



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:55 PM UTC

PDB ID : 8F5T / pdb_00008f5t
Title : Rabbit muscle pyruvate kinase in complex with sodium and magnesium
Authors : Holyoak, T.; Fenton, A.W.
Deposited on : 2022-11-15
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

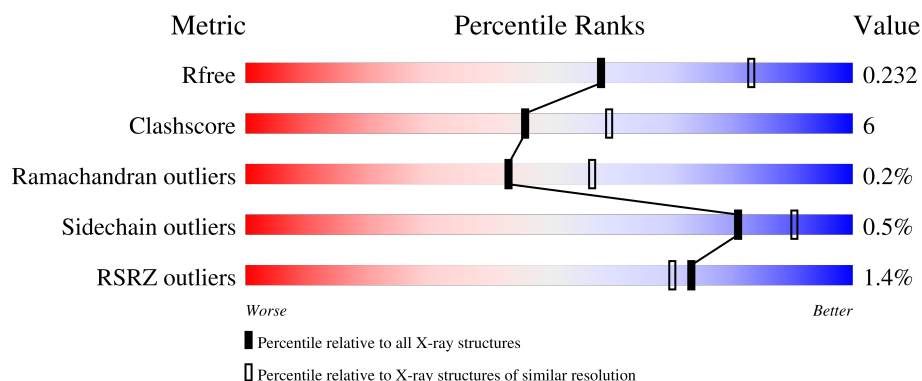
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 ≥ 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	531	86% 12% .
1	B	531	89% 8% .
1	C	531	86% 11% .
1	D	531	86% 11% .
1	E	531	5% 84% 14% .

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Mol	Chain	Length	Quality of chain
1	F	531	% 81% 16% ..
1	G	531	4% 83% 14% .
1	H	531	% 79% 18% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33531 atoms, of which 24 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 Pyruvate kinase PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	0	0
			3989	2507	709	745	28			
1	B	520	Total	C	N	O	S	0	0	0
			3989	2507	709	745	28			
1	C	520	Total	C	N	O	S	0	0	0
			3989	2507	709	745	28			
1	D	520	Total	C	N	O	S	0	0	0
			3989	2507	709	745	28			
1	E	520	Total	C	N	O	S	0	0	0
			3989	2507	709	745	28			
1	F	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	G	515	Total	C	N	O	S	0	0	0
			3958	2488	703	739	28			
1	H	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	ALA	SER	variant	UNP P11974
B	400	ALA	SER	variant	UNP P11974
C	400	ALA	SER	variant	UNP P11974
D	400	ALA	SER	variant	UNP P11974
E	400	ALA	SER	variant	UNP P11974
F	400	ALA	SER	variant	UNP P11974
G	400	ALA	SER	variant	UNP P11974
H	400	ALA	SER	variant	UNP P11974

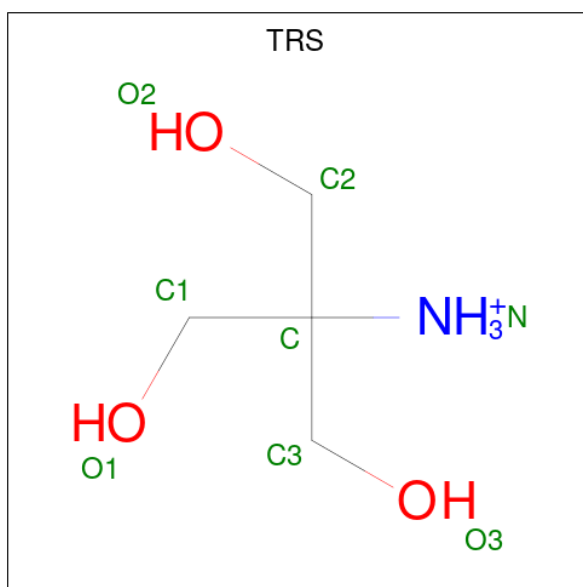
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

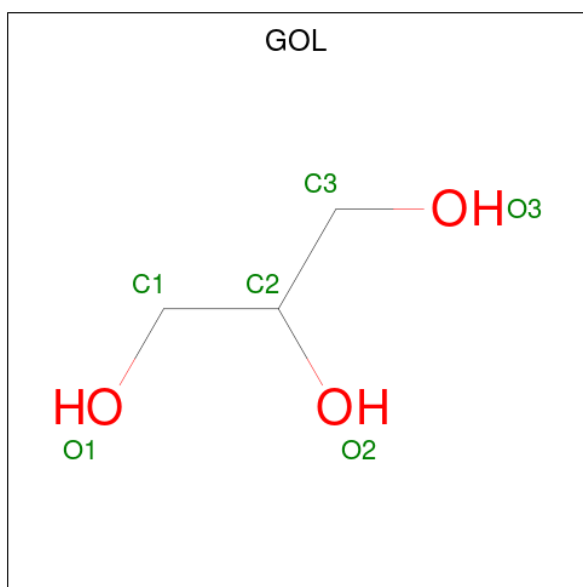
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	0
			8	4	1	3		
4	E	1	Total	C	N	O	0	0
			8	4	1	3		
4	F	1	Total	C	N	O	0	0
			8	4	1	3		
4	G	1	Total	C	N	O	0	0
			8	4	1	3		
4	H	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		

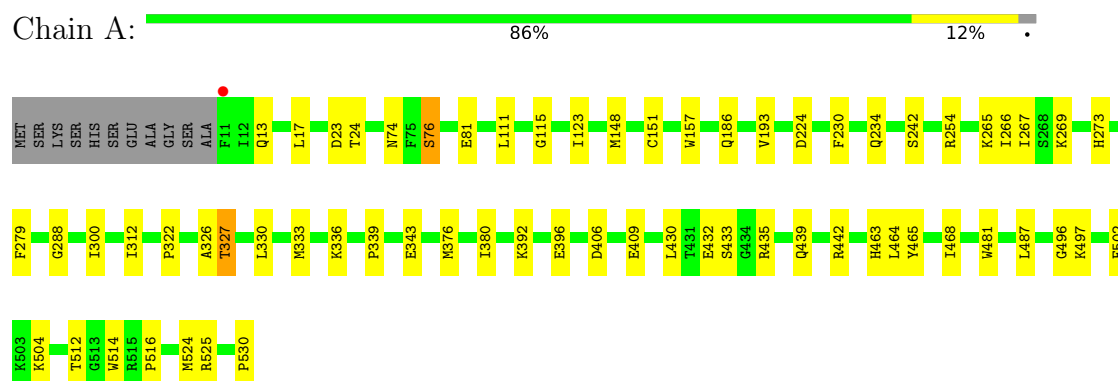
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	266	Total	O	0	0
			266	266		
6	B	262	Total	O	0	0
			262	262		
6	C	222	Total	O	0	0
			222	222		
6	D	215	Total	O	0	0
			215	215		
6	E	191	Total	O	0	0
			191	191		
6	F	171	Total	O	0	0
			171	171		
6	G	142	Total	O	0	0
			142	142		
6	H	97	Total	O	0	0
			97	97		

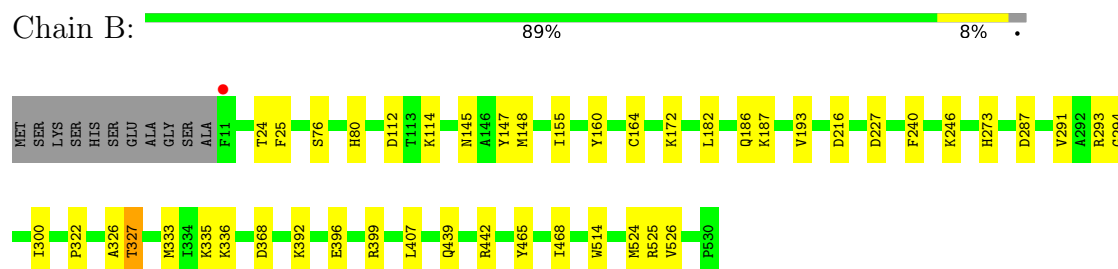
3 Residue-property plots

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.

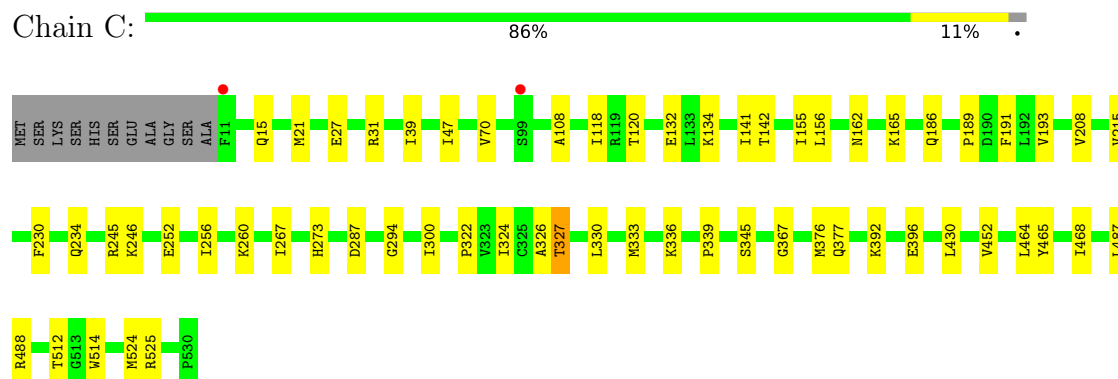
• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM

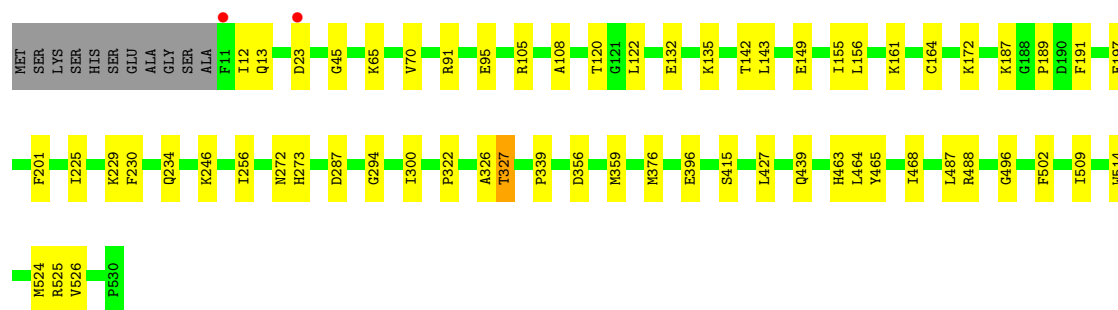


• Molecule 1: Pyruvate kinase PKM



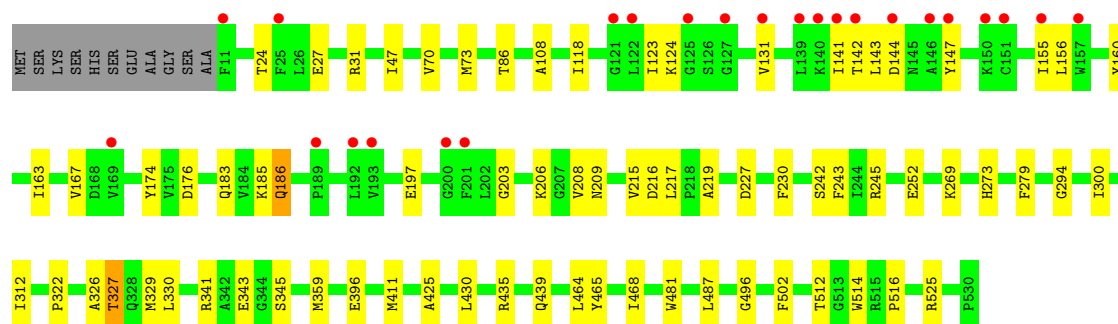
• Molecule 1: Pyruvate kinase PKM

Chain D:  86% 11%



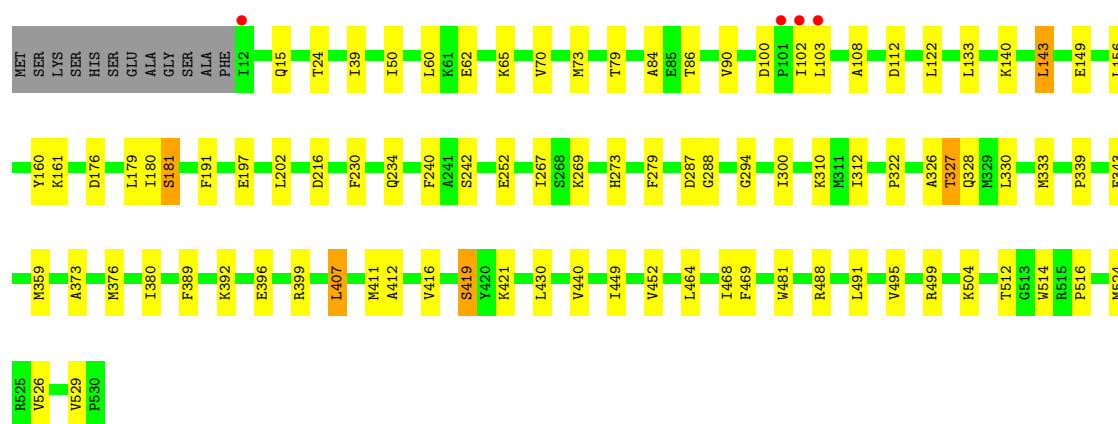
• Molecule 1: Pyruvate kinase PKM

Chain E:  5% 84% 14%



• Molecule 1: Pyruvate kinase PKM

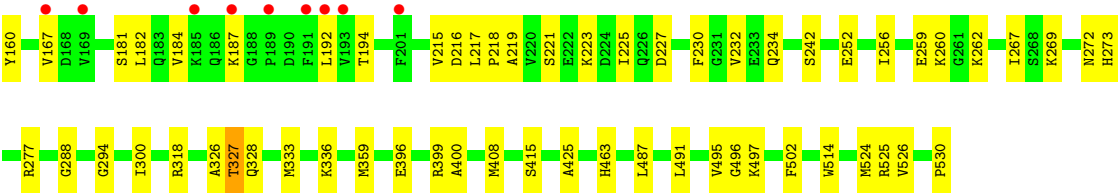
Chain F:  % 81% 16% ..



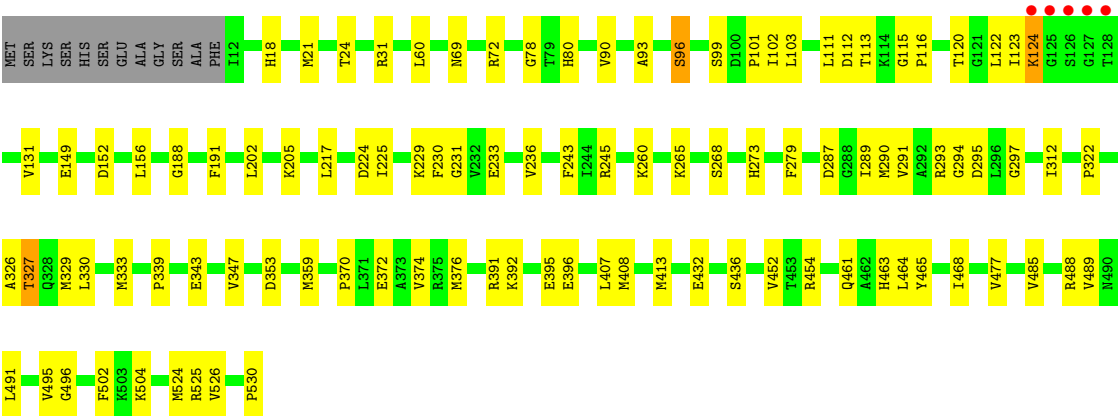
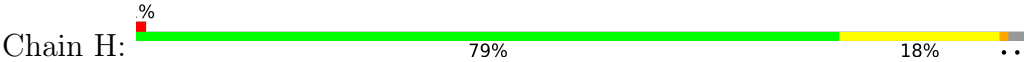
• Molecule 1: Pyruvate kinase PKM

Chain G:  4% 83% 14%





● Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.45Å 113.76Å 169.14Å 90.00° 94.05° 90.00°	Depositor
Resolution (Å)	47.16 – 2.41 47.16 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.16-2.41) 98.7 (47.16-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.232 0.185 , 0.232	Depositor DCC
R_{free} test set	10347 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.4	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	0.95	EDS
Total number of atoms	33531	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.12	0/4053	0.31	0/5467
1	B	0.12	0/4053	0.29	0/5467
1	C	0.11	0/4053	0.29	0/5467
1	D	0.11	0/4053	0.28	0/5467
1	E	0.11	0/4053	0.29	0/5467
1	F	0.10	0/4041	0.28	0/5451
1	G	0.10	0/4021	0.26	0/5424
1	H	0.11	0/4041	0.29	0/5451
All	All	0.11	0/32368	0.29	0/43661

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	3989	0	4065	41	0
1	B	3989	0	4065	28	0
1	C	3989	0	4065	41	0
1	D	3989	0	4065	48	0
1	E	3989	0	4065	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3978	0	4055	70	0
1	G	3958	0	4029	56	0
1	H	3978	0	4055	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	12	1	0
4	D	8	0	12	3	0
4	E	8	0	12	0	0
4	F	8	0	12	2	0
4	G	8	0	12	2	0
4	H	8	0	12	0	0
5	B	6	8	8	0	0
5	D	6	8	8	2	0
5	E	6	8	8	2	0
6	A	266	0	0	6	0
6	B	262	0	0	1	0
6	C	222	0	0	3	0
6	D	215	0	0	6	0
6	E	191	0	0	1	0
6	F	171	0	0	2	0
6	G	142	0	0	1	0
6	H	97	0	0	3	0
All	All	33507	24	32560	377	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 6.

All (377) 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:G:326:ALA:HB1	1:G:359:MET:HE2	1.52	0.90
1:F:524:MET:HE3	1:H:524:MET:HE3	1.56	0.87
1:C:524:MET:HE3	1:D:524:MET:HE3	1.56	0.87
1:C:21:MET:HE2	1:C:21:MET:HA	1.61	0.82
1:E:73:MET:HE1	1:E:86:THR:HG21	1.62	0.82
1:E:326:ALA:HB1	1:E:359:MET:HE2	1.61	0.81
1:A:13:GLN:HG2	1:A:17:LEU:HB2	1.64	0.80
1:G:160:TYR:OH	1:G:216:ASP:OD1	2.00	0.79
1:F:50:ILE:HB	1:F:73:MET:HE1	1.63	0.79
1:H:491:LEU:O	1:H:495:VAL:HG23	1.84	0.78
1:D:273:HIS:CE1	1:D:300:ILE:HG22	2.19	0.77
1:F:15:GLN:HG3	1:F:39:ILE:HG23	1.68	0.75
1:F:452:VAL:HG11	1:F:488:ARG:HB3	1.67	0.75
1:F:330:LEU:HD13	1:F:333:MET:CE	2.18	0.74
1:B:186:GLN:HB2	1:B:193:VAL:HB	1.70	0.72
1:F:143:LEU:HD22	1:F:161:LYS:HA	1.70	0.72
1:F:399:ARG:NH2	1:H:21:MET:O	2.23	0.72
1:E:273:HIS:CE1	1:E:300:ILE:HG22	2.24	0.71
1:C:525:ARG:HD3	1:D:514:TRP:CE3	2.25	0.71
1:C:142:THR:HB	1:C:155:ILE:HD11	1.72	0.71
1:E:142:THR:OG1	1:E:155:ILE:HD11	1.91	0.70
1:C:70:VAL:HG22	1:C:108:ALA:HB3	1.73	0.70
1:F:50:ILE:HB	1:F:73:MET:CE	2.21	0.69
1:B:76:SER:HA	1:B:114:LYS:HG3	1.74	0.69
1:E:525:ARG:HD3	1:G:514:TRP:CE3	2.27	0.68
1:A:186:GLN:HB3	1:A:193:VAL:HB	1.76	0.68
1:F:330:LEU:HD13	1:F:333:MET:HE2	1.75	0.68
1:E:118:ILE:HG22	1:E:208:VAL:HB	1.75	0.67
1:H:233:GLU:OE1	1:H:260:LYS:NZ	2.26	0.67
1:G:221:SER:O	1:G:225:ILE:HD12	1.96	0.66
1:D:23:ASP:OD1	6:D:701:HOH:O	2.12	0.66
1:B:294:GLY:CA	1:B:327:THR:HG21	2.26	0.66
1:A:525:ARG:HD3	1:B:514:TRP:CE3	2.32	0.65
1:C:514:TRP:CE3	1:D:525:ARG:HD3	2.31	0.65
1:H:408:MET:HE2	1:H:436:SER:HA	1.78	0.65
1:F:514:TRP:CE3	1:H:525:ARG:HD3	2.32	0.65
1:A:406:ASP:HB3	1:A:409:GLU:HB2	1.77	0.64
6:A:792:HOH:O	1:B:399:ARG:HD2	1.97	0.64
1:A:265:LYS:HE3	6:A:924:HOH:O	1.98	0.64
1:G:252:GLU:O	1:G:256:ILE:HG12	1.97	0.63
1:G:145:ASN:O	1:G:148:MET:HG2	1.98	0.63
1:D:122:LEU:HD12	1:D:149:GLU:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:ILE:O	1:E:167:VAL:HG22	1.98	0.63
1:H:339:PRO:HG3	1:H:376:MET:HG2	1.80	0.63
1:F:160:TYR:OH	1:F:216:ASP:OD1	2.07	0.63
1:E:118:ILE:CG2	1:E:208:VAL:HB	2.29	0.62
1:F:524:MET:HE3	1:H:524:MET:CE	2.28	0.62
1:H:295:ASP:OD2	6:H:701:HOH:O	2.16	0.62
1:H:102:ILE:HG22	1:H:103:LEU:HD22	1.82	0.62
1:C:273:HIS:CE1	1:C:300:ILE:HG22	2.35	0.61
1:G:232:VAL:HG11	1:G:260:LYS:HG2	1.83	0.61
1:G:415:SER:OG	1:G:524:MET:HG3	2.01	0.61
1:D:45:GLY:HA2	4:D:603:TRS:H22	1.82	0.61
1:G:326:ALA:CB	1:G:359:MET:HE2	2.26	0.61
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.36	0.60
1:E:439:GLN:HE21	5:E:604:GOL:H31	1.67	0.60
1:E:242:SER:HA	1:E:269:LYS:HD3	1.82	0.60
1:D:463:HIS:ND1	4:D:603:TRS:H32	2.17	0.59
1:D:225:ILE:O	1:D:229:LYS:HD3	2.01	0.59
1:G:114:LYS:HE3	1:G:117:GLU:OE2	2.02	0.59
1:G:327:THR:HG22	1:G:328:GLN:HG3	1.83	0.59
1:F:103:LEU:HA	1:F:499:ARG:HH12	1.68	0.59
1:B:273:HIS:CE1	1:B:300:ILE:HG22	2.38	0.58
1:F:273:HIS:CE1	1:F:300:ILE:HG22	2.38	0.58
1:C:15:GLN:HG3	1:C:39:ILE:HG23	1.84	0.58
1:A:463:HIS:ND1	4:A:603:TRS:H22	2.18	0.58
1:E:465:TYR:HB2	1:E:468:ILE:HD12	1.84	0.58
1:D:164:CYS:O	1:D:187:LYS:HE2	2.02	0.58
1:F:15:GLN:CG	1:F:39:ILE:HG23	2.34	0.57
1:F:73:MET:HE2	1:F:86:THR:HG21	1.86	0.57
1:F:430:LEU:HD22	1:F:512:THR:HG22	1.86	0.57
1:C:186:GLN:HB2	1:C:193:VAL:HB	1.86	0.57
1:D:496:GLY:HA3	1:D:502:PHE:CZ	2.40	0.57
1:D:65:LYS:NZ	6:D:705:HOH:O	2.36	0.57
1:A:524:MET:HE3	1:B:524:MET:HE3	1.86	0.57
1:E:203:GLY:HA3	1:E:206:LYS:HE2	1.86	0.57
1:G:273:HIS:CE1	1:G:300:ILE:HG22	2.40	0.57
1:F:491:LEU:O	1:F:495:VAL:HG23	2.03	0.57
1:A:392:LYS:O	1:A:396:GLU:HG3	2.05	0.56
1:D:322:PRO:HB3	1:D:464:LEU:O	2.04	0.56
1:A:273:HIS:HB2	6:A:876:HOH:O	2.03	0.56
1:A:514:TRP:CE3	1:B:525:ARG:HD3	2.40	0.56
1:G:487:LEU:HD23	1:G:487:LEU:C	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ARG:O	1:D:95:GLU:HG2	2.05	0.56
1:E:142:THR:HG22	1:E:144:ASP:H	1.71	0.56
1:C:326:ALA:O	1:C:327:THR:HB	2.06	0.56
1:F:327:THR:HG22	1:F:328:GLN:HG3	1.87	0.56
1:E:142:THR:HG21	1:E:147:TYR:CD1	2.42	0.55
1:F:396:GLU:CD	1:G:24:THR:HB	2.31	0.55
1:E:439:GLN:HE21	5:E:604:GOL:C3	2.18	0.55
1:G:463:HIS:CE1	4:G:603:TRS:H12	2.42	0.55
1:C:47:ILE:HG12	1:C:70:VAL:HB	1.89	0.55
1:F:287:ASP:O	1:F:322:PRO:HD2	2.05	0.55
1:H:322:PRO:HB3	1:H:464:LEU:O	2.06	0.55
1:B:326:ALA:O	1:B:327:THR:HB	2.06	0.55
1:B:465:TYR:HB2	1:B:468:ILE:HD12	1.89	0.55
1:C:392:LYS:O	1:C:396:GLU:HG3	2.07	0.54
1:G:294:GLY:CA	1:G:327:THR:HG21	2.38	0.54
1:G:463:HIS:ND1	4:G:603:TRS:H12	2.21	0.54
1:G:242:SER:HA	1:G:269:LYS:HD3	1.88	0.54
1:A:24:THR:HB	1:C:396:GLU:CD	2.33	0.53
1:D:294:GLY:CA	1:D:327:THR:HG21	2.39	0.53
1:E:326:ALA:O	1:E:327:THR:HB	2.08	0.53
1:E:70:VAL:HG22	1:E:108:ALA:HB3	1.91	0.53
1:A:123:ILE:HD13	1:A:151:CYS:HB2	1.91	0.53
1:E:27:GLU:HG2	6:E:795:HOH:O	2.08	0.53
1:F:24:THR:HB	1:G:396:GLU:CD	2.34	0.52
1:F:133:LEU:HD11	1:F:202:LEU:HD22	1.89	0.52
1:B:392:LYS:O	1:B:396:GLU:HG3	2.10	0.52
1:G:181:SER:O	1:G:182:LEU:HD23	2.09	0.52
1:G:184:VAL:HA	1:G:194:THR:HG22	1.91	0.52
1:F:333:MET:HE1	1:F:373:ALA:HA	1.92	0.52
1:G:326:ALA:HB1	1:G:359:MET:CE	2.33	0.52
1:H:353:ASP:OD2	6:H:702:HOH:O	2.18	0.52
1:E:142:THR:HG22	1:E:144:ASP:N	2.24	0.52
1:G:23:ASP:OD1	1:G:23:ASP:N	2.42	0.52
1:H:291:VAL:HG12	1:H:293:ARG:HG2	1.92	0.52
1:A:433:SER:OG	1:A:435:ARG:HG3	2.09	0.52
1:D:229:LYS:HE2	1:D:256:ILE:HG23	1.92	0.52
1:H:408:MET:HE2	1:H:436:SER:CA	2.38	0.52
1:G:73:MET:HE3	1:G:86:THR:CG2	2.40	0.51
1:H:391:ARG:O	1:H:395:GLU:HG3	2.10	0.51
1:G:273:HIS:HB3	1:G:277:ARG:NH1	2.25	0.51
1:A:487:LEU:C	1:A:487:LEU:HD23	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:GLN:HE21	5:D:604:GOL:C3	2.23	0.51
1:C:322:PRO:HB3	1:C:464:LEU:O	2.10	0.51
1:H:452:VAL:HG11	1:H:488:ARG:HB3	1.92	0.51
1:H:156:LEU:HD13	1:H:202:LEU:HD21	1.93	0.51
1:A:273:HIS:CE1	1:A:300:ILE:HG22	2.45	0.51
1:G:232:VAL:CG1	1:G:260:LYS:HG2	2.41	0.51
1:A:439:GLN:O	1:A:442:ARG:HG2	2.11	0.50
1:H:326:ALA:HB1	1:H:359:MET:HE2	1.92	0.50
1:E:487:LEU:C	1:E:487:LEU:HD23	2.36	0.50
1:F:60:LEU:HD13	1:F:90:VAL:HA	1.94	0.50
1:A:339:PRO:HG3	1:A:376:MET:HG2	1.93	0.50
1:D:326:ALA:HB1	1:D:359:MET:HE2	1.91	0.50
1:A:267:ILE:HD12	1:A:288:GLY:HA3	1.94	0.50
1:D:463:HIS:CE1	4:D:603:TRS:H32	2.46	0.50
1:G:187:LYS:HG3	1:G:192:LEU:HD21	1.93	0.50
1:G:167:VAL:HG21	1:G:192:LEU:HD11	1.93	0.50
1:A:330:LEU:HD23	1:A:343:GLU:HB3	1.94	0.50
1:D:246:LYS:HE3	6:D:795:HOH:O	2.12	0.50
1:B:160:TYR:OH	1:B:216:ASP:OD1	2.13	0.50
1:E:183:GLN:HB2	1:E:197:GLU:OE2	2.12	0.50
1:H:72:ARG:NH2	1:H:112:ASP:OD2	2.40	0.50
1:H:265:LYS:HG2	1:H:461:GLN:NE2	2.26	0.50
1:F:156:LEU:HD13	1:F:202:LEU:HD21	1.93	0.50
1:E:514:TRP:CE3	1:G:525:ARG:HD3	2.47	0.49
1:H:330:LEU:HD23	1:H:343:GLU:HB3	1.94	0.49
1:A:465:TYR:HB2	1:A:468:ILE:HD12	1.93	0.49
1:G:73:MET:HE3	1:G:86:THR:HG22	1.94	0.49
1:H:465:TYR:HB2	1:H:468:ILE:HD12	1.94	0.49
1:D:465:TYR:HB2	1:D:468:ILE:HD12	1.93	0.49
1:F:122:LEU:HB2	1:F:149:GLU:HA	1.93	0.49
1:G:225:ILE:HD12	1:G:225:ILE:H	1.78	0.49
1:D:12:ILE:HG22	1:D:13:GLN:O	2.12	0.49
1:D:70:VAL:HG22	1:D:108:ALA:HB3	1.95	0.49
1:F:133:LEU:HD12	1:F:180:ILE:HD13	1.94	0.49
1:H:408:MET:HE2	1:H:436:SER:O	2.12	0.49
1:G:425:ALA:HB1	1:G:502:PHE:HB3	1.94	0.49
1:F:176:ASP:O	1:F:179:LEU:HG	2.13	0.49
1:E:330:LEU:HD23	1:E:343:GLU:HB3	1.93	0.48
1:D:172:LYS:NZ	1:D:197:GLU:OE2	2.45	0.48
1:B:164:CYS:O	1:B:187:LYS:HE3	2.13	0.48
1:C:215:VAL:O	1:C:245:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:GLY:CA	1:E:327:THR:HG21	2.43	0.48
1:B:147:TYR:CD2	1:B:155:ILE:HD13	2.49	0.48
1:D:189:PRO:HD2	1:D:191:PHE:CE1	2.48	0.48
1:D:294:GLY:HA3	1:D:327:THR:HG21	1.95	0.48
1:G:47:ILE:HG12	1:G:70:VAL:HB	1.95	0.48
1:D:488:ARG:HD2	6:D:709:HOH:O	2.13	0.48
1:E:243:PHE:CE2	1:E:245:ARG:HD3	2.48	0.48
1:F:326:ALA:O	1:F:327:THR:HB	2.13	0.48
1:F:333:MET:CE	1:F:373:ALA:HA	2.43	0.48
1:F:70:VAL:HG22	1:F:108:ALA:HB3	1.94	0.48
1:H:188:GLY:HA3	1:H:191:PHE:CZ	2.48	0.48
1:B:145:ASN:O	1:B:148:MET:HG2	2.13	0.48
1:D:415:SER:OG	1:D:524:MET:HG3	2.13	0.48
1:C:230:PHE:CZ	1:C:234:GLN:HG3	2.49	0.48
1:H:72:ARG:NE	1:H:112:ASP:OD2	2.46	0.48
1:E:396:GLU:CD	1:H:24:THR:HB	2.38	0.48
1:G:497:LYS:NZ	1:G:530:PRO:OXT	2.46	0.48
1:E:176:ASP:OD1	1:E:206:LYS:HD2	2.14	0.48
1:E:279:PHE:CZ	1:E:312:ILE:HG23	2.48	0.48
1:H:287:ASP:O	1:H:322:PRO:HD2	2.14	0.48
1:D:339:PRO:HG3	1:D:376:MET:HG2	1.96	0.47
1:F:100:ASP:OD1	1:F:100:ASP:O	2.32	0.47
1:C:252:GLU:O	1:C:256:ILE:HG12	2.14	0.47
1:E:322:PRO:HB3	1:E:464:LEU:O	2.13	0.47
1:F:273:HIS:HB2	6:F:801:HOH:O	2.14	0.47
1:B:24:THR:HB	1:D:396:GLU:CD	2.39	0.47
1:G:425:ALA:CB	1:G:502:PHE:HB3	2.45	0.47
1:F:416:VAL:HA	1:F:419:SER:HB3	1.96	0.47
1:G:326:ALA:O	1:G:327:THR:HB	2.15	0.47
1:H:113:THR:HG23	1:H:224:ASP:OD1	2.15	0.47
1:H:116:PRO:HB2	1:H:217:LEU:HD13	1.95	0.47
1:F:330:LEU:HD23	1:F:343:GLU:HB3	1.95	0.47
1:A:326:ALA:O	1:A:327:THR:HB	2.14	0.47
1:H:273:HIS:HB2	6:H:761:HOH:O	2.13	0.47
1:H:115:GLY:HA2	1:H:224:ASP:OD2	2.15	0.47
1:E:185:LYS:C	1:E:186:GLN:HG3	2.40	0.47
1:E:219:ALA:HB3	1:E:252:GLU:HG2	1.97	0.47
1:D:143:LEU:HD22	1:D:161:LYS:HA	1.97	0.47
1:E:47:ILE:HG12	1:E:70:VAL:HB	1.96	0.47
1:A:481:TRP:CD2	1:A:516:PRO:HG3	2.50	0.46
1:D:272:ASN:HB2	6:D:730:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:MET:SD	1:G:524:MET:HE1	2.55	0.46
1:D:439:GLN:HE21	5:D:604:GOL:H31	1.80	0.46
1:F:468:ILE:O	4:F:603:TRS:O1	2.34	0.46
1:D:105:ARG:NH2	1:D:463:HIS:HE1	2.13	0.46
1:D:287:ASP:O	1:D:322:PRO:HD2	2.16	0.46
1:E:430:LEU:HD22	1:E:512:THR:HG22	1.98	0.46
1:G:223:LYS:NZ	1:G:227:ASP:OD2	2.40	0.46
1:H:392:LYS:O	1:H:396:GLU:HG3	2.15	0.46
1:E:326:ALA:CB	1:E:359:MET:HE2	2.37	0.46
1:G:60:LEU:HD13	1:G:90:VAL:HA	1.98	0.46
1:H:279:PHE:CZ	1:H:312:ILE:HG23	2.51	0.46
1:H:294:GLY:CA	1:H:327:THR:HG21	2.45	0.46
1:A:497:LYS:NZ	6:A:707:HOH:O	2.49	0.46
1:H:111:LEU:HD23	1:H:111:LEU:C	2.41	0.46
1:B:246:LYS:HE3	6:B:753:HOH:O	2.16	0.46
1:C:465:TYR:HB2	1:C:468:ILE:HD12	1.97	0.46
1:F:407:LEU:HG	1:H:526:VAL:HG11	1.98	0.46
1:D:487:LEU:C	1:D:487:LEU:HD23	2.41	0.46
1:F:84:ALA:HB2	1:F:230:PHE:HZ	1.81	0.46
1:F:181:SER:OG	1:F:197:GLU:HB2	2.15	0.46
1:G:230:PHE:CE2	1:G:234:GLN:HG3	2.50	0.46
1:F:103:LEU:N	1:F:103:LEU:HD23	2.31	0.46
1:F:140:LYS:HE3	1:F:191:PHE:CG	2.51	0.46
1:H:329:MET:HE2	1:H:347:VAL:HG22	1.98	0.46
1:B:335:LYS:NZ	1:B:368:ASP:OD2	2.31	0.45
1:C:430:LEU:HD22	1:C:512:THR:HG22	1.98	0.45
1:H:93:ALA:O	1:H:96:SER:HB3	2.15	0.45
1:A:242:SER:HA	1:A:269:LYS:HD3	1.98	0.45
1:B:287:ASP:O	1:B:322:PRO:HD2	2.16	0.45
1:F:376:MET:O	1:F:380:ILE:HG13	2.16	0.45
1:H:454:ARG:NH1	1:H:477:VAL:HG22	2.31	0.45
1:A:74:ASN:OD1	1:A:76:SER:HB2	2.16	0.45
1:A:376:MET:O	1:A:380:ILE:HG13	2.16	0.45
1:H:69:ASN:HB3	1:H:463:HIS:ND1	2.32	0.45
1:E:142:THR:HG22	1:E:143:LEU:N	2.32	0.45
1:C:21:MET:HA	1:C:21:MET:CE	2.41	0.45
1:H:370:PRO:O	1:H:374:VAL:HG23	2.17	0.45
1:A:230:PHE:CE2	1:A:234:GLN:HG3	2.52	0.45
1:C:267:ILE:HG21	1:C:324:ILE:HD12	1.98	0.45
1:G:219:ALA:HB3	1:G:252:GLU:HG2	1.98	0.45
1:A:148:MET:HE3	1:A:157:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ASP:O	1:C:322:PRO:HD2	2.17	0.45
1:G:491:LEU:O	1:G:495:VAL:HG23	2.16	0.45
1:H:60:LEU:HD13	1:H:90:VAL:HA	1.99	0.45
1:A:111:LEU:HD23	1:A:111:LEU:C	2.42	0.45
1:F:102:ILE:HG22	1:F:103:LEU:HD23	1.98	0.45
1:A:81:GLU:CD	1:A:81:GLU:H	2.24	0.44
1:B:439:GLN:O	1:B:442:ARG:HG2	2.17	0.44
1:C:118:ILE:CG2	1:C:208:VAL:HB	2.47	0.44
1:F:440:VAL:HG12	1:F:449:ILE:CD1	2.48	0.44
1:C:132:GLU:OE2	1:C:134:LYS:HE2	2.17	0.44
1:H:99:SER:O	1:H:101:PRO:HD3	2.18	0.44
1:H:504:LYS:HD3	1:H:530:PRO:O	2.17	0.44
1:F:73:MET:HE2	1:F:86:THR:CG2	2.46	0.44
1:G:267:ILE:HD12	1:G:288:GLY:HA3	1.99	0.44
1:H:333:MET:HE1	1:H:372:GLU:C	2.43	0.44
1:A:333:MET:HA	1:A:336:LYS:O	2.18	0.44
1:A:504:LYS:HD2	1:A:530:PRO:OXT	2.17	0.44
1:E:329:MET:O	1:E:330:LEU:HD23	2.17	0.44
1:G:259:GLU:O	1:G:262:LYS:HG2	2.17	0.44
1:G:318:ARG:HG3	1:G:400:ALA:HB1	1.99	0.44
1:H:18:HIS:CE1	1:H:31:ARG:HD3	2.53	0.44
1:H:113:THR:HG22	1:H:115:GLY:N	2.32	0.44
1:H:131:VAL:HG11	1:H:152:ASP:HA	1.98	0.44
1:B:147:TYR:CE2	1:B:155:ILE:HD13	2.53	0.44
1:F:514:TRP:CD2	1:H:525:ARG:HD3	2.53	0.44
1:F:526:VAL:HG21	1:H:407:LEU:HG	1.99	0.44
1:G:333:MET:HA	1:G:336:LYS:O	2.17	0.44
1:E:174:TYR:HB2	1:E:209:ASN:HB2	2.00	0.44
1:E:215:VAL:HG11	1:E:217:LEU:HD12	1.98	0.44
1:A:279:PHE:CZ	1:A:312:ILE:HG23	2.53	0.44
1:D:132:GLU:HB2	1:D:201:PHE:CE1	2.53	0.44
1:C:514:TRP:CD2	1:D:525:ARG:HD3	2.52	0.44
1:F:230:PHE:CE2	1:F:234:GLN:HG3	2.53	0.44
1:H:103:LEU:HD22	1:H:103:LEU:N	2.33	0.44
1:H:326:ALA:O	1:H:327:THR:HB	2.18	0.44
1:F:326:ALA:HB1	1:F:359:MET:HE2	2.00	0.43
1:F:389:PHE:CE2	1:F:392:LYS:HG3	2.53	0.43
1:C:273:HIS:HB2	6:C:805:HOH:O	2.18	0.43
1:C:330:LEU:HD11	1:C:377:GLN:HG3	1.99	0.43
1:C:487:LEU:C	1:C:487:LEU:HD23	2.42	0.43
1:B:294:GLY:N	1:B:327:THR:HG21	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:ASN:O	1:G:148:MET:HE2	2.18	0.43
1:C:162:ASN:OD1	1:C:165:LYS:NZ	2.43	0.43
1:F:504:LYS:HA	1:F:529:VAL:O	2.18	0.43
1:A:430:LEU:HD22	1:A:512:THR:HG22	2.00	0.43
1:D:526:VAL:O	1:D:526:VAL:HG13	2.18	0.43
1:E:24:THR:HB	1:H:396:GLU:CD	2.44	0.43
1:G:272:ASN:HB2	6:G:726:HOH:O	2.17	0.43
1:A:115:GLY:HA2	1:A:224:ASP:OD2	2.19	0.43
1:C:141:ILE:HA	1:C:156:LEU:O	2.18	0.43
1:C:189:PRO:HD2	1:C:191:PHE:CE2	2.53	0.43
1:D:135:LYS:HE2	1:D:197:GLU:O	2.19	0.42
1:E:160:TYR:OH	1:E:216:ASP:OD1	2.25	0.42
1:B:333:MET:HA	1:B:336:LYS:O	2.19	0.42
1:D:273:HIS:ND1	1:D:300:ILE:HG22	2.33	0.42
1:F:103:LEU:HA	1:F:499:ARG:NH1	2.35	0.42
1:G:217:LEU:HB3	1:G:218:PRO:HD2	2.01	0.42
1:C:27:GLU:O	1:C:31:ARG:HG3	2.19	0.42
1:D:120:THR:HB	1:D:156:LEU:HD11	2.02	0.42
1:H:231:GLY:O	1:H:236:VAL:HG22	2.19	0.42
1:H:279:PHE:CE1	1:H:312:ILE:HG23	2.55	0.42
1:C:339:PRO:HG3	1:C:376:MET:HG2	2.00	0.42
1:E:123:ILE:HG22	1:E:124:LYS:HG2	2.01	0.42
1:H:496:GLY:HA3	1:H:502:PHE:CZ	2.54	0.42
1:E:123:ILE:HG21	1:E:131:VAL:HG13	2.02	0.42
1:F:411:MET:SD	1:H:526:VAL:HG23	2.60	0.42
1:H:80:HIS:CE1	1:H:230:PHE:HB2	2.55	0.42
1:C:367:GLY:HA3	6:C:783:HOH:O	2.18	0.42
1:G:122:LEU:O	1:G:151:CYS:HB2	2.20	0.42
1:C:452:VAL:HG11	1:C:488:ARG:HB3	2.02	0.42
1:D:142:THR:HG21	1:D:155:ILE:HD11	2.01	0.42
1:F:252:GLU:OE1	1:F:252:GLU:HA	2.19	0.42
1:H:120:THR:O	1:H:205:LYS:HA	2.19	0.42
1:B:172:LYS:HA	1:B:182:LEU:O	2.19	0.42
1:E:341:ARG:NH2	1:H:297:GLY:HA3	2.35	0.42
1:H:290:MET:HE2	1:H:359:MET:SD	2.60	0.42
1:E:425:ALA:HB1	1:E:502:PHE:HB3	2.02	0.42
1:E:481:TRP:CD2	1:E:516:PRO:HG3	2.55	0.42
1:H:265:LYS:HA	1:H:265:LYS:HD3	1.88	0.42
1:C:120:THR:HB	1:C:156:LEU:HD11	2.02	0.42
1:E:227:ASP:O	1:E:230:PHE:HB3	2.20	0.42
1:F:79:THR:HG23	6:F:826:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:ILE:O	1:H:124:LYS:C	2.63	0.42
1:D:322:PRO:HA	1:D:356:ASP:OD2	2.19	0.41
1:E:27:GLU:O	1:E:31:ARG:HG3	2.20	0.41
1:F:279:PHE:CZ	1:F:312:ILE:HG23	2.55	0.41
1:F:294:GLY:CA	1:F:327:THR:HG21	2.50	0.41
1:A:13:GLN:HB3	6:A:863:HOH:O	2.20	0.41
1:B:112:ASP:HA	1:B:240:PHE:HB2	2.01	0.41
1:H:268:SER:HB2	1:H:289:ILE:HD13	2.01	0.41
1:A:322:PRO:HB3	1:A:464:LEU:O	2.21	0.41
1:C:246:LYS:NZ	6:C:713:HOH:O	2.52	0.41
1:C:525:ARG:HD3	1:D:514:TRP:CD2	2.54	0.41
1:E:496:GLY:HA3	1:E:502:PHE:CZ	2.55	0.41
1:G:526:VAL:O	1:G:526:VAL:HG13	2.20	0.41
1:F:242:SER:HA	1:F:269:LYS:HD3	2.02	0.41
1:G:215:VAL:CG1	1:G:217:LEU:HD12	2.51	0.41
1:B:526:VAL:O	1:B:526:VAL:HG13	2.20	0.41
1:D:230:PHE:CE2	1:D:234:GLN:HG3	2.55	0.41
1:F:62:GLU:OE2	1:F:65:LYS:HE2	2.20	0.41
1:B:80:HIS:NE2	1:B:227:ASP:OD1	2.44	0.41
1:B:291:VAL:HG12	1:B:293:ARG:HG2	2.03	0.41
1:C:333:MET:HA	1:C:336:LYS:O	2.19	0.41
1:D:273:HIS:HB2	6:D:848:HOH:O	2.20	0.41
1:F:412:ALA:O	1:F:416:VAL:HG23	2.21	0.41
1:F:469:PHE:HA	4:F:603:TRS:O1	2.21	0.41
1:G:187:LYS:HG3	1:G:192:LEU:CD2	2.51	0.41
1:H:122:LEU:HB2	1:H:149:GLU:HA	2.03	0.41
1:A:254:ARG:CZ	1:A:266:ILE:HD12	2.51	0.41
1:A:267:ILE:CD1	1:A:288:GLY:HA3	2.50	0.41
1:F:310:LYS:HB3	1:G:29:MET:HG2	2.03	0.41
1:F:481:TRP:CD2	1:F:516:PRO:HG3	2.56	0.41
1:H:123:ILE:HG22	1:H:124:LYS:HG2	2.02	0.41
1:H:225:ILE:O	1:H:229:LYS:HG3	2.21	0.41
1:C:294:GLY:CA	1:C:327:THR:HG21	2.50	0.41
1:E:118:ILE:HG12	1:E:160:TYR:HB2	2.03	0.41
1:G:408:MET:HE3	1:G:408:MET:O	2.21	0.41
1:H:243:PHE:CE2	1:H:245:ARG:HD3	2.56	0.40
1:F:112:ASP:HA	1:F:240:PHE:HB2	2.03	0.40
1:F:339:PRO:CD	1:F:376:MET:HE3	2.51	0.40
1:G:496:GLY:HA3	1:G:502:PHE:CZ	2.56	0.40
1:C:230:PHE:CE2	1:C:234:GLN:HG3	2.56	0.40
1:E:141:ILE:HA	1:E:156:LEU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:PRO:HB3	1:F:464:LEU:O	2.22	0.40
1:A:432:GLU:HB3	6:A:923:HOH:O	2.21	0.40
1:D:427:LEU:HA	1:D:509:ILE:O	2.21	0.40
1:F:421:LYS:HE2	1:H:413:MET:SD	2.62	0.40
1:F:440:VAL:HG12	1:F:449:ILE:HD13	2.04	0.40
1:F:267:ILE:HD12	1:F:288:GLY:HA3	2.04	0.40
1:H:485:VAL:O	1:H:489:VAL:HG23	2.21	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	518/531 (98%)	507 (98%)	10 (2%)	1 (0%)	43 57
1	B	518/531 (98%)	507 (98%)	10 (2%)	1 (0%)	43 57
1	C	518/531 (98%)	507 (98%)	10 (2%)	1 (0%)	43 57
1	D	518/531 (98%)	508 (98%)	9 (2%)	1 (0%)	43 57
1	E	518/531 (98%)	501 (97%)	16 (3%)	1 (0%)	43 57
1	F	517/531 (97%)	502 (97%)	14 (3%)	1 (0%)	43 57
1	G	511/531 (96%)	496 (97%)	14 (3%)	1 (0%)	43 57
1	H	517/531 (97%)	496 (96%)	18 (4%)	3 (1%)	21 30
All	All	4135/4248 (97%)	4024 (97%)	101 (2%)	10 (0%)	43 57

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	THR
1	B	327	THR
1	D	327	THR

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Mol	Chain	Res	Type
1	A	327	THR
1	E	327	THR
1	F	327	THR
1	G	327	THR
1	H	327	THR
1	H	124	LYS
1	H	78	GLY

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	426/434 (98%)	424 (100%)	2 (0%)	81	90
1	B	426/434 (98%)	424 (100%)	2 (0%)	81	90
1	C	426/434 (98%)	424 (100%)	2 (0%)	81	90
1	D	426/434 (98%)	426 (100%)	0	100	100
1	E	426/434 (98%)	423 (99%)	3 (1%)	76	87
1	F	425/434 (98%)	421 (99%)	4 (1%)	70	84
1	G	423/434 (98%)	421 (100%)	2 (0%)	81	90
1	H	425/434 (98%)	423 (100%)	2 (0%)	81	90
All	All	3403/3472 (98%)	3386 (100%)	17 (0%)	81	90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	76	SER
1	B	25	PHE
1	B	407	LEU
1	C	260	LYS
1	C	345	SER
1	E	186	GLN
1	E	345	SER

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Mol	Chain	Res	Type
1	E	435	ARG
1	F	143	LEU
1	F	181	SER
1	F	407	LEU
1	F	419	SER
1	G	131	VAL
1	G	399	ARG
1	H	96	SER
1	H	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	183	GLN
1	A	209	ASN
1	A	478	GLN
1	A	494	ASN
1	B	209	ASN
1	C	186	GLN
1	D	18	HIS
1	D	198	ASN
1	D	209	ASN
1	D	251	HIS
1	D	490	ASN
1	E	273	HIS
1	E	439	GLN
1	F	18	HIS
1	F	494	ASN
1	G	18	HIS
1	G	403	HIS
1	H	457	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 16 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	B	603	-	5,5,5	1.18	1 (20%)	5,5,5	1.39	1 (20%)
4	TRS	A	603	-	7,7,7	0.25	0	9,9,9	0.80	0
5	GOL	E	604	-	5,5,5	0.88	0	5,5,5	1.27	1 (20%)
4	TRS	E	603	-	7,7,7	0.32	0	9,9,9	0.28	0
4	TRS	H	603	-	7,7,7	0.30	0	9,9,9	0.49	0
4	TRS	D	603	-	7,7,7	0.27	0	9,9,9	0.43	0
4	TRS	F	603	-	7,7,7	0.33	0	9,9,9	0.35	0
5	GOL	D	604	-	5,5,5	1.04	0	5,5,5	1.28	1 (20%)
4	TRS	G	603	-	7,7,7	0.28	0	9,9,9	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	603	-	-	2/4/4/4	-
4	TRS	A	603	-	-	3/9/9/9	-
5	GOL	E	604	-	-	1/4/4/4	-
4	TRS	E	603	-	-	3/9/9/9	-
4	TRS	H	603	-	-	3/9/9/9	-
4	TRS	D	603	-	-	5/9/9/9	-
4	TRS	F	603	-	-	2/9/9/9	-
5	GOL	D	604	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TRS	G	603	-	-	6/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	603	GOL	O2-C2	-2.02	1.37	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	603	GOL	C3-C2-C1	-2.79	101.55	111.80
5	D	604	GOL	C3-C2-C1	-2.45	102.80	111.80
5	E	604	GOL	C3-C2-C1	-2.39	103.03	111.80

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	TRS	N-C-C3-O3
4	D	603	TRS	C1-C-C3-O3
4	D	603	TRS	C2-C-C3-O3
4	D	603	TRS	N-C-C3-O3
4	E	603	TRS	N-C-C2-O2
4	G	603	TRS	C2-C-C1-O1
4	G	603	TRS	C3-C-C1-O1
4	G	603	TRS	N-C-C3-O3
4	H	603	TRS	C3-C-C2-O2
4	H	603	TRS	N-C-C2-O2
5	B	603	GOL	C1-C2-C3-O3
5	D	604	GOL	O1-C1-C2-C3
4	A	603	TRS	C1-C-C3-O3
4	E	603	TRS	C3-C-C2-O2
4	G	603	TRS	C1-C-C3-O3
5	D	604	GOL	O1-C1-C2-O2
5	B	603	GOL	O2-C2-C3-O3
4	G	603	TRS	N-C-C1-O1
4	H	603	TRS	C1-C-C2-O2
4	A	603	TRS	C2-C-C3-O3
4	E	603	TRS	C1-C-C2-O2
4	D	603	TRS	C3-C-C2-O2
4	F	603	TRS	C2-C-C3-O3

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Mol	Chain	Res	Type	Atoms
4	G	603	TRS	C2-C-C3-O3
5	E	604	GOL	O1-C1-C2-C3
4	D	603	TRS	N-C-C2-O2
4	F	603	TRS	N-C-C3-O3

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	TRS	1	0
5	E	604	GOL	2	0
4	D	603	TRS	3	0
4	F	603	TRS	2	0
5	D	604	GOL	2	0
4	G	603	TRS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	520/531 (97%)	-0.46	1 (0%) 91 90	23, 33, 68, 91	0
1	B	520/531 (97%)	-0.41	1 (0%) 91 90	24, 37, 57, 100	0
1	C	520/531 (97%)	-0.43	2 (0%) 88 87	26, 39, 58, 83	0
1	D	520/531 (97%)	-0.27	2 (0%) 88 87	27, 41, 64, 87	0
1	E	520/531 (97%)	-0.07	24 (4%) 37 33	26, 40, 88, 119	0
1	F	519/531 (97%)	-0.10	4 (0%) 82 80	33, 49, 70, 106	0
1	G	515/531 (96%)	0.13	19 (3%) 45 41	30, 48, 106, 136	0
1	H	519/531 (97%)	-0.01	5 (0%) 79 77	28, 47, 69, 103	0
All	All	4153/4248 (97%)	-0.20	58 (1%) 73 70	23, 42, 75, 136	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	147	TYR	4.0
1	H	125	GLY	3.6
1	G	169	VAL	3.6
1	A	11	PHE	3.4
1	F	103	LEU	3.3
1	E	155	ILE	3.1
1	F	12	ILE	3.0
1	E	25	PHE	3.0
1	H	126	SER	3.0
1	H	127	GLY	3.0
1	G	122	LEU	2.9
1	G	156	LEU	2.9
1	E	121	GLY	2.9
1	G	191	PHE	2.8
1	E	140	LYS	2.8
1	H	128	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	192	LEU	2.8
1	E	193	VAL	2.7
1	G	137	ALA	2.7
1	E	125	GLY	2.7
1	F	102	ILE	2.7
1	C	99	SER	2.7
1	C	11	PHE	2.7
1	H	124	LYS	2.7
1	G	11	PHE	2.6
1	G	192	LEU	2.6
1	G	193	VAL	2.5
1	E	131	VAL	2.5
1	E	142	THR	2.5
1	G	201	PHE	2.5
1	E	150	LYS	2.4
1	E	122	LEU	2.4
1	G	185	LYS	2.4
1	E	11	PHE	2.4
1	D	23	ASP	2.4
1	D	11	PHE	2.4
1	G	147	TYR	2.4
1	G	167	VAL	2.4
1	E	200	GLY	2.3
1	G	189	PRO	2.3
1	E	139	LEU	2.3
1	E	146	ALA	2.2
1	G	155	ILE	2.2
1	B	11	PHE	2.2
1	E	189	PRO	2.2
1	G	129	ALA	2.2
1	E	201	PHE	2.2
1	G	148	MET	2.1
1	E	144	ASP	2.1
1	G	141	ILE	2.1
1	G	187	LYS	2.1
1	G	150	LYS	2.1
1	E	151	CYS	2.1
1	E	157	TRP	2.1
1	E	127	GLY	2.1
1	E	141	ILE	2.1
1	F	101	PRO	2.0
1	E	169	VAL	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.

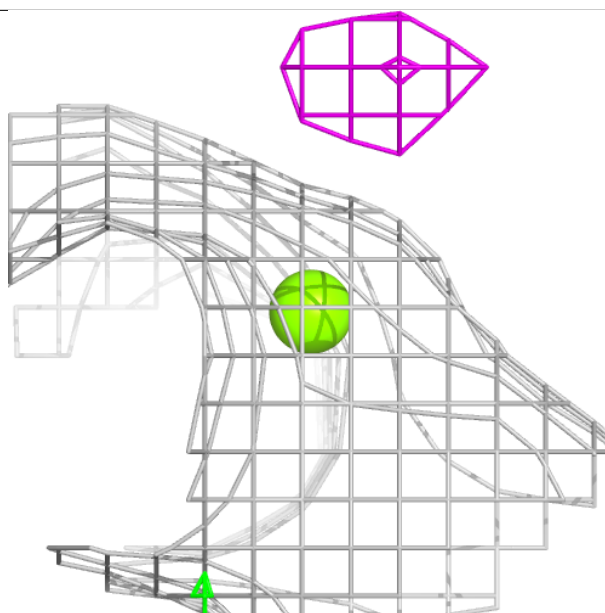
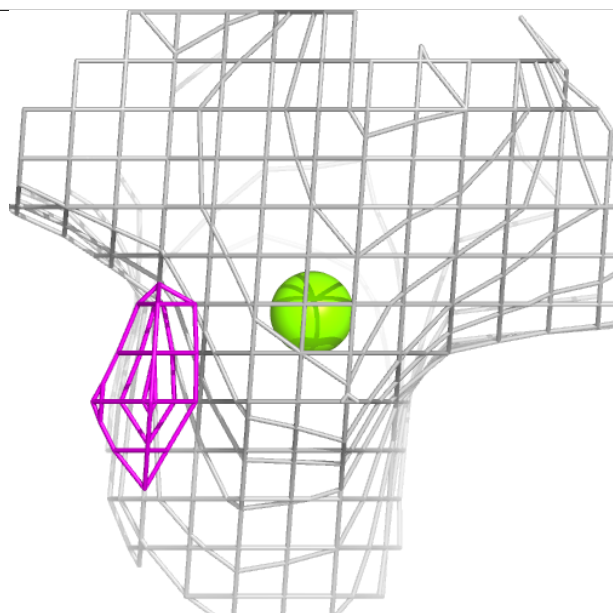
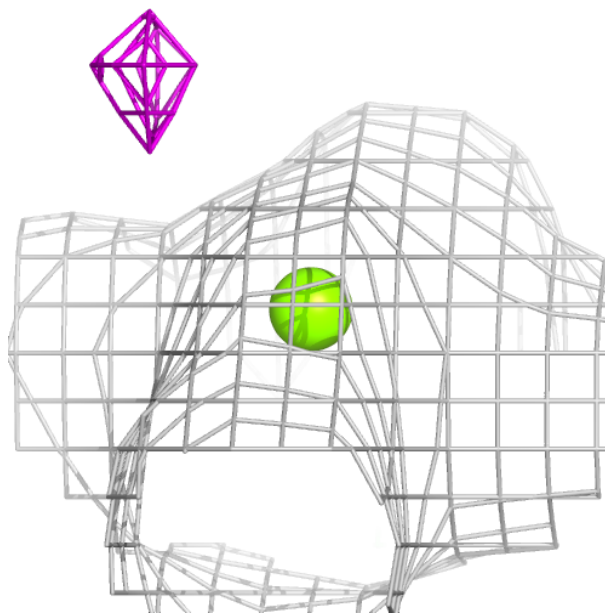
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TRS	F	603	8/8	0.82	0.18	58,68,72,81	0
4	TRS	G	603	8/8	0.83	0.17	52,57,61,65	0
5	GOL	D	604	6/6	0.85	0.17	55,69,83,83	0
5	GOL	E	604	6/6	0.87	0.14	45,61,70,73	0
4	TRS	D	603	8/8	0.89	0.11	41,47,51,55	0
5	GOL	B	603	6/6	0.89	0.19	41,55,66,66	0
4	TRS	E	603	8/8	0.89	0.13	45,49,51,59	0
4	TRS	A	603	8/8	0.89	0.13	34,39,42,47	0
4	TRS	H	603	8/8	0.90	0.12	50,55,60,66	0
2	MG	H	601	1/1	0.94	0.05	52,52,52,52	0
2	MG	G	601	1/1	0.94	0.06	68,68,68,68	0
3	NA	H	602	1/1	0.96	0.06	39,39,39,39	0
3	NA	F	602	1/1	0.96	0.10	43,43,43,43	0
3	NA	B	602	1/1	0.97	0.09	27,27,27,27	0
3	NA	D	602	1/1	0.98	0.11	34,34,34,34	0
3	NA	E	602	1/1	0.98	0.11	29,29,29,29	0
2	MG	C	601	1/1	0.98	0.03	36,36,36,36	0
3	NA	G	602	1/1	0.98	0.13	31,31,31,31	0
2	MG	D	601	1/1	0.98	0.04	44,44,44,44	0
2	MG	F	601	1/1	0.98	0.05	50,50,50,50	0
3	NA	C	602	1/1	0.98	0.10	31,31,31,31	0
2	MG	B	601	1/1	0.99	0.03	41,41,41,41	0
2	MG	E	601	1/1	0.99	0.03	50,50,50,50	0
2	MG	A	601	1/1	0.99	0.03	41,41,41,41	0
3	NA	A	602	1/1	1.00	0.08	25,25,25,25	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.

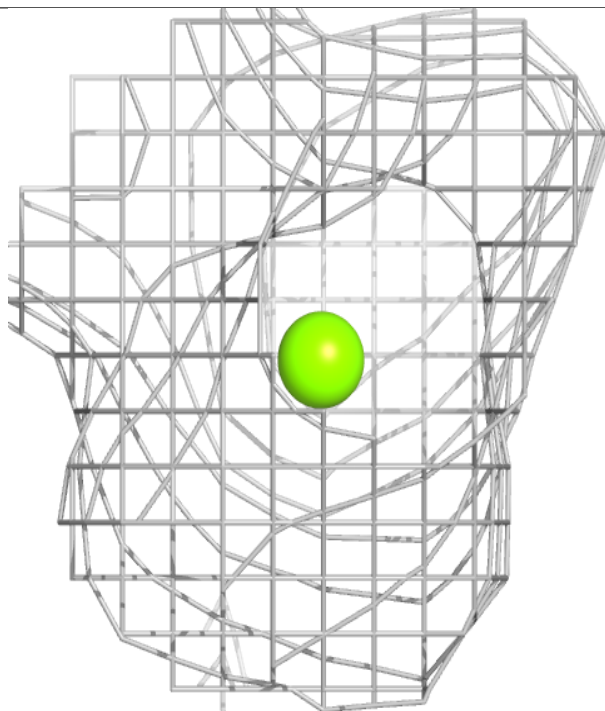
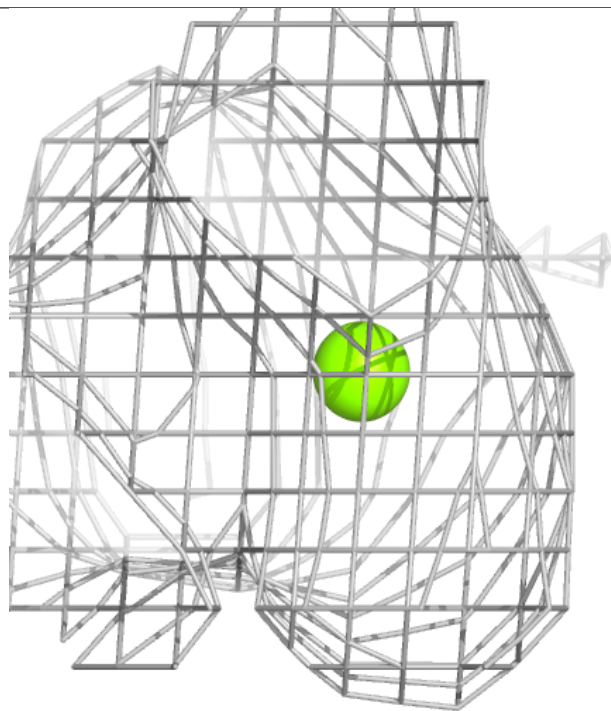
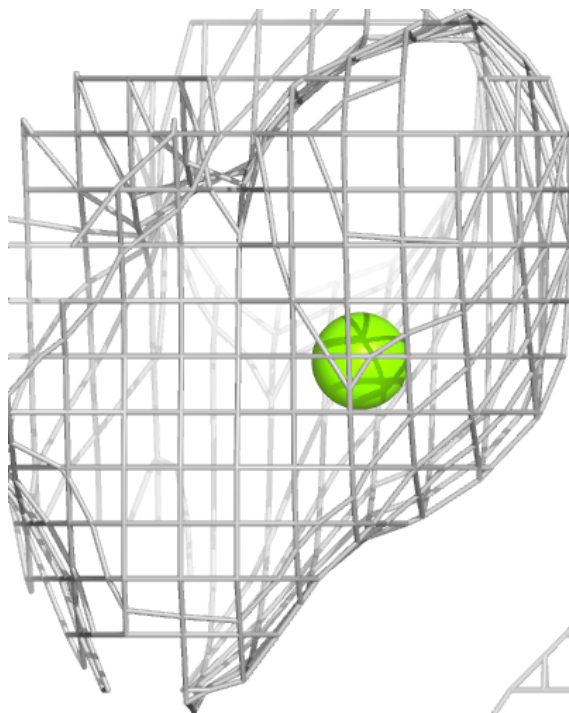
Electron density around MG H 601:

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



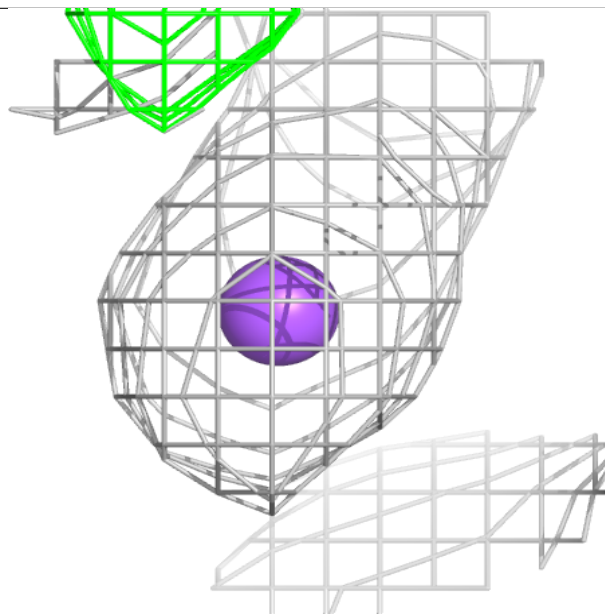
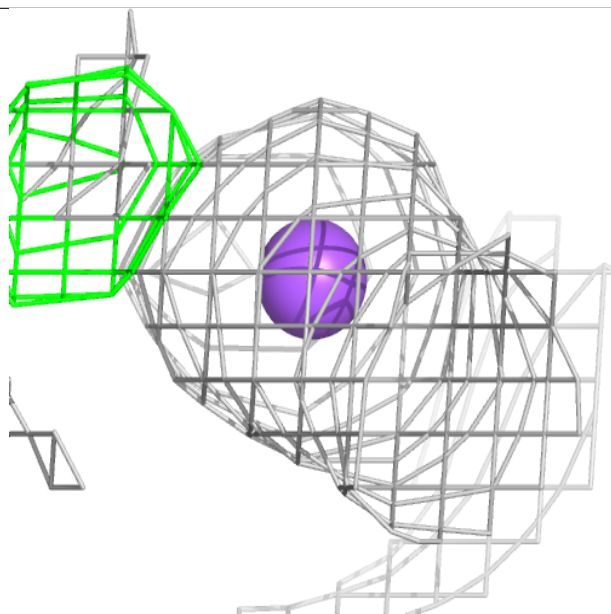
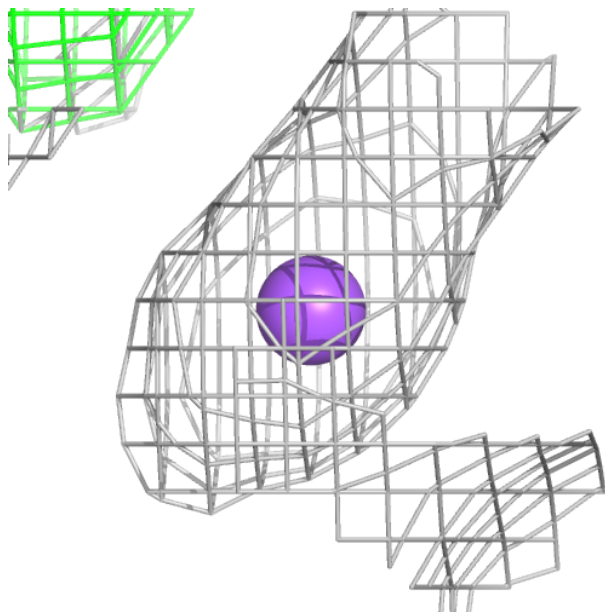
Electron density around MG G 601:

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



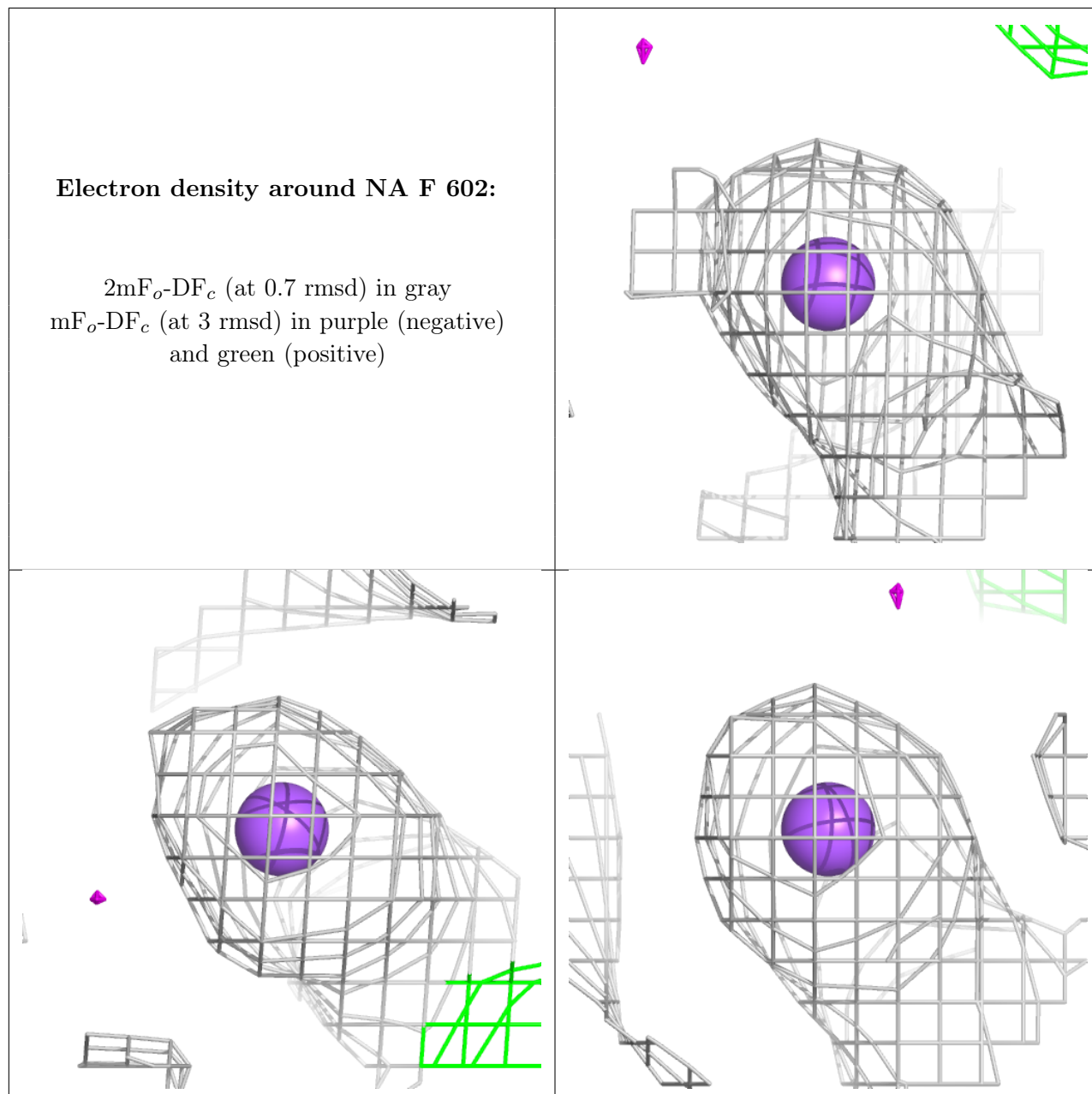
Electron density around NA H 602:

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



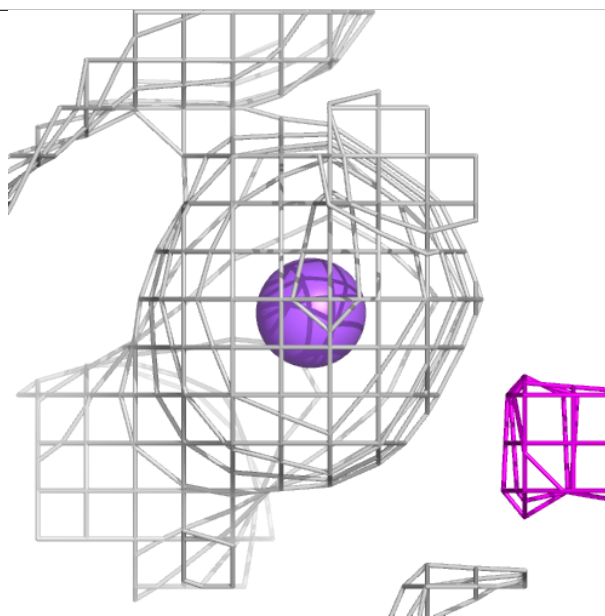
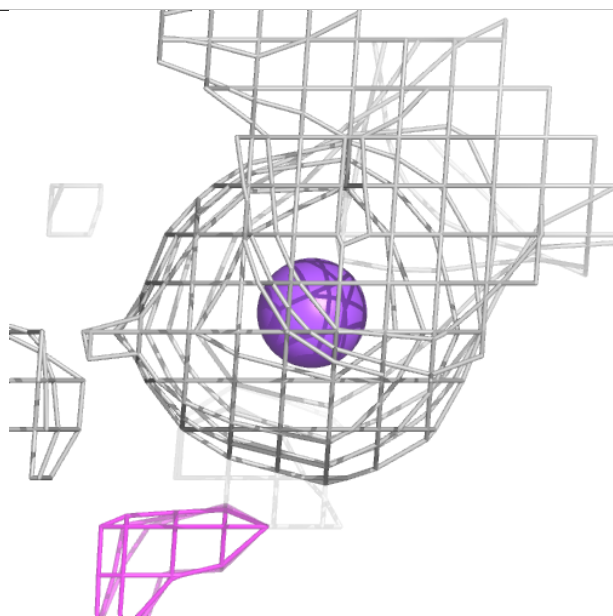
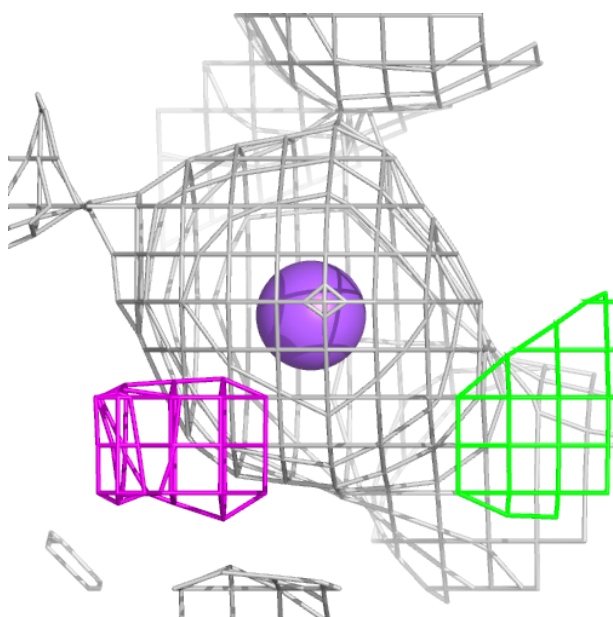
Electron density around NA F 602:

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



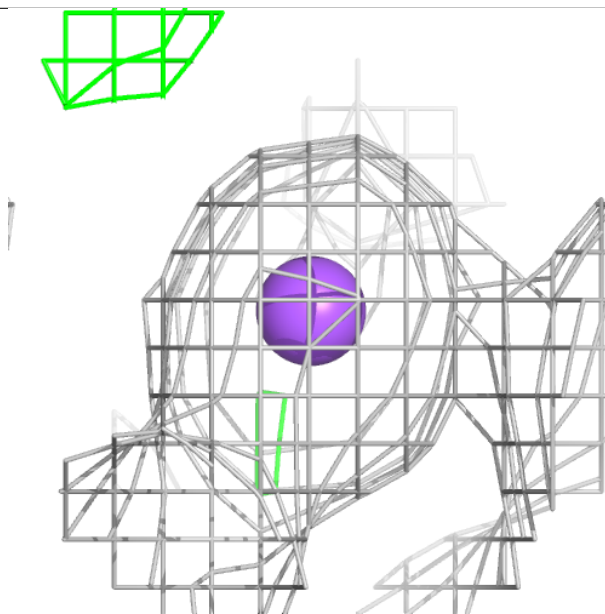
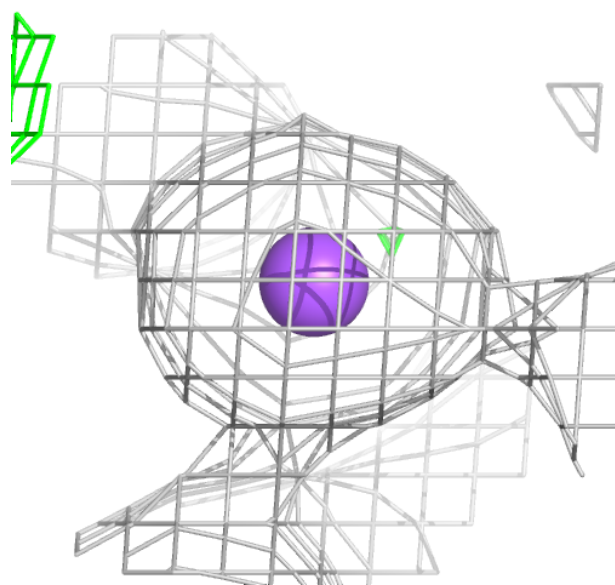
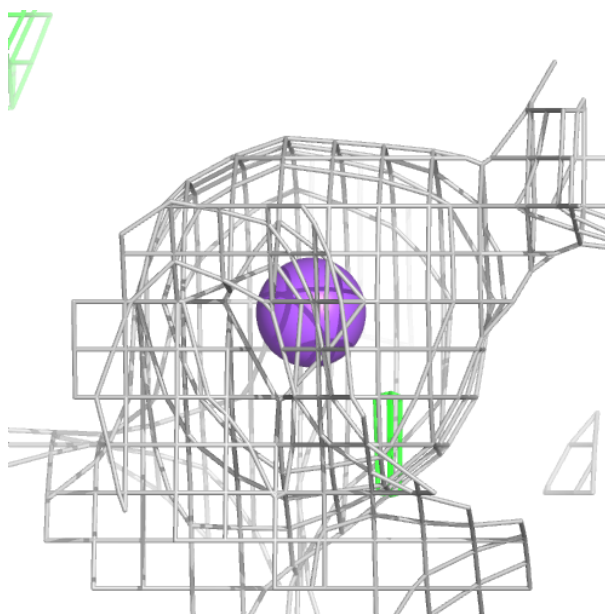
Electron density around NA B 602:

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



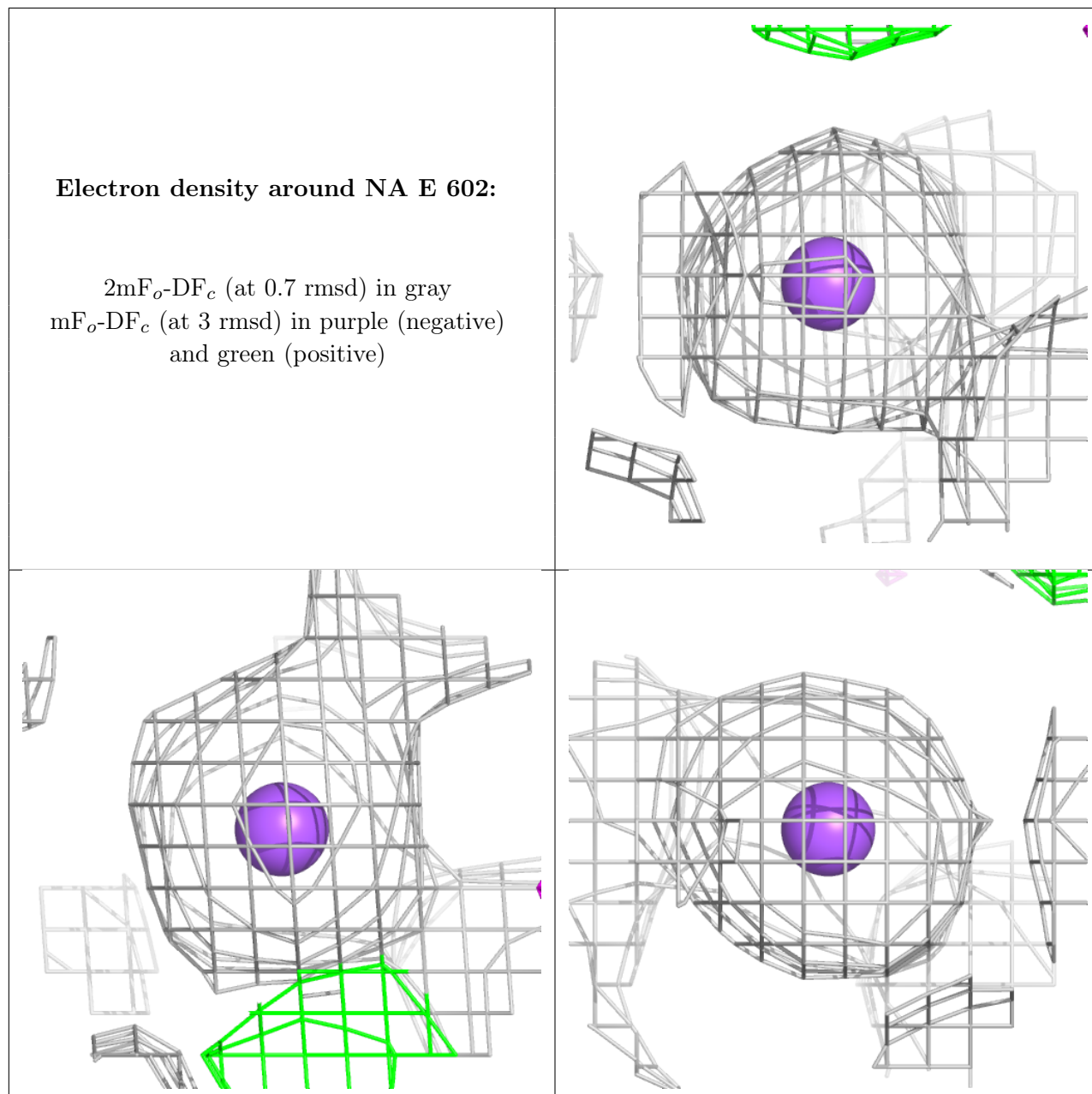
Electron density around NA D 602:

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



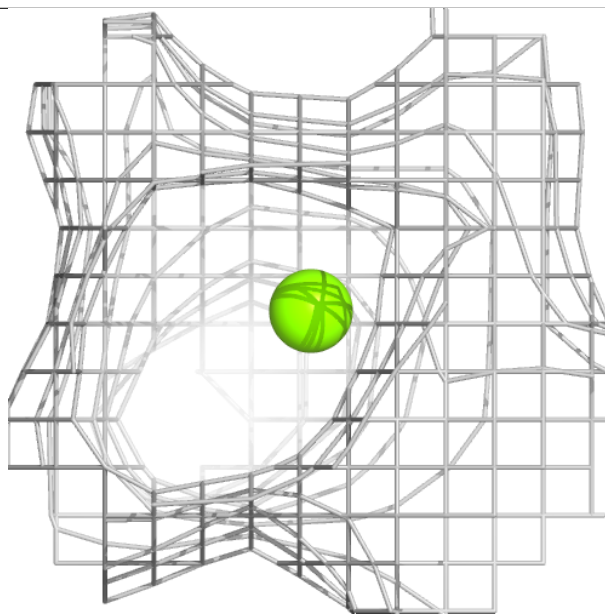
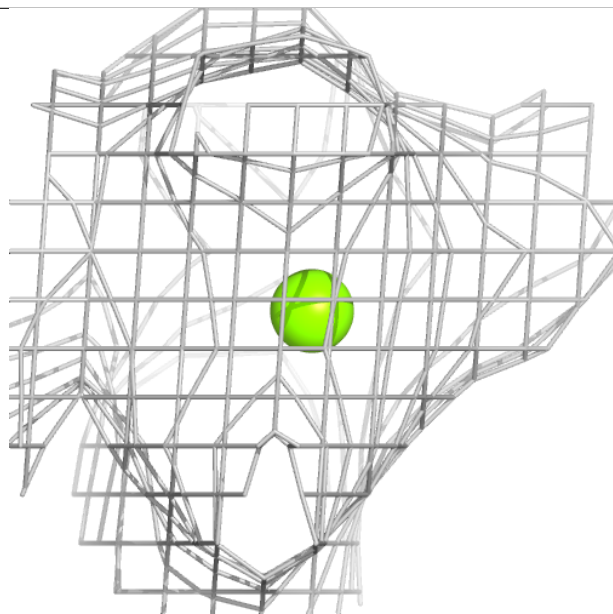
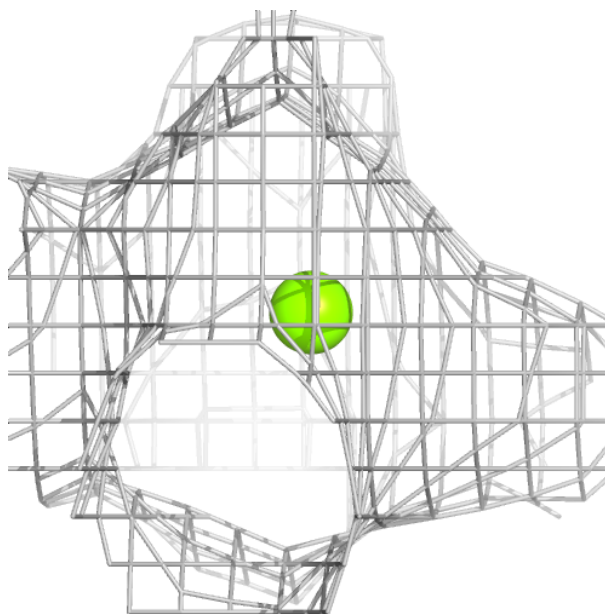
Electron density around NA E 602:

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



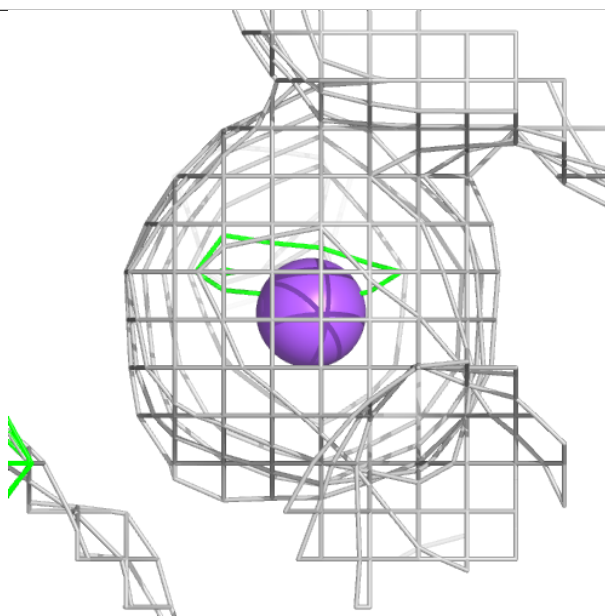
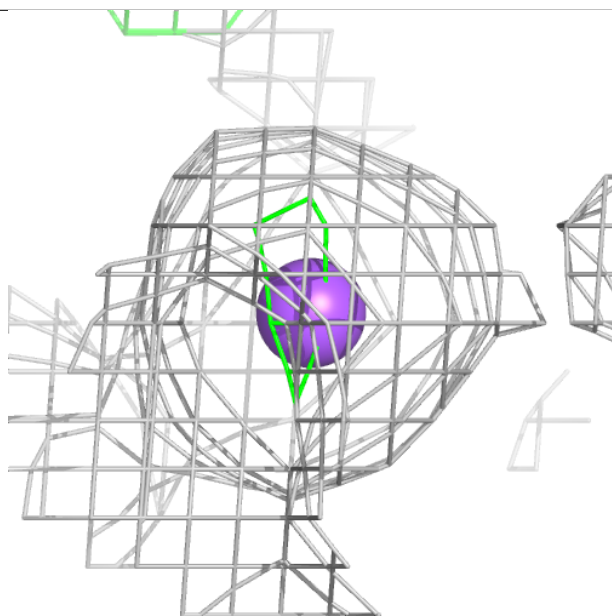
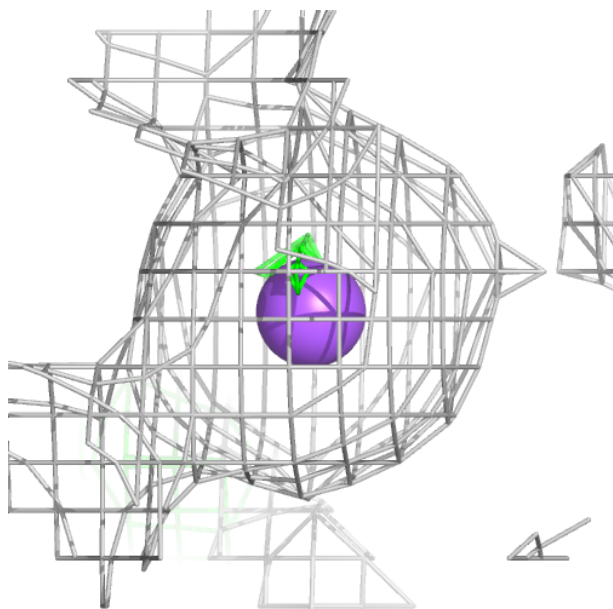
Electron density around MG C 601:

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



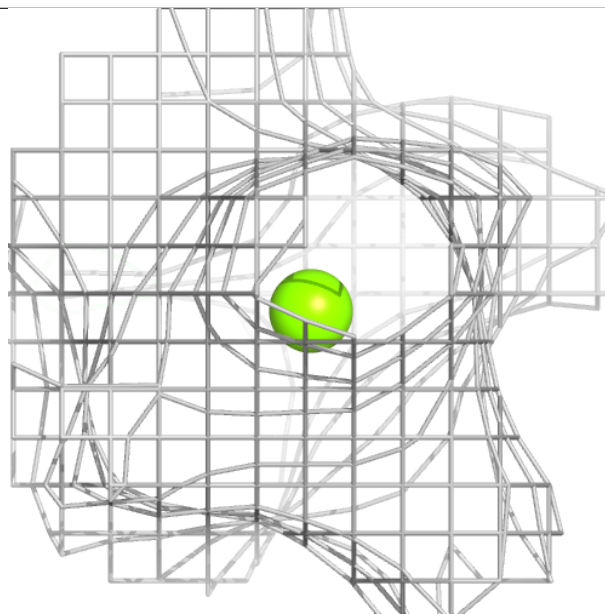
Electron density around NA G 602:

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



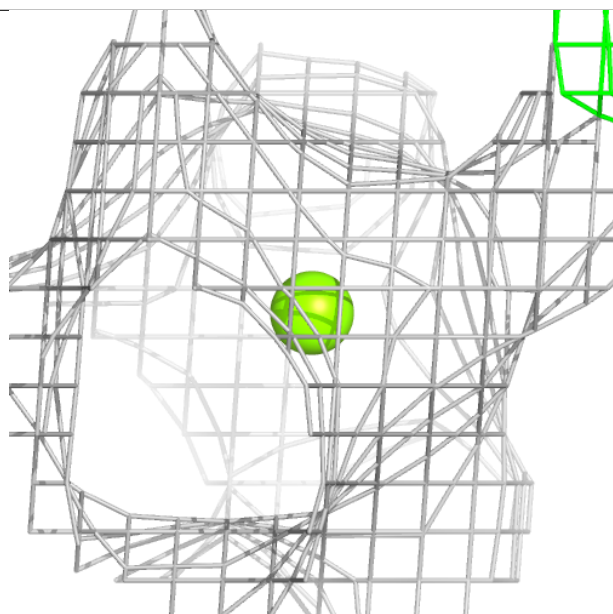
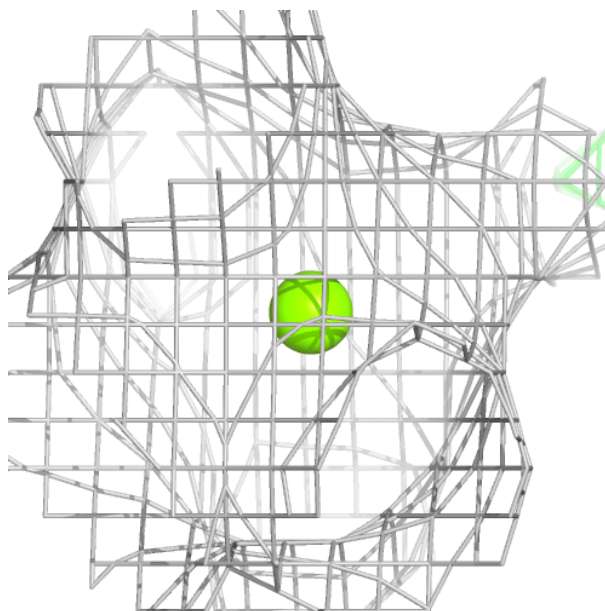
Electron density around MG D 601:

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



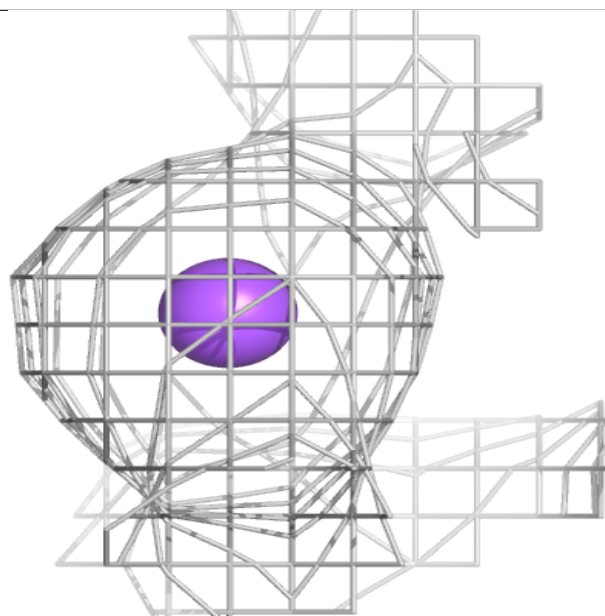
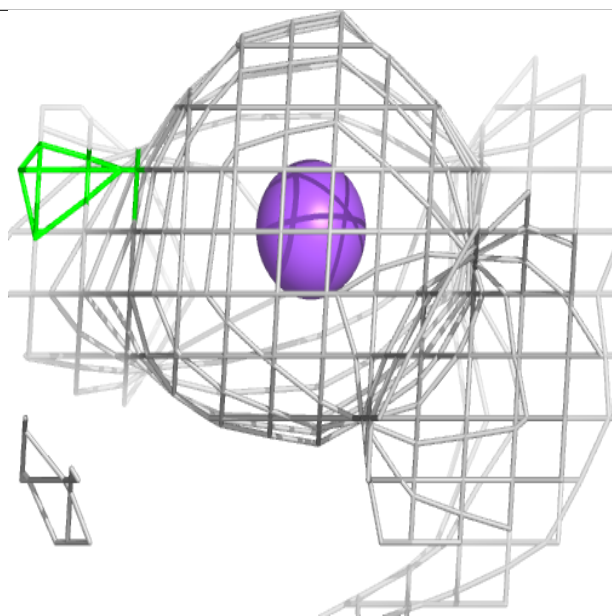
Electron density around MG F 601:

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



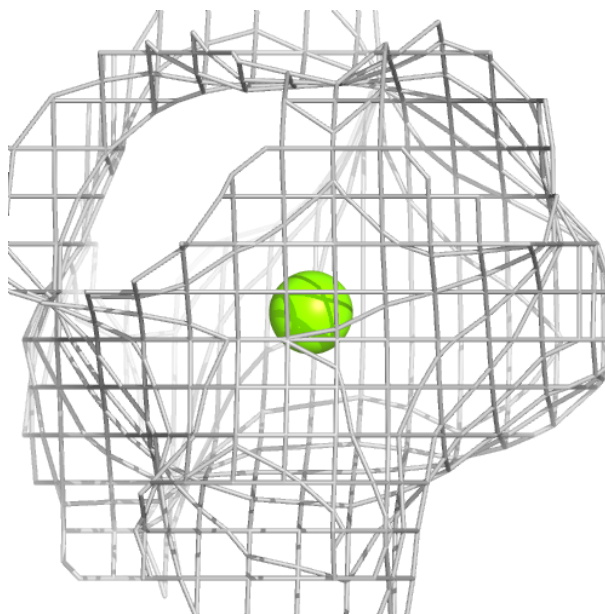
Electron density around NA C 602:

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



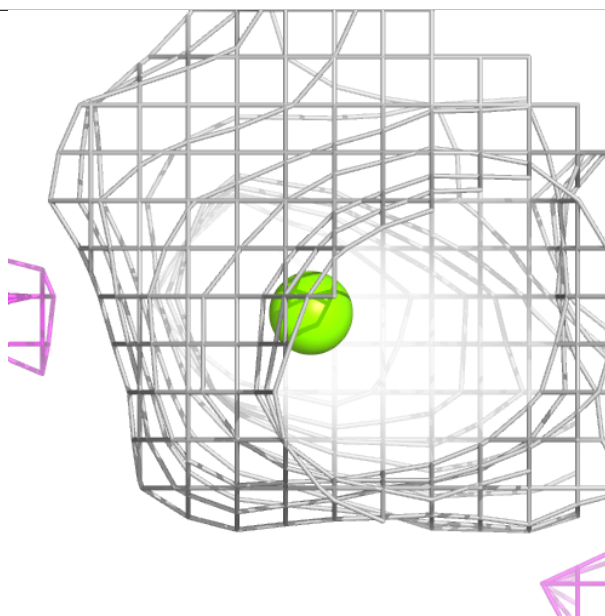
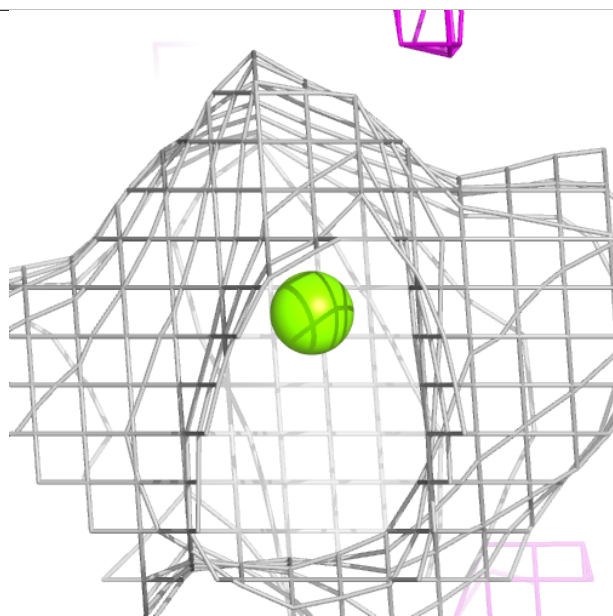
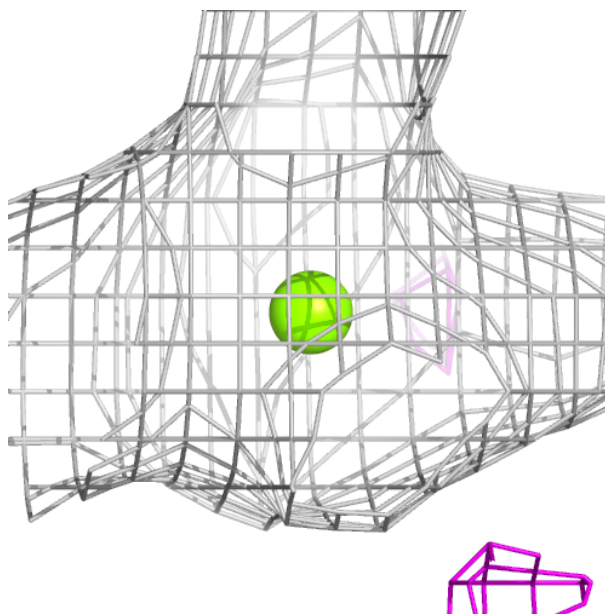
Electron density around MG B 601:

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



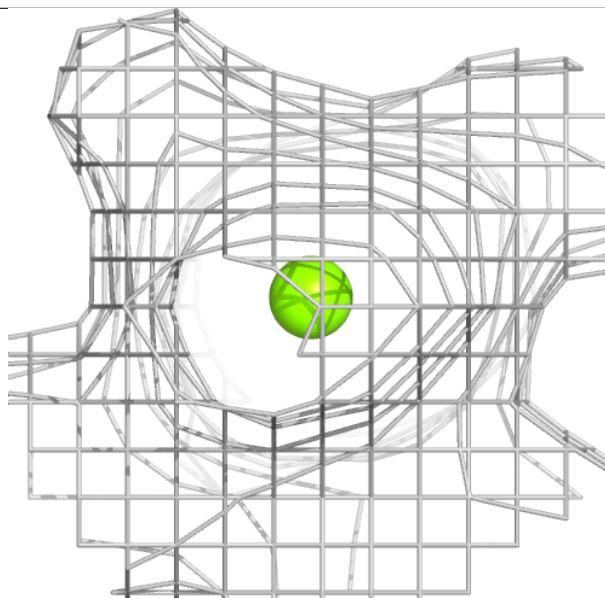
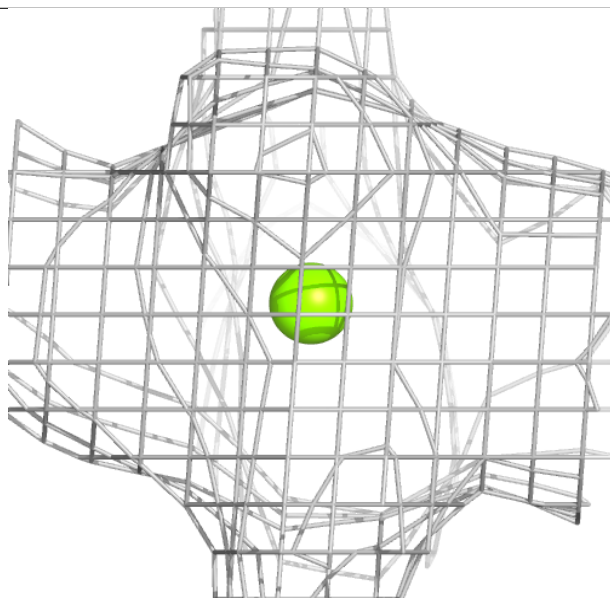
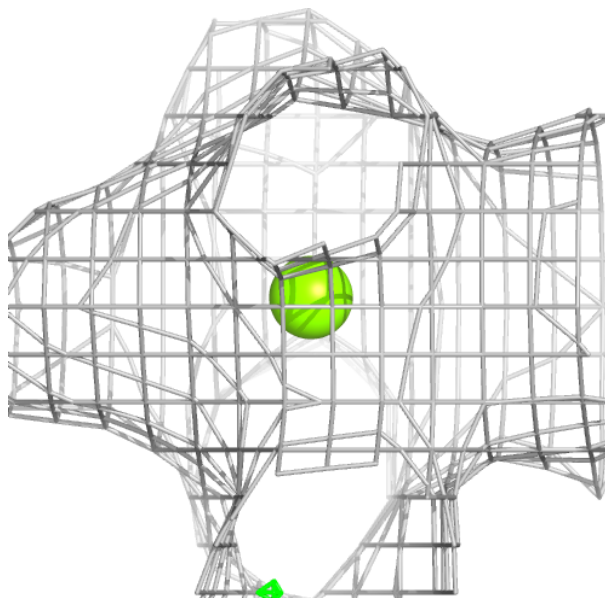
Electron density around MG E 601:

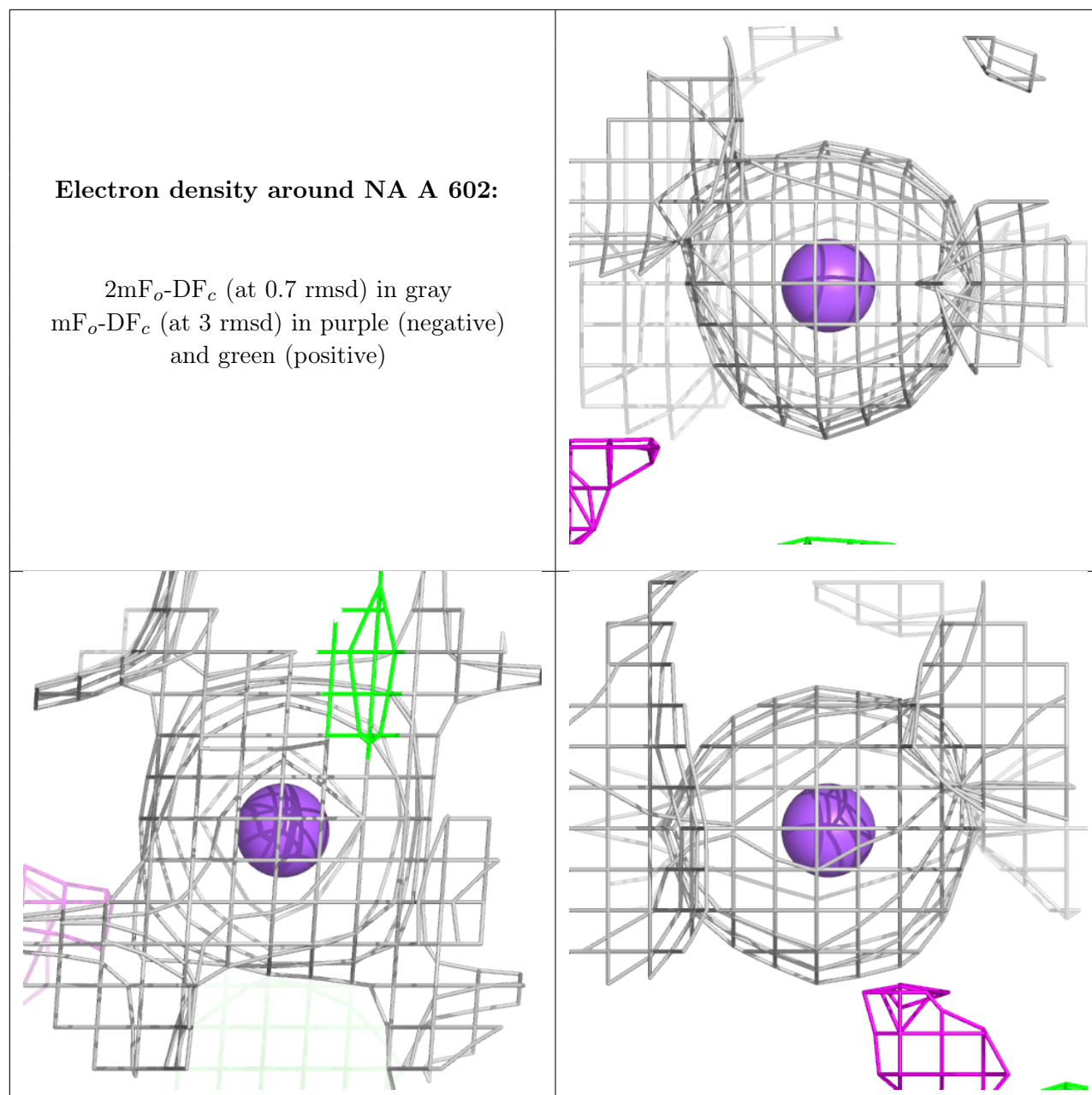
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.