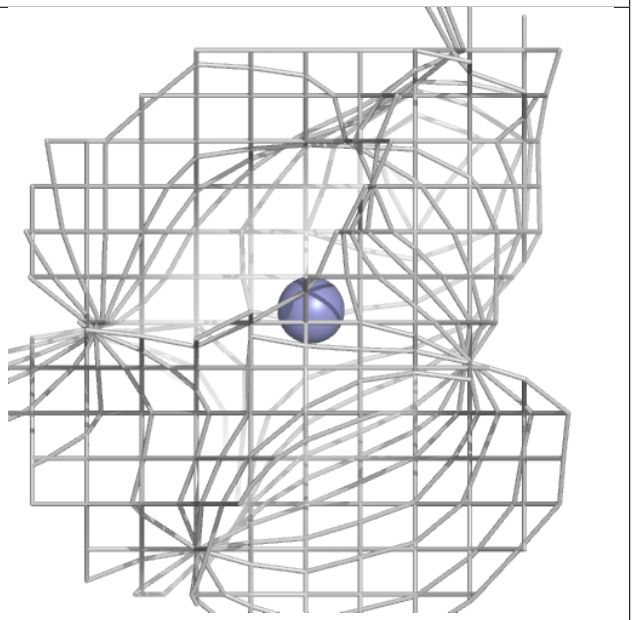


Electron density around ZN E 301:

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

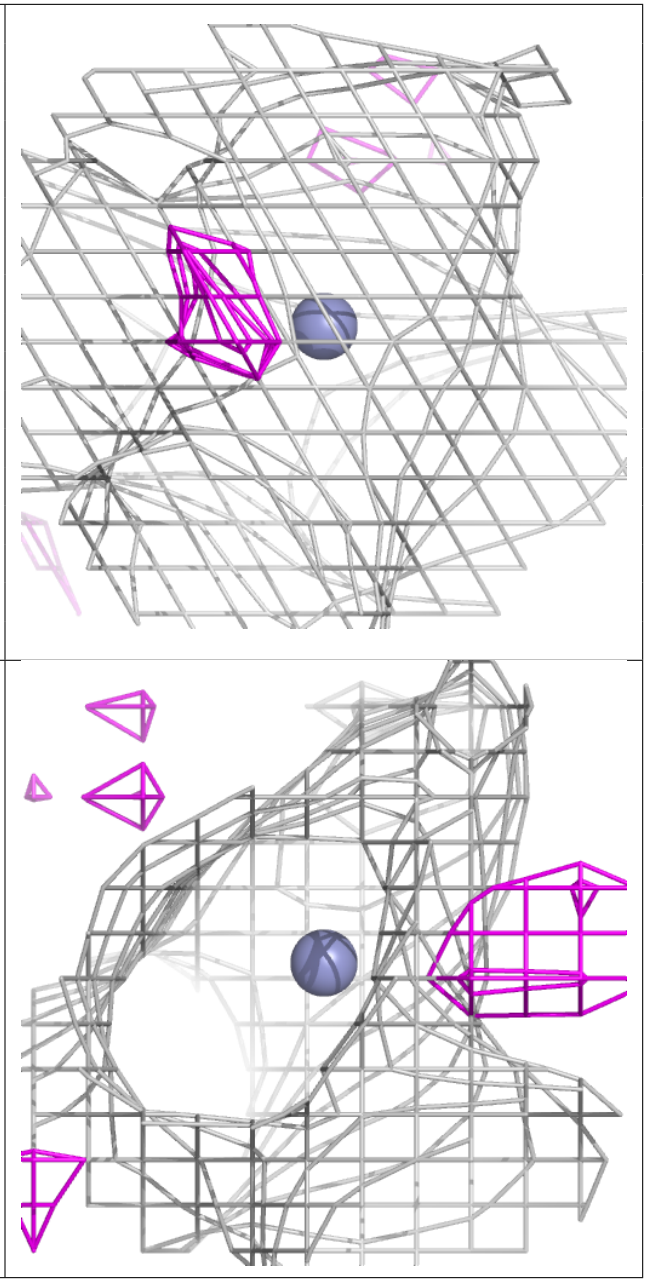






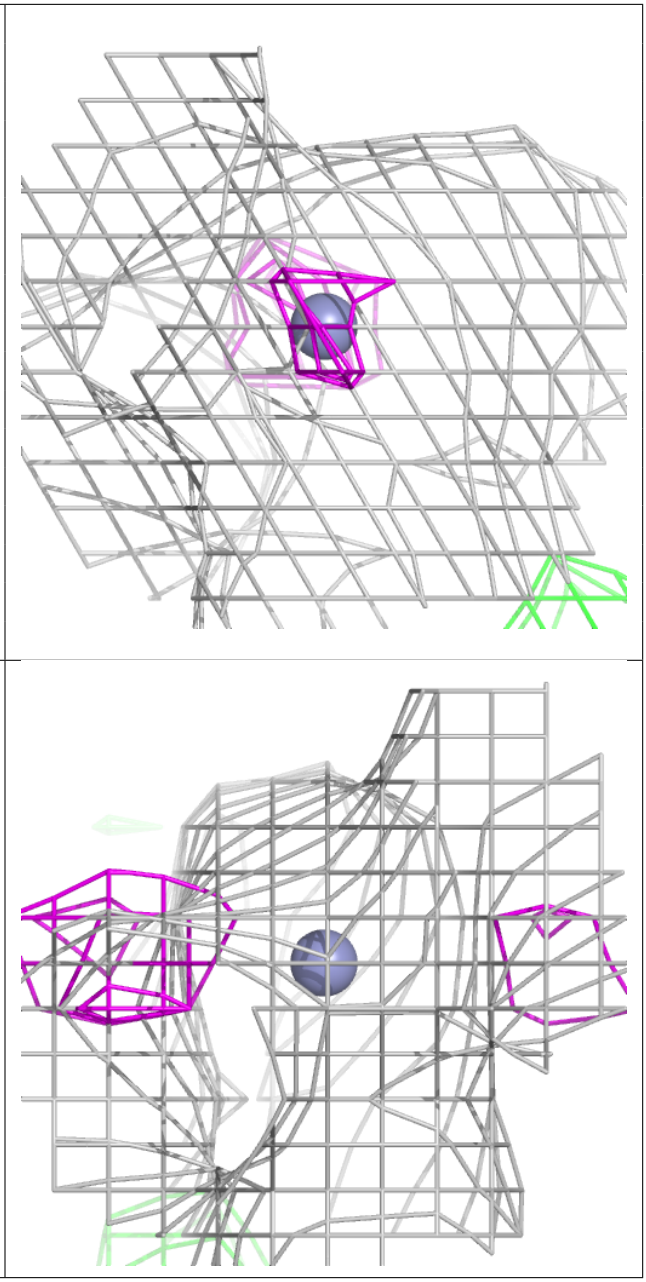
Electron density around ZN C 301:

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



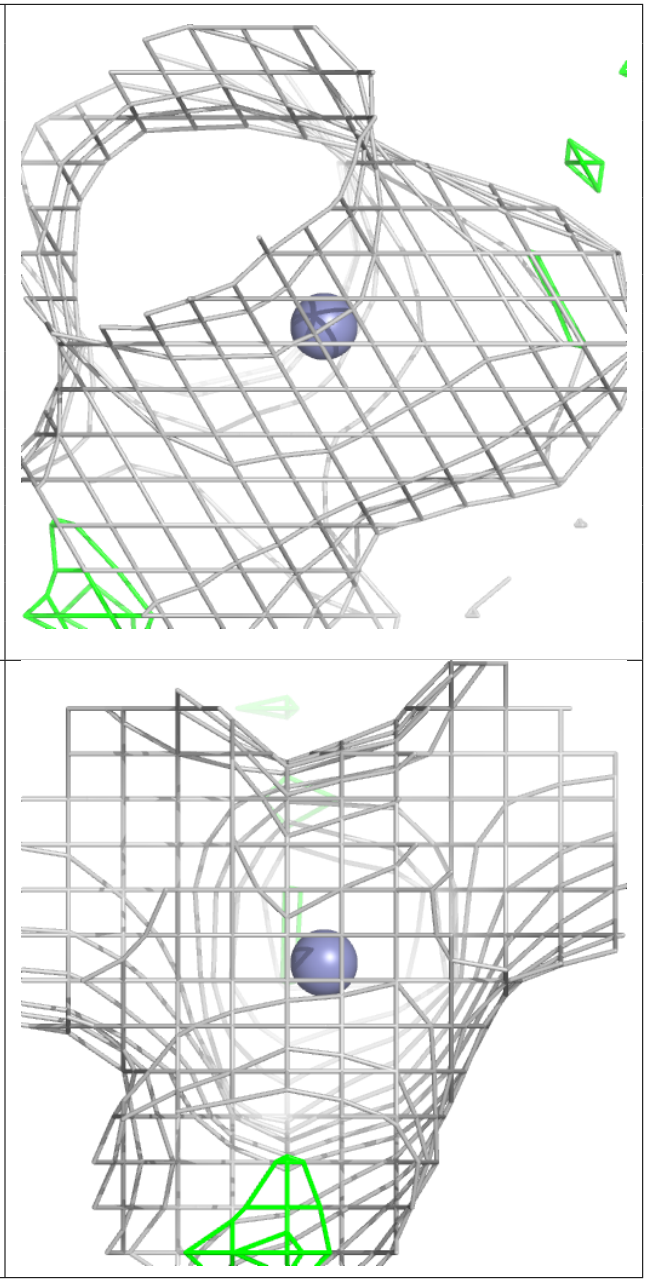
Electron density around ZN A 301:

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



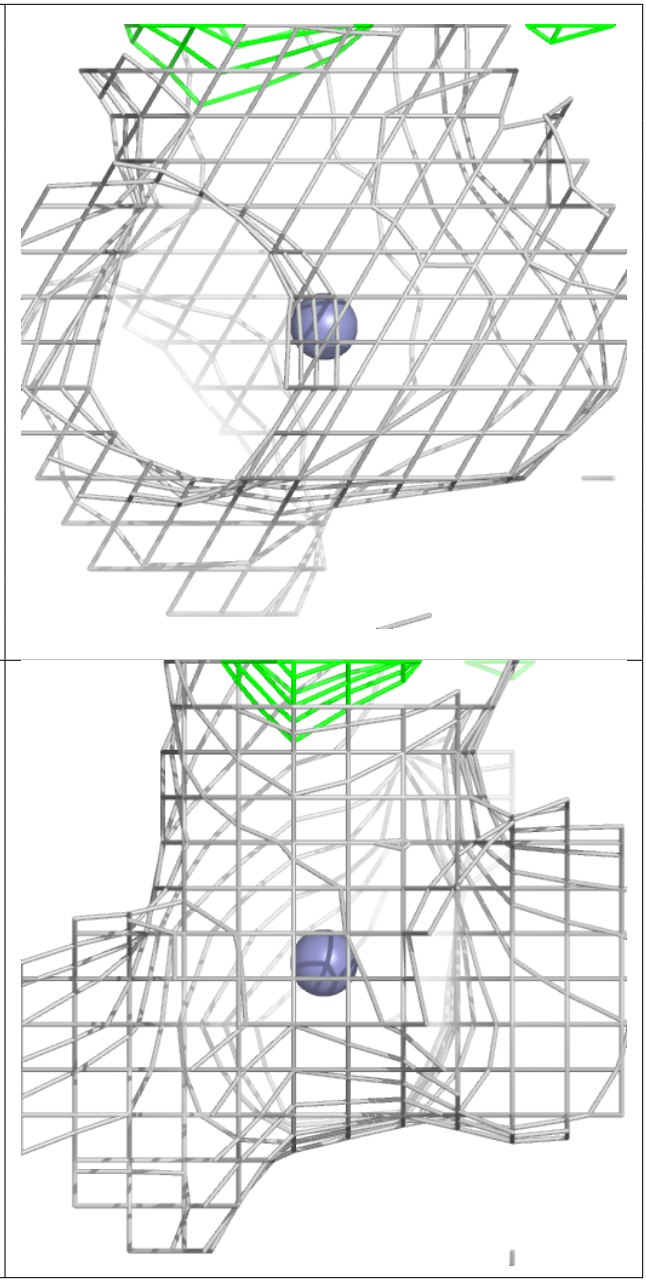
Electron density around ZN D 302:

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



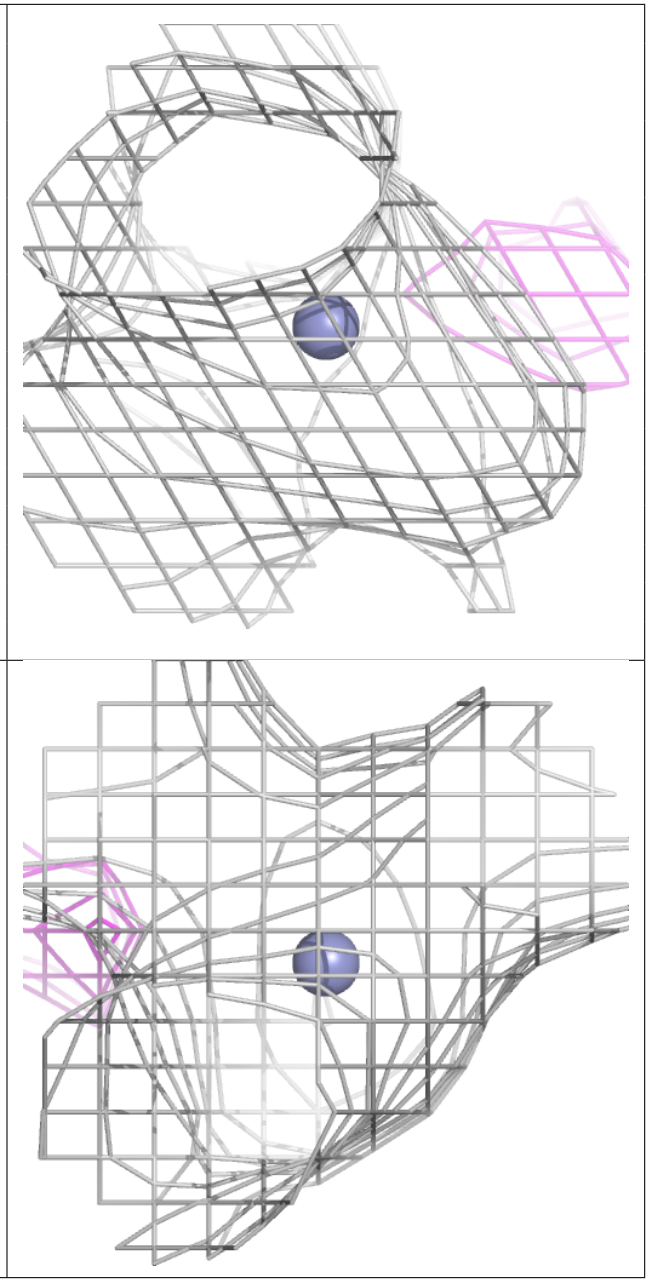
Electron density around ZN B 302:

$2mF_o$-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 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 (i)

There are no such residues in this entry.