



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:16 PM UTC

PDB ID : 6NL6 / pdb_00006nl6
Title : Crystal structure of mutant B1 immunoglobulin-binding domain of Streptococcal Protein G (T16F, T18A, V21E, T25L, K28Y, V29I, K31R, Q32H, Y33L, N35K, D36H, N37Q)
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Deposited on : 2019-01-08
Resolution : 1.40 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
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

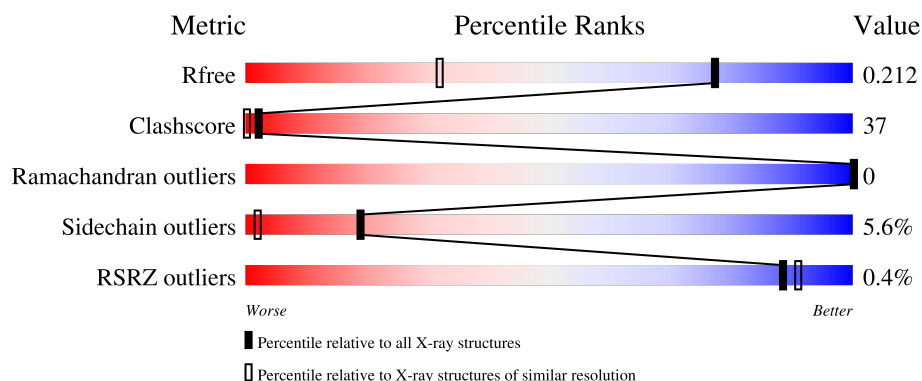
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	56	 43% 34% 21% .
1	B	56	 39% 46% 12% .
1	C	56	 2% 52% 23% 20% 5%
1	D	56	 39% 43% 16% .

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	CL	B	104	-	-	X	-
3	CL	B	105	-	-	X	-
3	CL	D	102	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2166 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Immunoglobulin G-binding protein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	56	Total	C	N	O	S	0	3	0
			464	298	73	91	2			
1	B	56	Total	C	N	O	S	0	3	0
			466	300	74	90	2			
1	C	56	Total	C	N	O	S	0	5	0
			476	307	74	93	2			
1	D	56	Total	C	N	O	S	0	7	0
			486	315	75	94	2			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P19909
A	16	PHE	THR	engineered mutation	UNP P19909
A	18	ALA	THR	engineered mutation	UNP P19909
A	21	GLU	VAL	engineered mutation	UNP P19909
A	25	LEU	THR	engineered mutation	UNP P19909
A	28	TYR	LYS	engineered mutation	UNP P19909
A	29	ILE	VAL	engineered mutation	UNP P19909
A	31	ARG	LYS	engineered mutation	UNP P19909
A	32	HIS	GLN	engineered mutation	UNP P19909
A	33	LEU	TYR	engineered mutation	UNP P19909
A	35	LYS	ASN	engineered mutation	UNP P19909
A	36	HIS	ASP	engineered mutation	UNP P19909
A	37	GLN	ASN	engineered mutation	UNP P19909
B	1	MET	-	initiating methionine	UNP P19909
B	16	PHE	THR	engineered mutation	UNP P19909
B	18	ALA	THR	engineered mutation	UNP P19909
B	21	GLU	VAL	engineered mutation	UNP P19909
B	25	LEU	THR	engineered mutation	UNP P19909
B	28	TYR	LYS	engineered mutation	UNP P19909
B	29	ILE	VAL	engineered mutation	UNP P19909
B	31	ARG	LYS	engineered mutation	UNP P19909

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	HIS	GLN	engineered mutation	UNP P19909
B	33	LEU	TYR	engineered mutation	UNP P19909
B	35	LYS	ASN	engineered mutation	UNP P19909
B	36	HIS	ASP	engineered mutation	UNP P19909
B	37	GLN	ASN	engineered mutation	UNP P19909
C	1	MET	-	initiating methionine	UNP P19909
C	16	PHE	THR	engineered mutation	UNP P19909
C	18	ALA	THR	engineered mutation	UNP P19909
C	21	GLU	VAL	engineered mutation	UNP P19909
C	25	LEU	THR	engineered mutation	UNP P19909
C	28	TYR	LYS	engineered mutation	UNP P19909
C	29	ILE	VAL	engineered mutation	UNP P19909
C	31	ARG	LYS	engineered mutation	UNP P19909
C	32	HIS	GLN	engineered mutation	UNP P19909
C	33	LEU	TYR	engineered mutation	UNP P19909
C	35	LYS	ASN	engineered mutation	UNP P19909
C	36	HIS	ASP	engineered mutation	UNP P19909
C	37	GLN	ASN	engineered mutation	UNP P19909
D	1	MET	-	initiating methionine	UNP P19909
D	16	PHE	THR	engineered mutation	UNP P19909
D	18	ALA	THR	engineered mutation	UNP P19909
D	21	GLU	VAL	engineered mutation	UNP P19909
D	25	LEU	THR	engineered mutation	UNP P19909
D	28	TYR	LYS	engineered mutation	UNP P19909
D	29	ILE	VAL	engineered mutation	UNP P19909
D	31	ARG	LYS	engineered mutation	UNP P19909
D	32	HIS	GLN	engineered mutation	UNP P19909
D	33	LEU	TYR	engineered mutation	UNP P19909
D	35	LYS	ASN	engineered mutation	UNP P19909
D	36	HIS	ASP	engineered mutation	UNP P19909
D	37	GLN	ASN	engineered mutation	UNP P19909

- 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	3	Total Zn 3 3	0	0
2	C	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Zn 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Cl 2	0	0
3	C	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0

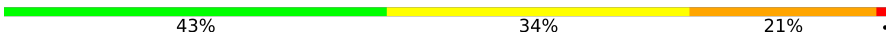
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total 65	O 65	0	0
4	B	70	Total 70	O 70	0	0
4	C	63	Total 63	O 63	0	0
4	D	66	Total 66	O 66	0	0

3 Residue-property plots [i](#)

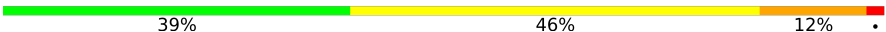
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

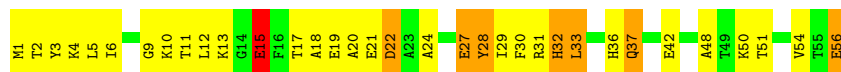
- Molecule 1: Immunoglobulin G-binding protein G

Chain A:  43% 34% 21% .



- Molecule 1: Immunoglobulin G-binding protein G

Chain B:  39% 46% 12% .

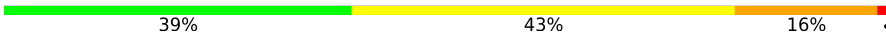


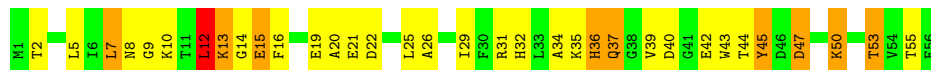
- Molecule 1: Immunoglobulin G-binding protein G

Chain C:  2% 52% 23% 20% 5% .



- Molecule 1: Immunoglobulin G-binding protein G

Chain D:  39% 43% 16% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	48.29Å 48.29Å 83.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.38 – 1.40 37.38 – 1.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (37.38-1.40) 98.9 (37.38-1.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.145 , 0.214 0.149 , 0.212	Depositor DCC
R_{free} test set	2175 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.227 for h,-h-k,-l 0.031 for -k,-h,-l	Xtriage
Reported twinning fraction	0.501 for H, K, L 0.499 for K, H, -L	Depositor
Outliers	0 of 42380 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2166	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 97.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7179e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, 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	2.24	17/483 (3.5%)	1.85	7/651 (1.1%)
1	B	2.23	23/485 (4.7%)	1.82	11/652 (1.7%)
1	C	2.27	20/501 (4.0%)	1.71	8/674 (1.2%)
1	D	2.20	18/517 (3.5%)	1.77	5/695 (0.7%)
All	All	2.23	78/1986 (3.9%)	1.79	31/2672 (1.2%)

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

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

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	GLN	CA-CB	12.42	1.75	1.53
1	B	20	ALA	N-CA	-11.67	1.31	1.46
1	A	20	ALA	N-CA	-10.92	1.32	1.46
1	D	37	GLN	CA-CB	9.44	1.70	1.53
1	A	29	ILE	CA-CB	8.69	1.63	1.54
1	A	9	GLY	N-CA	8.64	1.53	1.44
1	A	22	ASP	CA-CB	-8.58	1.42	1.53
1	A	6	ILE	C-O	-8.20	1.14	1.24
1	D	29	ILE	C-O	-7.94	1.14	1.24
1	C	32	HIS	ND1-CE1	-7.84	1.24	1.32
1	B	19	GLU	C-N	7.78	1.43	1.33
1	B	37	GLN	CD-OE1	-7.62	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	GLN	CD-OE1	-7.47	1.09	1.23
1	D	37	GLN	CD-NE2	-7.42	1.17	1.33
1	D	12	LEU	CA-C	7.18	1.61	1.52
1	C	36[A]	HIS	C-N	7.10	1.44	1.33
1	C	36[B]	HIS	C-N	7.10	1.44	1.33
1	B	29	ILE	CA-CB	7.06	1.61	1.54
1	B	6	ILE	C-O	-6.89	1.16	1.24
1	A	55	THR	C-O	-6.68	1.16	1.24
1	A	11	THR	N-CA	6.67	1.54	1.46
1	D	37	GLN	CG-CD	-6.65	1.35	1.52
1	C	26	ALA	CA-CB	-6.61	1.43	1.53
1	B	37	GLN	CA-CB	6.54	1.65	1.53
1	C	12	LEU	N-CA	6.53	1.54	1.45
1	D	43	TRP	N-CA	6.51	1.54	1.46
1	C	45	TYR	N-CA	6.49	1.53	1.46
1	B	22	ASP	CA-CB	-6.43	1.45	1.53
1	B	28	TYR	C-O	-6.34	1.16	1.24
1	C	7	LEU	CA-C	6.29	1.61	1.53
1	D	43	TRP	C-O	6.27	1.31	1.24
1	B	37	GLN	CB-CG	6.14	1.70	1.52
1	B	19	GLU	CA-C	6.10	1.60	1.52
1	B	42	GLU	CD-OE1	6.06	1.36	1.25
1	D	26	ALA	CA-CB	-6.02	1.44	1.53
1	C	39	VAL	CA-C	-5.96	1.45	1.52
1	D	55	THR	C-O	5.96	1.30	1.24
1	A	41	GLY	C-O	-5.93	1.16	1.23
1	C	28	TYR	CA-C	5.93	1.60	1.52
1	D	7	LEU	CA-C	5.89	1.60	1.52
1	C	43	TRP	C-O	5.80	1.30	1.24
1	C	10	LYS	C-O	5.80	1.29	1.23
1	B	30	PHE	N-CA	5.75	1.53	1.46
1	B	10	LYS	C-O	5.67	1.31	1.24
1	B	9	GLY	N-CA	5.65	1.50	1.44
1	B	11	THR	CA-CB	5.64	1.62	1.53
1	D	20	ALA	C-O	-5.62	1.17	1.23
1	A	54	VAL	CA-CB	5.61	1.61	1.54
1	D	20	ALA	N-CA	5.51	1.52	1.45
1	C	23	ALA	CA-C	5.46	1.60	1.52
1	A	19	GLU	C-N	5.46	1.40	1.33
1	D	53	THR	N-CA	5.45	1.52	1.46
1	A	37	GLN	CD-OE1	-5.43	1.13	1.23
1	A	29	ILE	C-O	5.43	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	TYR	CA-C	5.41	1.59	1.52
1	B	18	ALA	C-O	5.40	1.30	1.23
1	C	47	ASP	C-O	-5.40	1.17	1.24
1	C	56	GLU	C-OXT	-5.39	1.12	1.23
1	D	43	TRP	CA-C	-5.37	1.46	1.52
1	B	13	LYS	N-CA	-5.36	1.39	1.46
1	A	54	VAL	C-O	-5.33	1.18	1.24
1	D	36[A]	HIS	C-N	5.32	1.41	1.33
1	D	36[B]	HIS	C-N	5.32	1.41	1.33
1	C	16	PHE	CA-CB	-5.31	1.44	1.53
1	D	45	TYR	CA-CB	-5.31	1.44	1.53
1	B	31	ARG	N-CA	5.30	1.53	1.46
1	B	27	GLU	N-CA	5.30	1.52	1.46
1	A	2	THR	CA-C	-5.29	1.46	1.52
1	B	33	LEU	CA-CB	5.27	1.61	1.53
1	B	51	THR	CA-C	5.27	1.58	1.52
1	C	13	LYS	N-CA	5.22	1.52	1.46
1	C	20	ALA	N-CA	5.21	1.52	1.45
1	A	42	GLU	CD-OE1	5.19	1.35	1.25
1	A	47	ASP	CA-CB	5.18	1.61	1.53
1	B	11	THR	N-CA	5.16	1.52	1.46
1	B	17	THR	C-O	-5.11	1.17	1.24
1	C	37	GLN	C-N	5.11	1.38	1.33
1	D	32	HIS	CE1-NE2	5.08	1.37	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	LYS	N-CA-C	-9.05	97.00	111.04
1	B	37	GLN	CB-CG-CD	7.29	125.00	112.60
1	A	12	LEU	O-C-N	6.59	130.93	123.42
1	B	15	GLU	CB-CG-CD	6.31	123.32	112.60
1	C	10	LYS	N-CA-C	-5.93	101.85	111.04
1	B	27	GLU	O-C-N	5.84	128.17	122.09
1	B	18	ALA	O-C-N	5.75	129.83	123.33
1	B	42	GLU	CG-CD-OE2	-5.71	105.27	118.40
1	D	14	GLY	N-CA-C	5.70	118.91	110.42
1	A	37	GLN	CB-CG-CD	5.70	122.28	112.60
1	A	15	GLU	CB-CG-CD	5.67	122.24	112.60
1	B	56	GLU	CB-CA-C	-5.65	99.36	110.10
1	D	34	ALA	O-C-N	5.59	128.53	122.15
1	B	27	GLU	CA-C-O	-5.52	115.00	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ALA	N-CA-CB	5.48	118.27	110.16
1	C	17[A]	THR	CA-C-N	-5.30	112.61	121.94
1	C	17[A]	THR	C-N-CA	-5.30	112.61	121.94
1	C	17[B]	THR	CA-C-N	-5.30	112.61	121.94
1	C	17[B]	THR	C-N-CA	-5.30	112.61	121.94
1	A	21	GLU	CA-CB-CG	-5.26	103.58	114.10
1	A	33	LEU	N-CA-CB	5.25	117.84	110.12
1	D	50	LYS	N-CA-C	-5.19	104.74	111.74
1	B	17	THR	CA-C-O	-5.16	115.13	120.70
1	D	7	LEU	CD1-CG-CD2	5.15	122.12	110.80
1	C	43	TRP	O-C-N	5.13	129.32	123.27
1	A	13	LYS	N-CA-CB	-5.12	102.66	110.65
1	B	48	ALA	N-CA-C	-5.11	105.60	111.07
1	C	28	TYR	CA-C-N	-5.11	113.16	120.42
1	C	28	TYR	C-N-CA	-5.11	113.16	120.42
1	B	32	HIS	N-CA-C	-5.10	105.80	111.36
1	A	34	ALA	N-CA-C	-5.01	106.01	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	ILE	Mainchain
1	C	7	LEU	Mainchain

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	464	0	456	50	4
1	B	466	0	462	32	1
1	C	476	0	475	38	3
1	D	486	0	495	38	3
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	5	2
3	C	1	0	0	1	0
3	D	1	0	0	1	1
4	A	65	0	0	16	2
4	B	70	0	0	20	2
4	C	63	0	0	11	1
4	D	66	0	0	18	1
All	All	2166	0	1888	141	10

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 37.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLN:CA	1:C:37:GLN:CB	1.75	1.61
1:B:4:LYS:HB2	4:B:237:HOH:O	1.27	1.34
1:A:54:VAL:HB	4:A:205:HOH:O	1.28	1.25
1:C:36[B]:HIS:HE1	3:C:102:CL:CL	1.56	1.25
1:A:4:LYS:HB2	4:A:244:HOH:O	1.36	1.22
1:B:54:VAL:HB	4:B:204:HOH:O	1.36	1.22
1:D:36[B]:HIS:HE1	3:D:102:CL:CL	1.60	1.21
1:B:27:GLU:OE2	3:B:105:CL:CL	2.06	1.09
4:B:242:HOH:O	1:D:16:PHE:CG	2.08	1.07
1:A:27:GLU:OE2	3:B:104:CL:CL	2.09	1.06
1:A:50:LYS:HE2	4:A:220:HOH:O	1.56	1.03
1:D:39:VAL:HG11	4:D:251:HOH:O	1.58	1.01
1:C:47:ASP:HB3	4:C:220:HOH:O	1.64	0.98
1:A:1[B]:MET:CE	1:A:1[B]:MET:HA	1.95	0.96
4:A:234:HOH:O	1:C:16:PHE:CG	2.22	0.93
1:D:47:ASP:HB3	4:D:231:HOH:O	1.68	0.92
1:A:50:LYS:CE	4:A:220:HOH:O	2.18	0.88
1:B:12:LEU:HD11	4:B:242:HOH:O	1.76	0.85
1:A:12:LEU:HD11	4:A:234:HOH:O	1.76	0.85
4:A:234:HOH:O	1:C:16:PHE:CD1	2.27	0.85
1:A:1[B]:MET:HA	1:A:1[B]:MET:HE3	1.58	0.84
1:C:39:VAL:HG11	4:C:248:HOH:O	1.76	0.84
1:B:1[B]:MET:HG2	1:B:50[B]:LYS:HD2	1.58	0.84
4:B:242:HOH:O	1:D:16:PHE:CD1	2.25	0.83
1:B:37:GLN:HE21	1:D:37:GLN:HG2	1.42	0.82
1:A:33:LEU:HB2	4:A:209:HOH:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:LYS:CD	4:D:250:HOH:O	2.29	0.80
1:D:50:LYS:CG	4:D:250:HOH:O	2.31	0.78
1:B:1[A]:MET:HE2	4:B:210:HOH:O	1.82	0.78
1:A:37:GLN:HE21	1:C:37:GLN:HG2	1.49	0.77
1:B:1[B]:MET:SD	1:B:50[B]:LYS:NZ	2.56	0.75
4:B:208:HOH:O	1:D:12:LEU:HA	1.87	0.74
1:A:1[B]:MET:HA	1:A:1[B]:MET:HE2	1.68	0.73
1:D:50:LYS:HG3	4:D:250:HOH:O	1.87	0.73
1:C:40:ASP:O	4:C:201:HOH:O	2.06	0.73
1:A:1[B]:MET:HE2	1:A:2:THR:H	1.52	0.73
1:D:19:GLU:OE1	4:D:201:HOH:O	2.05	0.72
1:D:50:LYS:HD2	4:D:250:HOH:O	1.89	0.72
1:C:37:GLN:CB	1:C:37:GLN:HA	2.10	0.71
1:D:40:ASP:O	4:D:202:HOH:O	2.08	0.70
1:C:15[B]:GLU:CD	4:C:208:HOH:O	2.35	0.70
1:B:1[B]:MET:CG	1:B:50[B]:LYS:HD2	2.22	0.69
1:B:36[A]:HIS:CE1	4:B:230:HOH:O	2.46	0.69
1:C:37:GLN:CA	1:C:37:GLN:CG	2.70	0.69
1:B:36[A]:HIS:HE1	4:B:230:HOH:O	1.76	0.68
1:D:42:GLU:HG2	4:D:244:HOH:O	1.93	0.68
1:B:33:LEU:HB2	4:B:226:HOH:O	1.94	0.67
1:A:21:GLU:CD	4:D:202:HOH:O	2.37	0.67
1:A:32:HIS:CE1	1:A:36[B]:HIS:CE1	2.84	0.65
1:A:1[B]:MET:CE	1:A:1[B]:MET:CA	2.72	0.65
1:C:4[A]:LYS:CE	4:C:208:HOH:O	2.45	0.65
1:B:15:GLU:HG3	1:D:15[A]:GLU:HG3	1.77	0.65
1:A:15:GLU:HG3	1:C:15[A]:GLU:HG3	1.80	0.64
1:B:1[B]:MET:HG2	1:B:50[B]:LYS:CD	2.28	0.64
1:A:17[B]:THR:CG2	1:C:13:LYS:HB3	2.27	0.63
1:A:12:LEU:HD23	1:A:39:VAL:HG21	1.81	0.62
1:B:28:TYR:HD2	4:B:243:HOH:O	1.82	0.62
1:D:9:GLY:O	1:D:13:LYS:NZ	2.33	0.62
1:D:12:LEU:HB2	4:D:227:HOH:O	2.00	0.61
1:A:17[B]:THR:HG22	1:C:13:LYS:HB3	1.82	0.60
1:A:1[B]:MET:SD	4:A:220:HOH:O	2.57	0.60
1:C:56:GLU:O	4:C:202:HOH:O	2.17	0.60
1:B:27:GLU:CD	3:B:105:CL:CL	2.73	0.58
1:C:4[B]:LYS:HD3	1:C:15[B]:GLU:OE2	2.04	0.58
1:B:54:VAL:CB	4:B:204:HOH:O	2.14	0.57
1:A:27:GLU:CD	3:B:104:CL:CL	2.76	0.57
1:D:44[B]:THR:HG23	1:D:53:THR:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LYS:CB	4:B:237:HOH:O	2.10	0.57
1:A:32:HIS:CE1	1:A:36[B]:HIS:HE1	2.22	0.57
1:B:15:GLU:CG	1:D:15[A]:GLU:HG3	2.34	0.56
1:A:1[A]:MET:HE2	4:A:222:HOH:O	2.05	0.56
1:D:12:LEU:CA	4:D:213:HOH:O	2.54	0.56
1:A:4:LYS:CB	4:A:244:HOH:O	2.17	0.56
1:D:44[B]:THR:HG22	4:D:221:HOH:O	2.05	0.56
1:A:37:GLN:NE2	1:C:36[A]:HIS:HB2	2.21	0.55
1:C:7:LEU:HB3	4:C:248:HOH:O	2.07	0.55
1:A:8:ASN:ND2	4:A:201:HOH:O	2.17	0.54
1:B:3:TYR:CE1	1:B:50[B]:LYS:HD3	2.42	0.54
1:D:44[B]:THR:CG2	1:D:53:THR:HB	2.37	0.54
1:A:21:GLU:CG	4:D:202:HOH:O	2.55	0.53
1:A:15:GLU:CG	1:C:15[A]:GLU:HG3	2.38	0.53
1:A:54:VAL:CB	4:A:205:HOH:O	2.13	0.52
1:D:8:ASN:OD1	1:D:13:LYS:HE3	2.10	0.52
1:C:4[B]:LYS:HE3	4:C:256:HOH:O	2.09	0.52
1:B:5:LEU:HD11	4:B:204:HOH:O	2.09	0.51
1:A:12:LEU:HD23	1:A:39:VAL:CG2	2.41	0.51
1:C:2:THR:HA	1:C:19:GLU:HA	1.93	0.51
1:D:7:LEU:HB3	4:D:251:HOH:O	2.11	0.51
1:A:50:LYS:CD	4:A:220:HOH:O	2.56	0.51
1:D:44[B]:THR:OG1	1:D:45:TYR:N	2.44	0.50
1:B:12:LEU:CD1	4:B:242:HOH:O	2.43	0.50
1:C:37:GLN:CB	1:C:37:GLN:C	2.77	0.50
1:D:22:ASP:OD1	1:D:25:LEU:HG	2.12	0.49
1:A:1[B]:MET:HE2	1:A:1[B]:MET:CA	2.39	0.49
1:A:33:LEU:HD22	1:C:12:LEU:HD13	1.95	0.49
1:A:9:GLY:O	1:A:13:LYS:NZ	2.46	0.48
1:B:4:LYS:HE3	1:B:15:GLU:HB2	1.96	0.47
1:C:32:HIS:CE1	1:C:36[B]:HIS:HE1	2.22	0.47
4:B:242:HOH:O	1:D:16:PHE:CB	2.54	0.47
1:A:36[B]:HIS:HB2	1:C:37:GLN:HE22	1.78	0.47
1:A:1[B]:MET:HE2	1:A:2:THR:N	2.24	0.47
1:A:54:VAL:N	4:A:205:HOH:O	2.49	0.46
1:A:37:GLN:HE22	1:C:36[A]:HIS:HB2	1.79	0.46
1:A:37:GLN:NE2	1:C:36[B]:HIS:HB2	2.30	0.46
1:B:54:VAL:N	4:B:204:HOH:O	2.49	0.45
1:C:10:LYS:N	1:C:56:GLU:OE2	2.35	0.45
1:D:5:LEU:O	1:D:15[A]:GLU:HA	2.16	0.45
1:D:47:ASP:O	1:D:47:ASP:CG	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:HG2	4:D:202:HOH:O	2.16	0.45
1:B:37:GLN:NE2	1:D:36[B]:HIS:HB2	2.32	0.44
1:A:5:LEU:O	1:A:15:GLU:HA	2.17	0.44
1:C:42:GLU:HG2	4:C:250:HOH:O	2.17	0.44
1:C:32:HIS:CE1	1:C:36[B]:HIS:CE1	2.92	0.44
1:D:12:LEU:HD21	1:D:39:VAL:CG2	2.48	0.44
1:D:21:GLU:HB3	1:D:25:LEU:HD12	1.98	0.44
1:B:22:ASP:OD1	1:B:22:ASP:C	2.60	0.44
1:A:8:ASN:ND2	1:A:55:THR:HG23	2.32	0.43
3:B:105:CL:CL	4:B:251:HOH:O	2.59	0.43
1:C:15[A]:GLU:HG2	4:C:208:HOH:O	2.18	0.43
1:B:32:HIS:HA	4:B:250:HOH:O	2.18	0.43
1:A:36[A]:HIS:HB2	1:C:37:GLN:HE22	1.84	0.43
1:B:37:GLN:NE2	1:D:36[A]:HIS:HB2	2.33	0.43
1:C:43:TRP:HZ2	4:C:224:HOH:O	2.02	0.43
1:B:1[A]:MET:CE	1:B:21:GLU:O	2.66	0.42
1:D:42:GLU:CG	4:D:244:HOH:O	2.60	0.42
1:A:12:LEU:CD2	1:A:37:GLN:HB3	2.50	0.42
1:A:36[B]:HIS:HB2	1:C:37:GLN:NE2	2.35	0.42
1:C:5:LEU:O	1:C:15[A]:GLU:HA	2.20	0.41
1:A:33:LEU:O	1:A:36[B]:HIS:HB2	2.21	0.41
1:D:31:ARG:O	1:D:35[B]:LYS:HG3	2.20	0.41
1:A:22:ASP:OD1	1:A:22:ASP:C	2.63	0.41
1:D:12:LEU:HA	4:D:213:HOH:O	2.17	0.41
1:A:37:GLN:HG2	1:C:37:GLN:HE21	1.85	0.41
1:B:1[B]:MET:SD	1:B:50[B]:LYS:HD2	2.60	0.41
4:B:242:HOH:O	1:D:16:PHE:HB3	2.21	0.41
1:B:1[B]:MET:HG3	1:B:2:THR:N	2.35	0.41
1:A:8:ASN:HB2	4:A:248:HOH:O	2.21	0.40
1:D:2:THR:HA	1:D:19:GLU:HA	2.03	0.40

All (10) 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:32:HIS:NE2	3:B:105:CL:CL[3_455]	1.76	0.44
1:A:32:HIS:CE1	3:B:105:CL:CL[3_455]	1.82	0.38
1:B:56:GLU:OE1	1:C:22:ASP:OD2[2_664]	1.84	0.36
1:A:56:GLU:OE1	1:D:22:ASP:OD2[1_565]	1.93	0.27
4:A:243:HOH:O	4:D:246:HOH:O[1_565]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:GLU:OE2	4:B:206:HOH:O[3_445]	2.07	0.13
4:B:240:HOH:O	4:C:239:HOH:O[2_664]	2.13	0.07
1:C:27:GLU:OE2	3:D:102:CL:CL[3_565]	2.15	0.05
1:A:56:GLU:OXT	1:D:21:GLU:OE1[1_565]	2.18	0.02
1:C:42:GLU:OE2	4:A:219:HOH:O[3_565]	2.19	0.01

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	56/56 (100%)	54 (96%)	2 (4%)	0	100	100
1	B	56/56 (100%)	53 (95%)	3 (5%)	0	100	100
1	C	58/56 (104%)	57 (98%)	1 (2%)	0	100	100
1	D	60/56 (107%)	59 (98%)	1 (2%)	0	100	100
All	All	230/224 (103%)	223 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	48/45 (107%)	46 (96%)	2 (4%)	26	4
1	B	48/45 (107%)	47 (98%)	1 (2%)	47	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	50/45 (111%)	46 (92%)	4 (8%)	11 0
1	D	52/45 (116%)	47 (90%)	5 (10%)	8 0
All	All	198/180 (110%)	186 (94%)	12 (6%)	19 1

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	50	LYS
1	B	15	GLU
1	C	12	LEU
1	C	13	LYS
1	C	15[A]	GLU
1	C	15[B]	GLU
1	D	12	LEU
1	D	13	LYS
1	D	15[A]	GLU
1	D	15[B]	GLU
1	D	47	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	37	GLN
1	B	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	56/56 (100%)	-0.00	0 100 100	9, 14, 26, 32	3 (5%)
1	B	56/56 (100%)	-0.09	0 100 100	8, 14, 24, 31	3 (5%)
1	C	56/56 (100%)	-0.07	1 (1%) 67 71	8, 14, 28, 32	5 (8%)
1	D	56/56 (100%)	0.00	0 100 100	7, 14, 31, 43	7 (12%)
All	All	224/224 (100%)	-0.04	1 (0%) 88 91	7, 14, 28, 43	18 (8%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	THR	2.2

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	CL	B	105	1/1	0.98	0.07	19,19,19,19	0

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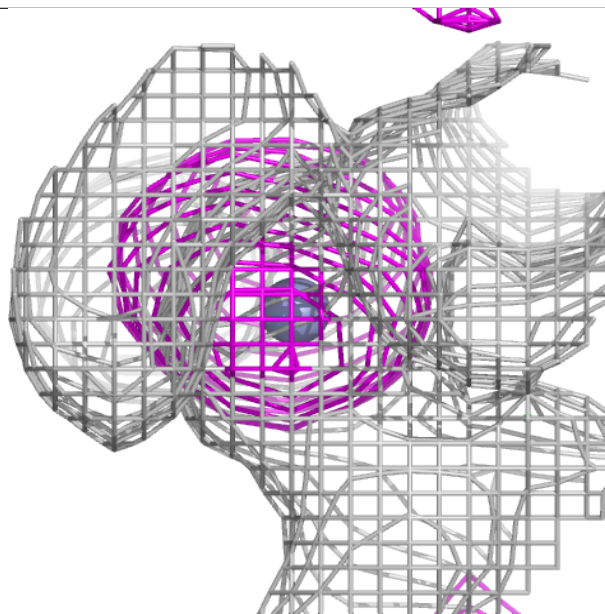
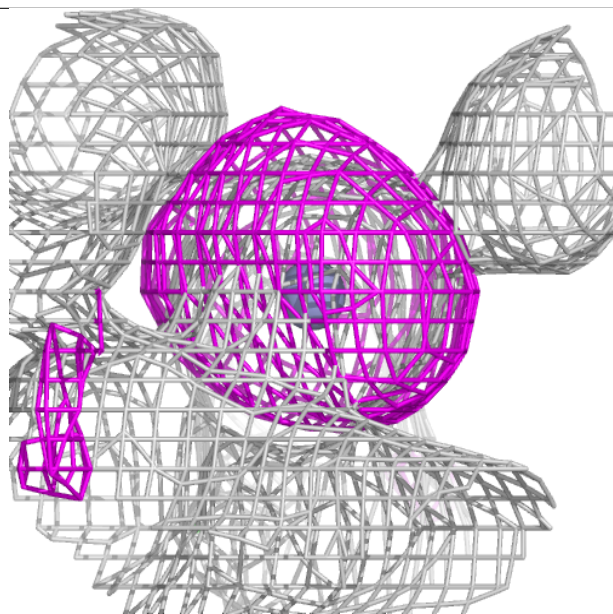
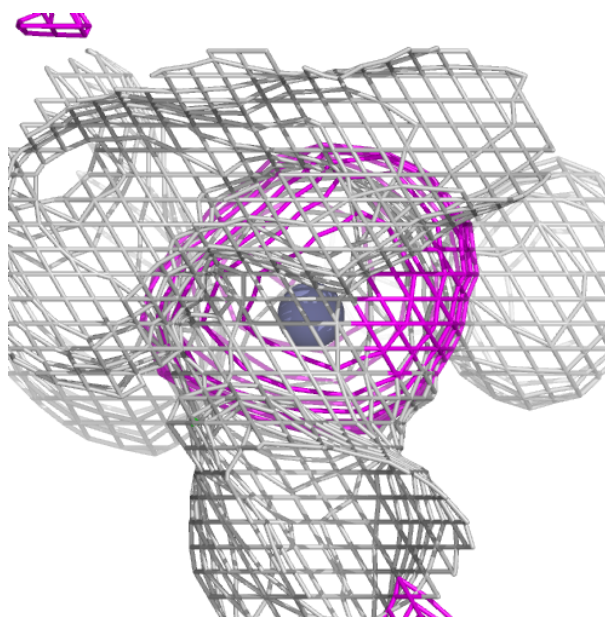
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	101	1/1	0.99	0.14	23,23,23,23	0
2	ZN	D	101	1/1	0.99	0.14	20,20,20,20	0
2	ZN	B	103	1/1	0.99	0.13	18,18,18,18	0
3	CL	C	102	1/1	0.99	0.04	22,22,22,22	0
3	CL	D	102	1/1	0.99	0.06	20,20,20,20	0
3	CL	B	104	1/1	1.00	0.05	20,20,20,20	0
2	ZN	A	101	1/1	1.00	0.11	16,16,16,16	0
2	ZN	B	101	1/1	1.00	0.13	19,19,19,19	0
2	ZN	B	102	1/1	1.00	0.11	19,19,19,19	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.

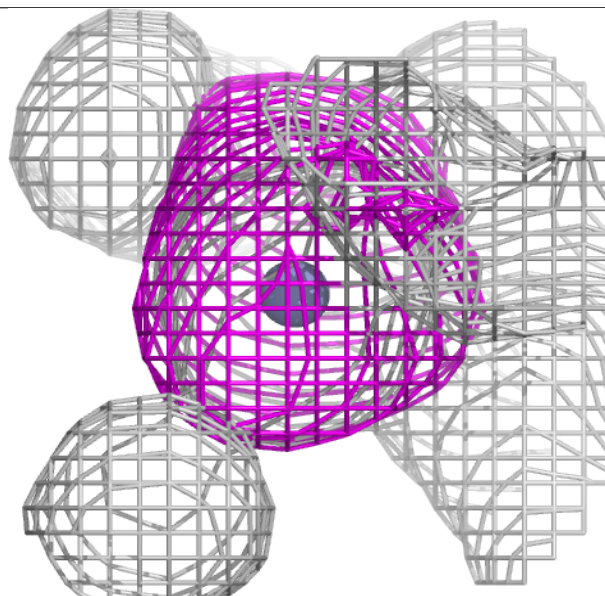
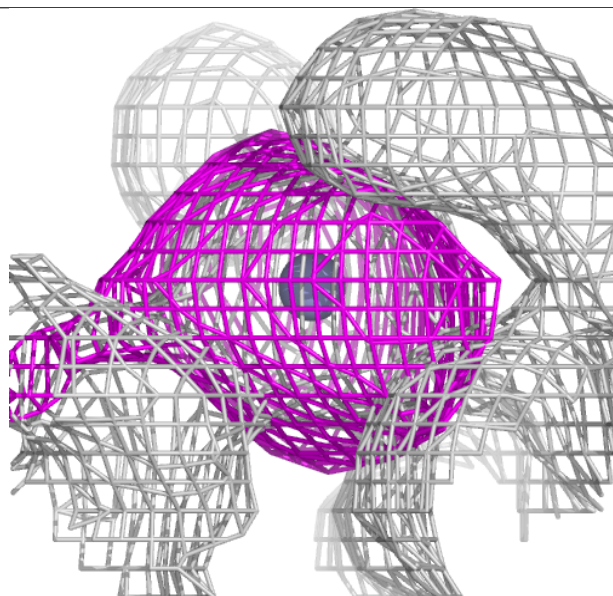
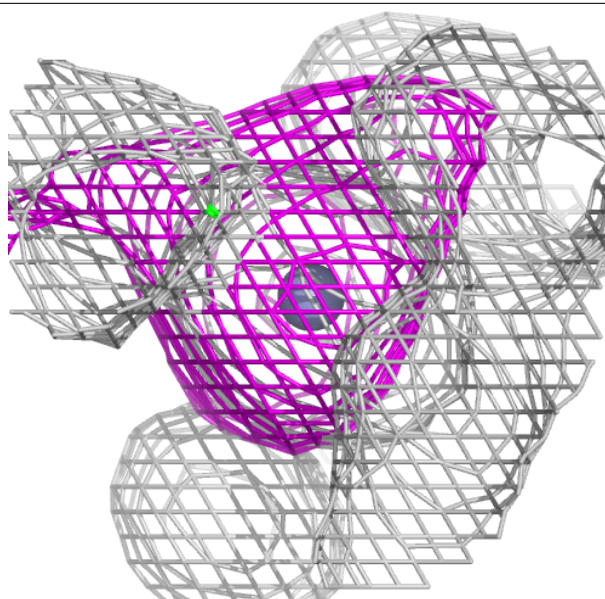
Electron density around ZN C 101:

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



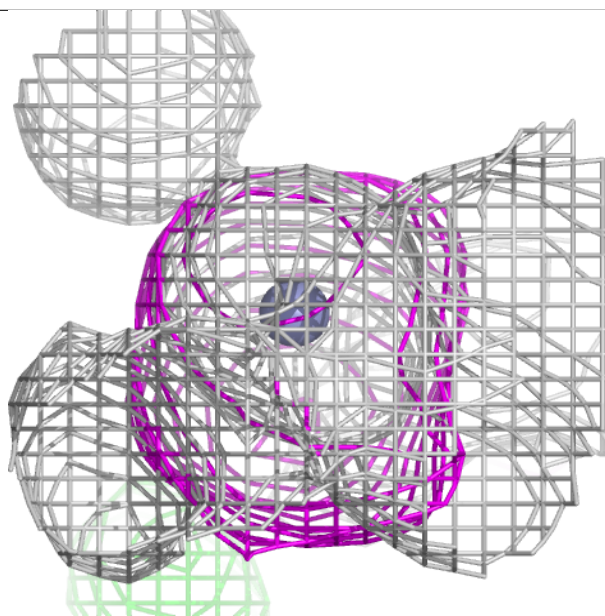
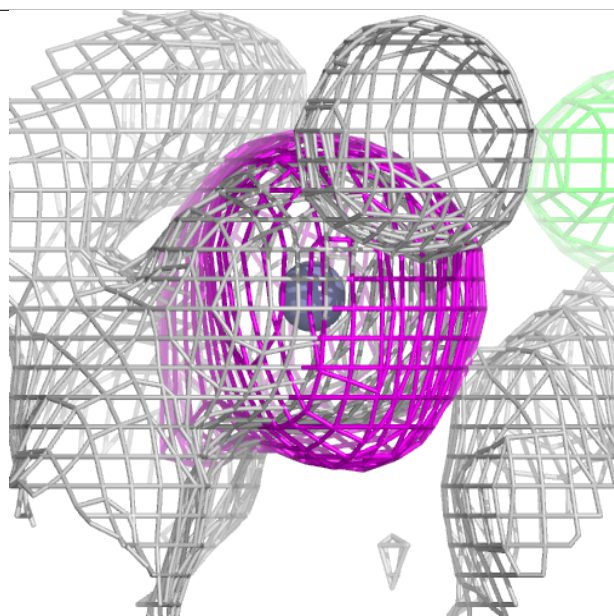
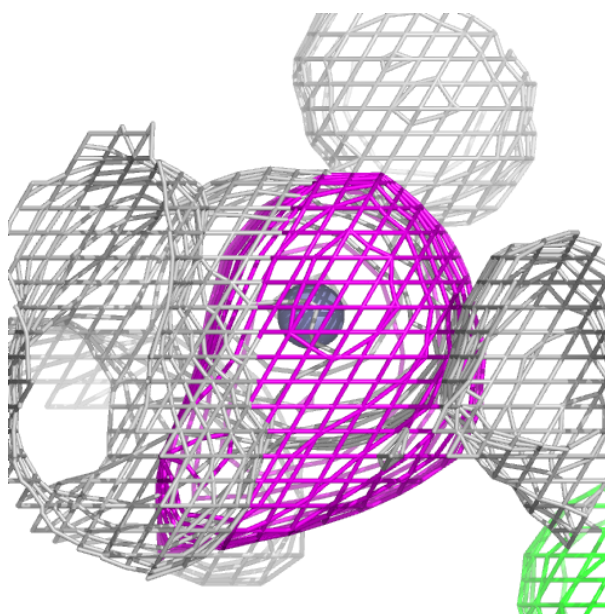
Electron density around ZN D 101:

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



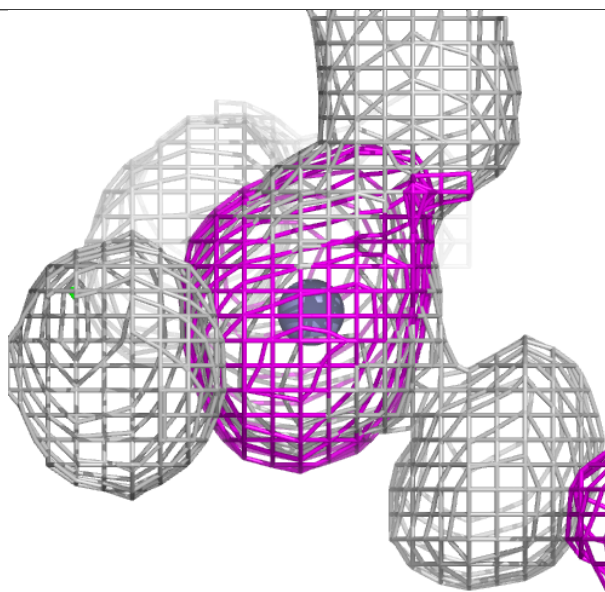
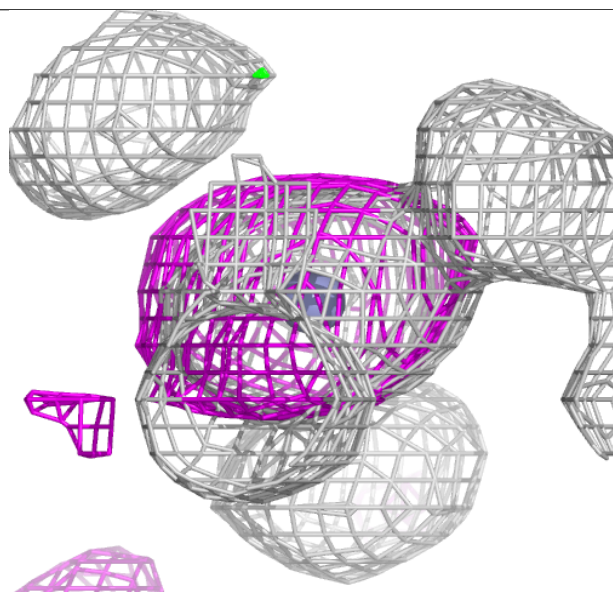
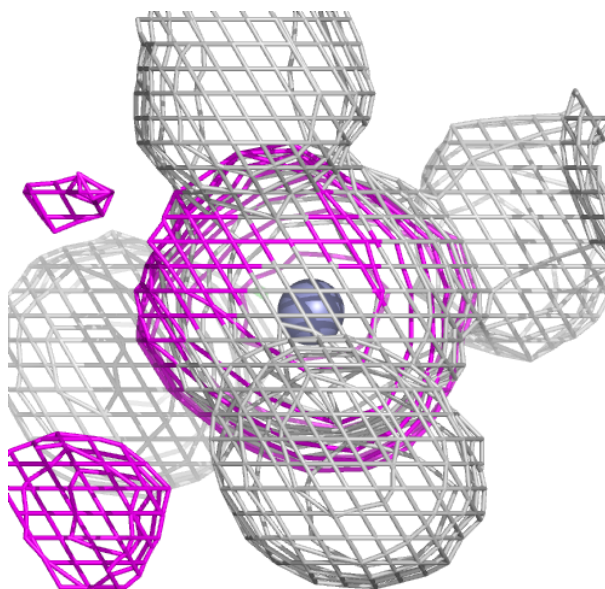
Electron density around ZN B 103:

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



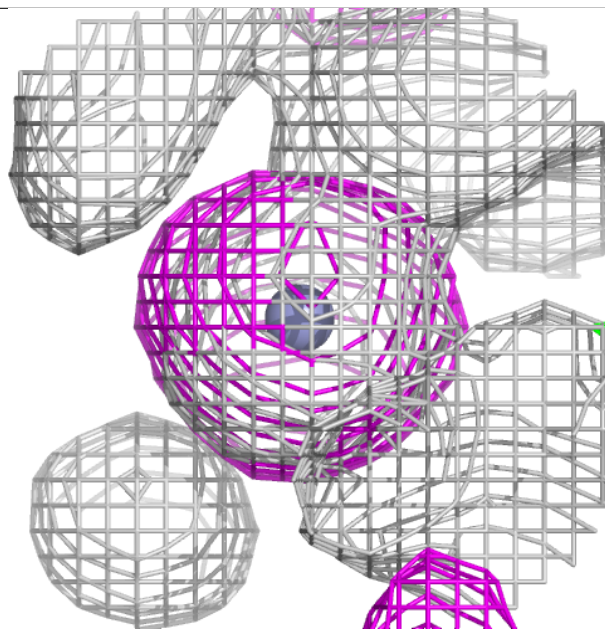
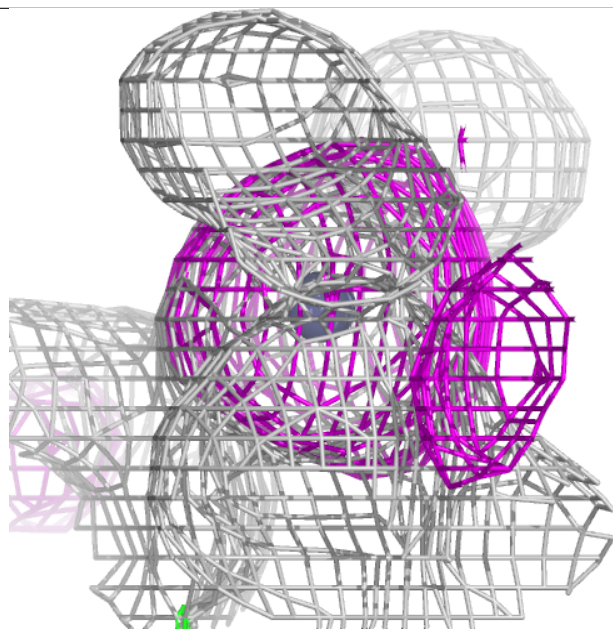
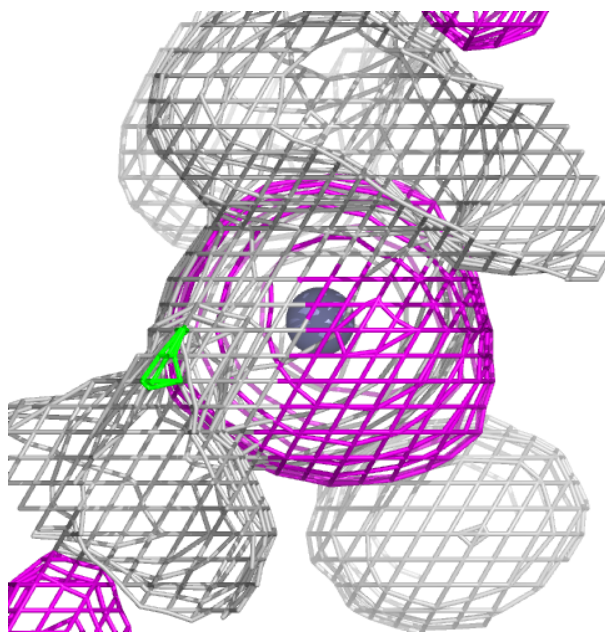
Electron density around ZN A 101:

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



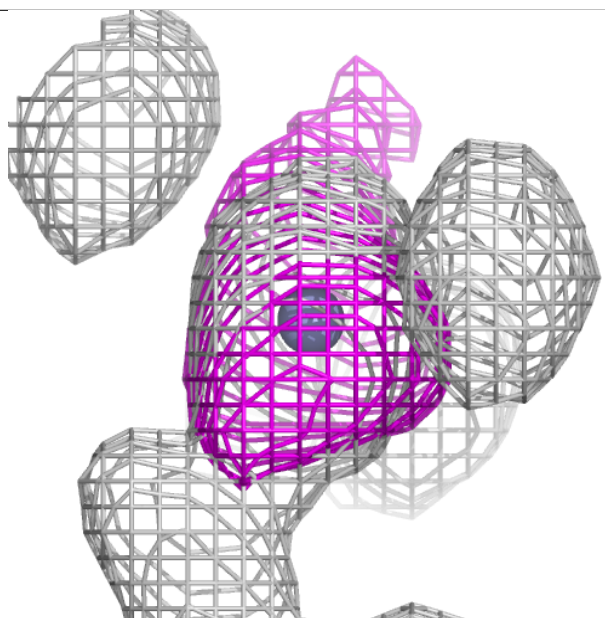
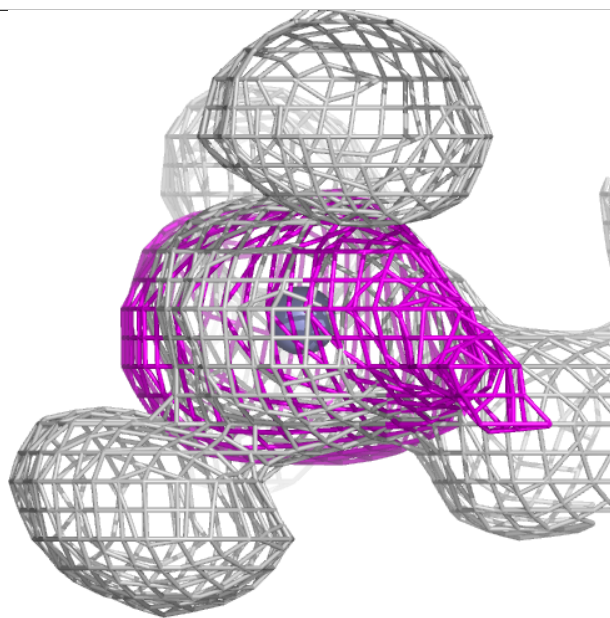
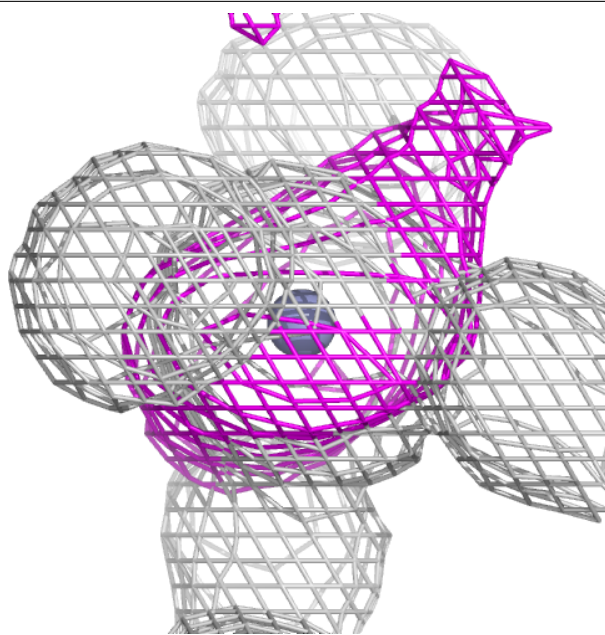
Electron density around ZN B 101:

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



Electron density around ZN B 102:

$2mF_o - DF_c$ (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.