



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:04 PM UTC

PDB ID : 8CQ6 / pdb_00008cq6
Title : Bifunctional cyclohexadienyl dehydratase/chorismate mutase from Duganella sacchari
Authors : Khatanbaatar, T.; Cordara, G.; Krengel, U.
Deposited on : 2023-03-03
Resolution : 2.44 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

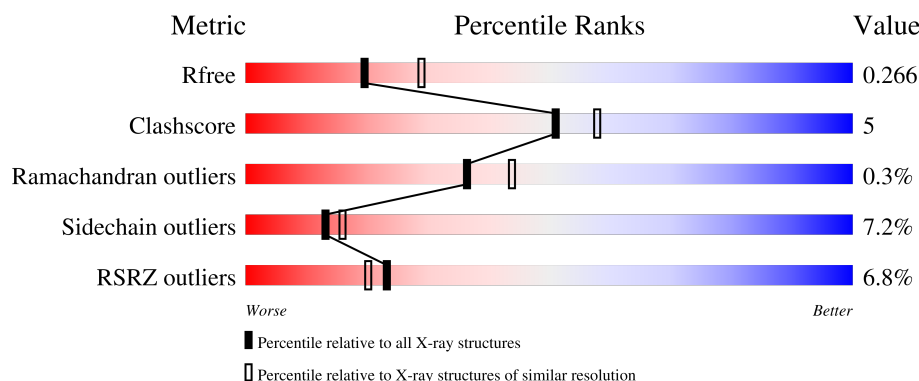
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	416	4% 74% 16% • 9%
1	B	416	5% 73% 17% • 8%
1	C	416	10% 72% 18% • 6%
1	D	416	6% 74% 17% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12234 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 chorismate mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2954	1865	530	552	7			
1	B	384	Total	C	N	O	S	0	6	0
			3034	1916	546	565	7			
1	C	389	Total	C	N	O	S	0	7	0
			3098	1957	563	571	7			
1	D	389	Total	C	N	O	S	0	3	0
			3067	1938	558	564	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	LEU	-	expression tag	UNP A0A1M7QNNQ8
A	410	GLU	-	expression tag	UNP A0A1M7QNNQ8
A	411	HIS	-	expression tag	UNP A0A1M7QNNQ8
A	412	HIS	-	expression tag	UNP A0A1M7QNNQ8
A	413	HIS	-	expression tag	UNP A0A1M7QNNQ8
A	414	HIS	-	expression tag	UNP A0A1M7QNNQ8
A	415	HIS	-	expression tag	UNP A0A1M7QNNQ8
A	416	HIS	-	expression tag	UNP A0A1M7QNNQ8
B	409	LEU	-	expression tag	UNP A0A1M7QNNQ8
B	410	GLU	-	expression tag	UNP A0A1M7QNNQ8
B	411	HIS	-	expression tag	UNP A0A1M7QNNQ8
B	412	HIS	-	expression tag	UNP A0A1M7QNNQ8
B	413	HIS	-	expression tag	UNP A0A1M7QNNQ8
B	414	HIS	-	expression tag	UNP A0A1M7QNNQ8
B	415	HIS	-	expression tag	UNP A0A1M7QNNQ8
B	416	HIS	-	expression tag	UNP A0A1M7QNNQ8
C	409	LEU	-	expression tag	UNP A0A1M7QNNQ8
C	410	GLU	-	expression tag	UNP A0A1M7QNNQ8
C	411	HIS	-	expression tag	UNP A0A1M7QNNQ8
C	412	HIS	-	expression tag	UNP A0A1M7QNNQ8
C	413	HIS	-	expression tag	UNP A0A1M7QNNQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	414	HIS	-	expression tag	UNP A0A1M7QNNQ8
C	415	HIS	-	expression tag	UNP A0A1M7QNNQ8
C	416	HIS	-	expression tag	UNP A0A1M7QNNQ8
D	409	LEU	-	expression tag	UNP A0A1M7QNNQ8
D	410	GLU	-	expression tag	UNP A0A1M7QNNQ8
D	411	HIS	-	expression tag	UNP A0A1M7QNNQ8
D	412	HIS	-	expression tag	UNP A0A1M7QNNQ8
D	413	HIS	-	expression tag	UNP A0A1M7QNNQ8
D	414	HIS	-	expression tag	UNP A0A1M7QNNQ8
D	415	HIS	-	expression tag	UNP A0A1M7QNNQ8
D	416	HIS	-	expression tag	UNP A0A1M7QNNQ8

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	B	2	Total Na 2 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	18	Total O 18 18	0	0

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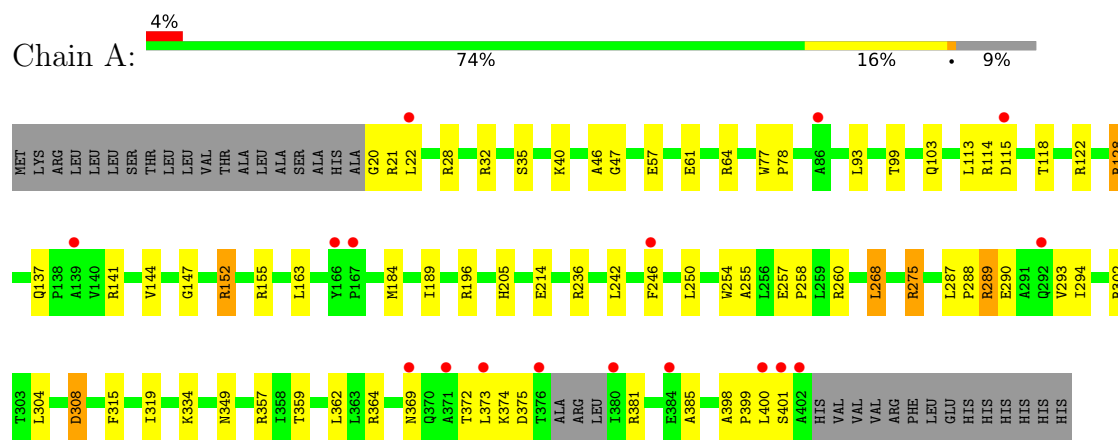
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	15	Total	O	0	0
			15	15		
4	D	21	Total	O	0	0
			21	21		

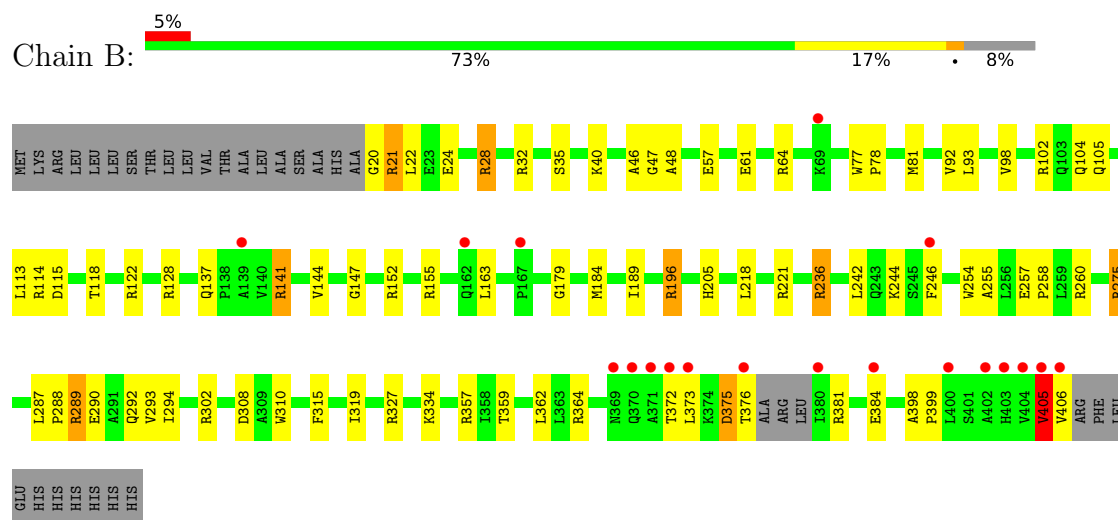
3 Residue-property plots [i](#)

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.

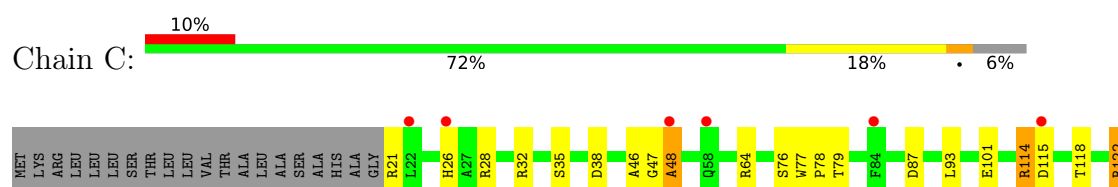
• Molecule 1: chorismate mutase

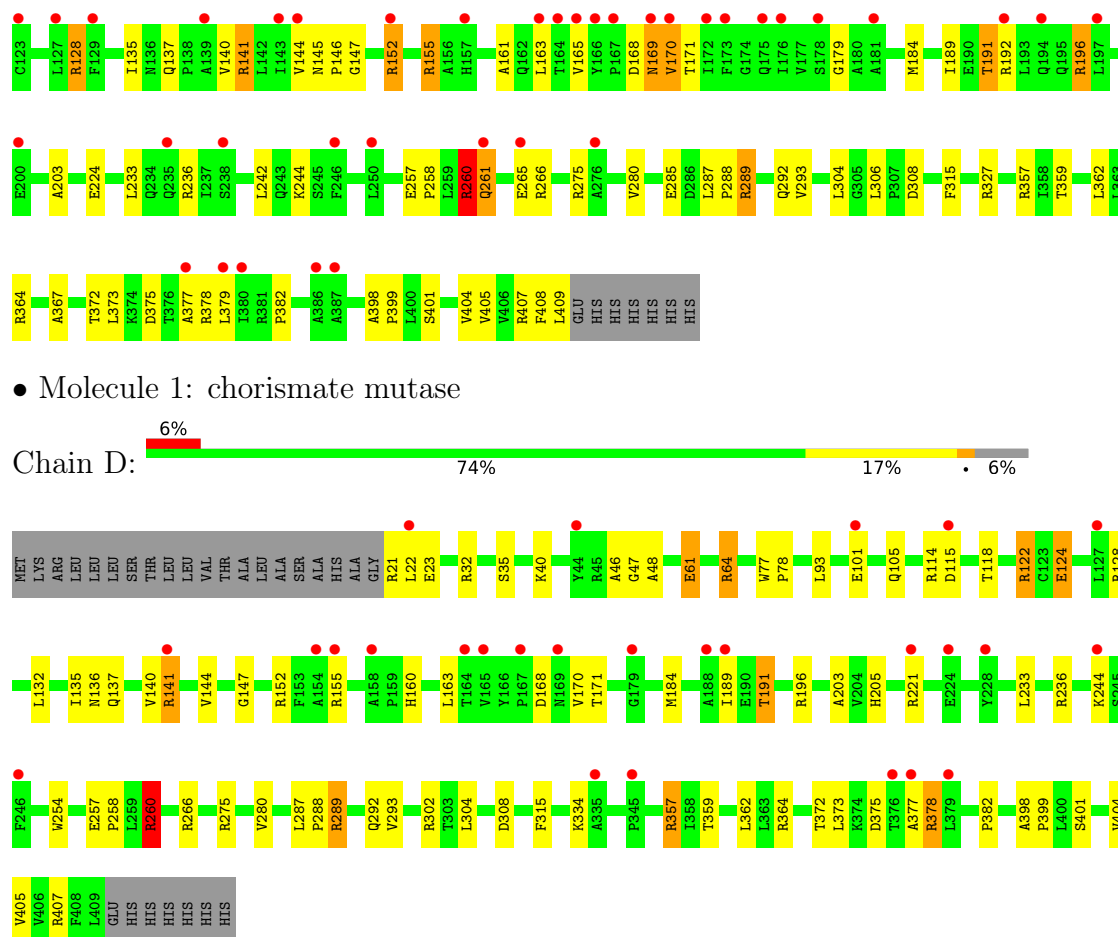


• Molecule 1: chorismate mutase



• Molecule 1: chorismate mutase





• Molecule 1: chorismate mutase

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.11Å 111.93Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.90 – 2.44 99.90 – 2.44	Depositor EDS
% Data completeness (in resolution range)	60.3 (99.90-2.44) 60.4 (99.90-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.225 , 0.265 0.226 , 0.266	Depositor DCC
R_{free} test set	2573 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12234	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 48.01 % 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 9.1447e-05. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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	0.49	0/3013	0.85	0/4101
1	B	0.49	0/3094	0.85	0/4212
1	C	0.47	0/3161	0.86	0/4302
1	D	0.48	0/3130	0.85	0/4260
All	All	0.48	0/12398	0.85	0/16875

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	24
1	B	0	24
1	C	0	29
1	D	0	25
All	All	0	102

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (102) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ARG	Sidechain
1	A	115	ASP	Peptide
1	A	122	ARG	Sidechain
1	A	128	ARG	Sidechain
1	A	141	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	147	GLY	Peptide
1	A	152	ARG	Sidechain
1	A	155	ARG	Sidechain
1	A	196	ARG	Sidechain
1	A	20	GLY	Peptide
1	A	21	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	275	ARG	Sidechain
1	A	289	ARG	Sidechain
1	A	302	ARG	Sidechain
1	A	32	ARG	Sidechain
1	A	357	ARG	Sidechain
1	A	364	ARG	Sidechain
1	A	375	ASP	Peptide
1	A	400	LEU	Peptide
1	A	401	SER	Peptide
1	A	46	ALA	Peptide
1	A	47	GLY	Peptide
1	A	64	ARG	Sidechain
1	B	114	ARG	Sidechain
1	B	115	ASP	Peptide
1	B	122	ARG	Sidechain
1	B	141	ARG	Sidechain
1	B	147	GLY	Peptide
1	B	152	ARG	Sidechain
1	B	155	ARG	Sidechain
1	B	196	ARG	Sidechain
1	B	20	GLY	Peptide
1	B	21	ARG	Sidechain
1	B	221	ARG	Sidechain
1	B	236	ARG	Sidechain
1	B	275	ARG	Sidechain
1	B	28	ARG	Sidechain
1	B	289	ARG	Sidechain
1	B	302	ARG	Sidechain
1	B	32	ARG	Sidechain
1	B	357	ARG	Sidechain
1	B	364	ARG	Sidechain
1	B	375	ASP	Peptide
1	B	405	VAL	Peptide
1	B	46	ALA	Peptide
1	B	47	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	64	ARG	Sidechain
1	C	114	ARG	Sidechain
1	C	115	ASP	Peptide
1	C	122	ARG	Sidechain
1	C	128	ARG	Sidechain
1	C	141	ARG	Sidechain
1	C	147	GLY	Peptide
1	C	152[A]	ARG	Sidechain
1	C	155	ARG	Sidechain
1	C	168	ASP	Peptide
1	C	196	ARG	Sidechain
1	C	21	ARG	Sidechain
1	C	236	ARG	Sidechain
1	C	260	ARG	Sidechain
1	C	266	ARG	Sidechain
1	C	275	ARG	Sidechain
1	C	28[A]	ARG	Sidechain
1	C	289	ARG	Sidechain
1	C	32	ARG	Sidechain
1	C	327	ARG	Sidechain
1	C	357	ARG	Sidechain
1	C	364	ARG	Sidechain
1	C	375	ASP	Peptide
1	C	377	ALA	Peptide
1	C	378	ARG	Sidechain
1	C	407	ARG	Sidechain
1	C	46	ALA	Peptide
1	C	47	GLY	Peptide
1	C	48	ALA	Peptide
1	C	64	ARG	Sidechain
1	D	115	ASP	Peptide
1	D	122	ARG	Sidechain
1	D	141[A]	ARG	Sidechain
1	D	147	GLY	Peptide
1	D	152	ARG	Sidechain
1	D	155	ARG	Sidechain
1	D	196	ARG	Sidechain
1	D	21	ARG	Sidechain
1	D	221[A]	ARG	Sidechain
1	D	236	ARG	Sidechain
1	D	260	ARG	Sidechain
1	D	266	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	275	ARG	Sidechain
1	D	289	ARG	Sidechain
1	D	302	ARG	Sidechain
1	D	32	ARG	Sidechain
1	D	357	ARG	Sidechain
1	D	364	ARG	Sidechain
1	D	375	ASP	Peptide
1	D	377	ALA	Peptide
1	D	378	ARG	Sidechain
1	D	407	ARG	Sidechain
1	D	46	ALA	Peptide
1	D	47	GLY	Peptide
1	D	64	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2954	0	2954	25	0
1	B	3034	0	3037	39	0
1	C	3098	0	3110	39	0
1	D	3067	0	3078	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	17	0	0	0	0
4	B	18	0	0	1	0
4	C	15	0	0	1	0
4	D	21	0	0	0	0
All	All	12234	0	12179	126	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 5.

All (126) 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:B:24[B]:GLU:HA	1:B:24[B]:GLU:OE1	1.38	1.19
1:B:375:ASP:HB3	1:B:376:THR:HG23	1.64	0.79
1:A:113:LEU:HD13	1:A:246:PHE:CZ	2.19	0.78
1:B:113:LEU:HD13	1:B:246:PHE:CZ	2.19	0.78
1:A:214:GLU:OE2	1:D:114:ARG:HD3	1.89	0.72
1:D:135:ILE:O	1:D:140:VAL:HG21	1.90	0.72
1:B:24[B]:GLU:OE1	1:B:24[B]:GLU:CA	2.28	0.72
1:D:260:ARG:NH2	1:D:382:PRO:O	2.23	0.72
1:C:135:ILE:O	1:C:140:VAL:HG21	1.89	0.71
1:C:260:ARG:NH2	1:C:382:PRO:O	2.23	0.71
1:C:76:SER:OG	1:C:79:THR:HG22	1.92	0.70
1:C:137:GLN:O	1:C:140:VAL:HG22	1.92	0.69
1:D:137:GLN:O	1:D:140:VAL:HG22	1.93	0.68
1:C:38:ASP:HB2	1:C:169:ASN:ND2	2.10	0.67
1:D:136:ASN:HD21	1:D:160:HIS:H	1.45	0.64
1:B:113:LEU:HD13	1:B:246:PHE:CE2	2.33	0.64
1:A:113:LEU:HD13	1:A:246:PHE:CE2	2.33	0.63
1:C:169:ASN:OD1	4:C:601:HOH:O	2.15	0.63
1:B:81:MET:HE3	1:B:102:ARG:HG2	1.86	0.57
1:D:170:VAL:HG23	1:D:171:THR:HG23	1.87	0.57
1:D:168:ASP:OD1	1:D:170:VAL:HG22	2.06	0.56
1:B:310:TRP:CH2	1:B:405:VAL:HG22	2.41	0.56
1:A:268:LEU:HD22	1:A:385:ALA:HB2	1.89	0.55
1:A:260:ARG:NH2	1:A:381:ARG:O	2.39	0.55
1:B:260:ARG:NH2	1:B:381:ARG:O	2.40	0.55
1:C:196:ARG:HD3	1:D:124:GLU:HG2	1.89	0.55
1:C:306:LEU:HD21	1:C:367:ALA:HB2	1.91	0.53
1:C:191:THR:CG2	1:C:203:ALA:CB	2.88	0.51
1:A:308:ASP:OD1	1:A:308:ASP:N	2.43	0.51
1:B:141:ARG:NH2	1:B:179:GLY:O	2.44	0.51
1:B:315:PHE:CZ	1:B:359:THR:HG23	2.46	0.50
1:C:141:ARG:NH2	1:C:179:GLY:O	2.44	0.50
1:C:304:LEU:HD23	1:D:304:LEU:HD23	1.92	0.50
1:D:144:VAL:HG22	1:D:163:LEU:HD11	1.93	0.50
1:B:292[B]:GLN:HG3	1:B:293[B]:VAL:N	2.23	0.50
1:C:169:ASN:ND2	1:C:169:ASN:C	2.70	0.50
1:C:287:LEU:N	1:C:288:PRO:CD	2.75	0.49
1:D:191:THR:CG2	1:D:203:ALA:CB	2.90	0.49
1:A:315:PHE:CZ	1:A:359:THR:HG23	2.47	0.49
1:B:40:LYS:HD3	1:B:254:TRP:CE3	2.47	0.49
1:A:214:GLU:OE2	1:D:114:ARG:CD	2.60	0.48
1:B:144:VAL:HG22	1:B:163:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HG22	1:A:163:LEU:HD11	1.95	0.48
1:C:78:PRO:HG3	1:C:146:PRO:HG2	1.95	0.48
1:C:315:PHE:CZ	1:C:359:THR:HG23	2.49	0.47
1:D:287:LEU:N	1:D:288:PRO:CD	2.77	0.47
1:D:315:PHE:CZ	1:D:359:THR:HG23	2.49	0.47
1:C:87:ASP:O	1:C:87:ASP:OD1	2.32	0.47
1:C:261[B]:GLN:O	1:C:265:GLU:HG2	2.14	0.47
1:A:40:LYS:HD3	1:A:254:TRP:CE3	2.50	0.47
1:B:287:LEU:N	1:B:288:PRO:CD	2.78	0.47
1:A:287:LEU:N	1:A:288:PRO:CD	2.78	0.47
1:A:293:VAL:HG11	1:A:319:ILE:HD11	1.98	0.46
1:C:280:VAL:HG12	1:C:280:VAL:O	2.16	0.46
1:C:261[A]:GLN:O	1:C:265:GLU:HG2	2.15	0.46
1:D:191:THR:CG2	1:D:203:ALA:HB1	2.46	0.46
1:C:144:VAL:HG22	1:C:163:LEU:HD11	1.97	0.45
1:D:61:GLU:OE1	1:D:64:ARG:NH1	2.47	0.45
1:C:315:PHE:CE2	1:C:359:THR:HG23	2.51	0.45
1:C:191:THR:CG2	1:C:203:ALA:HB1	2.46	0.45
1:D:315:PHE:CE2	1:D:359:THR:HG23	2.52	0.45
1:C:145:ASN:HD22	1:C:184:MET:HE1	1.82	0.45
1:D:280:VAL:HG12	1:D:280:VAL:O	2.17	0.45
1:B:81:MET:HG3	1:B:105:GLN:NE2	2.32	0.44
1:C:155:ARG:HH21	1:C:163:LEU:HD23	1.82	0.44
1:B:375:ASP:C	1:B:376:THR:HG1	2.23	0.44
1:B:48:ALA:HB2	1:B:384:GLU:OE1	2.17	0.44
1:B:293[B]:VAL:HG11	1:B:319:ILE:HD11	1.98	0.44
1:B:290:GLU:O	1:B:294[A]:ILE:HD13	2.18	0.44
1:C:192:ARG:NH2	1:D:124:GLU:O	2.51	0.44
1:A:290:GLU:O	1:A:294:ILE:HD13	2.17	0.43
1:D:362:LEU:C	1:D:362:LEU:HD23	2.43	0.43
1:B:144:VAL:HA	1:B:184:MET:HE3	2.00	0.43
1:A:99:THR:O	1:A:103:GLN:HG3	2.18	0.43
1:C:289:ARG:HD2	1:C:293:VAL:HG23	2.01	0.43
1:B:293[A]:VAL:HG11	1:B:319:ILE:HD11	1.99	0.43
1:C:140:VAL:HG23	1:C:161:ALA:HB1	2.01	0.43
1:C:362:LEU:C	1:C:362:LEU:HD23	2.44	0.43
1:C:401:SER:O	1:C:405:VAL:HG23	2.18	0.43
1:D:362:LEU:HD23	1:D:362:LEU:O	2.19	0.43
1:B:310:TRP:CH2	1:B:399:PRO:O	2.71	0.42
1:B:289:ARG:HD2	1:B:293[A]:VAL:HG23	2.02	0.42
1:C:77:TRP:N	1:C:78:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ASN:O	1:C:170:VAL:HB	2.18	0.42
1:A:315:PHE:CE2	1:A:359:THR:HG23	2.54	0.42
1:B:77:TRP:N	1:B:78:PRO:CD	2.83	0.42
1:B:257:GLU:N	1:B:258:PRO:CD	2.83	0.42
1:A:398:ALA:N	1:A:399:PRO:CD	2.83	0.42
1:C:398:ALA:N	1:C:399:PRO:CD	2.83	0.42
1:D:398:ALA:N	1:D:399:PRO:CD	2.83	0.42
1:D:401:SER:O	1:D:405:VAL:HG23	2.19	0.42
1:A:257:GLU:N	1:A:258:PRO:CD	2.82	0.42
1:B:315:PHE:CE2	1:B:359:THR:HG23	2.54	0.42
1:B:362:LEU:HD23	1:B:362:LEU:C	2.45	0.42
1:D:40:LYS:HD3	1:D:254:TRP:CE3	2.55	0.42
1:B:98:VAL:HG11	1:C:114:ARG:HD3	2.02	0.42
1:B:289:ARG:HD2	1:B:293[B]:VAL:HG23	2.02	0.42
1:A:205:HIS:O	1:A:205:HIS:ND1	2.53	0.42
1:A:362:LEU:C	1:A:362:LEU:HD23	2.45	0.42
1:B:398:ALA:N	1:B:399:PRO:CD	2.83	0.42
1:A:77:TRP:N	1:A:78:PRO:CD	2.83	0.42
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.95	0.41
1:B:255:ALA:O	1:B:258:PRO:HD2	2.20	0.41
1:B:327:ARG:NH1	4:B:601:HOH:O	2.47	0.41
1:C:257:GLU:N	1:C:258:PRO:CD	2.83	0.41
1:D:257:GLU:N	1:D:258:PRO:CD	2.84	0.41
1:A:289:ARG:HD2	1:A:293:VAL:HG23	2.01	0.41
1:B:362:LEU:HD23	1:B:362:LEU:O	2.21	0.41
1:C:362:LEU:HD23	1:C:362:LEU:O	2.20	0.41
1:D:144:VAL:HA	1:D:184:MET:HE3	2.02	0.41
1:B:57:GLU:O	1:B:61:GLU:HG3	2.21	0.41
1:B:81:MET:CE	1:B:102:ARG:HG2	2.50	0.41
1:C:26[B]:HIS:O	1:C:26[B]:HIS:ND1	2.54	0.41
1:C:144:VAL:HA	1:C:184:MET:HE3	2.02	0.41
1:C:169:ASN:C	1:C:171:THR:H	2.28	0.41
1:D:205:HIS:O	1:D:205:HIS:ND1	2.54	0.41
1:A:144:VAL:HA	1:A:184:MET:HE3	2.02	0.40
1:B:310:TRP:CZ3	1:B:399:PRO:O	2.74	0.40
1:D:289:ARG:HD2	1:D:293:VAL:HG23	2.02	0.40
1:A:57:GLU:O	1:A:61:GLU:HG3	2.20	0.40
1:B:92:VAL:HB	1:B:218:LEU:HB3	2.03	0.40
1:C:408:PHE:C	1:C:409:LEU:HD12	2.47	0.40
1:B:205:HIS:O	1:B:205:HIS:ND1	2.54	0.40
1:A:255:ALA:O	1:A:258:PRO:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:TRP:N	1:D:78:PRO:CD	2.83	0.40
1:B:236:ARG:HH11	1:B:236:ARG:HG2	1.86	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	376/416 (90%)	364 (97%)	12 (3%)	0	100	100
1	B	386/416 (93%)	373 (97%)	12 (3%)	1 (0%)	36	44
1	C	394/416 (95%)	378 (96%)	13 (3%)	3 (1%)	16	18
1	D	390/416 (94%)	374 (96%)	15 (4%)	1 (0%)	36	44
All	All	1546/1664 (93%)	1489 (96%)	52 (3%)	5 (0%)	36	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	VAL
1	C	169	ASN
1	D	48	ALA
1	C	48	ALA
1	C	170	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	304/335 (91%)	284 (93%)	20 (7%)	15	19
1	B	313/335 (93%)	293 (94%)	20 (6%)	16	21
1	C	319/335 (95%)	294 (92%)	25 (8%)	11	13
1	D	316/335 (94%)	289 (92%)	27 (8%)	10	11
All	All	1252/1340 (93%)	1160 (93%)	92 (7%)	13	15

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	28	ARG
1	A	35	SER
1	A	93	LEU
1	A	118	THR
1	A	128	ARG
1	A	137	GLN
1	A	152	ARG
1	A	189	ILE
1	A	242	LEU
1	A	268	LEU
1	A	275	ARG
1	A	304	LEU
1	A	308	ASP
1	A	334	LYS
1	A	349	ASN
1	A	369	ASN
1	A	372	THR
1	A	373	LEU
1	A	374	LYS
1	B	21	ARG
1	B	22	LEU
1	B	28	ARG
1	B	35	SER
1	B	93	LEU
1	B	104	GLN
1	B	118	THR
1	B	128	ARG
1	B	137	GLN
1	B	189	ILE
1	B	196	ARG

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Mol	Chain	Res	Type
1	B	242	LEU
1	B	244	LYS
1	B	275	ARG
1	B	308	ASP
1	B	334	LYS
1	B	372	THR
1	B	373	LEU
1	B	405	VAL
1	B	406	VAL
1	C	35	SER
1	C	93	LEU
1	C	101	GLU
1	C	118	THR
1	C	122	ARG
1	C	128	ARG
1	C	152[A]	ARG
1	C	152[B]	ARG
1	C	165	VAL
1	C	189	ILE
1	C	191	THR
1	C	224	GLU
1	C	233	LEU
1	C	242	LEU
1	C	244	LYS
1	C	260	ARG
1	C	261[A]	GLN
1	C	261[B]	GLN
1	C	285	GLU
1	C	292	GLN
1	C	308	ASP
1	C	372	THR
1	C	373	LEU
1	C	379	LEU
1	C	404	VAL
1	D	22	LEU
1	D	23	GLU
1	D	35	SER
1	D	61	GLU
1	D	93	LEU
1	D	101	GLU
1	D	105	GLN
1	D	118	THR

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Mol	Chain	Res	Type
1	D	122	ARG
1	D	124	GLU
1	D	128	ARG
1	D	132	LEU
1	D	141[A]	ARG
1	D	141[B]	ARG
1	D	189	ILE
1	D	191	THR
1	D	233	LEU
1	D	244	LYS
1	D	260	ARG
1	D	292	GLN
1	D	308	ASP
1	D	334	LYS
1	D	357	ARG
1	D	372	THR
1	D	373	LEU
1	D	378	ARG
1	D	404	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	162	GLN
1	A	169	ASN
1	A	281	GLN
1	A	300	GLN
1	A	340	HIS
1	A	370	GLN
1	A	395	GLN
1	B	105	GLN
1	B	126	GLN
1	B	137	GLN
1	B	162	GLN
1	B	169	ASN
1	B	281	GLN
1	B	300	GLN
1	B	340	HIS
1	B	370	GLN
1	B	395	GLN
1	C	105	GLN

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Mol	Chain	Res	Type
1	C	145	ASN
1	C	157	HIS
1	C	169	ASN
1	C	300	GLN
1	C	340	HIS
1	C	370	GLN
1	D	103	GLN
1	D	136	ASN
1	D	162	GLN
1	D	169	ASN
1	D	292	GLN
1	D	300	GLN
1	D	337	GLN
1	D	340	HIS
1	D	354	GLN
1	D	395	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 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

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	380/416 (91%)	0.47	17 (4%)	38	35	33, 53, 82, 117	0
1	B	384/416 (92%)	0.53	19 (4%)	35	32	19, 54, 87, 146	6 (1%)
1	C	389/416 (93%)	0.87	43 (11%)	10	8	24, 63, 94, 121	7 (1%)
1	D	389/416 (93%)	0.57	26 (6%)	24	20	30, 56, 82, 124	3 (0%)
All	All	1542/1664 (92%)	0.61	105 (6%)	23	20	19, 56, 89, 146	16 (1%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	ALA	7.3
1	B	406	VAL	6.8
1	C	26[A]	HIS	6.3
1	C	170	VAL	6.2
1	B	380	ILE	5.8
1	A	380	ILE	5.6
1	B	376	THR	4.9
1	D	154	ALA	4.5
1	D	379	LEU	4.3
1	D	221[A]	ARG	4.1
1	C	181	ALA	4.0
1	C	246	PHE	4.0
1	C	379	LEU	4.0
1	B	371	ALA	3.8
1	C	139	ALA	3.8
1	D	141[A]	ARG	3.8
1	A	371	ALA	3.7
1	D	158	ALA	3.7
1	C	377	ALA	3.6
1	C	169	ASN	3.6
1	A	376	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	369	ASN	3.6
1	B	373	LEU	3.5
1	B	246	PHE	3.5
1	D	167	PRO	3.4
1	C	152[A]	ARG	3.4
1	D	377	ALA	3.3
1	B	403	HIS	3.3
1	C	144	VAL	3.3
1	C	115	ASP	3.2
1	C	163	LEU	3.2
1	B	405	VAL	3.2
1	B	402	ALA	3.1
1	D	188	ALA	3.1
1	C	250	LEU	3.1
1	D	22	LEU	3.0
1	C	164	THR	3.0
1	C	175	GLN	3.0
1	C	176	ILE	3.0
1	C	22	LEU	2.9
1	D	115	ASP	2.9
1	C	143	ILE	2.9
1	C	167	PRO	2.8
1	C	127	LEU	2.8
1	A	115	ASP	2.8
1	C	123	CYS	2.8
1	C	178	SER	2.7
1	D	164	THR	2.7
1	C	165	VAL	2.7
1	B	372	THR	2.7
1	C	387	ALA	2.7
1	D	155	ARG	2.7
1	C	261[A]	GLN	2.7
1	B	167	PRO	2.6
1	A	373	LEU	2.6
1	A	292	GLN	2.6
1	C	386	ALA	2.6
1	A	167	PRO	2.6
1	A	400	LEU	2.6
1	D	127	LEU	2.6
1	B	369	ASN	2.6
1	D	224	GLU	2.5
1	B	404	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	276	ALA	2.5
1	D	345	PRO	2.5
1	B	139	ALA	2.5
1	B	162	GLN	2.5
1	C	172	ILE	2.4
1	B	400	LEU	2.4
1	D	189	ILE	2.4
1	D	246	PHE	2.4
1	D	335	ALA	2.4
1	C	200	GLU	2.4
1	C	238	SER	2.4
1	D	244	LYS	2.4
1	D	44	TYR	2.4
1	C	129	PHE	2.4
1	D	179	GLY	2.4
1	A	22	LEU	2.4
1	D	169	ASN	2.4
1	C	197	LEU	2.3
1	D	228	TYR	2.3
1	A	139	ALA	2.3
1	B	69	LYS	2.3
1	A	246	PHE	2.3
1	A	401	SER	2.3
1	C	157	HIS	2.3
1	A	384	GLU	2.2
1	C	380	ILE	2.2
1	B	384	GLU	2.2
1	D	165	VAL	2.2
1	C	48	ALA	2.2
1	C	173	PHE	2.1
1	B	370	GLN	2.1
1	D	376	THR	2.1
1	C	84	PHE	2.1
1	C	58	GLN	2.1
1	A	86	ALA	2.1
1	C	192	ARG	2.1
1	A	166	TYR	2.1
1	C	166	TYR	2.1
1	C	265	GLU	2.0
1	D	101	GLU	2.0
1	C	194	GLN	2.0
1	C	235	GLN	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](#)

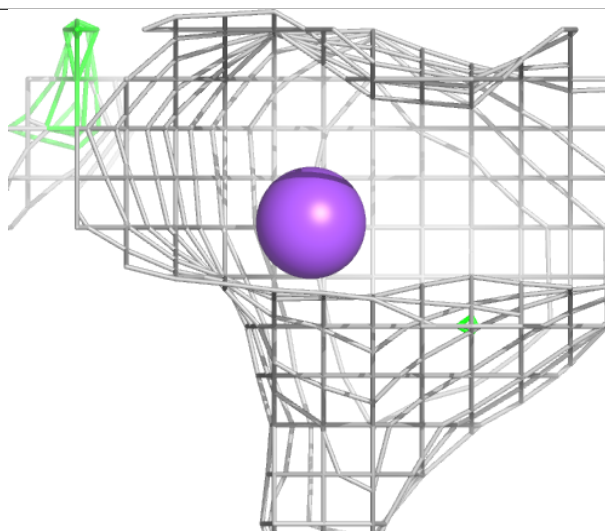
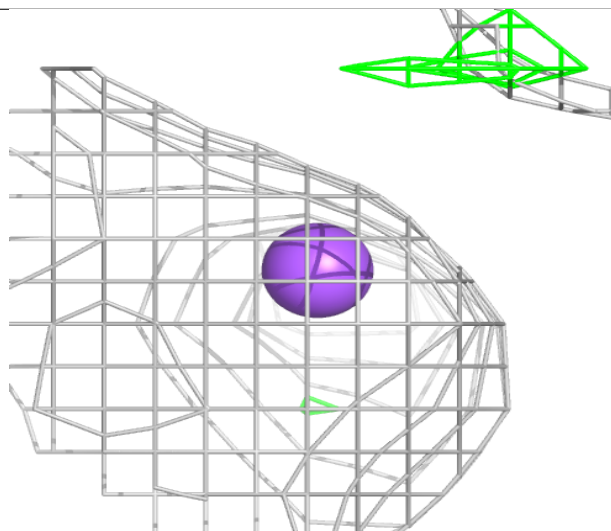
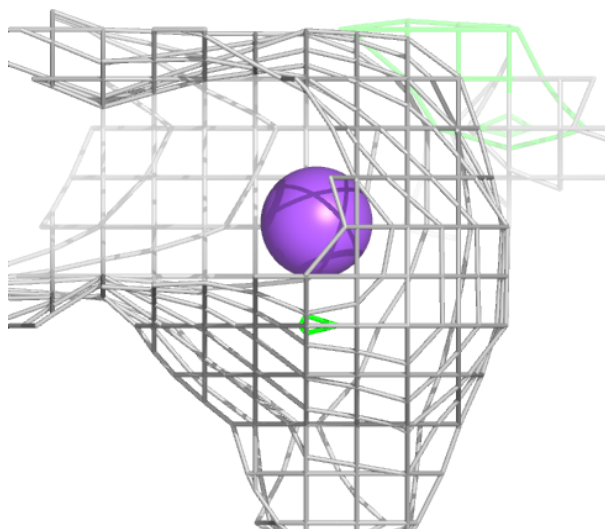
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	A	502	1/1	0.82	0.19	64,64,64,64	0
2	NA	A	501	1/1	0.91	0.13	51,51,51,51	0
3	CL	B	503	1/1	0.91	0.09	51,51,51,51	0
2	NA	B	501	1/1	0.94	0.10	46,46,46,46	0
3	CL	C	501	1/1	0.95	0.06	51,51,51,51	0
2	NA	B	502	1/1	0.96	0.14	51,51,51,51	0
3	CL	A	505	1/1	0.97	0.06	48,48,48,48	0
3	CL	A	503	1/1	0.97	0.07	51,51,51,51	0
3	CL	A	504	1/1	0.97	0.07	62,62,62,62	0
3	CL	D	501	1/1	0.98	0.09	44,44,44,44	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.

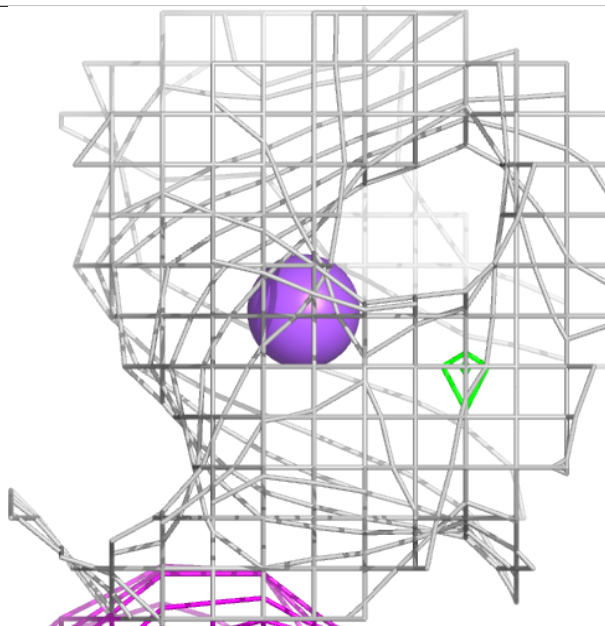
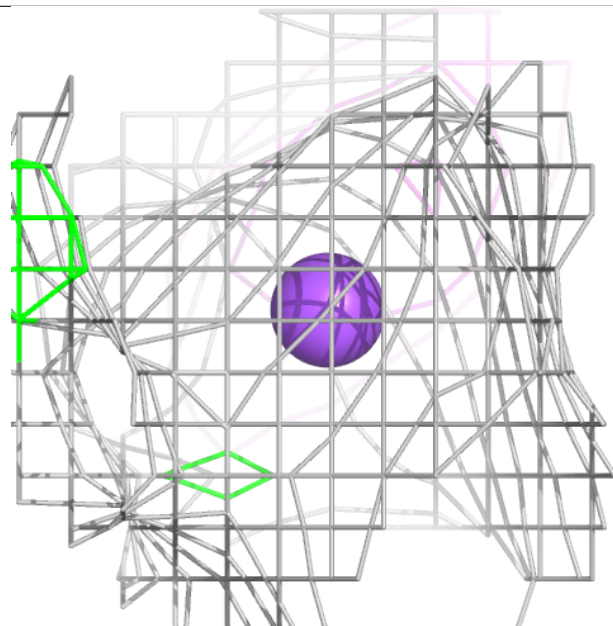
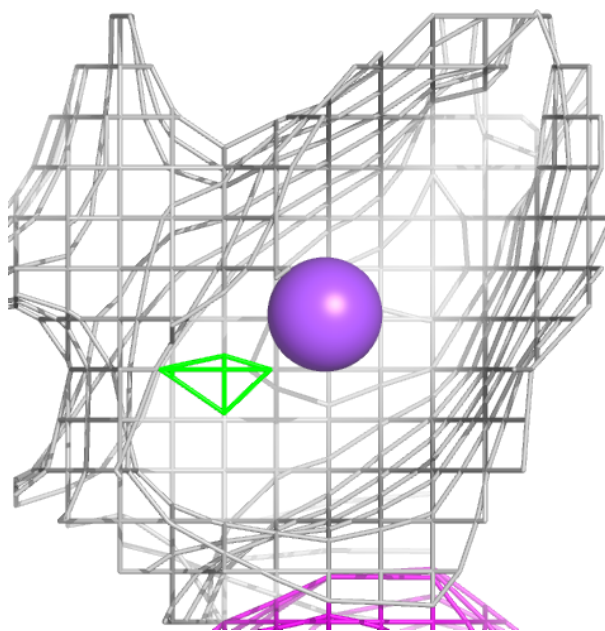
Electron density around NA A 502:

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



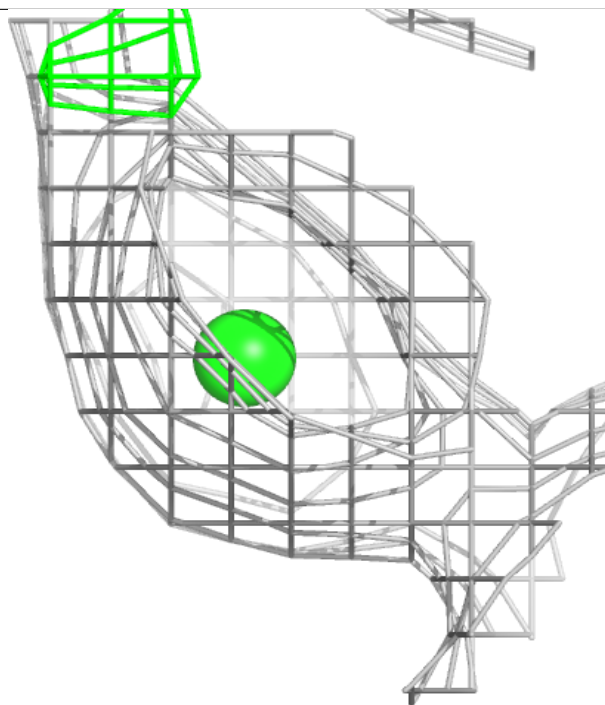
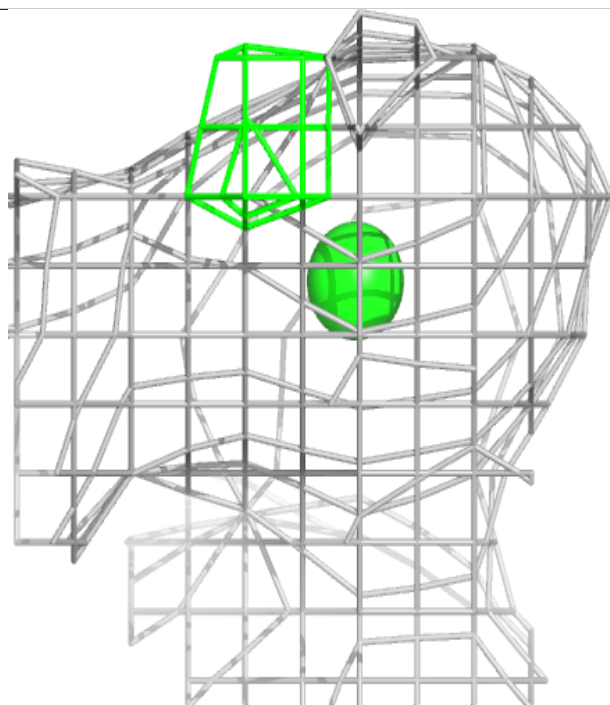
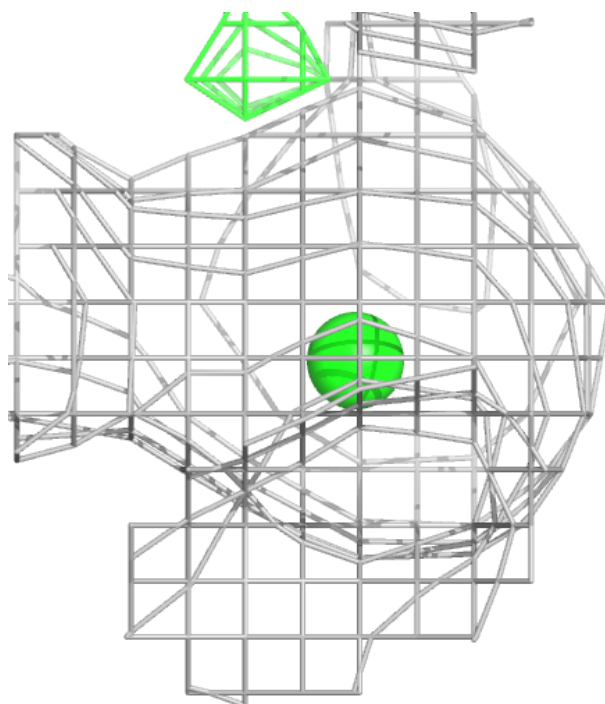
Electron density around NA A 501:

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



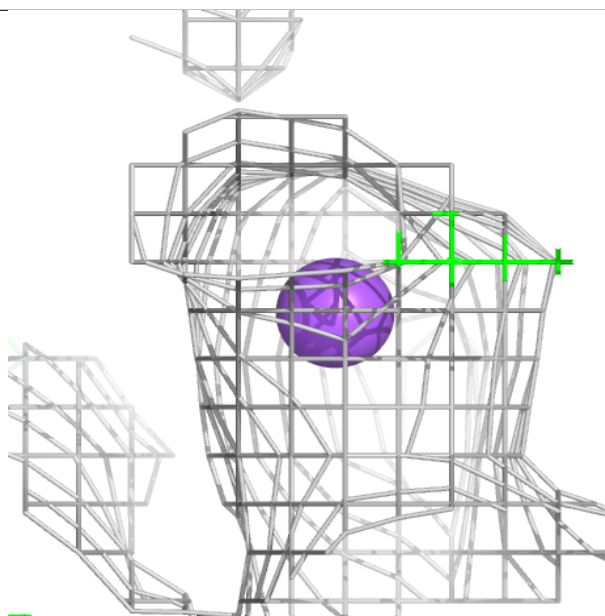
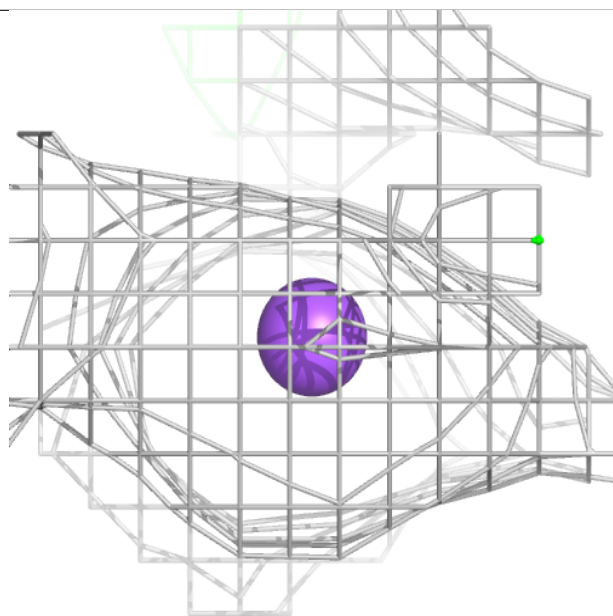
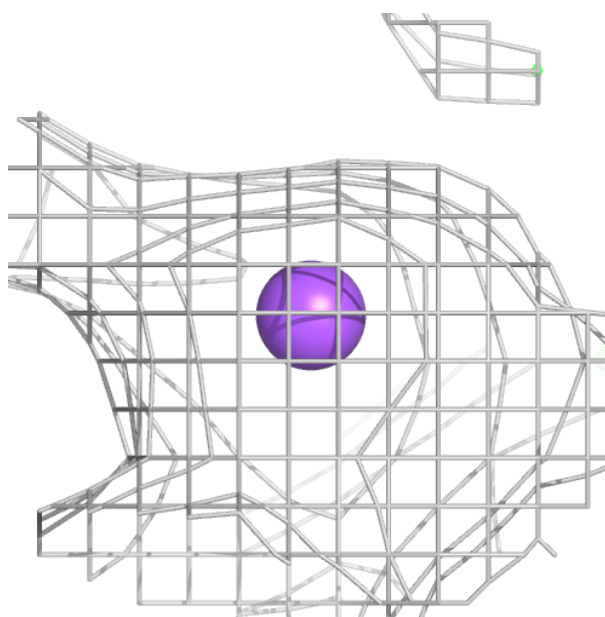
Electron density around CL B 503:

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



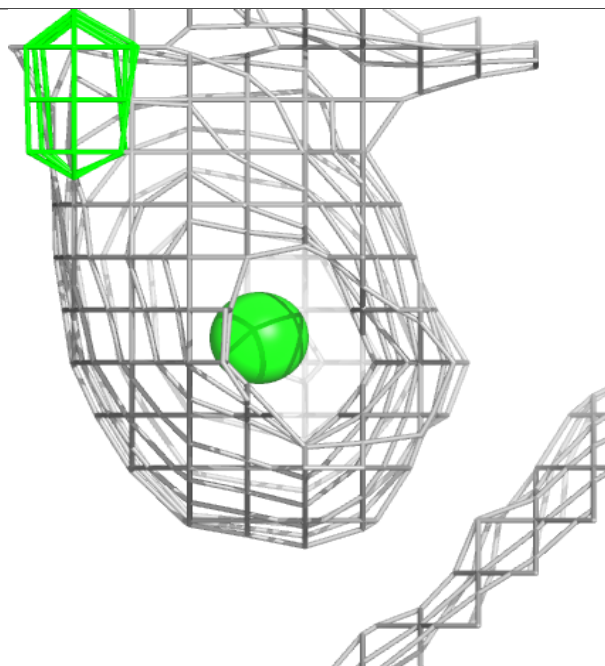
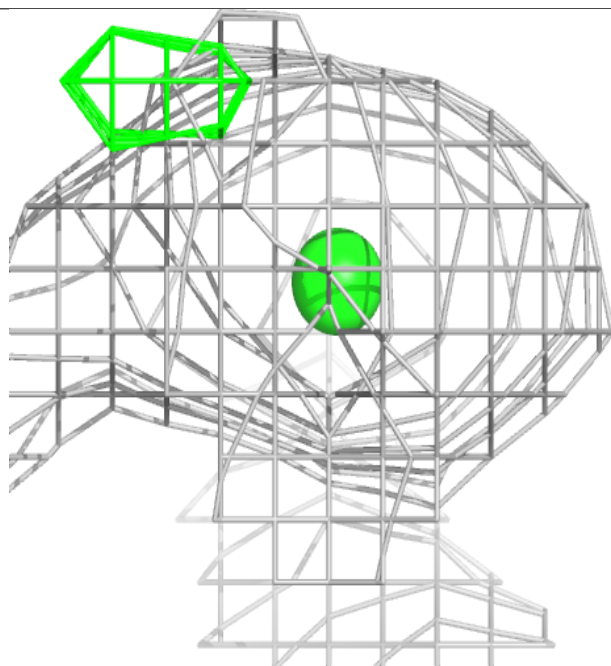
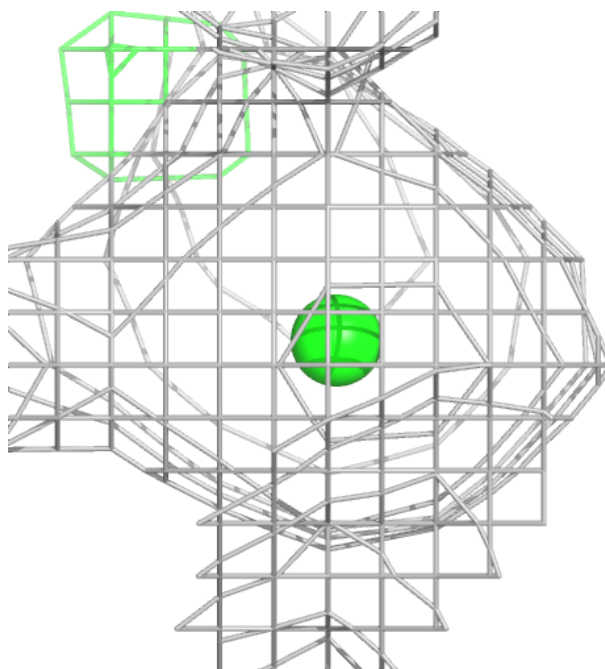
Electron density around NA B 501:

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



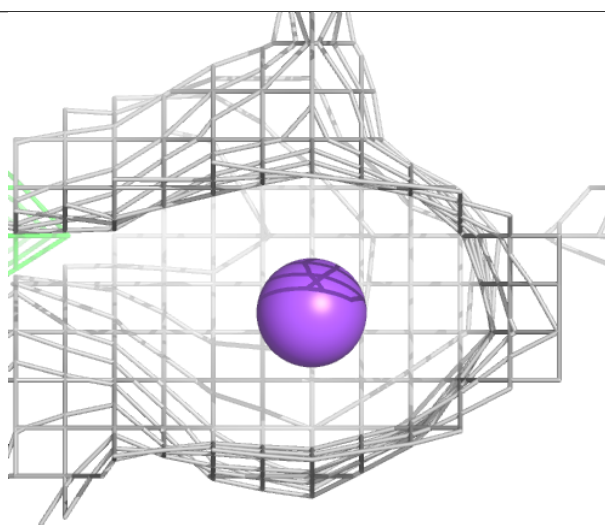
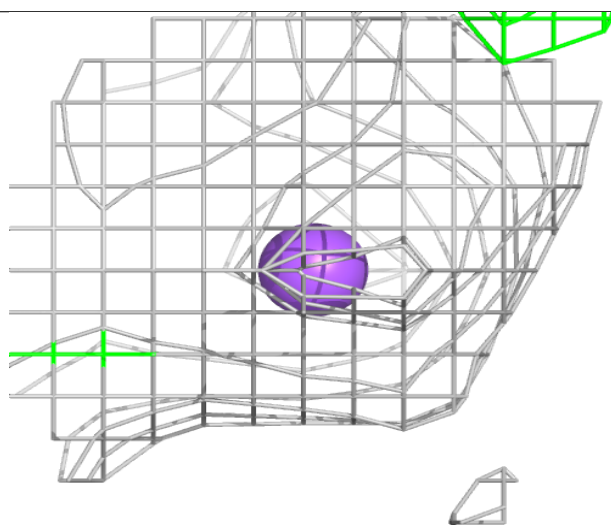
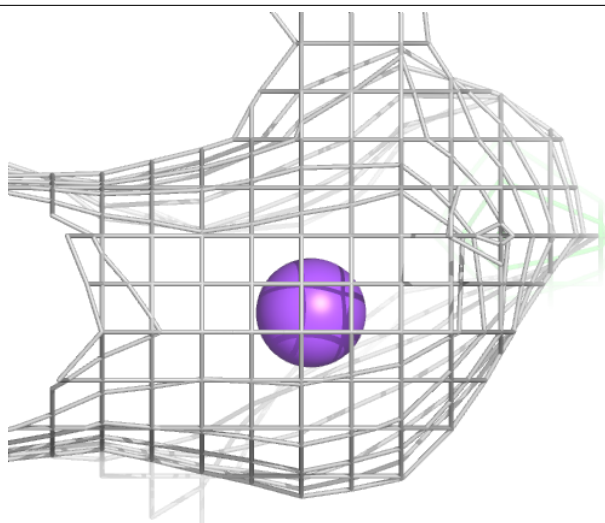
Electron density around CL C 501:

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



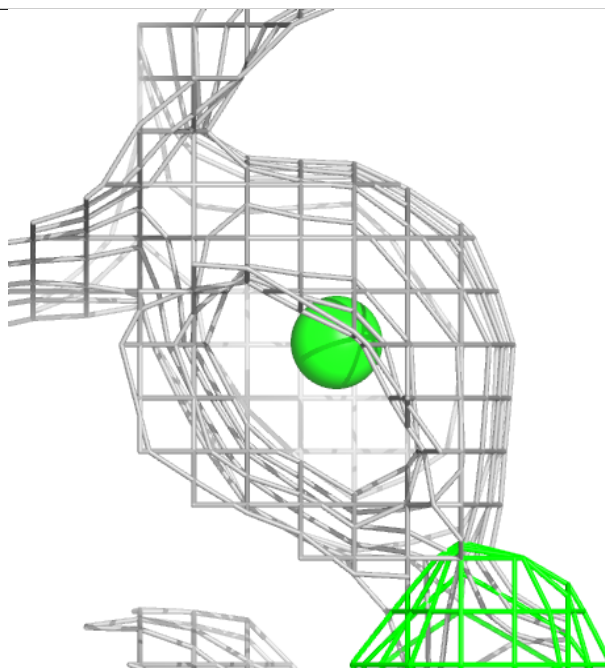
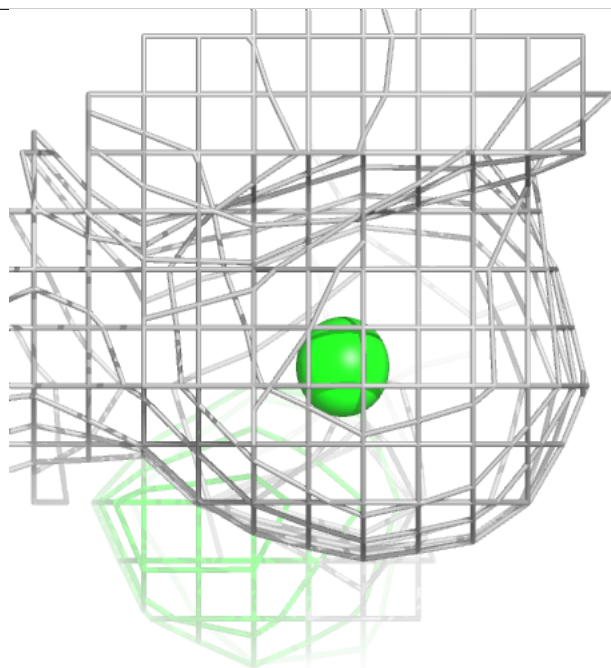
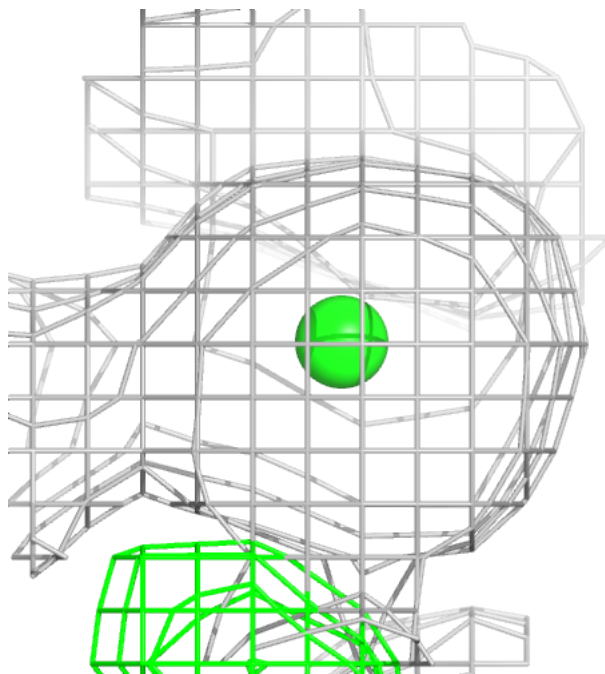
Electron density around NA B 502:

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



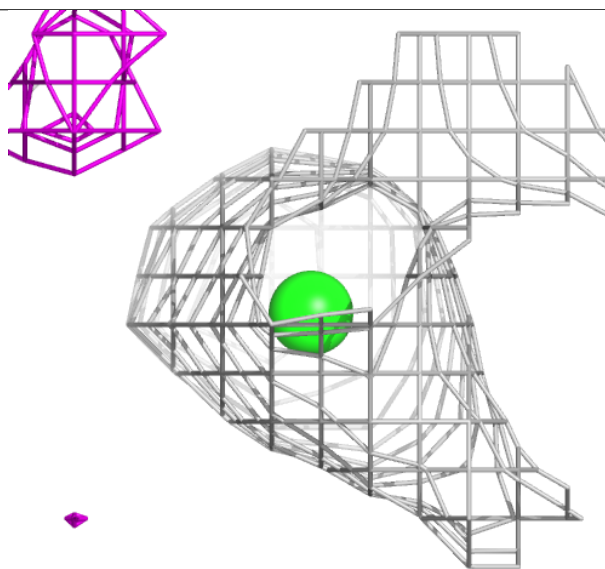
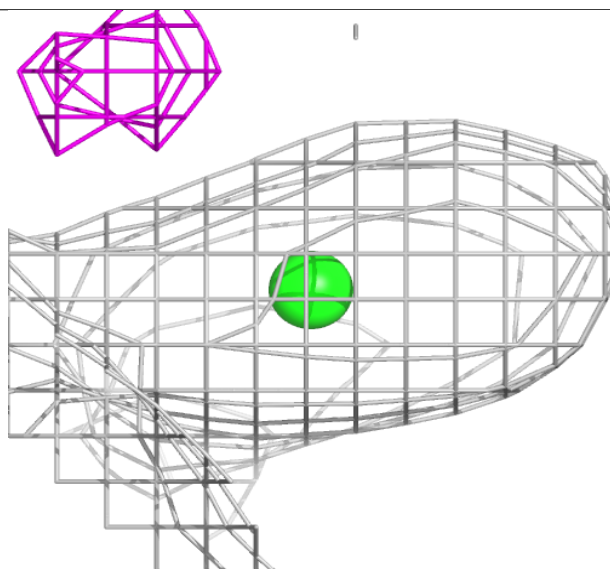
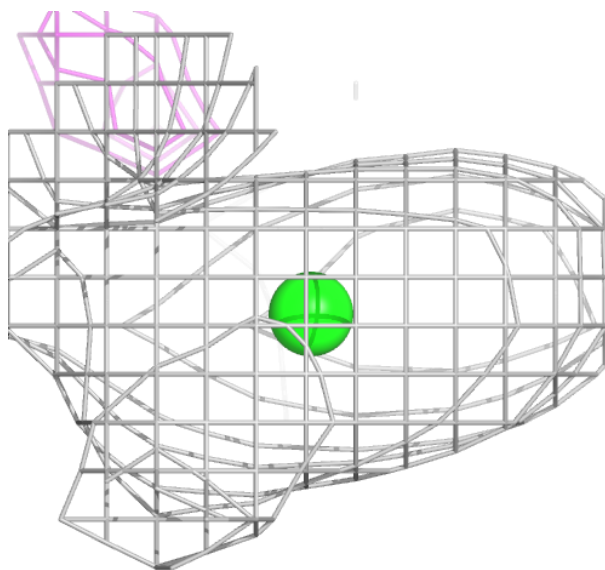
Electron density around CL A 505:

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



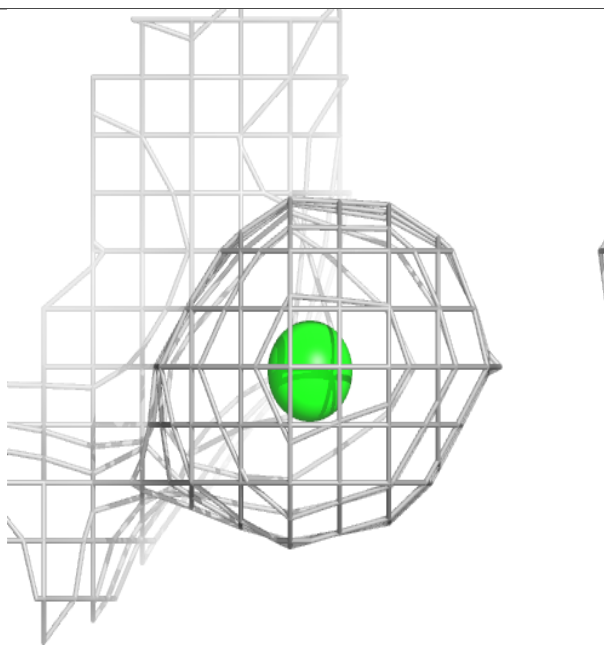
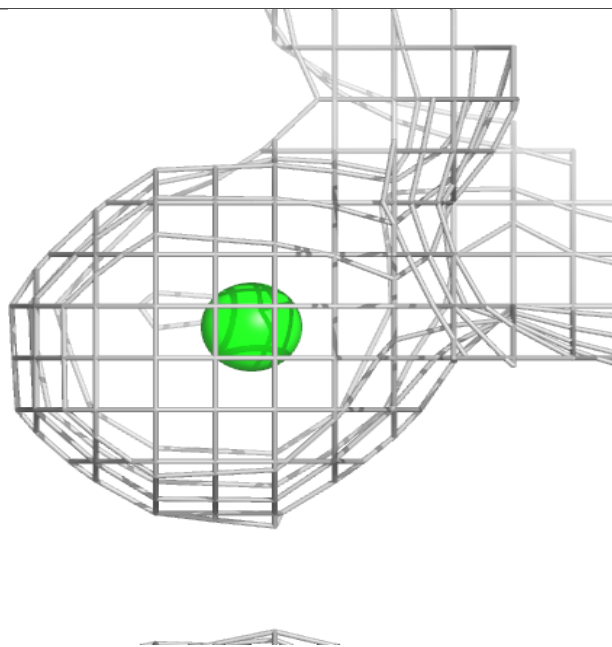
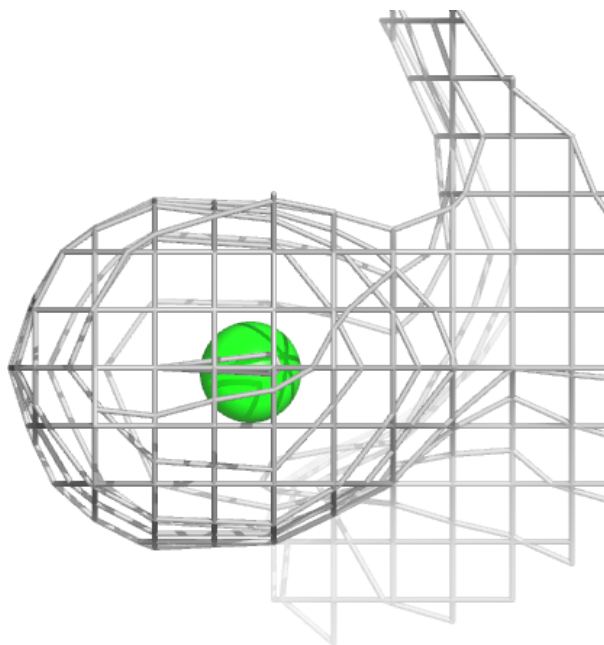
Electron density around CL A 503:

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



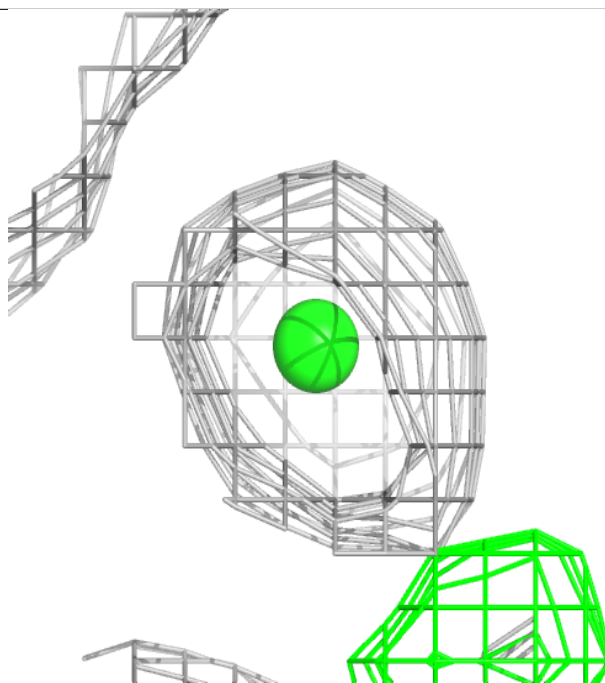
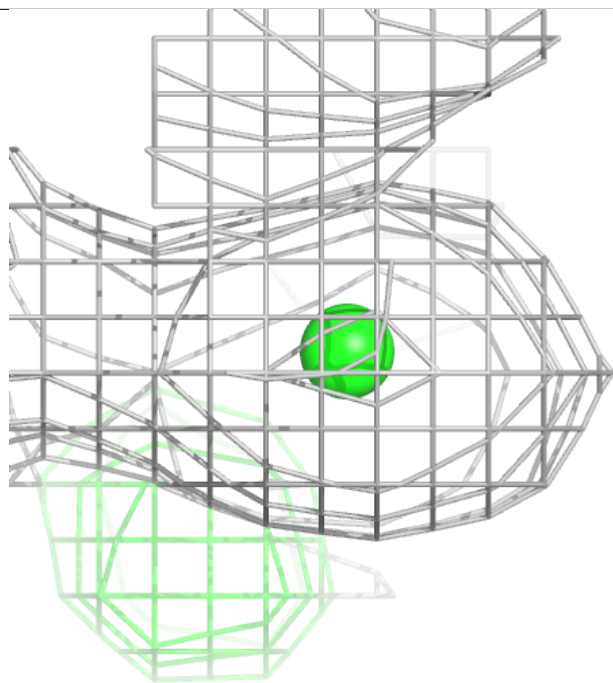
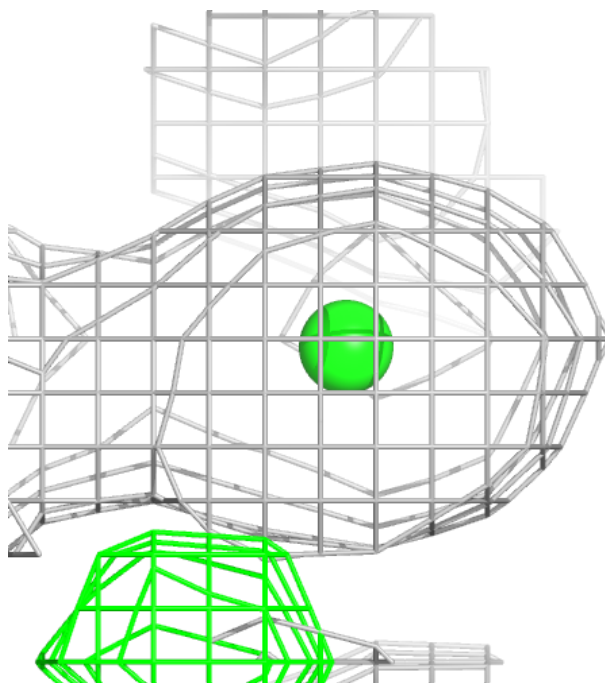
Electron density around CL A 504:

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



Electron density around CL D 501:

$2mF_o-DF_c$ (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.