



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2025 – 10:10 am BST

PDB ID : 9FID / pdb\_00009fid  
Title : X-ray structure of furin (PCSK3) in complex with the PC1/3 (PCSK1) prodomain mutant R78K,R80A  
Authors : Dahms, S.O.; Brandstetter, H.  
Deposited on : 2024-05-29  
Resolution : 2.40 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

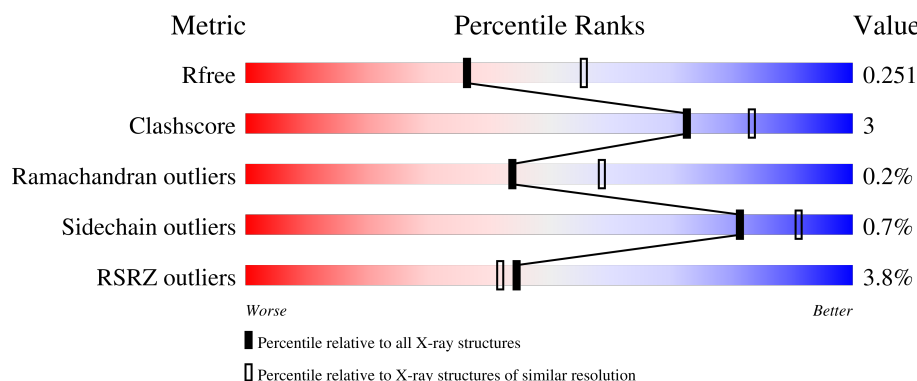
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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	482	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>•</div> </div> </div>
1	B	482	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>
1	C	482	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
2	D	95	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>6%</div> <div>25%</div> </div> </div>
2	E	95	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>5%</div> <div>26%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	95	<div><div></div><div>14%</div><div>73%</div><div>•</div><div>24%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24133 atoms, of which 11681 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 Furin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	H	N	O	S	251	0	0
			6866	2183	3341	631	697	14			
1	B	465	Total	C	H	N	O	S	292	0	0
			6919	2199	3367	636	703	14			
1	C	460	Total	C	H	N	O	S	231	0	0
			6854	2180	3335	630	695	14			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	expression tag	UNP P09958
A	576	GLY	-	expression tag	UNP P09958
A	577	SER	-	expression tag	UNP P09958
A	578	LEU	-	expression tag	UNP P09958
A	579	VAL	-	expression tag	UNP P09958
A	580	PRO	-	expression tag	UNP P09958
A	581	ARG	-	expression tag	UNP P09958
A	582	GLY	-	expression tag	UNP P09958
A	583	SER	-	expression tag	UNP P09958
A	584	HIS	-	expression tag	UNP P09958
A	585	HIS	-	expression tag	UNP P09958
A	586	HIS	-	expression tag	UNP P09958
A	587	HIS	-	expression tag	UNP P09958
A	588	HIS	-	expression tag	UNP P09958
A	589	HIS	-	expression tag	UNP P09958
B	575	SER	-	expression tag	UNP P09958
B	576	GLY	-	expression tag	UNP P09958
B	577	SER	-	expression tag	UNP P09958
B	578	LEU	-	expression tag	UNP P09958
B	579	VAL	-	expression tag	UNP P09958
B	580	PRO	-	expression tag	UNP P09958
B	581	ARG	-	expression tag	UNP P09958
B	582	GLY	-	expression tag	UNP P09958

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Chain	Residue	Modelled	Actual	Comment	Reference
B	583	SER	-	expression tag	UNP P09958
B	584	HIS	-	expression tag	UNP P09958
B	585	HIS	-	expression tag	UNP P09958
B	586	HIS	-	expression tag	UNP P09958
B	587	HIS	-	expression tag	UNP P09958
B	588	HIS	-	expression tag	UNP P09958
B	589	HIS	-	expression tag	UNP P09958
C	575	SER	-	expression tag	UNP P09958
C	576	GLY	-	expression tag	UNP P09958
C	577	SER	-	expression tag	UNP P09958
C	578	LEU	-	expression tag	UNP P09958
C	579	VAL	-	expression tag	UNP P09958
C	580	PRO	-	expression tag	UNP P09958
C	581	ARG	-	expression tag	UNP P09958
C	582	GLY	-	expression tag	UNP P09958
C	583	SER	-	expression tag	UNP P09958
C	584	HIS	-	expression tag	UNP P09958
C	585	HIS	-	expression tag	UNP P09958
C	586	HIS	-	expression tag	UNP P09958
C	587	HIS	-	expression tag	UNP P09958
C	588	HIS	-	expression tag	UNP P09958
C	589	HIS	-	expression tag	UNP P09958

- Molecule 2 is a protein called Neuroendocrine convertase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	71	Total	C	H	N	O	94	0	0
			1126	367	546	101	112			
2	E	70	Total	C	H	N	O	115	0	0
			1116	364	541	100	111			
2	F	72	Total	C	H	N	O	108	0	0
			1137	370	551	102	114			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	16	MET	-	initiating methionine	UNP P29120
D	17	GLY	-	expression tag	UNP P29120
D	18	HIS	-	expression tag	UNP P29120
D	19	HIS	-	expression tag	UNP P29120
D	20	HIS	-	expression tag	UNP P29120
D	21	HIS	-	expression tag	UNP P29120

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	HIS	-	expression tag	UNP P29120
D	23	HIS	-	expression tag	UNP P29120
D	24	SER	-	expression tag	UNP P29120
D	25	GLY	-	expression tag	UNP P29120
D	26	HIS	-	expression tag	UNP P29120
D	27	MET	-	expression tag	UNP P29120
D	78	LYS	ARG	engineered mutation	UNP P29120
D	80	ALA	ARG	engineered mutation	UNP P29120
E	16	MET	-	initiating methionine	UNP P29120
E	17	GLY	-	expression tag	UNP P29120
E	18	HIS	-	expression tag	UNP P29120
E	19	HIS	-	expression tag	UNP P29120
E	20	HIS	-	expression tag	UNP P29120
E	21	HIS	-	expression tag	UNP P29120
E	22	HIS	-	expression tag	UNP P29120
E	23	HIS	-	expression tag	UNP P29120
E	24	SER	-	expression tag	UNP P29120
E	25	GLY	-	expression tag	UNP P29120
E	26	HIS	-	expression tag	UNP P29120
E	27	MET	-	expression tag	UNP P29120
E	78	LYS	ARG	engineered mutation	UNP P29120
E	80	ALA	ARG	engineered mutation	UNP P29120
F	16	MET	-	initiating methionine	UNP P29120
F	17	GLY	-	expression tag	UNP P29120
F	18	HIS	-	expression tag	UNP P29120
F	19	HIS	-	expression tag	UNP P29120
F	20	HIS	-	expression tag	UNP P29120
F	21	HIS	-	expression tag	UNP P29120
F	22	HIS	-	expression tag	UNP P29120
F	23	HIS	-	expression tag	UNP P29120
F	24	SER	-	expression tag	UNP P29120
F	25	GLY	-	expression tag	UNP P29120
F	26	HIS	-	expression tag	UNP P29120
F	27	MET	-	expression tag	UNP P29120
F	78	LYS	ARG	engineered mutation	UNP P29120
F	80	ALA	ARG	engineered mutation	UNP P29120

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Ca 2	0	0
3	C	2	Total 2	Ca 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	B	1	Total 1	Na 1	0	0
4	C	1	Total 1	Na 1	0	0

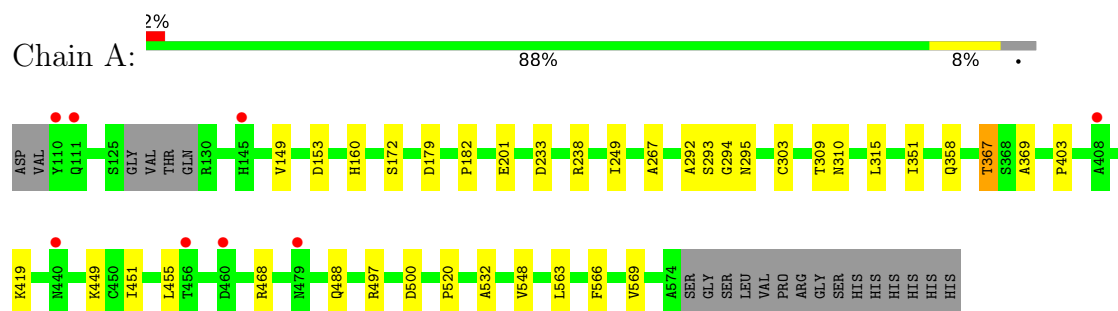
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total 36	O 36	0	0
5	D	3	Total 3	O 3	0	0
5	B	26	Total 26	O 26	0	0
5	E	1	Total 1	O 1	0	0
5	C	37	Total 37	O 37	0	0
5	F	3	Total 3	O 3	0	0

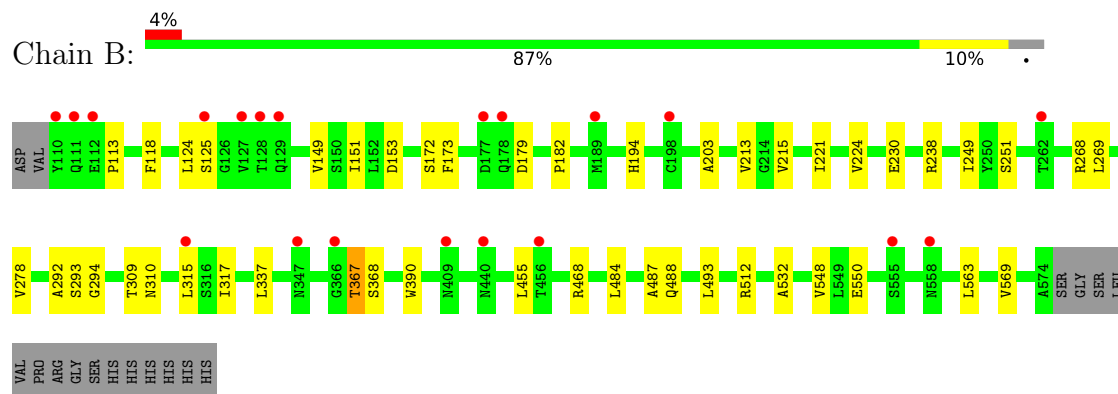
### 3 Residue-property plots [i](#)

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.

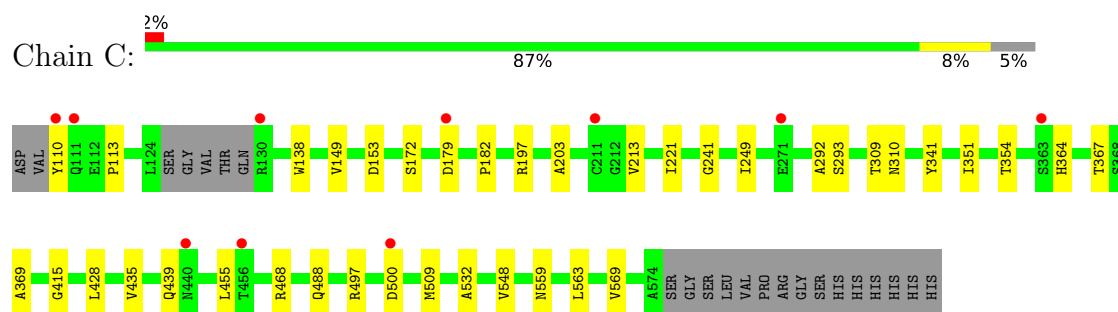
#### • Molecule 1: Furin



#### • Molecule 1: Furin



#### • Molecule 1: Furin



#### • Molecule 2: Neuroendocrine convertase 1







● Molecule 2: Neuroendocrine convertase 1



● Molecule 2: Neuroendocrine convertase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.48Å 196.98Å 99.87Å 90.00° 106.82° 90.00°	Depositor
Resolution (Å)	43.78 – 2.40 43.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	75.2 (43.78-2.40) 75.2 (43.78-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.227 , 0.252 0.226 , 0.251	Depositor DCC
$R_{free}$ test set	3075 reflections (3.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA, NA

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	0.11	0/3606	0.33	0/4914
1	B	0.12	0/3634	0.33	0/4954
1	C	0.14	0/3600	0.33	0/4906
2	D	0.13	0/593	0.36	0/797
2	E	0.13	0/588	0.36	0/790
2	F	0.12	0/599	0.36	0/805
All	All	0.12	0/12620	0.33	0/17166

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3525	3341	3338	21	0
1	B	3552	3367	3366	27	0
1	C	3519	3335	3333	20	0
2	D	580	546	546	3	0
2	E	575	541	541	4	0
2	F	586	551	551	2	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	36	0	0	0	0
5	B	26	0	0	0	0
5	C	37	0	0	0	0
5	D	3	0	0	0	0
5	E	1	0	0	0	0
5	F	3	0	0	0	0
All	All	12452	11681	11675	72	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 3.

All (72) 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:A:292:ALA:HB1	1:A:367:THR:HG23	1.51	0.90
1:A:292:ALA:HB1	1:A:367:THR:CG2	2.14	0.78
1:C:293:SER:HA	1:C:309:THR:HG21	1.68	0.76
1:A:293:SER:HA	1:A:309:THR:HG21	1.66	0.76
1:B:292:ALA:HB1	1:B:367:THR:HG23	1.70	0.73
1:C:292:ALA:HB1	1:C:367:THR:HG22	1.74	0.69
1:B:293:SER:HA	1:B:309:THR:HG21	1.74	0.68
1:B:310:ASN:ND2	1:B:532:ALA:O	2.28	0.67
1:A:310:ASN:ND2	1:A:532:ALA:O	2.27	0.66
1:C:468:ARG:HG2	1:C:548:VAL:HG22	1.77	0.66
1:A:294:GLY:H	1:A:367:THR:HG21	1.59	0.66
1:C:497:ARG:NH1	1:C:500:ASP:OD1	2.28	0.65
1:B:512:ARG:NH2	1:B:550:GLU:OE1	2.28	0.64
2:D:58:LEU:HD11	2:D:71:LYS:HG3	1.78	0.64
1:A:497:ARG:NH2	1:A:520:PRO:O	2.30	0.62
1:B:294:GLY:H	1:B:367:THR:HG21	1.64	0.61
1:C:310:ASN:ND2	1:C:532:ALA:O	2.35	0.59
1:C:351:ILE:HG13	1:C:369:ALA:HB1	1.85	0.57
1:A:488:GLN:HB2	1:A:569:VAL:HB	1.88	0.56
1:C:149:VAL:HG22	1:C:249:ILE:HB	1.85	0.56
1:B:113:PRO:HB3	1:B:213:VAL:HG11	1.88	0.56
1:B:238:ARG:HH21	2:E:69:LEU:HD23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ARG:HH21	2:D:69:LEU:HD23	1.72	0.54
1:A:468:ARG:HG2	1:A:548:VAL:HG22	1.90	0.54
1:A:455:LEU:HD11	1:A:563:LEU:HG	1.90	0.54
1:B:172:SER:HB3	1:B:182:PRO:HG3	1.90	0.53
1:B:493:LEU:HD12	1:B:493:LEU:C	2.34	0.53
1:A:172:SER:HB3	1:A:182:PRO:HG3	1.90	0.52
1:B:118:PHE:CZ	1:B:125:SER:HB3	2.44	0.52
1:A:149:VAL:HG22	1:A:249:ILE:HB	1.90	0.52
1:C:172:SER:HB3	1:C:182:PRO:HG3	1.91	0.51
1:C:500:ASP:OD2	1:C:559:ASN:ND2	2.43	0.51
2:F:57:LEU:HD11	2:F:68:TYR:HB3	1.93	0.50
1:B:149:VAL:HG22	1:B:249:ILE:HB	1.94	0.49
1:B:484:LEU:HD21	1:B:487:ALA:HB2	1.95	0.49
1:B:124:LEU:HD21	1:B:215:VAL:HG22	1.96	0.48
1:C:203:ALA:HB3	1:C:221:ILE:HB	1.96	0.47
1:B:268:ARG:HD2	2:E:98:TRP:CE2	2.49	0.47
1:C:488:GLN:HB2	1:C:569:VAL:HB	1.96	0.47
1:A:403:PRO:HG2	1:A:419:LYS:HB2	1.96	0.47
1:C:113:PRO:HB3	1:C:213:VAL:HG11	1.96	0.47
1:B:203:ALA:HB3	1:B:221:ILE:HB	1.96	0.47
1:B:468:ARG:HG2	1:B:548:VAL:HG22	1.95	0.47
1:C:351:ILE:HB	1:C:364:HIS:HB3	1.96	0.46
1:B:455:LEU:HD11	1:B:563:LEU:HG	1.98	0.46
1:B:151:ILE:HG12	1:B:221:ILE:HD11	1.98	0.45
1:C:341:TYR:CE2	1:C:428:LEU:HD21	2.51	0.45
1:B:488:GLN:HB2	1:B:569:VAL:HB	1.98	0.45
2:D:35:TRP:HZ2	2:D:83:ALA:HB3	1.82	0.45
1:A:351:ILE:HG13	1:A:369:ALA:HB1	1.98	0.44
1:A:201:GLU:OE1	1:A:351:ILE:HG21	2.17	0.44
1:B:269:LEU:HD11	2:E:36:ALA:CB	2.47	0.44
1:B:173:PHE:O	1:B:224:VAL:HA	2.18	0.44
1:A:497:ARG:NH1	1:A:500:ASP:OD1	2.52	0.43
1:B:151:ILE:HD13	1:B:251:SER:HB3	2.01	0.43
1:B:278:VAL:HB	1:B:390:TRP:CE2	2.54	0.43
1:C:415:GLY:HA3	1:C:509:MET:HE3	2.01	0.43
1:C:435:VAL:O	1:C:439:GLN:HG3	2.18	0.42
1:C:455:LEU:HD11	1:C:563:LEU:HG	2.00	0.42
1:C:110:TYR:OH	1:C:138:TRP:HB3	2.20	0.42
1:A:233:ASP:CG	1:A:267:ALA:HB3	2.44	0.42
1:A:455:LEU:HG	1:A:566:PHE:HB3	2.01	0.42
1:C:197:ARG:HA	1:C:354:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLY:O	2:F:63:SER:OG	2.35	0.42
1:A:295:ASN:OD1	1:A:367:THR:HB	2.20	0.41
1:A:449:LYS:HE2	1:A:451:ILE:HD11	2.02	0.41
1:B:194:HIS:CE1	1:B:368:SER:HB2	2.56	0.41
2:E:49:ILE:HD11	2:E:95:ARG:HB2	2.02	0.41
1:B:315:LEU:CD2	1:B:317:ILE:HD11	2.51	0.41
1:A:160:HIS:CD2	1:A:358:GLN:HA	2.57	0.40
1:B:315:LEU:HD21	1:B:317:ILE:HD11	2.03	0.40
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	457/482 (95%)	444 (97%)	12 (3%)	1 (0%)	44	59
1	B	463/482 (96%)	449 (97%)	13 (3%)	1 (0%)	44	59
1	C	456/482 (95%)	442 (97%)	13 (3%)	1 (0%)	44	59
2	D	67/95 (70%)	66 (98%)	1 (2%)	0	100	100
2	E	66/95 (70%)	66 (100%)	0	0	100	100
2	F	68/95 (72%)	67 (98%)	1 (2%)	0	100	100
All	All	1577/1731 (91%)	1534 (97%)	40 (2%)	3 (0%)	44	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	153	ASP
1	C	153	ASP
1	A	153	ASP

### 5.3.2 Protein sidechains ⓘ

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	372/390 (95%)	368 (99%)	4 (1%)	70	84
1	B	375/390 (96%)	372 (99%)	3 (1%)	79	90
1	C	371/390 (95%)	370 (100%)	1 (0%)	91	96
2	D	58/79 (73%)	57 (98%)	1 (2%)	56	75
2	E	58/79 (73%)	58 (100%)	0	100	100
2	F	59/79 (75%)	59 (100%)	0	100	100
All	All	1293/1407 (92%)	1284 (99%)	9 (1%)	81	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ASP
1	A	303	CYS
1	A	315	LEU
1	A	367	THR
2	D	97	ILE
1	B	179	ASP
1	B	230	GLU
1	B	367	THR
1	C	179	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	218	ASN
1	A	300	HIS
1	A	364	HIS
1	B	218	ASN
1	B	364	HIS
1	B	521	HIS
1	C	218	ASN

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Mol	Chain	Res	Type
1	C	325	ASN
1	C	364	HIS
1	C	521	HIS

### 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 9 ligands modelled in this entry, 9 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	461/482 (95%)	0.23	8 (1%) 69 65	12, 35, 47, 62	36 (7%)
1	B	465/482 (96%)	0.35	20 (4%) 40 38	13, 36, 46, 76	42 (9%)
1	C	460/482 (95%)	0.29	10 (2%) 62 59	17, 35, 46, 62	33 (7%)
2	D	71/95 (74%)	0.48	2 (2%) 55 51	15, 37, 47, 63	14 (19%)
2	E	70/95 (73%)	0.89	7 (10%) 14 12	21, 43, 63, 91	16 (22%)
2	F	72/95 (75%)	1.05	13 (18%) 4 4	18, 46, 65, 87	16 (22%)
All	All	1599/1731 (92%)	0.36	60 (3%) 44 42	12, 36, 50, 91	157 (9%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	ASN	6.4
2	F	84	PHE	4.3
1	C	130	ARG	4.1
1	B	128	THR	4.1
1	B	111	GLN	4.0
2	E	103	TYR	3.8
2	E	84	PHE	3.8
1	C	111	GLN	3.6
2	F	72	HIS	3.5
2	D	65	GLU	3.5
2	F	85	HIS	3.5
2	F	94	ASP	3.4
1	B	110	TYR	3.3
2	F	53	LEU	3.2
1	B	127	VAL	3.2
1	B	189	MET	3.2
1	B	129	GLN	3.1
1	A	456	THR	3.1
1	B	555	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	479	ASN	2.9
2	E	54	GLY	2.9
2	F	54	GLY	2.8
1	A	440	ASN	2.8
1	B	178	GLN	2.8
1	C	110	TYR	2.7
2	E	41	GLY	2.7
1	B	177	ASP	2.6
1	C	211	CYS	2.6
1	A	408	ALA	2.6
1	A	110	TYR	2.5
1	B	366	GLY	2.5
1	B	409	ASN	2.5
1	B	440	ASN	2.5
1	C	500	ASP	2.4
2	F	52	GLU	2.4
1	C	179	ASP	2.3
2	E	72	HIS	2.3
1	B	347	ASN	2.3
2	F	49	ILE	2.3
1	A	145	HIS	2.2
2	F	62	GLY	2.2
1	A	111	GLN	2.2
1	B	315	LEU	2.2
2	F	45	ALA	2.2
1	B	125	SER	2.1
1	C	363	SER	2.1
1	B	456	THR	2.1
2	D	32	VAL	2.1
1	C	456	THR	2.1
2	F	108	SER	2.1
1	A	460	ASP	2.1
2	E	92	ASP	2.1
1	B	198	CYS	2.1
1	B	558	ASN	2.1
2	F	92	ASP	2.1
1	B	262	THR	2.0
1	B	112	GLU	2.0
1	C	271	GLU	2.0
2	F	104	GLU	2.0
2	E	53	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](#)

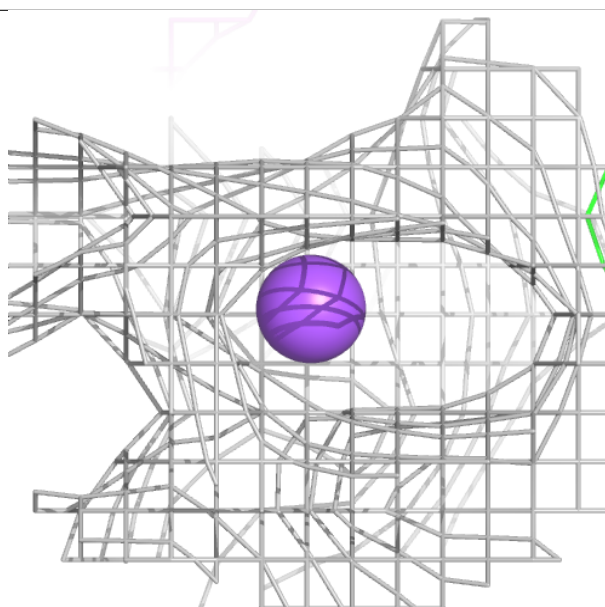
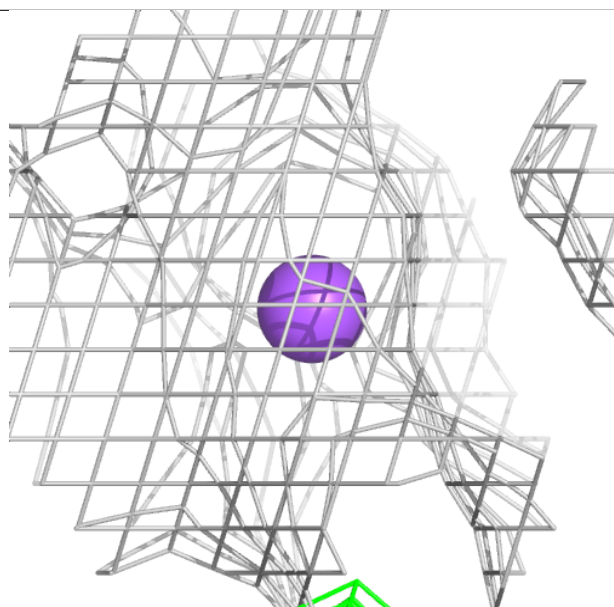
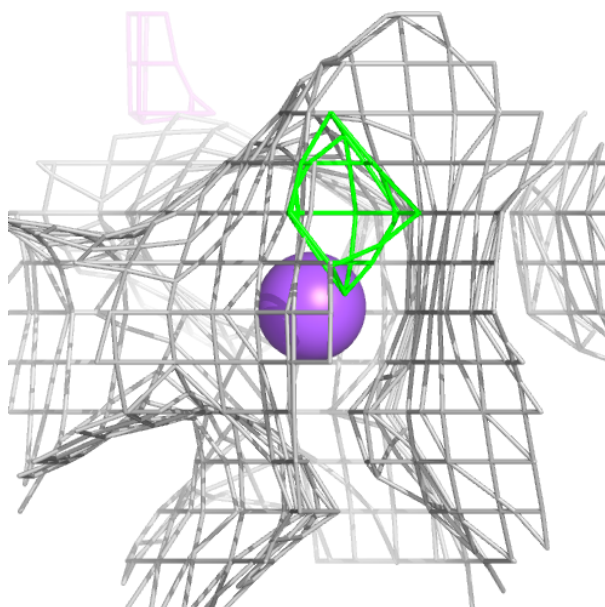
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	NA	A	602	1/1	0.90	0.08	33,33,33,33	0
4	NA	C	602	1/1	0.91	0.08	29,29,29,29	0
3	CA	A	601	1/1	0.93	0.15	62,62,62,62	0
3	CA	A	600	1/1	0.96	0.04	31,31,31,31	0
3	CA	C	600	1/1	0.96	0.13	51,51,51,51	0
3	CA	B	601	1/1	0.97	0.04	40,40,40,40	0
4	NA	B	602	1/1	0.98	0.04	32,32,32,32	0
3	CA	C	601	1/1	0.98	0.07	35,35,35,35	0
3	CA	B	600	1/1	0.99	0.06	42,42,42,42	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.

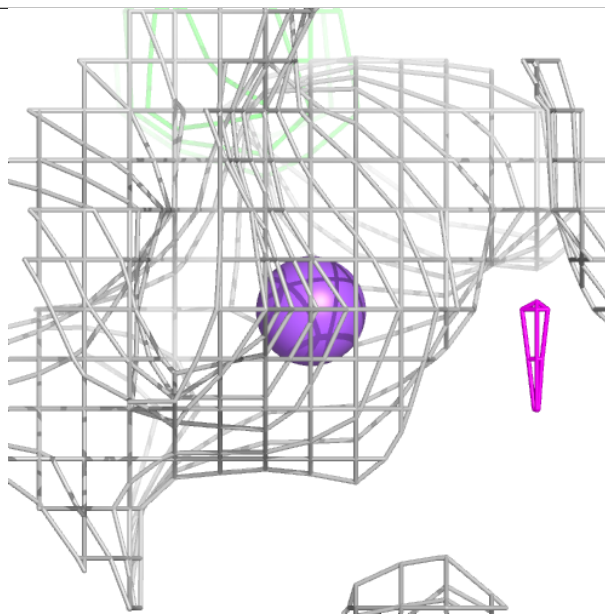
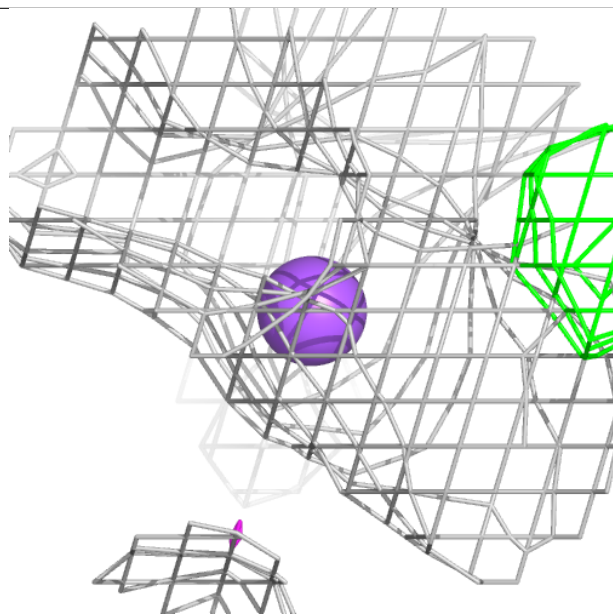
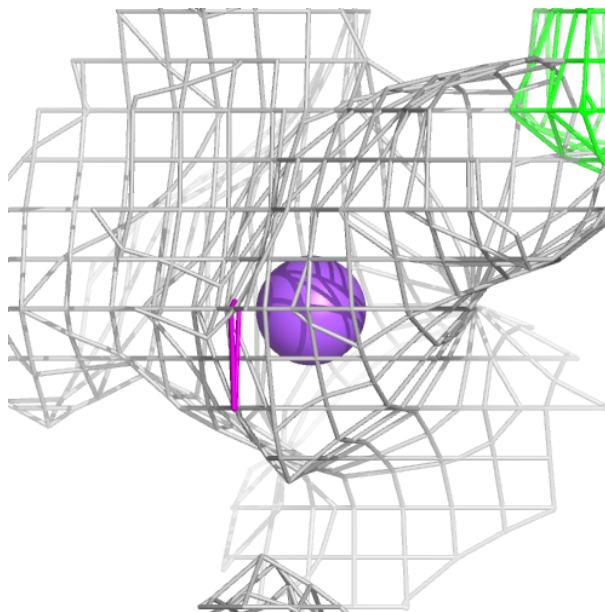
**Electron density around NA A 602:**

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



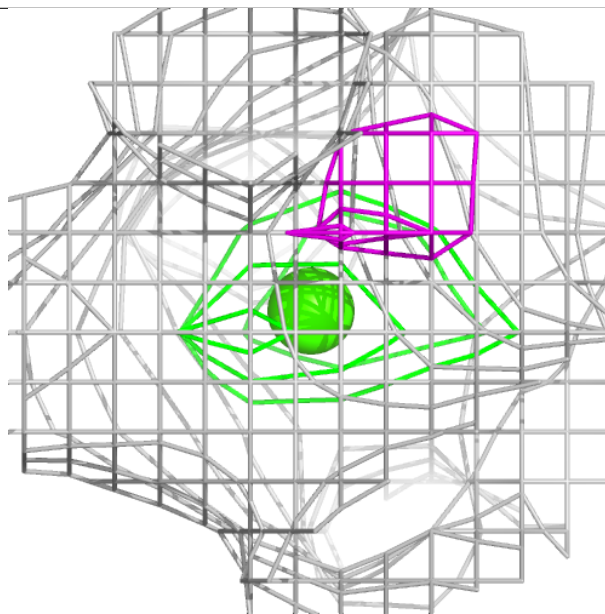
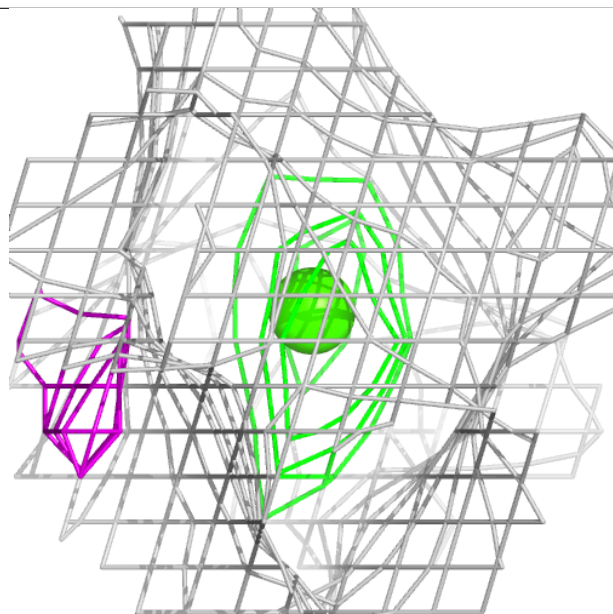
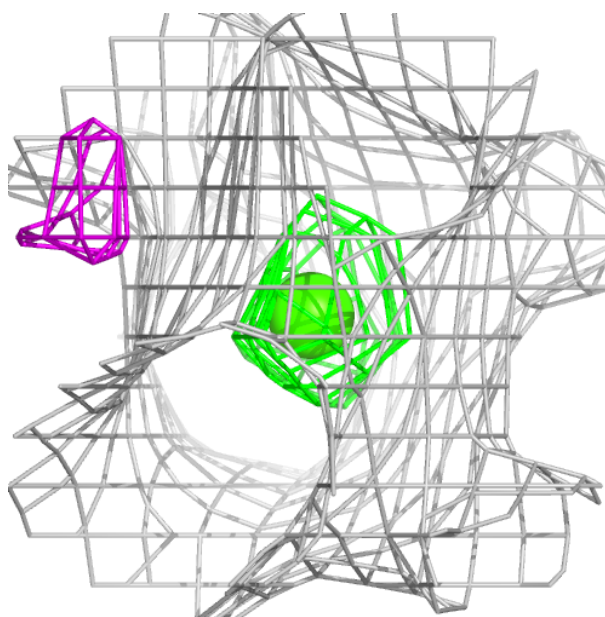
**Electron density around NA C 602:**

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



**Electron density around CA A 601:**

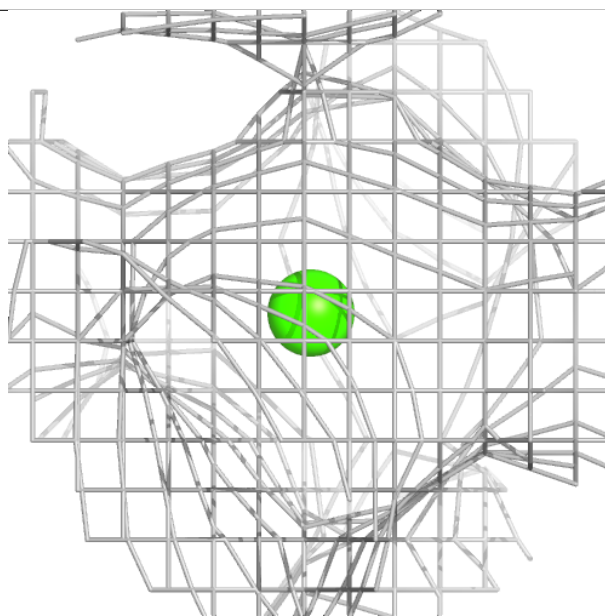
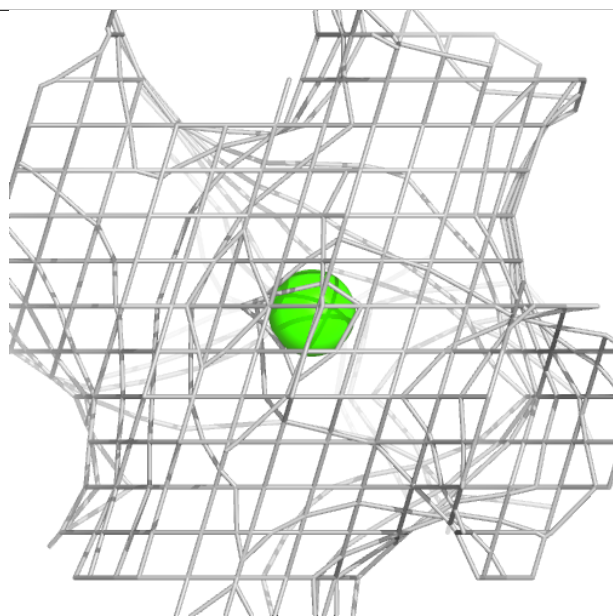
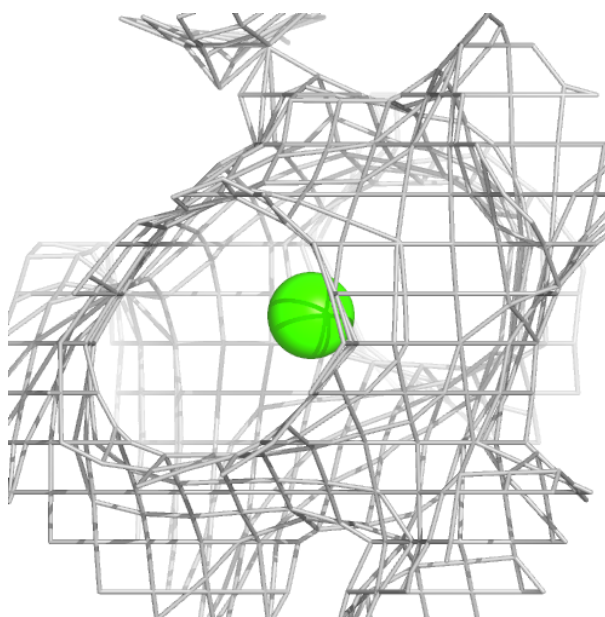
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





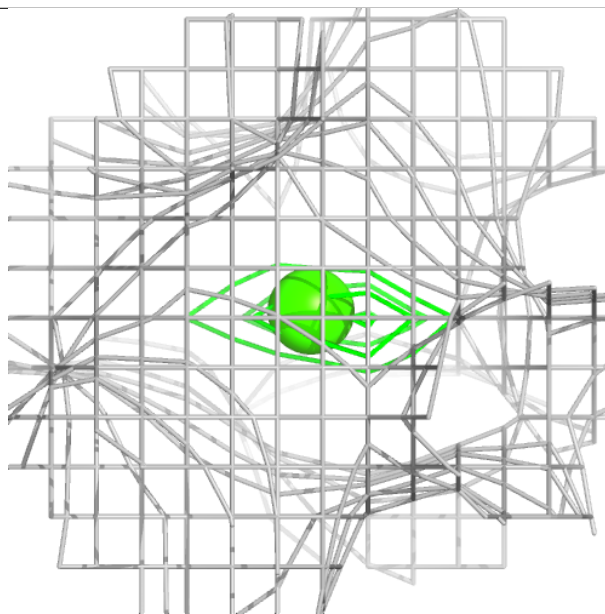
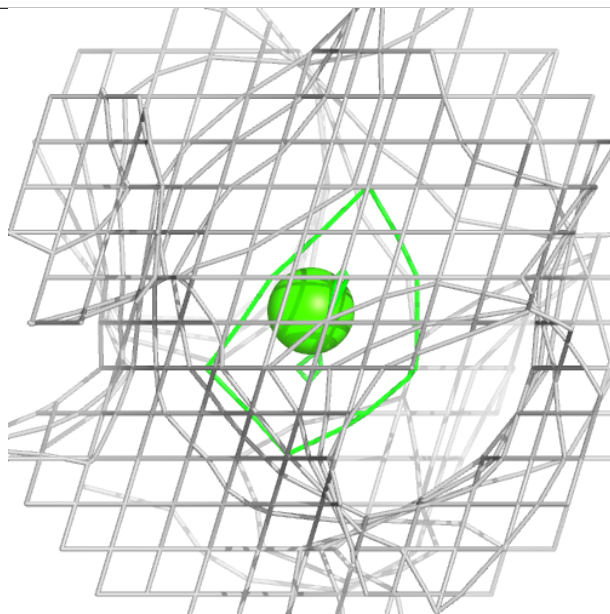
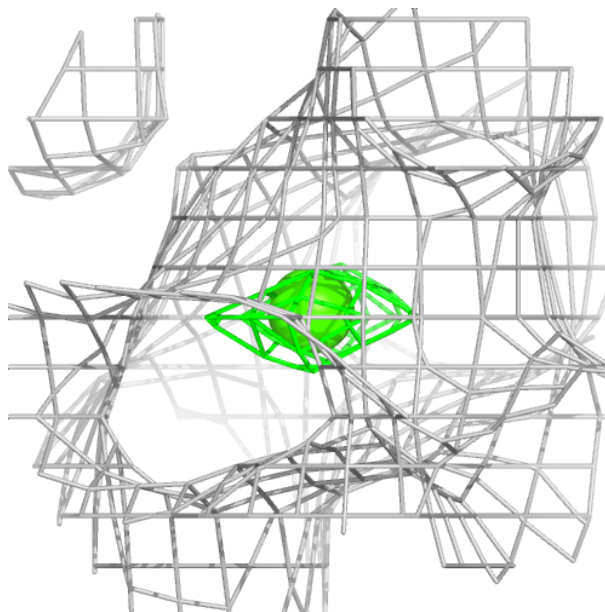
**Electron density around CA A 600:**

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



**Electron density around CA C 600:**

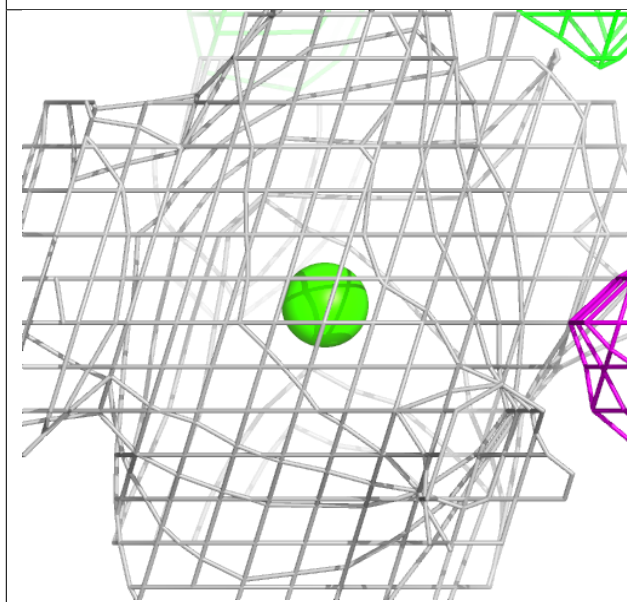
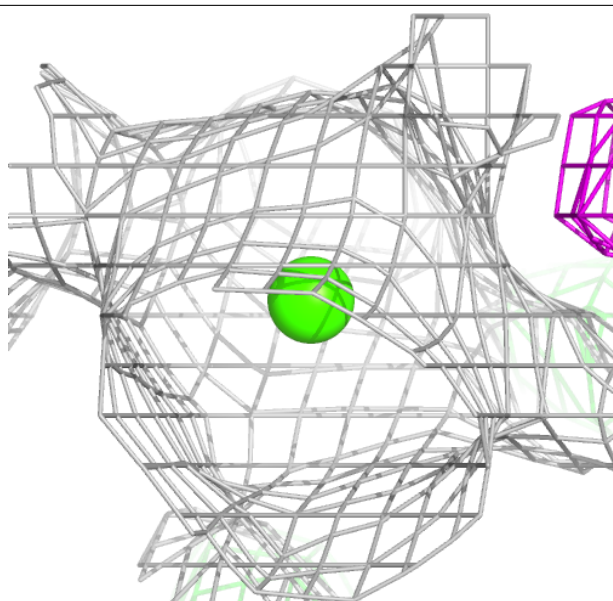
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





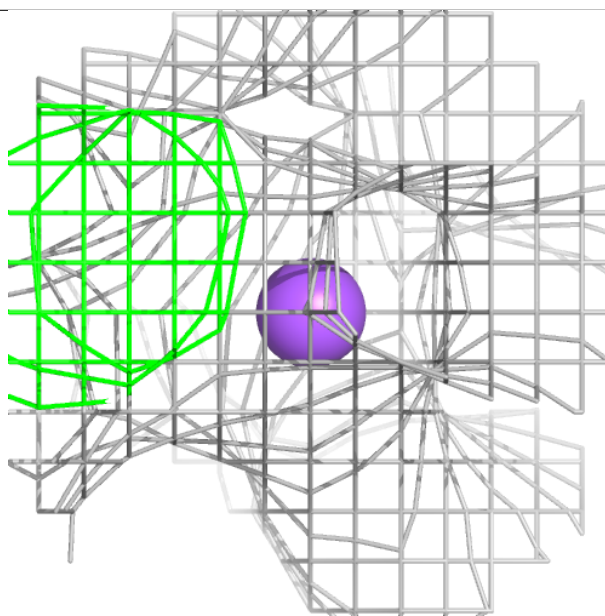
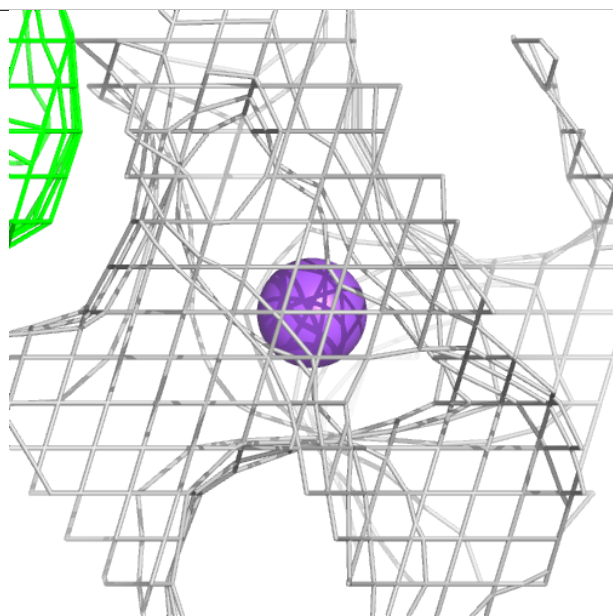
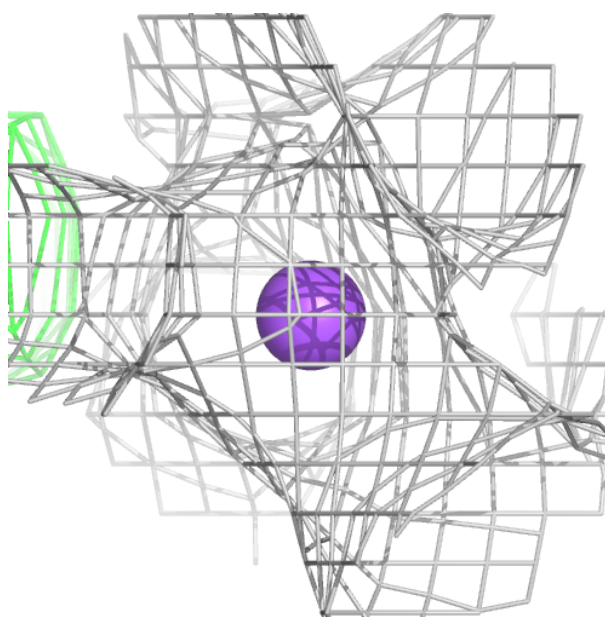
**Electron density around CA B 601:**

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



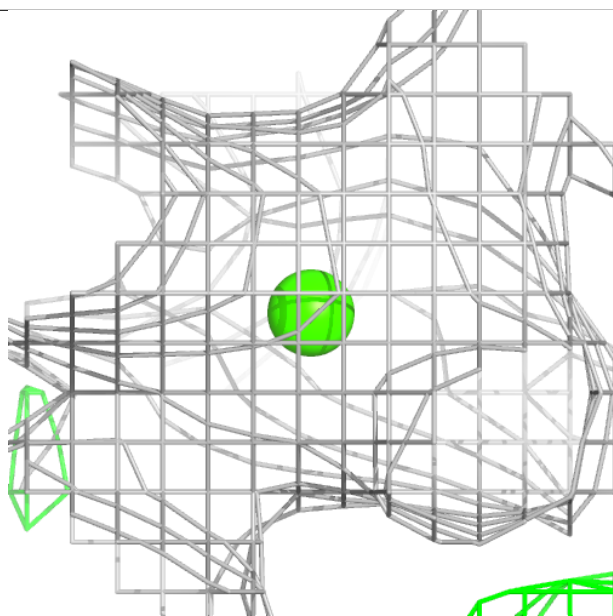
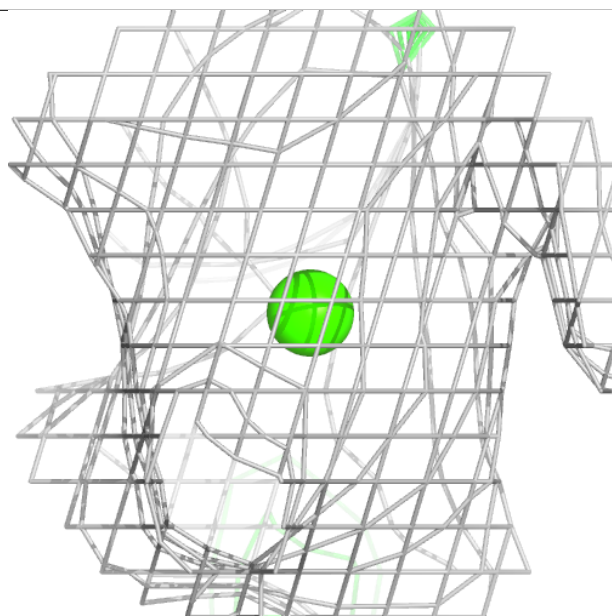
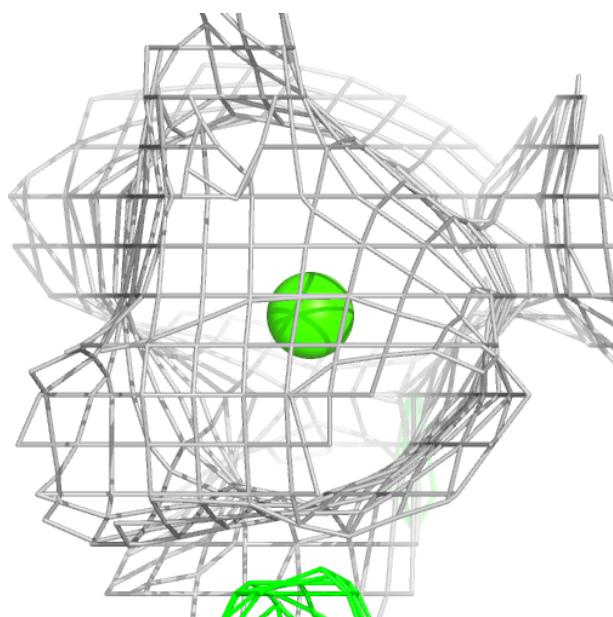
**Electron density around NA B 602:**

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



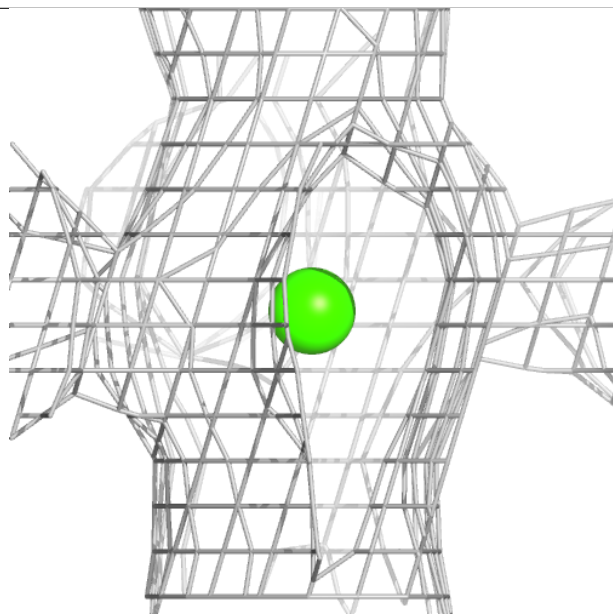
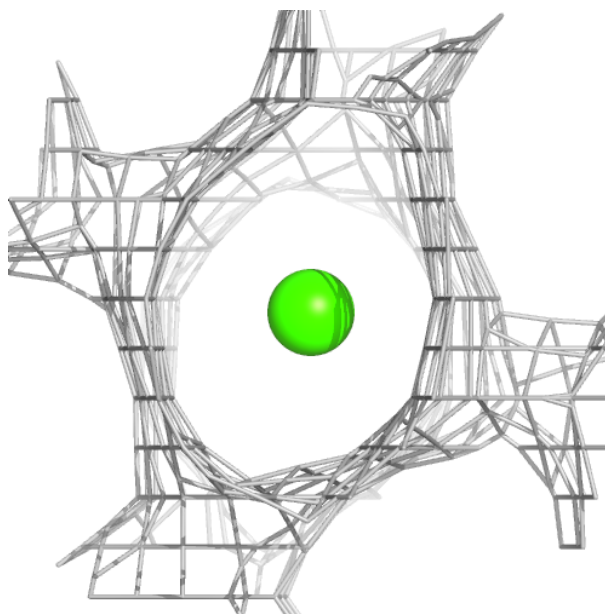
**Electron density around CA C 601:**

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



**Electron density around CA B 600:**

$2mF_o-DF_c$  (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.