



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:44 PM UTC

PDB ID : 6DKD / pdb_00006dkd
Title : Yeast Ddi2 Cyanamide Hydratase
Authors : Moore, S.A.; Xiao, W.; Li, J.
Deposited on : 2018-05-29
Resolution : 3.00 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

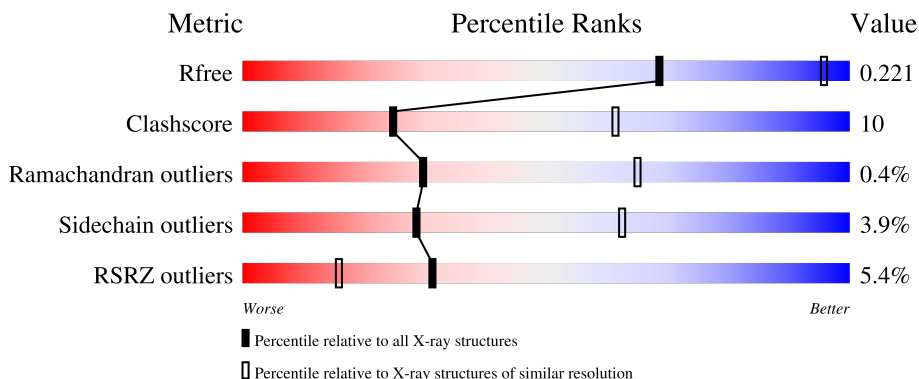
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



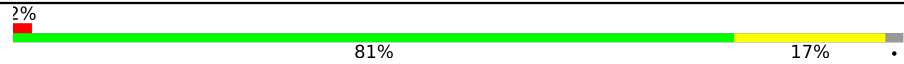

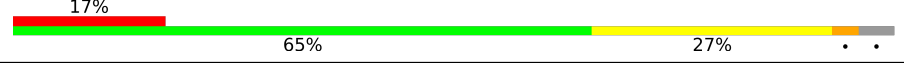

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	 75% 20%
1	B	234	 82% 15%
1	C	234	 83% 13%
1	D	234	 87% 11%
1	E	234	 81% 16%

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

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32110 atoms, of which 15747 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	3512	1129	1738	301	338	6	0	0	0
1	B	230	3542	1137	1753	305	341	6	0	0	0
1	C	230	3576	1145	1773	309	343	6	0	0	0
1	D	229	3567	1142	1769	308	342	6	0	0	0
1	E	229	3567	1142	1769	308	342	6	0	0	0
1	F	230	3555	1139	1761	308	341	6	0	0	0
1	G	229	3533	1134	1749	304	340	6	0	0	0
1	H	225	3408	1096	1683	297	327	5	0	0	0
1	I	226	3529	1129	1752	305	337	6	0	0	0

There are 81 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
A	137	ASN	HIS	engineered mutation	UNP A7A1Y4
B	-7	GLY	-	expression tag	UNP A7A1Y4
B	-6	PRO	-	expression tag	UNP A7A1Y4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	LEU	-	expression tag	UNP A7A1Y4
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
B	137	ASN	HIS	engineered mutation	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
C	137	ASN	HIS	engineered mutation	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
D	137	ASN	HIS	engineered mutation	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
E	137	ASN	HIS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	137	ASN	HIS	engineered mutation	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
G	-2	PRO	-	expression tag	UNP A7A1Y4
G	-1	GLU	-	expression tag	UNP A7A1Y4
G	0	PHE	-	expression tag	UNP A7A1Y4
G	137	ASN	HIS	engineered mutation	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
H	137	ASN	HIS	engineered mutation	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
I	137	ASN	HIS	engineered mutation	UNP A7A1Y4

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

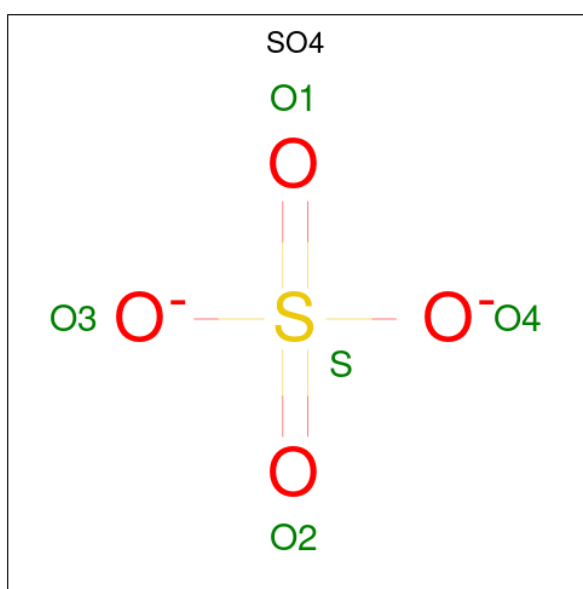
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	F	1	Total 1	Zn 1	0	0
2	G	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	I	1	Total 1	Zn 1	0	0

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



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

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

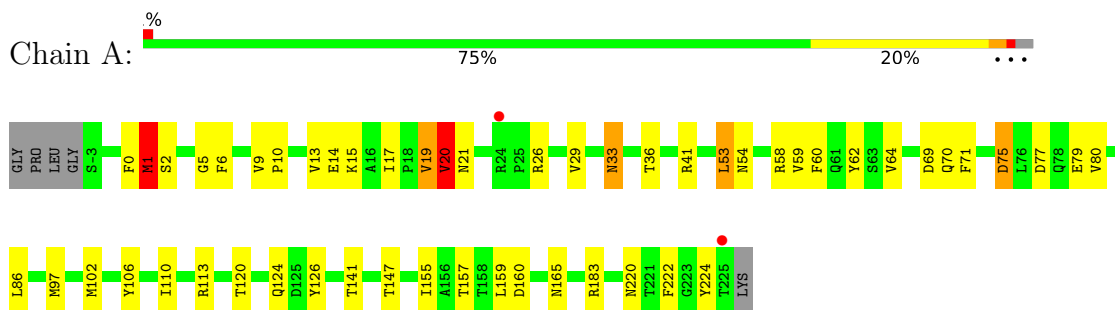
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0
4	B	19	Total O 19 19	0	0
4	C	36	Total O 36 36	0	0
4	D	37	Total O 37 37	0	0
4	E	42	Total O 42 42	0	0
4	F	18	Total O 18 18	0	0
4	G	12	Total O 12 12	0	0

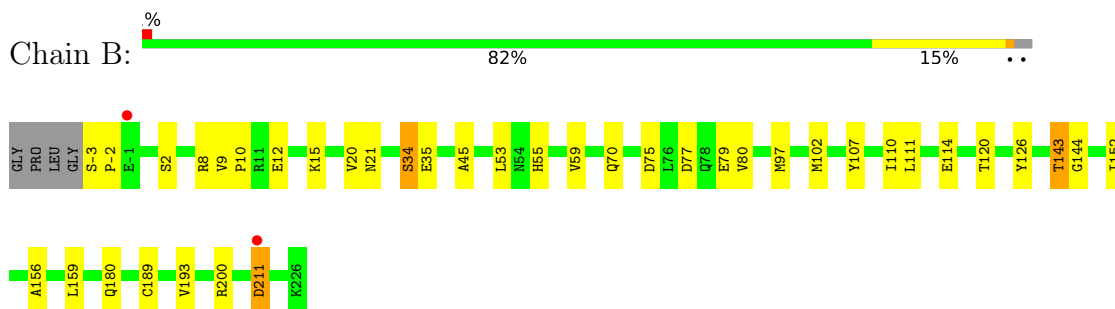
3 Residue-property plots [i](#)

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.

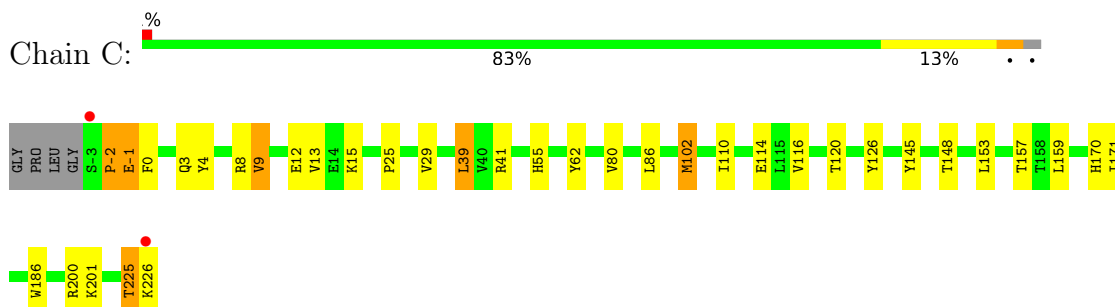
- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein

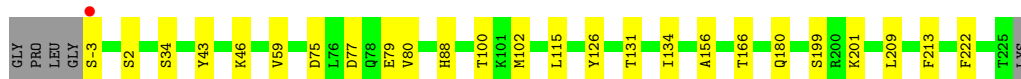


- Molecule 1: DNA damage-inducible protein

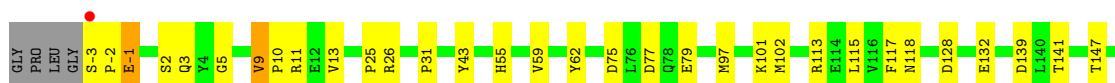
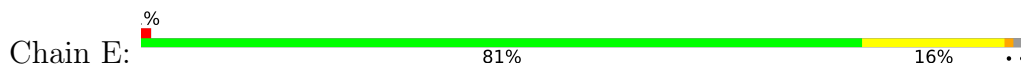


- Molecule 1: DNA damage-inducible protein

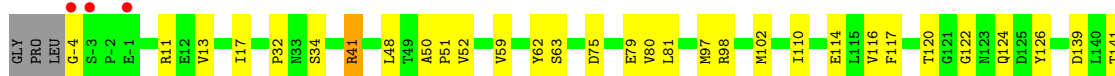
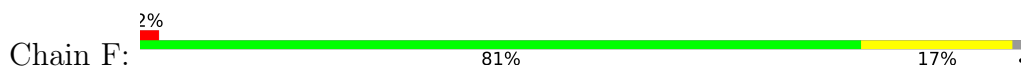




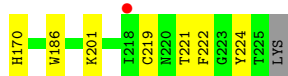
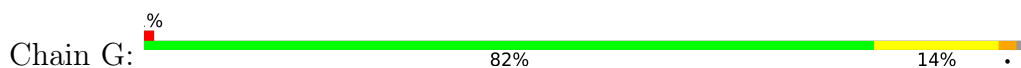
- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein



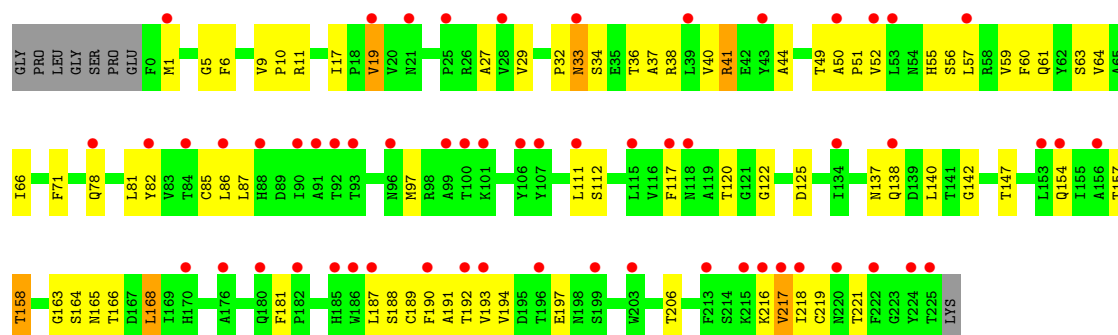
- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein



- Molecule 1: DNA damage-inducible protein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.64Å 264.64Å 119.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.77 – 3.00 39.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.77-3.00) 96.5 (39.77-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.194 , 0.221 0.198 , 0.221	Depositor DCC
R_{free} test set	2310 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtrriage
Anisotropy	0.507	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32110	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/1815	0.56	0/2483
1	B	0.25	0/1830	0.54	0/2502
1	C	0.28	0/1844	0.56	0/2518
1	D	0.26	0/1839	0.53	0/2511
1	E	0.29	0/1839	0.60	1/2511 (0.0%)
1	F	0.25	0/1835	0.52	0/2507
1	G	0.23	0/1825	0.51	0/2495
1	H	0.32	0/1764	0.62	1/2416 (0.0%)
1	I	0.24	0/1817	0.56	0/2480
All	All	0.26	0/16408	0.56	2/22423 (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	C	0	1
1	D	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	-3	SER	C-N-CD	-7.47	104.17	120.60
1	H	143	THR	N-CA-C	-5.41	98.64	108.65

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	-2	PRO	Peptide
1	D	-3	SER	Peptide
1	F	-4	GLY	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	1774	1738	1726	46	0
1	B	1789	1753	1743	24	0
1	C	1803	1773	1769	20	0
1	D	1798	1769	1767	15	0
1	E	1798	1769	1767	26	0
1	F	1794	1761	1755	22	0
1	G	1784	1749	1741	20	0
1	H	1725	1683	1664	79	0
1	I	1777	1752	1752	68	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	10	0	0	0	0
3	B	20	0	0	0	0
3	C	25	0	0	0	0
3	D	35	0	0	0	0
3	E	20	0	0	2	0
3	F	15	0	0	1	0
3	G	10	0	0	0	0
4	A	13	0	0	1	0
4	B	19	0	0	0	0
4	C	36	0	0	3	0
4	D	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	42	0	0	3	0
4	F	18	0	0	0	0
4	G	12	0	0	0	0
All	All	16363	15747	15684	313	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (313) 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:E:118:ASN:ND2	4:E:401:HOH:O	1.91	1.02
1:I:190:PHE:CD1	1:I:217:VAL:HG21	2.01	0.96
1:I:32:PRO:HB2	1:I:37:ALA:HB1	1.50	0.94
1:H:76:LEU:HD11	1:H:80:VAL:HG11	1.52	0.92
1:H:4:TYR:HA	1:H:80:VAL:HG21	1.54	0.88
1:I:36:THR:HG21	1:I:120:THR:HG22	1.58	0.85
1:H:17:ILE:HD11	1:H:71:PHE:CZ	2.13	0.84
1:H:59:VAL:HG13	1:H:156:ALA:CB	2.10	0.82
1:H:59:VAL:HG13	1:H:156:ALA:HB3	1.63	0.81
1:H:97:MET:HE1	1:H:197:GLU:OE1	1.82	0.79
1:I:34:SER:O	1:I:38:ARG:N	2.16	0.79
1:I:154:GLN:O	1:I:158:THR:OG1	1.99	0.78
1:H:10:PRO:HB2	1:H:16:ALA:HB2	1.65	0.78
1:H:11:ARG:HA	1:H:151:LEU:HD13	1.66	0.78
1:H:116:VAL:HG21	1:H:130:VAL:HG11	1.66	0.77
1:A:75:ASP:N	1:A:75:ASP:OD1	2.18	0.77
1:I:33:ASN:O	1:I:33:ASN:ND2	2.18	0.76
1:H:116:VAL:O	1:H:120:THR:CG2	2.33	0.76
1:H:17:ILE:HD11	1:H:71:PHE:CE1	2.20	0.76
1:B:2:SER:OG	1:B:75:ASP:OD2	2.02	0.75
1:H:76:LEU:HD11	1:H:80:VAL:CG1	2.15	0.75
1:I:190:PHE:CE1	1:I:217:VAL:HG21	2.22	0.74
1:A:26:ARG:NH2	1:A:69:ASP:OD1	2.20	0.74
1:H:77:ASP:OD1	1:H:79:GLU:N	2.19	0.74
1:I:66:ILE:HD13	1:I:168:LEU:HD21	1.69	0.73
1:B:55:HIS:O	1:B:59:VAL:HG23	1.88	0.73
1:H:64:VAL:CG2	1:H:81:LEU:HD21	2.19	0.73
1:I:137:ASN:HD21	1:I:157:THR:HG21	1.55	0.72
1:H:120:THR:OG1	1:H:120:THR:O	2.05	0.71
1:A:80:VAL:HG22	1:A:126:TYR:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:MET:HE2	1:H:201:LYS:NZ	2.06	0.71
1:E:2:SER:OG	1:E:75:ASP:OD2	2.08	0.70
1:E:26:ARG:NH1	4:E:405:HOH:O	2.24	0.70
1:A:220:ASN:O	4:A:401:HOH:O	2.10	0.70
1:I:165:ASN:O	1:I:168:LEU:HD22	1.93	0.69
1:A:19:VAL:O	1:A:20:VAL:HG23	1.93	0.68
1:H:116:VAL:O	1:H:120:THR:HG23	1.92	0.68
1:F:34:SER:OG	1:F:79:GLU:OE1	2.08	0.67
1:A:62:TYR:CD1	1:A:159:LEU:HD23	2.30	0.67
1:F:116:VAL:O	1:F:120:THR:HG23	1.94	0.67
1:G:45:ALA:HA	1:G:53:LEU:HD22	1.76	0.66
1:D:2:SER:OG	1:D:75:ASP:OD2	2.13	0.66
1:H:112:SER:HB3	1:H:130:VAL:HG12	1.77	0.66
1:B:211:ASP:OD1	1:B:211:ASP:N	2.29	0.65
1:C:102:MET:HE1	1:C:110:ILE:HD12	1.79	0.65
1:H:97:MET:HE2	1:H:201:LYS:HZ2	1.61	0.64
1:H:2:SER:HB2	1:H:7:VAL:CG2	2.28	0.64
1:H:20:VAL:HG12	1:H:21:ASN:N	2.12	0.64
1:I:189:CYS:O	1:I:193:VAL:HG23	1.98	0.64
1:I:34:SER:O	1:I:38:ARG:HB2	1.98	0.63
1:I:32:PRO:HG2	1:I:82:TYR:CD2	2.34	0.62
1:B:80:VAL:HG22	1:B:126:TYR:CE1	2.34	0.62
1:E:132:GLU:OE1	4:E:402:HOH:O	2.16	0.62
1:H:107:TYR:CE2	1:H:111:LEU:HD11	2.35	0.62
1:A:222:PHE:HD2	1:A:224:TYR:CD1	2.17	0.62
1:H:64:VAL:HG23	1:H:81:LEU:HD21	1.81	0.62
1:A:159:LEU:O	1:A:224:TYR:OH	2.17	0.61
1:I:63:SER:CB	1:I:81:LEU:HD21	2.29	0.61
1:H:80:VAL:HG22	1:H:126:TYR:CE1	2.36	0.61
1:A:222:PHE:HD2	1:A:224:TYR:CE1	2.18	0.61
1:B:143:THR:HG23	1:B:144:GLY:N	2.14	0.61
1:H:64:VAL:HG22	1:H:81:LEU:HD21	1.83	0.60
1:I:33:ASN:HD22	1:I:33:ASN:C	2.09	0.60
1:C:116:VAL:O	1:C:120:THR:HG23	2.00	0.60
1:I:63:SER:HB3	1:I:81:LEU:HD21	1.82	0.60
1:H:100:THR:HG21	1:H:107:TYR:CD2	2.37	0.59
1:A:26:ARG:HH21	1:A:69:ASP:CG	2.11	0.59
1:I:36:THR:O	1:I:40:VAL:HG23	2.02	0.59
1:A:59:VAL:HA	1:A:62:TYR:HD2	1.67	0.59
1:I:66:ILE:CD1	1:I:168:LEU:HD21	2.33	0.59
1:A:19:VAL:C	1:A:20:VAL:HG23	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:PHE:O	1:H:64:VAL:HG23	2.03	0.58
1:H:63:SER:HB2	1:H:81:LEU:HD11	1.84	0.58
1:H:140:LEU:HD23	1:H:154:GLN:NE2	2.18	0.58
1:B:-3:SER:CB	1:B:-2:PRO:CD	2.82	0.58
1:I:190:PHE:CE1	1:I:194:VAL:CG2	2.87	0.58
1:I:41:ARG:HB2	1:I:82:TYR:OH	2.02	0.58
1:H:20:VAL:CG1	1:H:21:ASN:N	2.66	0.58
1:C:201:LYS:NZ	4:C:402:HOH:O	2.37	0.57
1:H:169:ILE:HD11	1:H:173:THR:CG2	2.33	0.57
1:B:59:VAL:HG13	1:B:156:ALA:CB	2.34	0.57
1:C:62:TYR:CD2	1:C:159:LEU:HD23	2.39	0.57
1:H:10:PRO:O	1:H:151:LEU:HD22	2.05	0.57
1:I:188:SER:HA	1:I:218:ILE:CD1	2.34	0.57
1:H:11:ARG:HD2	1:H:154:GLN:OE1	2.05	0.56
1:A:58:ARG:HB3	1:A:62:TYR:HE2	1.70	0.56
1:B:77:ASP:OD1	1:B:79:GLU:N	2.38	0.56
1:C:39:LEU:C	1:C:39:LEU:HD23	2.30	0.56
1:I:32:PRO:HG2	1:I:82:TYR:CG	2.40	0.56
1:H:80:VAL:HG12	1:H:149:LEU:HD13	1.88	0.56
1:I:40:VAL:HG12	1:I:86:LEU:HD12	1.88	0.56
1:H:112:SER:HB3	1:H:130:VAL:CG1	2.35	0.56
1:A:120:THR:HG21	1:A:126:TYR:CD2	2.41	0.55
1:H:63:SER:CB	1:H:81:LEU:HD11	2.36	0.55
1:B:120:THR:HG21	1:B:126:TYR:CD2	2.42	0.54
1:F:62:TYR:CD2	1:F:159:LEU:HD23	2.42	0.54
1:G:80:VAL:HG22	1:G:126:TYR:CE1	2.42	0.54
1:A:59:VAL:HG11	1:A:157:THR:HG22	1.90	0.54
1:H:11:ARG:HD2	1:H:154:GLN:HE22	1.73	0.54
1:B:59:VAL:HG13	1:B:156:ALA:HB3	1.90	0.54
1:I:168:LEU:C	1:I:168:LEU:HD23	2.33	0.54
1:A:33:ASN:O	1:A:33:ASN:ND2	2.34	0.54
1:A:58:ARG:HB3	1:A:62:TYR:CE2	2.43	0.54
1:G:9:VAL:HG23	1:G:10:PRO:HD2	1.88	0.54
1:H:112:SER:CB	1:H:130:VAL:HG12	2.38	0.54
1:H:169:ILE:HD11	1:H:173:THR:HB	1.90	0.54
1:I:64:VAL:HG22	1:I:78:GLN:CD	2.33	0.53
1:F:80:VAL:HG22	1:F:126:TYR:CE1	2.44	0.53
1:B:45:ALA:HA	1:B:53:LEU:HD12	1.91	0.53
1:E:62:TYR:CD2	1:E:159:LEU:HD23	2.44	0.53
1:E:75:ASP:OD1	1:E:75:ASP:N	2.39	0.53
1:H:84:THR:OG1	1:H:149:LEU:HD21	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:VAL:HG22	1:I:61:GLN:OE1	2.09	0.53
1:A:33:ASN:C	1:A:33:ASN:HD22	2.15	0.53
1:I:64:VAL:HG22	1:I:78:GLN:OE1	2.09	0.53
1:F:11:ARG:NH2	1:F:141:THR:C	2.67	0.52
1:H:20:VAL:CG1	1:H:21:ASN:H	2.23	0.52
1:A:53:LEU:C	1:A:53:LEU:HD12	2.35	0.52
1:I:32:PRO:HD2	1:I:82:TYR:CE1	2.44	0.52
1:C:41:ARG:NH2	4:C:403:HOH:O	2.41	0.52
1:E:97:MET:HE1	1:E:197:GLU:OE1	2.10	0.52
1:I:9:VAL:HG22	1:I:10:PRO:HD2	1.92	0.52
1:B:53:LEU:O	1:B:53:LEU:HD23	2.09	0.52
1:I:57:LEU:HD13	1:I:181:PHE:CD1	2.45	0.52
1:B:21:ASN:O	1:B:70:GLN:NE2	2.37	0.52
1:B:189:CYS:O	1:B:193:VAL:HG23	2.10	0.52
1:I:17:ILE:HD11	1:I:71:PHE:CZ	2.45	0.51
1:H:107:TYR:CZ	1:H:111:LEU:HD21	2.45	0.51
1:C:200:ARG:NH1	4:C:405:HOH:O	2.43	0.51
1:D:131:THR:HG21	1:E:102:MET:HE1	1.91	0.51
1:H:125:ASP:OD1	1:H:125:ASP:N	2.44	0.51
1:I:64:VAL:CG2	1:I:78:GLN:OE1	2.59	0.51
1:H:48:LEU:HD23	1:H:52:VAL:HG12	1.93	0.51
1:A:62:TYR:CD1	1:A:159:LEU:CD2	2.94	0.51
1:A:41:ARG:HA	1:A:86:LEU:HD13	1.93	0.50
1:H:59:VAL:HG13	1:H:156:ALA:HB1	1.88	0.50
1:G:102:MET:HE1	1:G:110:ILE:HD12	1.94	0.50
1:A:183:ARG:NH1	1:A:224:TYR:CD2	2.80	0.50
1:C:80:VAL:HG22	1:C:126:TYR:CE1	2.47	0.50
1:H:50:ALA:HB3	1:H:51:PRO:HD3	1.93	0.50
1:A:58:ARG:O	1:A:62:TYR:CD2	2.64	0.50
1:H:12:GLU:OE1	1:H:143:THR:HA	2.11	0.50
1:I:1:MET:HE3	1:I:6:PHE:O	2.12	0.50
1:H:64:VAL:HG22	1:H:81:LEU:CD2	2.41	0.50
1:C:-2:PRO:HA	1:C:4:TYR:OH	2.11	0.49
1:F:117:PHE:CE1	1:F:124:GLN:OE1	2.65	0.49
1:I:64:VAL:HG22	1:I:78:GLN:NE2	2.28	0.49
1:C:153:LEU:O	1:C:157:THR:HG23	2.12	0.49
1:I:11:ARG:HH21	1:I:142:GLY:C	2.20	0.49
1:I:216:LYS:HA	1:I:219:CYS:HB2	1.94	0.49
1:E:97:MET:HE2	1:E:196:THR:HG22	1.94	0.49
1:B:53:LEU:HD23	1:B:53:LEU:C	2.38	0.49
1:A:102:MET:HE1	1:A:110:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:ARG:HB3	3:E:303:SO4:O1	2.13	0.49
1:I:60:PHE:CE1	1:I:78:GLN:OE1	2.66	0.49
1:A:9:VAL:CG2	1:A:10:PRO:HD2	2.43	0.48
1:D:201:LYS:NZ	4:D:403:HOH:O	2.45	0.48
1:I:190:PHE:CE1	1:I:194:VAL:HG21	2.49	0.48
1:D:88:HIS:HA	1:D:134:ILE:HG12	1.96	0.48
1:G:12:GLU:O	1:G:13:VAL:HB	2.14	0.48
1:H:70:GLN:C	1:H:72:PRO:HD3	2.38	0.48
1:I:19:VAL:O	1:I:19:VAL:CG1	2.60	0.48
1:B:9:VAL:HG23	1:B:10:PRO:HD2	1.96	0.48
1:H:11:ARG:HD2	1:H:154:GLN:NE2	2.28	0.48
1:H:131:THR:O	1:H:135:ILE:HD13	2.14	0.48
1:E:9:VAL:HG23	1:E:10:PRO:HD2	1.95	0.48
1:F:11:ARG:NH2	1:F:142:GLY:N	2.62	0.48
1:I:66:ILE:HG23	1:I:168:LEU:HG	1.94	0.48
1:E:102:MET:O	1:E:201:LYS:HE2	2.13	0.48
1:B:143:THR:CG2	1:B:144:GLY:N	2.77	0.48
1:H:6:PHE:HZ	1:H:125:ASP:O	1.97	0.48
1:I:117:PHE:CD1	1:I:122:GLY:HA2	2.49	0.48
1:A:0:PHE:O	1:A:2:SER:N	2.46	0.47
1:H:140:LEU:HD23	1:H:154:GLN:CD	2.39	0.47
1:I:1:MET:HG2	1:I:6:PHE:HB2	1.97	0.47
1:A:17:ILE:HD11	1:A:71:PHE:CZ	2.50	0.47
1:H:25:PRO:HB3	1:H:172:ASP:HB2	1.97	0.47
1:F:11:ARG:NH1	1:F:139:ASP:O	2.48	0.47
1:A:183:ARG:CZ	1:A:224:TYR:CD2	2.98	0.47
1:I:32:PRO:HB2	1:I:37:ALA:CB	2.34	0.47
1:C:12:GLU:HB2	1:C:15:LYS:HG3	1.96	0.47
1:B:34:SER:O	1:B:35:GLU:C	2.57	0.46
1:I:41:ARG:HD3	1:I:82:TYR:OH	2.15	0.46
1:A:77:ASP:OD1	1:A:79:GLU:N	2.48	0.46
1:C:9:VAL:HG11	1:C:148:THR:HG22	1.96	0.46
1:E:55:HIS:O	1:E:59:VAL:HG23	2.16	0.46
1:H:101:LYS:NZ	1:I:125:ASP:OD2	2.41	0.46
1:A:54:ASN:O	1:A:58:ARG:HG3	2.15	0.46
1:D:100:THR:OG1	1:E:128:ASP:OD2	2.26	0.46
1:G:224:TYR:CD1	1:G:224:TYR:N	2.84	0.46
1:G:2:SER:HB3	1:G:7:VAL:CG2	2.45	0.46
1:A:53:LEU:HD12	1:A:53:LEU:O	2.16	0.46
1:B:12:GLU:OE1	1:B:15:LYS:NZ	2.41	0.46
1:E:113:ARG:O	1:E:117:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:63:SER:HB2	1:I:81:LEU:HD21	1.95	0.46
1:F:62:TYR:CG	1:F:159:LEU:HD23	2.51	0.46
1:H:1:MET:O	1:H:6:PHE:CD2	2.70	0.45
1:H:2:SER:CB	1:H:7:VAL:CG2	2.94	0.45
1:D:77:ASP:OD1	1:D:79:GLU:N	2.41	0.45
1:H:166:THR:HG21	1:H:222:PHE:CE1	2.51	0.45
1:F:75:ASP:OD1	1:F:75:ASP:N	2.40	0.45
1:H:116:VAL:CG1	1:H:127:ALA:HA	2.46	0.45
1:A:0:PHE:O	1:A:1:MET:C	2.59	0.45
1:G:48:LEU:HD22	1:G:52:VAL:HG11	1.97	0.45
1:A:17:ILE:HG22	1:A:17:ILE:O	2.17	0.45
1:C:25:PRO:HG3	1:C:170:HIS:CE1	2.52	0.45
1:I:158:THR:HG22	1:I:164:SER:OG	2.16	0.44
1:I:187:LEU:O	1:I:218:ILE:HD13	2.17	0.44
1:A:13:VAL:C	1:A:15:LYS:H	2.25	0.44
1:A:160:ASP:HA	1:A:224:TYR:HE2	1.82	0.44
1:I:50:ALA:HB3	1:I:51:PRO:HD3	1.99	0.44
1:F:48:LEU:HD22	1:F:52:VAL:HG11	1.99	0.44
1:B:102:MET:HE1	1:B:110:ILE:HD12	1.99	0.44
1:A:1:MET:CE	1:B:200:ARG:HG2	2.48	0.44
1:A:5:GLY:O	1:A:147:THR:HB	2.17	0.44
1:A:21:ASN:O	1:A:70:GLN:NE2	2.49	0.44
1:C:41:ARG:HA	1:C:86:LEU:HD13	1.99	0.44
1:E:-1:GLU:N	1:E:3:GLN:OE1	2.51	0.44
1:G:74:TRP:CZ3	1:G:148:THR:HB	2.53	0.44
1:C:-1:GLU:HG3	1:C:0:PHE:N	2.33	0.44
1:D:80:VAL:HG22	1:D:126:TYR:CE1	2.53	0.44
1:I:158:THR:HG22	1:I:164:SER:CB	2.48	0.44
1:F:17:ILE:O	1:F:17:ILE:HG22	2.18	0.43
1:F:102:MET:HE1	1:F:110:ILE:HD12	2.00	0.43
1:I:55:HIS:O	1:I:59:VAL:HG23	2.18	0.43
1:D:43:TYR:CD2	1:D:115:LEU:HD21	2.53	0.43
1:G:102:MET:O	1:G:201:LYS:HE2	2.18	0.43
1:A:19:VAL:C	1:A:20:VAL:CG2	2.90	0.43
1:I:11:ARG:NH2	1:I:142:GLY:O	2.50	0.43
1:I:87:LEU:HD13	1:I:112:SER:HB3	2.00	0.43
1:I:191:ALA:CB	1:I:218:ILE:HD11	2.48	0.43
1:I:59:VAL:HG12	1:I:85:CYS:SG	2.57	0.43
1:F:200:ARG:NH1	3:F:302:SO4:O4	2.46	0.43
1:H:116:VAL:HG11	1:H:127:ALA:HA	2.01	0.43
1:I:40:VAL:HG12	1:I:86:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:VAL:HG12	1:G:85:CYS:SG	2.58	0.43
1:H:77:ASP:OD1	1:H:77:ASP:C	2.62	0.43
1:H:87:LEU:O	1:H:90:ILE:HG22	2.18	0.43
1:I:190:PHE:HB3	1:I:217:VAL:HG11	2.01	0.43
1:H:169:ILE:CD1	1:H:173:THR:HB	2.48	0.43
1:I:163:GLY:O	1:I:166:THR:HG23	2.18	0.43
1:A:60:PHE:O	1:A:64:VAL:HG23	2.18	0.43
1:A:106:TYR:N	1:A:106:TYR:CD1	2.85	0.43
1:F:63:SER:HB2	1:F:81:LEU:HD21	2.01	0.43
1:H:11:ARG:HD2	1:H:154:GLN:CD	2.44	0.42
1:H:71:PHE:N	1:H:72:PRO:HD3	2.34	0.42
1:H:169:ILE:HD11	1:H:173:THR:CB	2.48	0.42
1:I:138:GLN:HA	1:I:140:LEU:HG	2.01	0.42
1:C:8:ARG:HD2	1:C:145:TYR:CD2	2.54	0.42
1:H:120:THR:OG1	1:H:123:ASN:CB	2.68	0.42
1:A:183:ARG:HH11	1:A:183:ARG:HG2	1.84	0.42
1:B:152:ILE:HD12	1:B:152:ILE:HA	1.91	0.42
1:F:32:PRO:O	1:F:41:ARG:NH2	2.51	0.42
1:F:59:VAL:HG13	1:F:156:ALA:CB	2.48	0.42
1:F:98:ARG:HA	1:F:200:ARG:NH2	2.34	0.42
1:E:25:PRO:HG3	1:E:170:HIS:CE1	2.54	0.42
1:G:2:SER:HB2	1:G:75:ASP:OD1	2.20	0.42
1:H:97:MET:HE2	1:H:201:LYS:HZ3	1.82	0.42
1:H:117:PHE:HB2	1:H:127:ALA:CB	2.50	0.42
1:H:174:VAL:CG1	1:H:224:TYR:HD1	2.32	0.42
1:I:197:GLU:HG2	1:I:206:THR:HB	2.02	0.42
1:E:62:TYR:CG	1:E:159:LEU:HD23	2.54	0.42
1:I:219:CYS:O	1:I:221:THR:HG23	2.20	0.42
1:D:131:THR:CG2	1:E:102:MET:CE	2.98	0.42
1:G:92:THR:HA	1:G:97:MET:HE3	2.02	0.42
1:C:225:THR:O	1:C:226:LYS:C	2.62	0.42
1:D:209:LEU:HD13	1:D:213:PHE:CE2	2.55	0.42
1:I:111:LEU:HD23	1:I:111:LEU:HA	1.95	0.42
1:E:77:ASP:OD1	1:E:79:GLU:N	2.49	0.42
1:G:165:ASN:HB3	1:G:168:LEU:CD1	2.50	0.42
1:F:117:PHE:CZ	1:F:122:GLY:HA2	2.54	0.42
1:G:12:GLU:C	1:G:13:VAL:HG23	2.45	0.42
1:H:41:ARG:HA	1:H:86:LEU:HD13	2.02	0.42
1:D:131:THR:HG21	1:E:102:MET:CE	2.50	0.41
1:E:5:GLY:O	1:E:147:THR:HB	2.19	0.41
1:E:77:ASP:OD1	1:E:77:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:MET:O	1:F:201:LYS:HE2	2.19	0.41
1:H:2:SER:HB2	1:H:7:VAL:HG21	1.99	0.41
1:H:109:GLY:HA3	1:H:135:ILE:HD12	2.01	0.41
1:I:190:PHE:O	1:I:194:VAL:HG23	2.19	0.41
1:D:166:THR:HG21	1:D:222:PHE:CE1	2.55	0.41
1:A:113:ARG:NH2	1:A:124:GLN:NE2	2.68	0.41
1:G:55:HIS:CG	1:G:186:TRP:CZ2	3.08	0.41
1:H:109:GLY:HA3	1:H:135:ILE:CD1	2.50	0.41
1:E:31:PRO:HD3	3:E:305:SO4:O2	2.19	0.41
1:I:158:THR:HG22	1:I:164:SER:HB2	2.02	0.41
1:C:-1:GLU:HB3	1:C:3:GLN:OE1	2.20	0.41
1:F:59:VAL:HG13	1:F:156:ALA:HB3	2.01	0.41
1:E:43:TYR:CE1	1:E:115:LEU:HD11	2.55	0.41
1:F:50:ALA:HB3	1:F:51:PRO:HD3	2.02	0.41
1:A:9:VAL:HG22	1:A:10:PRO:HD2	2.03	0.41
1:C:55:HIS:CG	1:C:186:TRP:CZ2	3.09	0.41
1:E:11:ARG:HG2	1:E:11:ARG:HH11	1.86	0.41
1:G:12:GLU:O	1:G:13:VAL:CB	2.69	0.41
1:G:166:THR:HG21	1:G:222:PHE:CE1	2.56	0.41
1:I:56:SER:HB3	1:I:86:LEU:HA	2.03	0.41
1:B:8:ARG:HG2	1:D:199:SER:OG	2.20	0.41
1:C:62:TYR:CG	1:C:159:LEU:HD23	2.56	0.41
1:H:169:ILE:HG12	1:H:173:THR:HB	2.02	0.41
1:A:155:ILE:HG23	1:A:165:ASN:OD1	2.21	0.40
1:H:88:HIS:HA	1:H:134:ILE:HD13	2.03	0.40
1:G:219:CYS:O	1:G:221:THR:HG23	2.21	0.40
1:H:116:VAL:HG21	1:H:130:VAL:CG1	2.45	0.40
1:I:5:GLY:O	1:I:147:THR:HB	2.21	0.40
1:I:44:ALA:HB1	1:I:86:LEU:HD22	2.03	0.40
1:I:49:THR:OG1	1:I:52:VAL:HG23	2.21	0.40
1:B:107:TYR:CE2	1:B:111:LEU:HD11	2.55	0.40
1:H:117:PHE:CE1	1:H:124:GLN:NE2	2.90	0.40
1:A:1:MET:HG3	1:A:6:PHE:HB2	2.03	0.40
1:D:75:ASP:OD1	1:D:75:ASP:N	2.54	0.40
1:H:169:ILE:CG1	1:H:173:THR:HB	2.50	0.40
1:D:59:VAL:HG13	1:D:156:ALA:HB3	2.02	0.40
1:G:25:PRO:HG3	1:G:170:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/234 (97%)	216 (95%)	8 (4%)	3 (1%)	9	38
1	B	228/234 (97%)	222 (97%)	5 (2%)	1 (0%)	30	65
1	C	228/234 (97%)	221 (97%)	6 (3%)	1 (0%)	30	65
1	D	227/234 (97%)	220 (97%)	7 (3%)	0	100	100
1	E	227/234 (97%)	220 (97%)	6 (3%)	1 (0%)	30	65
1	F	228/234 (97%)	223 (98%)	5 (2%)	0	100	100
1	G	227/234 (97%)	219 (96%)	7 (3%)	1 (0%)	30	65
1	H	223/234 (95%)	208 (93%)	14 (6%)	1 (0%)	30	65
1	I	224/234 (96%)	214 (96%)	9 (4%)	1 (0%)	30	65
All	All	2039/2106 (97%)	1963 (96%)	67 (3%)	9 (0%)	30	65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	C	-1	GLU
1	E	-2	PRO
1	H	119	ALA
1	A	20	VAL
1	B	34	SER
1	I	27	ALA
1	A	14	GLU
1	G	-2	PRO

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	192/202 (95%)	182 (95%)	10 (5%)	21	55
1	B	194/202 (96%)	187 (96%)	7 (4%)	31	65
1	C	197/202 (98%)	189 (96%)	8 (4%)	27	61
1	D	197/202 (98%)	193 (98%)	4 (2%)	48	76
1	E	197/202 (98%)	190 (96%)	7 (4%)	31	65
1	F	195/202 (96%)	187 (96%)	8 (4%)	27	61
1	G	194/202 (96%)	187 (96%)	7 (4%)	31	65
1	H	183/202 (91%)	174 (95%)	9 (5%)	22	56
1	I	195/202 (96%)	187 (96%)	8 (4%)	27	61
All	All	1744/1818 (96%)	1676 (96%)	68 (4%)	28	62

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	VAL
1	A	20	VAL
1	A	29	VAL
1	A	33	ASN
1	A	36	THR
1	A	53	LEU
1	A	75	ASP
1	A	97	MET
1	A	141	THR
1	B	20	VAL
1	B	97	MET
1	B	114	GLU
1	B	143	THR
1	B	159	LEU
1	B	180	GLN
1	B	211	ASP
1	C	9	VAL
1	C	13	VAL
1	C	29	VAL
1	C	39	LEU
1	C	102	MET
1	C	114	GLU

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Mol	Chain	Res	Type
1	C	171	ILE
1	C	225	THR
1	D	34	SER
1	D	46	LYS
1	D	102	MET
1	D	180	GLN
1	E	-1	GLU
1	E	9	VAL
1	E	13	VAL
1	E	101	LYS
1	E	139	ASP
1	E	141	THR
1	E	211	ASP
1	F	13	VAL
1	F	41	ARG
1	F	97	MET
1	F	114	GLU
1	F	171	ILE
1	F	175	SER
1	F	180	GLN
1	F	225	THR
1	G	2	SER
1	G	9	VAL
1	G	17	ILE
1	G	59	VAL
1	G	95	LYS
1	G	141	THR
1	G	165	ASN
1	H	28	VAL
1	H	41	ARG
1	H	93	THR
1	H	97	MET
1	H	100	THR
1	H	120	THR
1	H	125	ASP
1	H	126	TYR
1	H	135	ILE
1	I	19	VAL
1	I	33	ASN
1	I	41	ARG
1	I	97	MET
1	I	158	THR

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Mol	Chain	Res	Type
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	ASN
1	B	198	ASN
1	C	138	GLN
1	E	78	GLN
1	E	118	ASN
1	E	165	ASN
1	F	165	ASN
1	G	165	ASN
1	H	78	GLN
1	I	124	GLN
1	I	137	ASN
1	I	205	HIS

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 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 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	A	302	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	G	303	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	G	301	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	E	302	-	4,4,4	0.22	0	6,6,6	0.25	0
3	SO4	F	302	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	F	303	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	E	304	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	D	303	-	4,4,4	0.22	0	6,6,6	0.16	0
3	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	B	302	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	C	303	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	A	303	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	B	303	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	D	307	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	C	304	-	4,4,4	0.23	0	6,6,6	0.18	0
3	SO4	D	305	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	305	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	D	302	-	4,4,4	0.22	0	6,6,6	0.11	0
3	SO4	E	303	-	4,4,4	0.22	0	6,6,6	0.20	0
3	SO4	D	306	-	4,4,4	0.23	0	6,6,6	0.19	0
3	SO4	E	305	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	F	304	-	4,4,4	0.23	0	6,6,6	0.18	0
3	SO4	D	304	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	D	308	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	B	304	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	C	305	-	4,4,4	0.24	0	6,6,6	0.21	0
3	SO4	C	306	-	4,4,4	0.24	0	6,6,6	0.06	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	SO4	1	0
3	E	303	SO4	1	0
3	E	305	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%)	-0.25	2 (0%) 81 61	60, 80, 114, 144	0
1	B	230/234 (98%)	-0.36	2 (0%) 81 61	53, 75, 103, 134	0
1	C	230/234 (98%)	-0.49	2 (0%) 81 61	41, 60, 85, 150	0
1	D	229/234 (97%)	-0.56	1 (0%) 88 76	42, 59, 84, 126	0
1	E	229/234 (97%)	-0.55	2 (0%) 81 61	43, 56, 86, 133	0
1	F	230/234 (98%)	-0.46	4 (1%) 69 45	48, 65, 93, 132	0
1	G	229/234 (97%)	-0.29	2 (0%) 81 61	54, 85, 115, 148	0
1	H	225/234 (96%)	1.15	39 (17%) 4 3	97, 158, 214, 265	0
1	I	226/234 (96%)	1.49	58 (25%) 1 1	106, 199, 254, 305	0
All	All	2057/2106 (97%)	-0.04	112 (5%) 31 16	41, 75, 208, 305	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	35	GLU	7.3
1	C	226	LYS	6.4
1	E	-3	SER	5.9
1	H	36	THR	5.4
1	I	187	LEU	4.9
1	H	6	PHE	4.7
1	I	28	VAL	4.7
1	F	-3	SER	4.5
1	I	90	ILE	4.4
1	I	84	THR	4.3
1	H	121	GLY	4.3
1	I	190	PHE	4.2
1	H	145	TYR	4.2
1	I	96	ASN	4.1
1	D	-3	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	I	138	GLN	4.0
1	I	176	ALA	3.9
1	G	-3	SER	3.9
1	H	126	TYR	3.8
1	H	119	ALA	3.8
1	H	38	ARG	3.7
1	H	224	TYR	3.7
1	I	43	TYR	3.7
1	I	107	TYR	3.6
1	I	106	TYR	3.6
1	H	120	THR	3.6
1	I	196	THR	3.6
1	A	225	THR	3.5
1	I	218	ILE	3.5
1	H	0	PHE	3.5
1	I	213	PHE	3.5
1	I	92	THR	3.4
1	I	86	LEU	3.4
1	I	101	LYS	3.4
1	I	222	PHE	3.4
1	I	224	TYR	3.4
1	C	-3	SER	3.3
1	I	91	ALA	3.3
1	H	10	PRO	3.2
1	I	57	LEU	3.2
1	H	14	GLU	3.2
1	H	4	TYR	3.2
1	I	185	HIS	3.2
1	H	39	LEU	3.2
1	I	33	ASN	3.2
1	E	225	THR	3.1
1	I	52	VAL	3.0
1	I	182	PRO	3.0
1	I	39	LEU	2.9
1	H	129	ALA	2.9
1	F	225	THR	2.9
1	I	100	THR	2.9
1	I	220	ASN	2.9
1	H	114	GLU	2.8
1	I	225	THR	2.8
1	H	1	MET	2.8
1	I	82	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	42	GLU	2.7
1	H	74	TRP	2.7
1	H	22	ALA	2.6
1	I	170	HIS	2.6
1	H	147	THR	2.5
1	I	192	THR	2.5
1	H	143	THR	2.5
1	I	93	THR	2.5
1	F	-1	GLU	2.5
1	I	111	LEU	2.4
1	F	-4	GLY	2.4
1	I	217	VAL	2.4
1	H	32	PRO	2.4
1	I	118	ASN	2.4
1	I	99	ALA	2.3
1	H	137	ASN	2.3
1	H	139	ASP	2.3
1	I	180	GLN	2.3
1	H	112	SER	2.3
1	I	78	GLN	2.3
1	I	25	PRO	2.3
1	I	50	ALA	2.3
1	I	117	PHE	2.3
1	H	98	ARG	2.3
1	I	153	LEU	2.2
1	I	199	SER	2.2
1	B	211	ASP	2.2
1	H	17	ILE	2.2
1	I	134	ILE	2.2
1	H	102	MET	2.2
1	I	186	TRP	2.2
1	H	77	ASP	2.2
1	I	203	TRP	2.2
1	H	136	ARG	2.2
1	I	88	HIS	2.2
1	I	19	VAL	2.1
1	H	110	ILE	2.1
1	H	15	LYS	2.1
1	H	133	ALA	2.1
1	H	83	VAL	2.1
1	I	193	VAL	2.1
1	G	218	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	-1	GLU	2.1
1	H	223	GLY	2.1
1	I	53	LEU	2.1
1	A	24	ARG	2.1
1	H	79	GLU	2.1
1	I	156	ALA	2.1
1	I	154	GLN	2.1
1	I	216	LYS	2.0
1	H	118	ASN	2.0
1	I	215	LYS	2.0
1	I	1	MET	2.0
1	I	21	ASN	2.0
1	I	115	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
3	SO4	D	302	5/5	0.41	0.17	189,195,198,203	0
3	SO4	D	305	5/5	0.42	0.19	200,205,213,214	0
2	ZN	I	500	1/1	0.74	0.18	132,132,132,132	1
3	SO4	B	303	5/5	0.79	0.18	124,136,144,151	0
3	SO4	C	306	5/5	0.79	0.19	114,118,122,123	5
3	SO4	D	308	5/5	0.79	0.17	105,107,110,111	5
3	SO4	B	302	5/5	0.81	0.14	157,158,170,174	0
3	SO4	B	304	5/5	0.81	0.20	134,139,154,156	0
3	SO4	F	302	5/5	0.82	0.26	114,122,127,132	0
3	SO4	E	304	5/5	0.83	0.21	100,104,106,113	0

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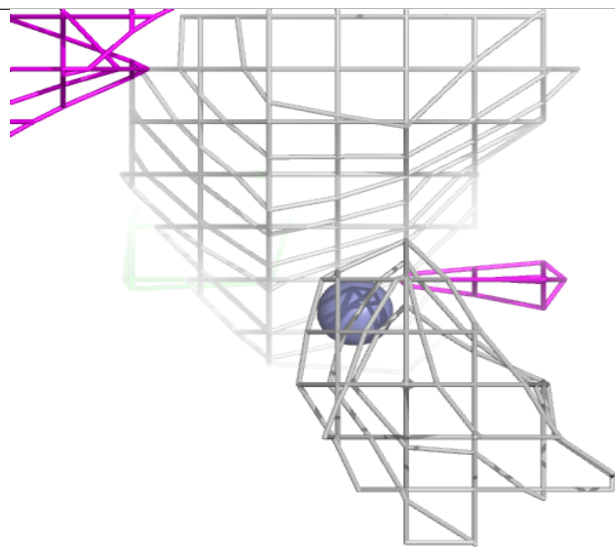
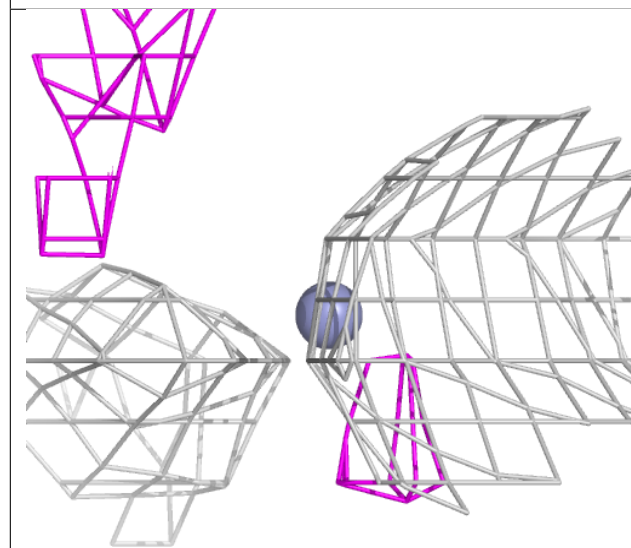
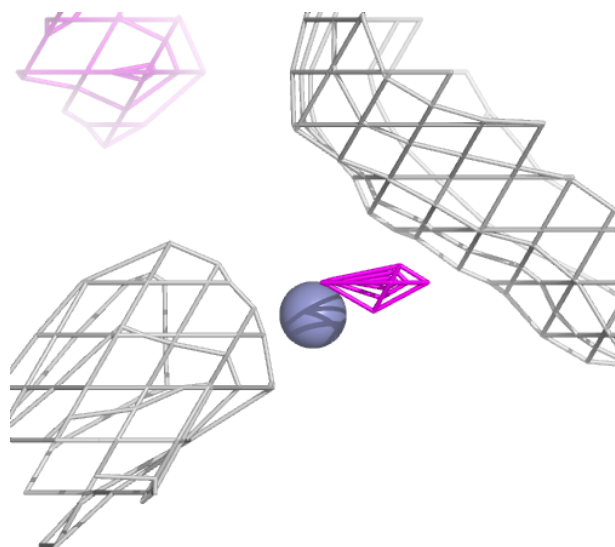
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	E	305	5/5	0.84	0.24	92,94,103,107	5
3	SO4	C	302	5/5	0.85	0.15	106,109,114,116	0
3	SO4	A	302	5/5	0.86	0.20	106,114,118,119	0
3	SO4	B	305	5/5	0.86	0.21	164,165,171,212	0
3	SO4	G	303	5/5	0.86	0.12	115,115,119,121	0
3	SO4	F	303	5/5	0.87	0.17	134,147,160,160	0
3	SO4	A	303	5/5	0.88	0.16	114,115,118,126	0
3	SO4	D	306	5/5	0.88	0.21	109,115,120,120	0
3	SO4	C	304	5/5	0.88	0.18	101,103,104,107	0
3	SO4	D	303	5/5	0.88	0.17	94,101,105,111	0
3	SO4	C	303	5/5	0.89	0.27	126,132,137,154	0
3	SO4	D	304	5/5	0.90	0.19	105,106,108,108	0
3	SO4	G	301	5/5	0.90	0.14	102,107,113,114	0
3	SO4	D	307	5/5	0.90	0.19	149,149,157,165	0
3	SO4	C	305	5/5	0.91	0.13	100,107,108,119	0
2	ZN	B	301	1/1	0.91	0.11	85,85,85,85	1
2	ZN	D	301	1/1	0.91	0.10	73,73,73,73	1
3	SO4	F	304	5/5	0.92	0.15	105,108,109,109	0
2	ZN	G	302	1/1	0.92	0.10	99,99,99,99	1
3	SO4	E	303	5/5	0.92	0.12	110,116,119,121	0
2	ZN	A	301	1/1	0.93	0.08	85,85,85,85	1
2	ZN	F	301	1/1	0.93	0.10	86,86,86,86	1
2	ZN	E	301	1/1	0.95	0.08	71,71,71,71	1
2	ZN	C	301	1/1	0.96	0.06	79,79,79,79	1
2	ZN	H	500	1/1	0.97	0.05	135,135,135,135	1
3	SO4	E	302	5/5	0.97	0.06	56,58,68,72	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.

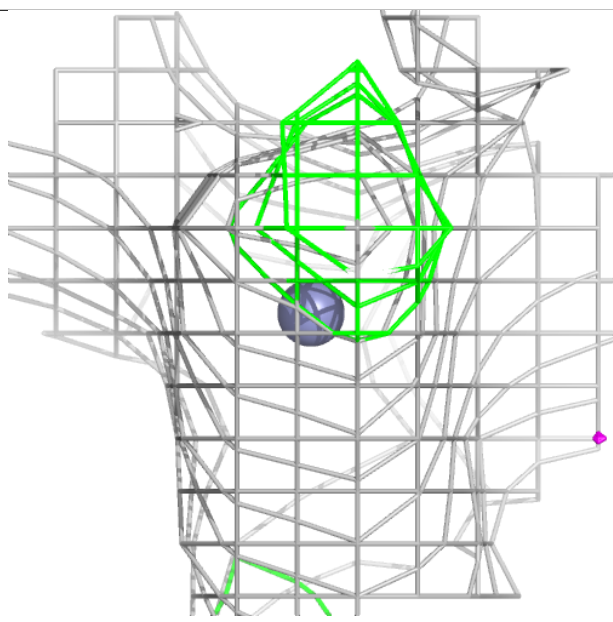
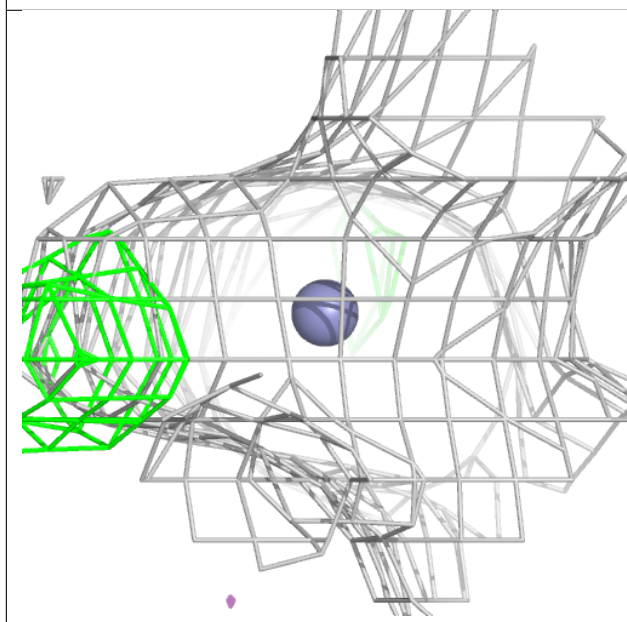
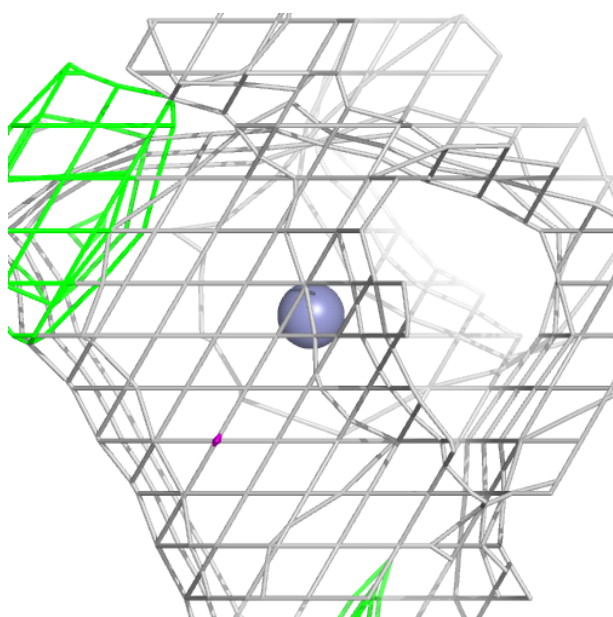
Electron density around ZN I 500:

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



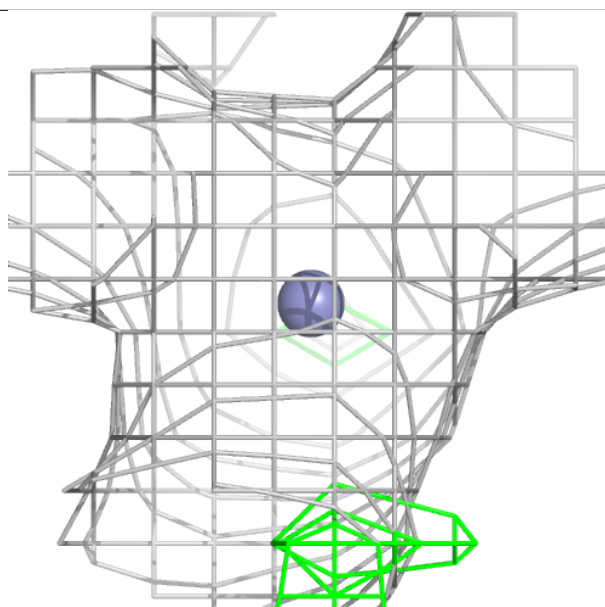
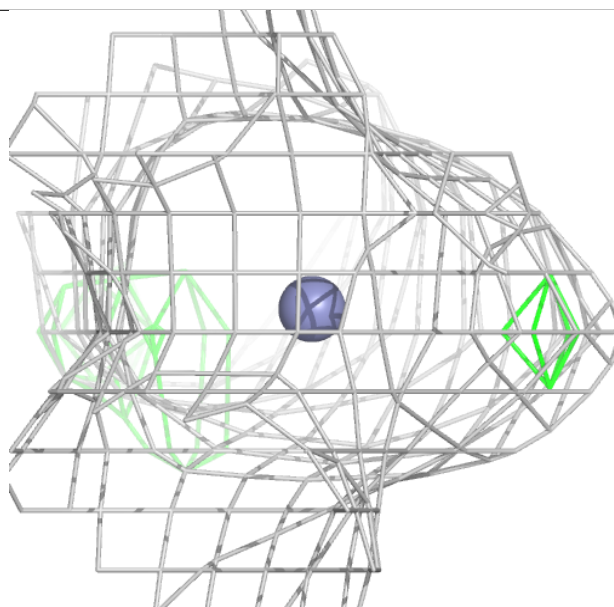
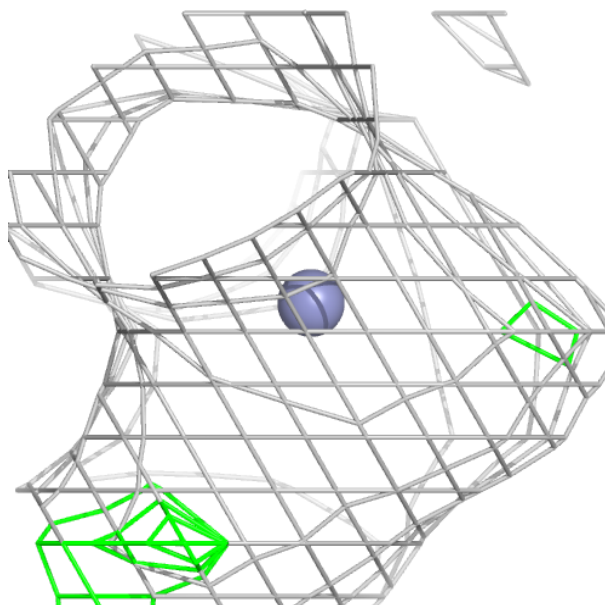
Electron density around ZN B 301:

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



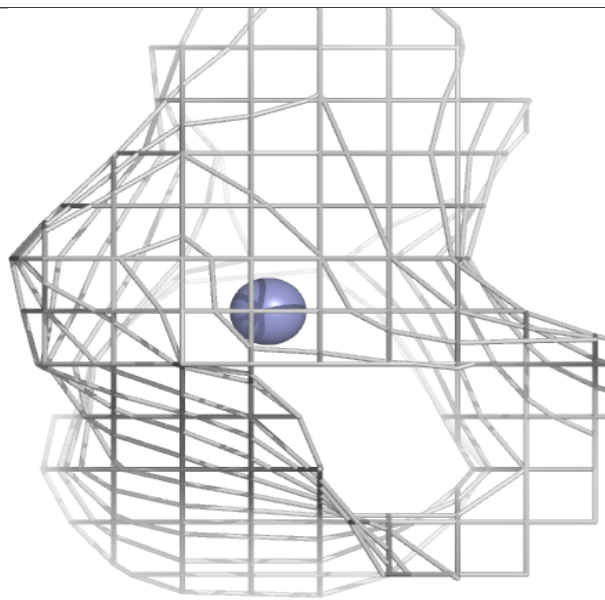
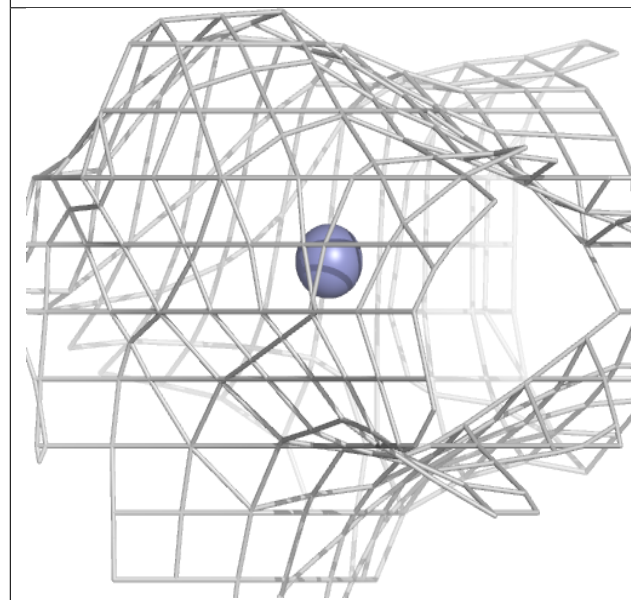
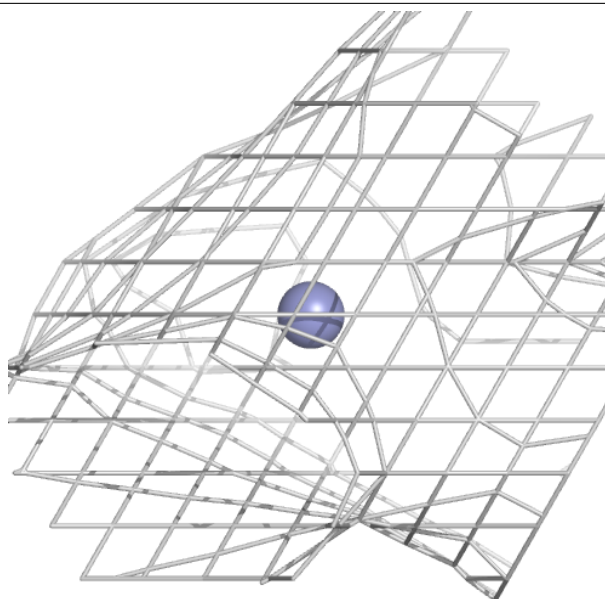
Electron density around ZN D 301:

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



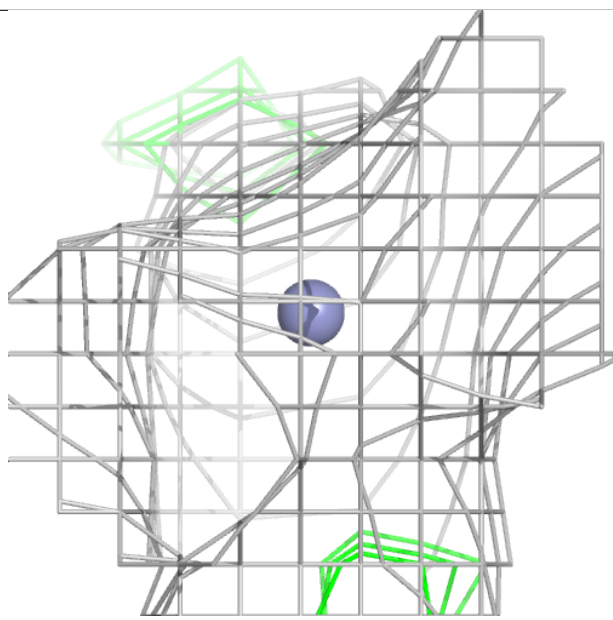
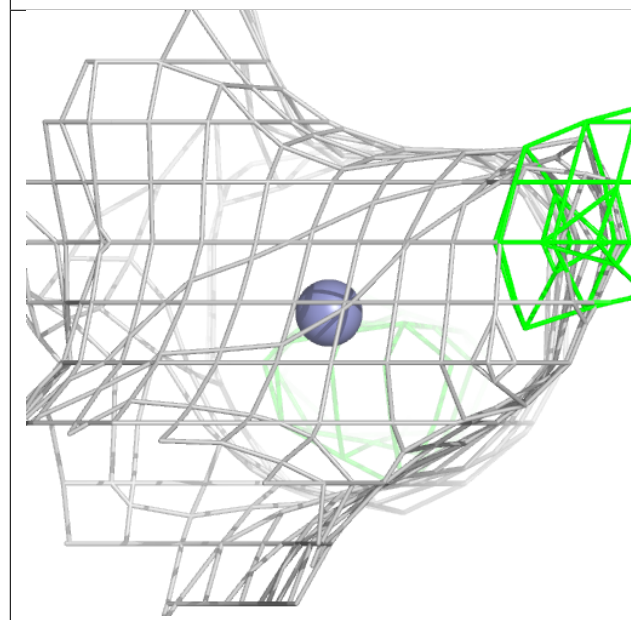
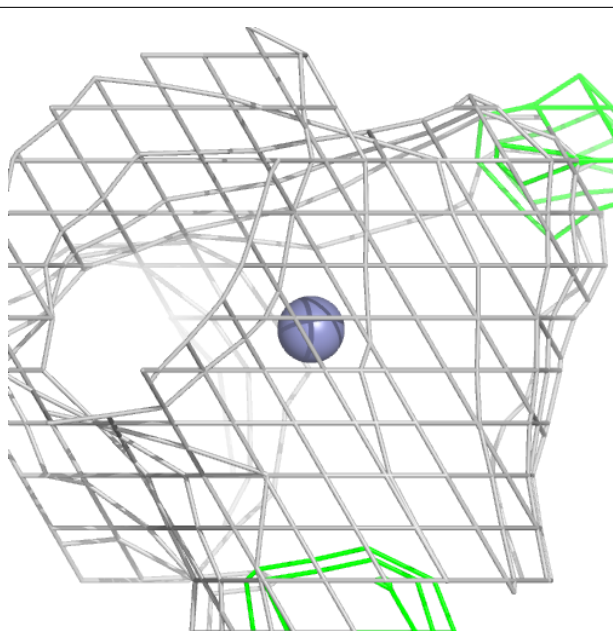
Electron density around ZN G 302:

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



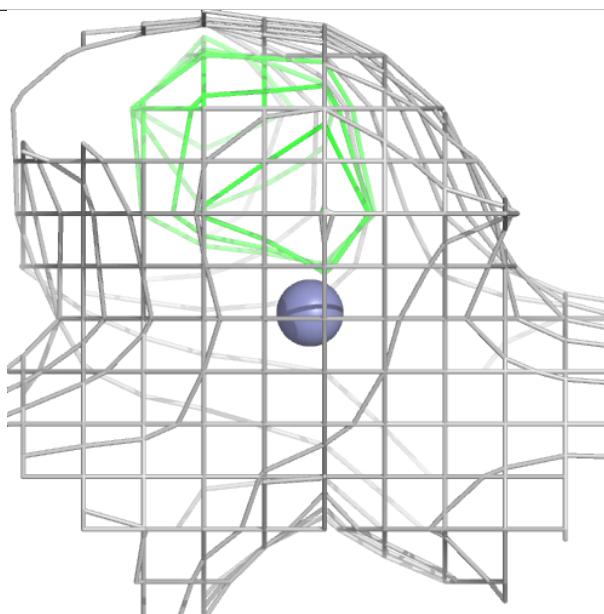
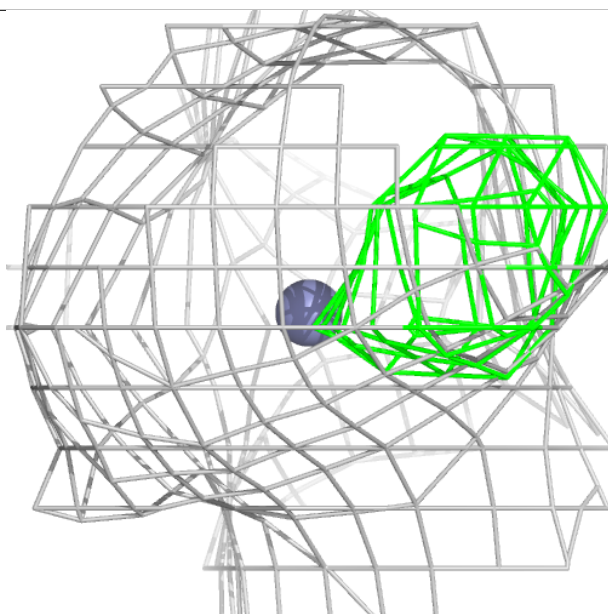
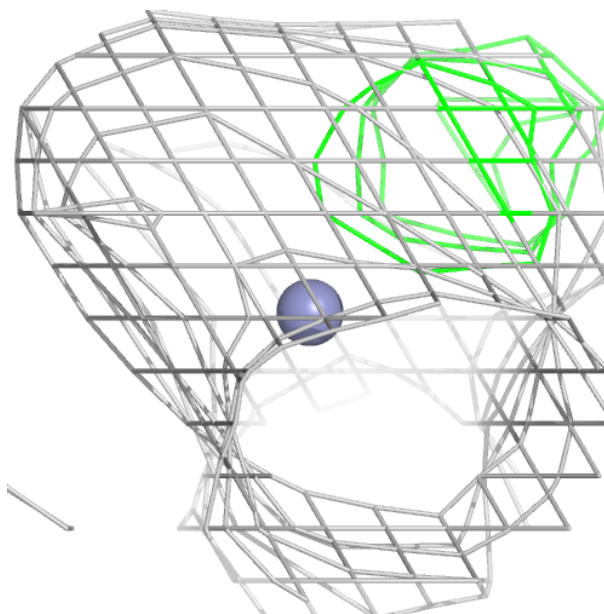
Electron density around ZN A 301:

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



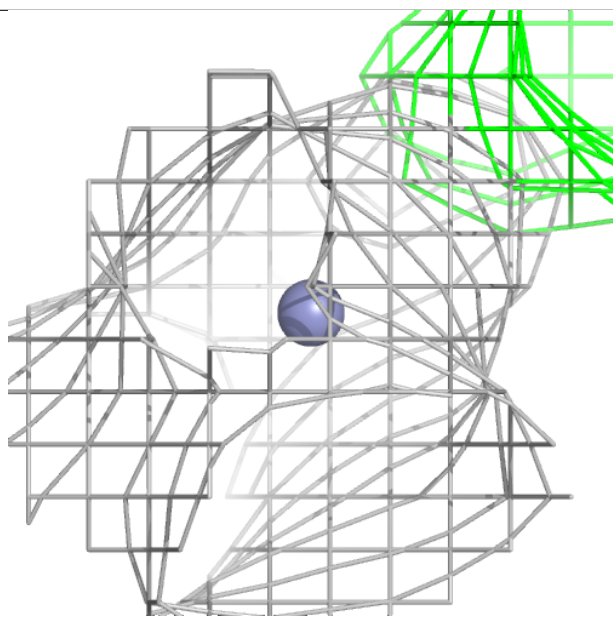
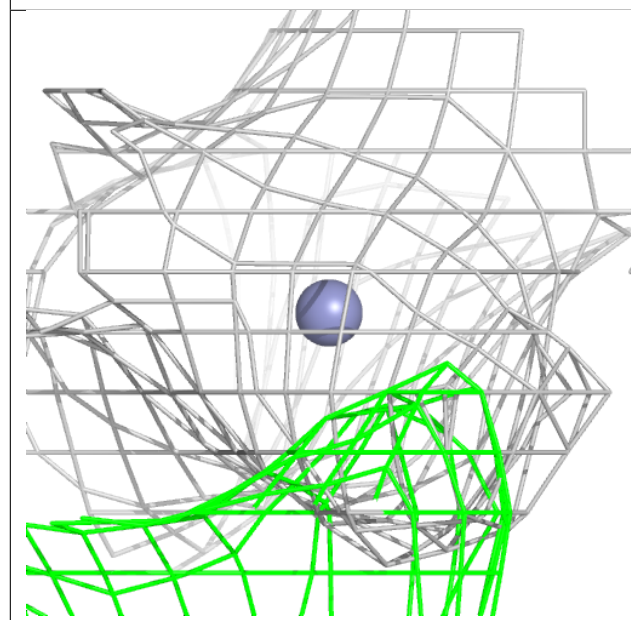
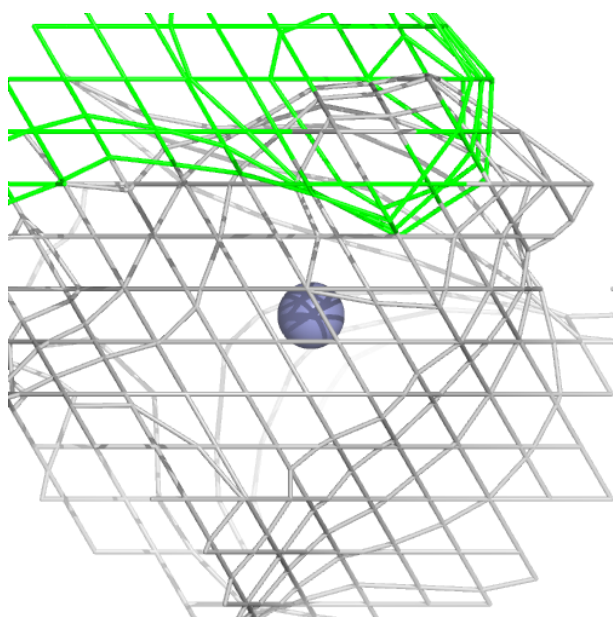
Electron density around ZN F 301:

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



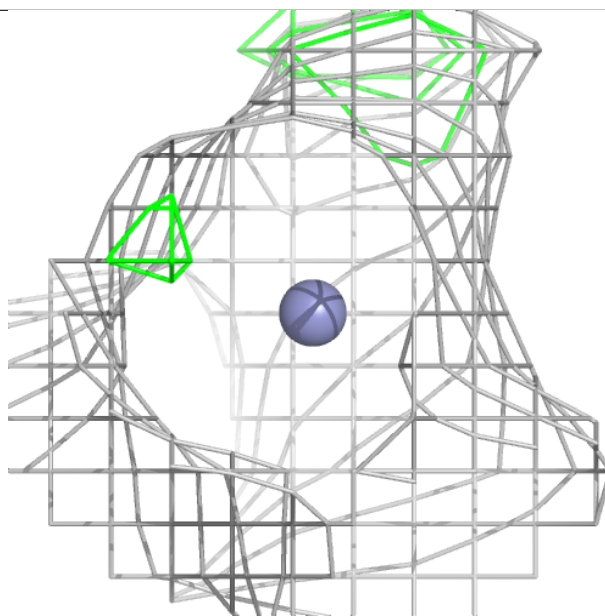
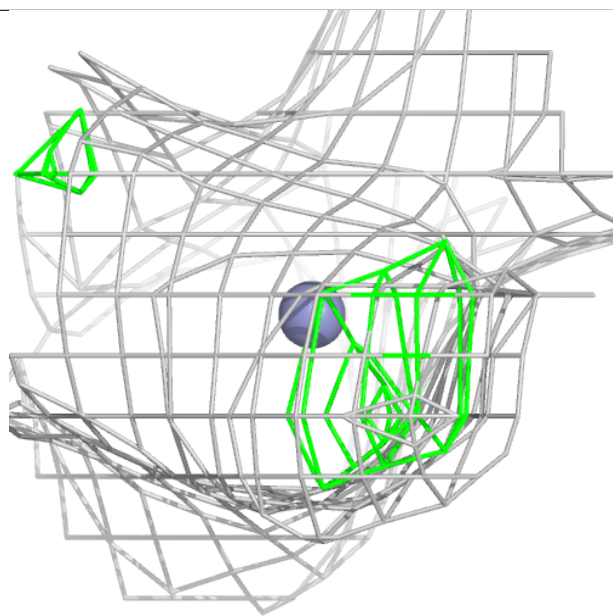
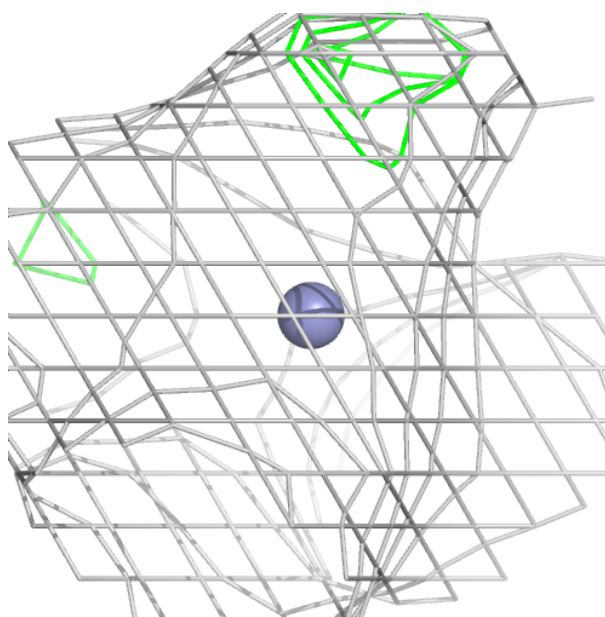
Electron density around ZN E 301:

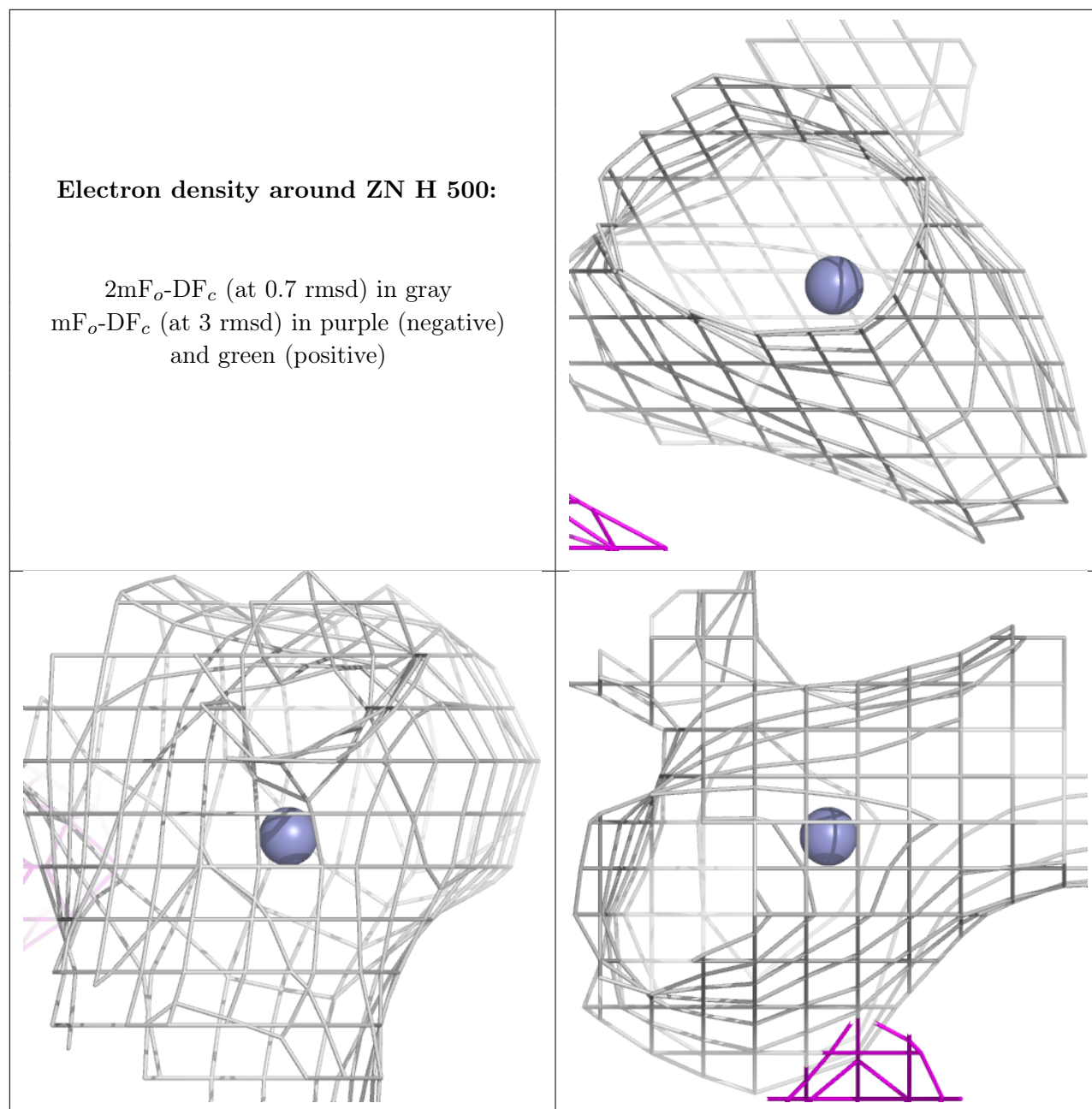
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.