Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 02:06 PM JST

PDB ID	:	7XA7
Title	:	Crystal structure of SARS-CoV-2 receptor-binding domain in complex with intermediate horseshoe bat ACE2
Authors	:	Tang, L.F.; Zhang, D.; Han, P.; Qi, J.X.
Deposited on	:	2022-03-17
Resolution	:	3.31 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:

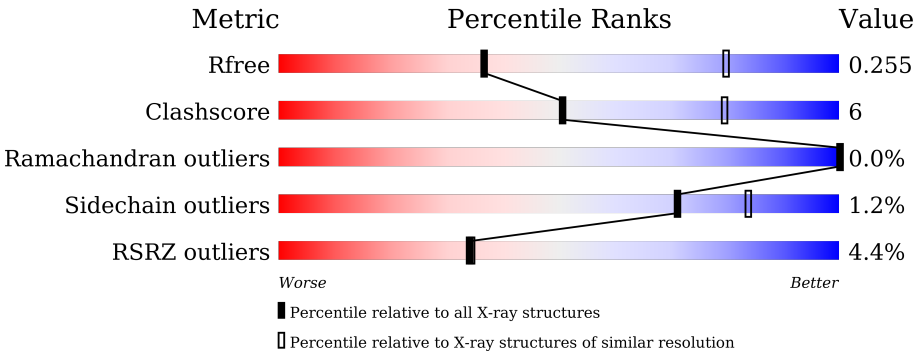
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 <=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	598	2% 82% 18%
1	C	598	3% 83% 16%
1	E	598	3% 85% 15%
1	G	598	4% 84% 16%
2	B	223	4% 79% 8% 13%
2	D	223	14% 72% 15% 13%

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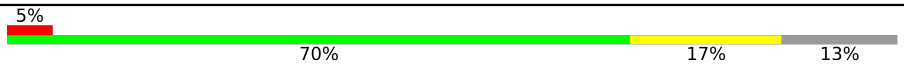
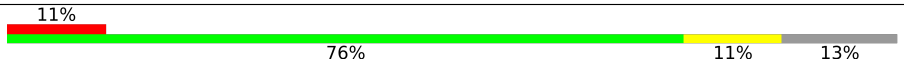
Mol	Chain	Length	Quality of chain
2	F	223	
2	H	223	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25842 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4890	3124	817	919	30			
1	C	596	Total	C	N	O	S	0	0	0
			4890	3124	817	919	30			
1	E	596	Total	C	N	O	S	0	0	0
			4890	3124	817	919	30			
1	G	596	Total	C	N	O	S	0	0	0
			4890	3124	817	919	30			

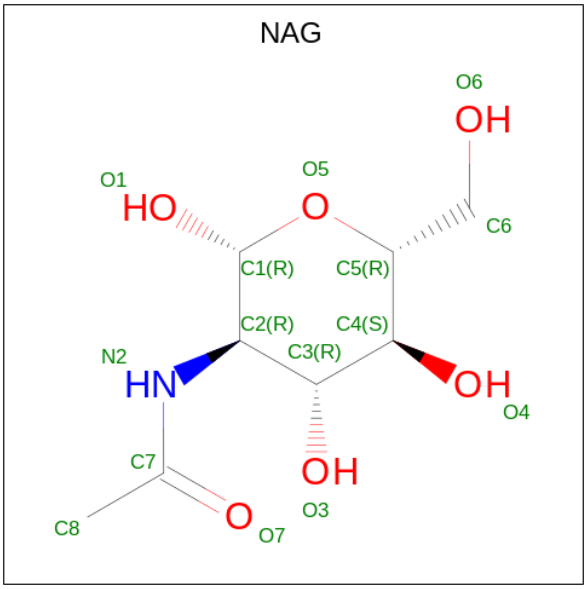
- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1545	991	258	288	8			
2	D	195	Total	C	N	O	S	0	0	0
			1545	991	258	288	8			
2	F	195	Total	C	N	O	S	0	0	0
			1545	991	258	288	8			
2	H	195	Total	C	N	O	S	0	0	0
			1545	991	258	288	8			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0
4	H	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	9	Total O 9 9	0	0
5	B	3	Total O 3 3	0	0
5	C	11	Total O 11 11	0	0
5	D	1	Total O 1 1	0	0
5	E	9	Total O 9 9	0	0
5	F	5	Total O 5 5	0	0

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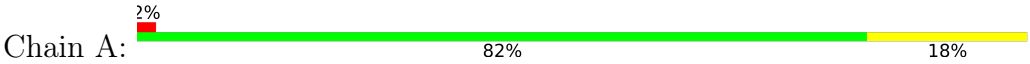
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	4	Total O 4 4	0	0

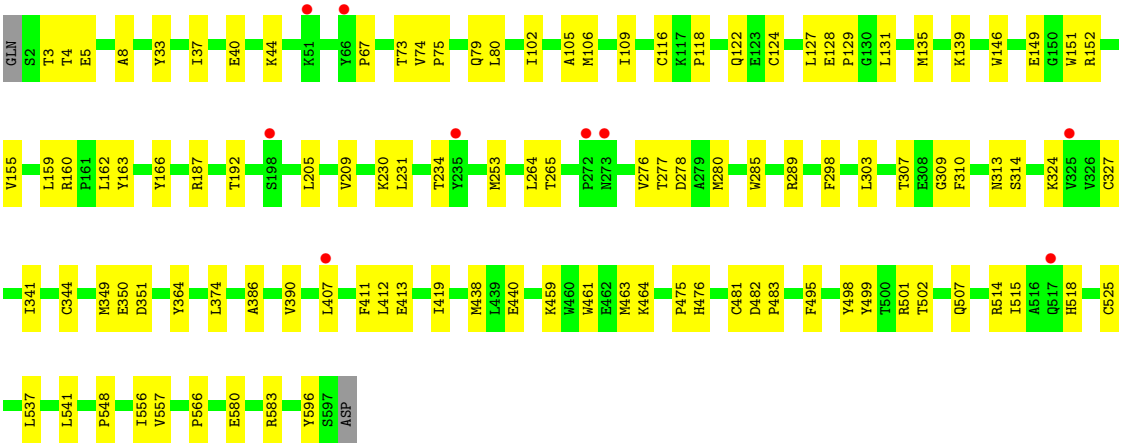
3 Residue-property plots

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: Angiotensin-converting enzyme

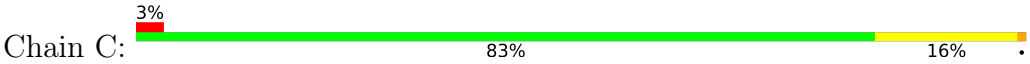
Chain A:

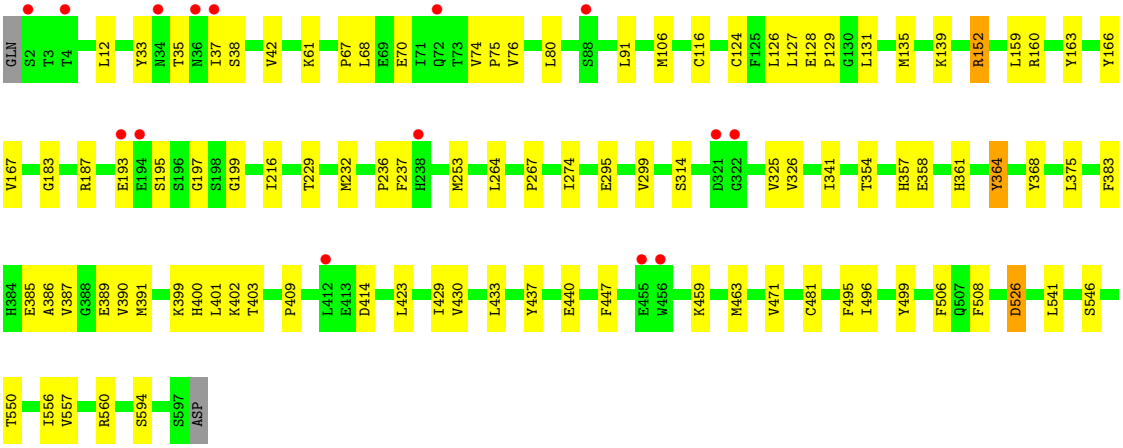




• Molecule 1: Angiotensin-converting enzyme

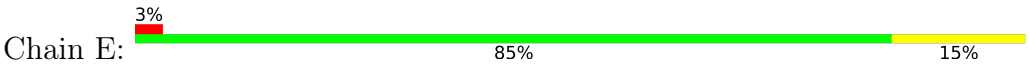
Chain C:

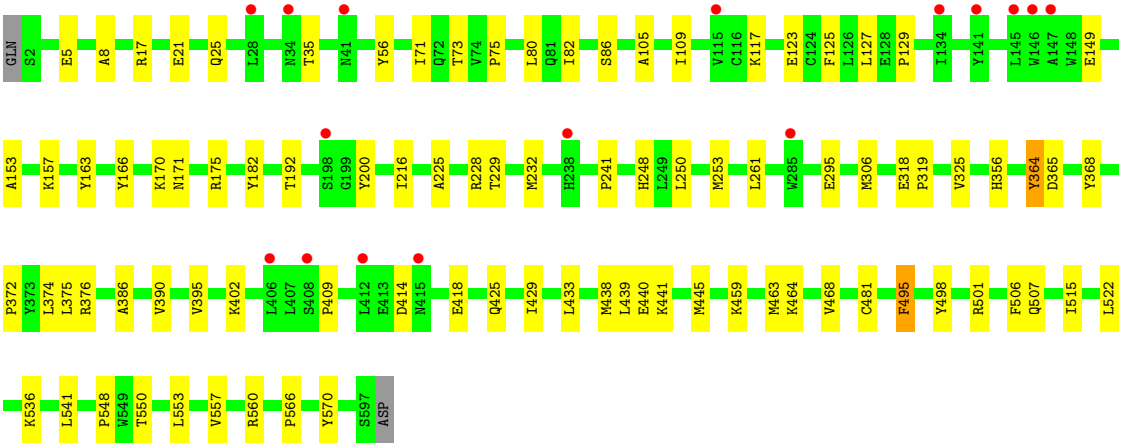




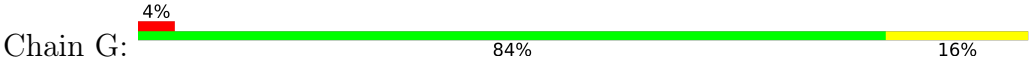
• Molecule 1: Angiotensin-converting enzyme

Chain E:

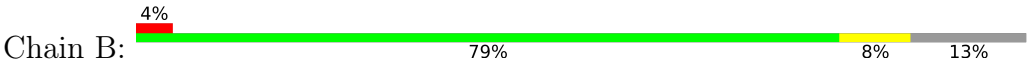


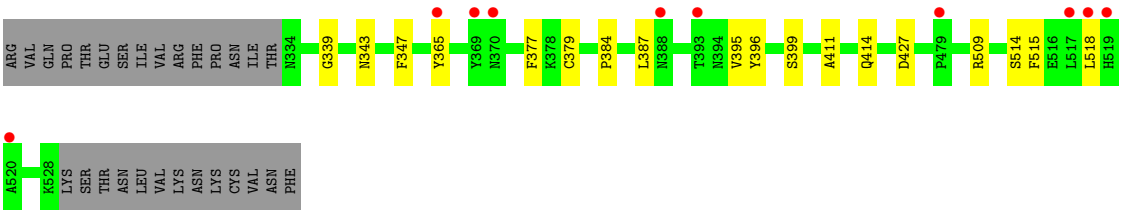


• Molecule 1: Angiotensin-converting enzyme

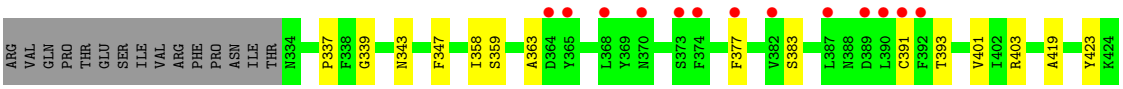


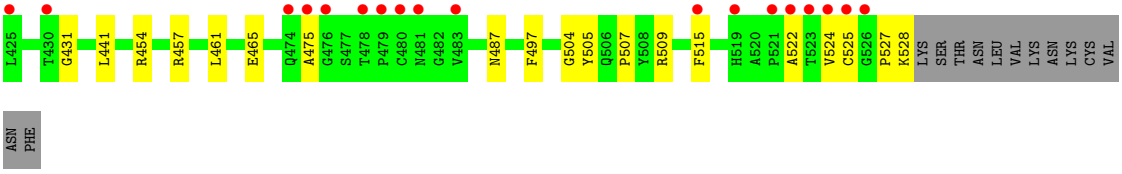
• Molecule 2: Spike protein S1



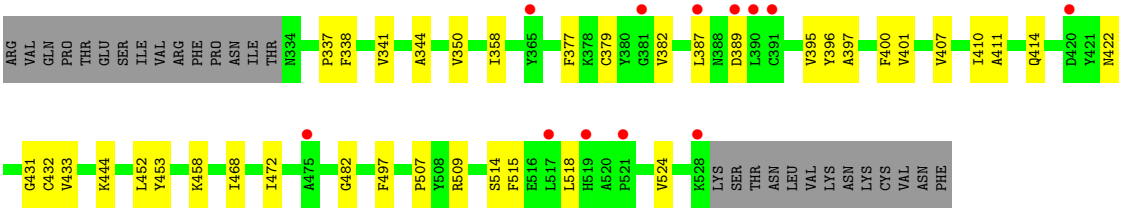


• Molecule 2: Spike protein S1

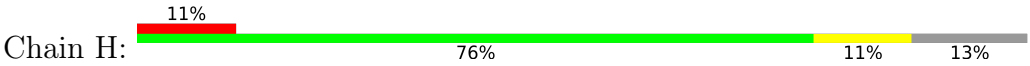


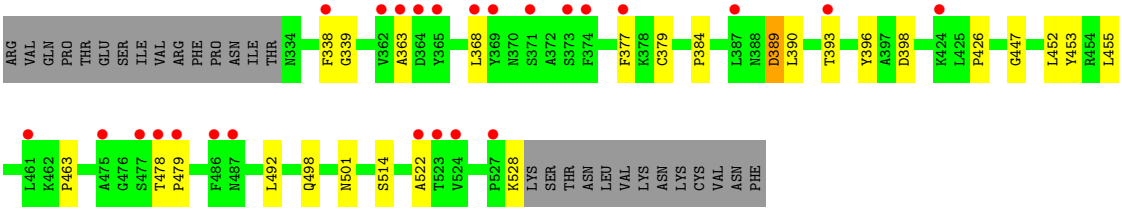


• Molecule 2: Spike protein S1



• Molecule 2: Spike protein S1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.94Å 130.85Å 564.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.28 – 3.31 40.28 – 3.31	Depositor EDS
% Data completeness (in resolution range)	96.1 (40.28-3.31) 88.9 (40.28-3.31)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.19rc3_4028	Depositor
R, R_{free}	0.233 , 0.254 0.234 , 0.255	Depositor DCC
R_{free} test set	2000 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å^2)	78.1	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	25842	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, NAG

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	0.24	0/5031	0.43	0/6827
1	C	0.24	0/5031	0.43	0/6827
1	E	0.24	0/5031	0.44	0/6827
1	G	0.24	0/5031	0.44	0/6827
2	B	0.25	0/1589	0.47	0/2162
2	D	0.25	0/1589	0.45	0/2162
2	F	0.25	0/1589	0.46	0/2162
2	H	0.25	0/1589	0.46	0/2162
All	All	0.24	0/26480	0.44	0/35956

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

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	4890	0	4676	61	0
1	C	4890	0	4676	52	0
1	E	4890	0	4676	47	0
1	G	4890	0	4676	59	0
2	B	1545	0	1465	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1545	0	1465	18	0
2	F	1545	0	1465	24	0
2	H	1545	0	1465	15	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	B	14	0	13	2	0
4	D	14	0	13	0	0
4	F	14	0	13	0	0
4	H	14	0	13	1	0
5	A	9	0	0	0	0
5	B	3	0	0	0	0
5	C	11	0	0	2	0
5	D	1	0	0	0	0
5	E	9	0	0	0	0
5	F	5	0	0	0	0
5	G	4	0	0	0	0
All	All	25842	0	24616	285	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 (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:THR:HG23	1:E:548:PRO:HB3	1.63	0.78
1:E:459:LYS:HG3	1:E:463:MET:HE3	1.65	0.77
1:A:73:THR:HG22	1:A:75:PRO:HD2	1.65	0.77
1:A:74:VAL:HG23	1:A:75:PRO:HD3	1.71	0.72
1:A:277:THR:HG22	1:A:349:MET:H	1.58	0.68
1:E:117:LYS:HD2	1:E:123:GLU:HB3	1.75	0.67
1:G:74:VAL:HG23	1:G:75:PRO:HD3	1.76	0.67
2:F:396:TYR:HB2	2:F:514:SER:HB2	1.77	0.66
1:E:73:THR:HG22	1:E:75:PRO:HD2	1.78	0.65
1:G:212:ILE:HG23	1:G:564:VAL:HG21	1.78	0.65
1:G:498:TYR:HA	1:G:501:ARG:HG2	1.80	0.64
1:E:250:LEU:HA	1:E:261:LEU:HD11	1.80	0.63
1:A:109:ILE:HG22	1:A:155:VAL:HG23	1.81	0.63
1:E:82:ILE:HD11	1:E:374:LEU:HB3	1.80	0.63
1:G:127:LEU:HA	1:G:131:LEU:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:HD11	1:C:326:VAL:HG13	1.81	0.62
1:A:234:THR:HG21	1:A:264:LEU:HD22	1.80	0.62
1:C:35:THR:HA	1:C:325:VAL:HG12	1.81	0.61
1:E:192:THR:HB	1:E:200:TYR:H	1.65	0.60
2:F:337:PRO:HD2	2:F:358:ILE:HG23	1.84	0.60
1:G:443:ARG:HD3	1:G:489:VAL:HG13	1.83	0.60
1:C:116:CYS:HA	1:C:124:CYS:HA	1.84	0.59
1:A:407:LEU:HD21	1:A:411:PHE:HD2	1.67	0.59
1:G:556:ILE:HG23	1:G:557:VAL:HG13	1.84	0.58
1:A:139:LYS:HD3	1:A:264:LEU:HD21	1.84	0.58
1:G:564:VAL:HG12	1:G:568:LEU:HG	1.86	0.58
1:G:439:LEU:HD12	1:G:460:TRP:HH2	1.70	0.56
2:H:426:PRO:HG3	2:H:463:PRO:HB3	1.87	0.56
2:H:453:TYR:HE2	2:H:455:LEU:HD13	1.71	0.56
1:C:229:THR:HA	1:C:232:MET:HE2	1.87	0.56
1:G:106:MET:HG2	1:G:159:LEU:HD22	1.88	0.55
1:A:556:ILE:HG23	1:A:557:VAL:HG13	1.87	0.55
1:E:192:THR:HG22	1:E:192:THR:O	2.06	0.55
2:B:339:GLY:HA2	4:B:601:NAG:O7	2.08	0.54
1:G:256:ARG:HD2	1:G:495:PHE:HZ	1.71	0.54
2:D:454:ARG:HD2	2:D:457:ARG:HB2	1.89	0.54
1:G:461:TRP:HA	1:G:464:LYS:HB2	1.90	0.54
1:C:375:LEU:HD13	1:C:546:SER:HA	1.89	0.53
1:C:429:ILE:HD13	1:C:506:PHE:HZ	1.72	0.53
2:B:379:CYS:HB2	2:B:384:PRO:HG3	1.89	0.53
2:B:384:PRO:HA	2:B:387:LEU:HD23	1.89	0.53
1:E:522:LEU:HD22	1:E:570:TYR:HD2	1.72	0.53
2:F:350:VAL:HG22	2:F:422:ASN:HB3	1.91	0.53
1:G:229:THR:HA	1:G:232:MET:HE2	1.90	0.53
1:G:554:LYS:HD2	1:G:560:ARG:HG3	1.91	0.53
2:B:365:TYR:CD2	2:B:387:LEU:HB3	2.44	0.53
1:C:267:PRO:HD3	1:C:423:LEU:HD22	1.90	0.53
2:D:431:GLY:HA2	2:D:515:PHE:HD2	1.73	0.53
1:E:425:GLN:HB3	1:E:429:ILE:HD12	1.91	0.53
1:E:440:GLU:HG2	1:E:495:PHE:HB3	1.90	0.53
1:C:106:MET:HG2	1:C:159:LEU:HD22	1.90	0.52
1:C:274:ILE:HD11	1:C:401:LEU:HD12	1.89	0.52
1:G:135:MET:HG2	1:G:253:MET:HA	1.91	0.52
1:A:152:ARG:HB3	1:A:476:HIS:HE1	1.73	0.52
1:G:439:LEU:HD12	1:G:460:TRP:CH2	2.45	0.52
2:D:401:VAL:HG22	2:D:509:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:461:LEU:HG	2:D:465:GLU:HB3	1.93	0.51
1:C:236:PRO:HB2	1:C:237:PHE:HD1	1.74	0.51
1:E:216:ILE:HD13	1:E:433:LEU:HD13	1.92	0.51
1:C:135:MET:HG3	1:C:253:MET:HG2	1.92	0.51
1:A:105:ALA:O	1:A:109:ILE:HG13	2.10	0.51
1:G:35:THR:HA	1:G:325:VAL:HG12	1.93	0.51
1:C:314:SER:HB2	1:C:341:ILE:H	1.76	0.51
1:C:361:HIS:HE1	1:C:385:GLU:HA	1.75	0.51
2:D:393:THR:HA	2:D:522:ALA:HA	1.92	0.51
2:D:475:ALA:HB3	2:D:487:ASN:HB3	1.93	0.50
1:G:414:ASP:O	1:G:418:GLU:HG2	2.11	0.50
1:C:126:LEU:HD12	1:C:127:LEU:H	1.77	0.50
1:E:105:ALA:O	1:E:109:ILE:HG13	2.11	0.50
1:A:3:THR:HG22	1:A:5:GLU:H	1.77	0.50
2:D:347:PHE:HB3	2:D:401:VAL:HG23	1.94	0.50
1:C:160:ARG:HB2	1:C:481:CYS:HB2	1.92	0.50
1:E:402:LYS:HD2	1:E:409:PRO:HA	1.93	0.50
1:G:250:LEU:HA	1:G:261:LEU:HD11	1.94	0.50
2:D:337:PRO:HD2	2:D:358:ILE:HD12	1.94	0.50
1:A:116:CYS:HA	1:A:124:CYS:HA	1.95	0.49
1:G:60:SER:HA	1:G:83:LEU:HG	1.93	0.49
1:A:507:GLN:HG2	1:A:566:PRO:HG2	1.94	0.49
1:G:475:PRO:HD3	1:G:596:TYR:CG	2.48	0.49
1:A:307:THR:HG23	1:A:310:PHE:H	1.76	0.49
1:A:459:LYS:O	1:A:463:MET:HG3	2.12	0.49
1:C:74:VAL:HG13	1:C:75:PRO:HD3	1.94	0.49
1:C:556:ILE:HG23	1:C:557:VAL:HG13	1.93	0.49
2:D:403:ARG:HG2	2:D:504:GLY:O	2.12	0.49
2:F:472:ILE:HD13	2:F:482:GLY:HA2	1.94	0.49
1:G:465:ARG:HE	1:G:471:VAL:HG23	1.77	0.49
2:H:498:GLN:HB2	2:H:501:ASN:HD21	1.78	0.49
2:B:347:PHE:CE2	2:B:399:SER:HB2	2.48	0.49
2:H:452:LEU:HD12	2:H:492:LEU:HB3	1.95	0.49
1:C:430:VAL:HA	1:C:433:LEU:HD12	1.94	0.49
1:G:429:ILE:HD13	1:G:506:PHE:HZ	1.77	0.49
1:A:187:ARG:HG2	1:A:205:LEU:HD23	1.95	0.48
1:E:170:LYS:HD2	1:E:182:TYR:CZ	2.48	0.48
1:G:501:ARG:HG3	1:G:502:THR:N	2.28	0.48
1:A:314:SER:HB2	1:A:341:ILE:H	1.78	0.48
1:E:228:ARG:HG2	1:E:232:MET:HE3	1.95	0.48
2:H:379:CYS:HB2	2:H:384:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:MET:HE1	1:A:464:LYS:HE2	1.95	0.48
1:C:267:PRO:HD3	1:C:423:LEU:CD2	2.44	0.48
1:A:192:THR:HB	1:A:548:PRO:HB3	1.96	0.48
2:F:395:VAL:HG23	2:F:524:VAL:HG11	1.95	0.48
1:E:171:ASN:O	1:E:175:ARG:HG3	2.13	0.48
1:G:564:VAL:HG12	1:G:564:VAL:O	2.14	0.48
1:E:507:GLN:HG3	1:E:566:PRO:HG2	1.95	0.48
1:G:503:ILE:HD12	1:G:564:VAL:HG22	1.95	0.48
1:A:102:ILE:HG23	1:A:162:LEU:HB3	1.96	0.48
1:E:356:HIS:CD2	1:E:395:VAL:HG11	2.49	0.48
1:G:373:TYR:HA	1:G:376:ARG:HD2	1.96	0.48
1:C:550:THR:HB	1:C:560:ARG:HG2	1.96	0.47
1:E:550:THR:HB	1:E:560:ARG:HG2	1.95	0.47
1:A:163:TYR:HA	1:A:166:TYR:HB3	1.96	0.47
1:A:4:THR:HG21	1:A:67:PRO:HD2	1.97	0.47
2:D:359:SER:HA	2:D:524:VAL:CG2	2.44	0.47
1:C:459:LYS:HE3	1:C:463:MET:HE2	1.96	0.47
1:C:386:ALA:O	1:C:390:VAL:HG13	2.15	0.47
2:H:396:TYR:HB2	2:H:514:SER:HB2	1.97	0.47
1:A:230:LYS:HB2	1:A:265:THR:HG22	1.97	0.47
1:E:163:TYR:HA	1:E:166:TYR:HB3	1.97	0.47
1:E:386:ALA:O	1:E:390:VAL:HG23	2.15	0.46
1:E:429:ILE:HD13	1:E:506:PHE:HZ	1.79	0.46
1:A:151:TRP:O	1:A:155:VAL:HG12	2.15	0.46
1:A:386:ALA:O	1:A:390:VAL:HG23	2.15	0.46
1:A:106:MET:HG2	1:A:159:LEU:HD22	1.98	0.46
1:C:12:LEU:HD12	1:C:76:VAL:HG13	1.97	0.46
1:G:116:CYS:HA	1:G:124:CYS:HA	1.98	0.46
1:A:209:VAL:HG13	1:A:499:TYR:CE1	2.51	0.46
1:A:276:VAL:O	1:A:280:MET:HG3	2.16	0.46
1:E:56:TYR:HE2	1:E:86:SER:HB2	1.80	0.46
2:B:343:ASN:ND2	4:B:601:NAG:O7	2.49	0.46
1:A:127:LEU:HA	1:A:131:LEU:HB2	1.98	0.46
1:E:127:LEU:HD11	1:E:253:MET:HG3	1.98	0.46
1:G:471:VAL:HG21	1:G:594:SER:HA	1.98	0.46
2:H:389:ASP:HA	2:H:528:LYS:HD2	1.98	0.46
1:G:334:LEU:HB2	1:G:338:ASP:HB3	1.98	0.46
1:A:40:GLU:O	1:A:44:LYS:HG3	2.17	0.45
1:C:139:LYS:HE2	1:C:264:LEU:HD21	1.98	0.45
2:D:403:ARG:HD2	2:D:505:TYR:HA	1.98	0.45
1:C:440:GLU:HG2	1:C:496:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:344:ALA:O	2:F:509:ARG:NH1	2.47	0.45
1:C:402:LYS:HD2	1:C:409:PRO:HA	1.97	0.45
1:C:195:SER:HB2	1:C:199:GLY:HA2	1.98	0.45
2:F:407:VAL:O	2:F:410:ILE:HG22	2.17	0.45
1:G:356:HIS:CD2	1:G:395:VAL:HG11	2.51	0.45
2:F:468:ILE:HG12	2:F:468:ILE:O	2.16	0.45
1:E:225:ALA:O	1:E:229:THR:HG23	2.17	0.45
1:A:327:CYS:HB3	1:A:344:CYS:HB2	1.65	0.45
1:C:38:SER:O	1:C:42:VAL:HG23	2.17	0.45
1:C:128:GLU:HA	1:C:129:PRO:HA	1.78	0.45
2:D:431:GLY:HA2	2:D:515:PHE:CD2	2.51	0.45
2:F:410:ILE:HG23	2:F:433:VAL:HG11	1.99	0.45
1:C:183:GLY:O	1:C:187:ARG:HG3	2.17	0.45
2:F:444:LYS:HD2	2:F:444:LYS:HA	1.76	0.45
1:A:514:ARG:HE	1:A:514:ARG:HB2	1.66	0.45
1:G:257:PHE:HB3	1:G:259:THR:HG22	1.99	0.45
2:F:518:LEU:HD23	2:F:518:LEU:HA	1.87	0.44
1:A:79:GLN:HG2	1:A:374:LEU:HB2	1.98	0.44
1:A:475:PRO:HD3	1:A:596:TYR:CG	2.53	0.44
2:D:528:LYS:HE3	2:D:528:LYS:HB2	1.68	0.44
1:G:212:ILE:HG23	1:G:564:VAL:CG2	2.45	0.44
1:G:364:TYR:CG	1:G:541:LEU:HD22	2.52	0.44
2:H:390:LEU:HD12	2:H:390:LEU:HA	1.83	0.44
1:A:440:GLU:HG2	1:A:495:PHE:HB3	2.00	0.44
2:D:497:PHE:CG	2:D:507:PRO:HG3	2.53	0.44
1:A:461:TRP:HA	1:A:464:LYS:HB2	1.99	0.44
2:F:411:ALA:HB3	2:F:414:GLN:HE21	1.82	0.44
1:C:236:PRO:HB2	1:C:237:PHE:CD1	2.53	0.44
1:G:73:THR:OG1	1:G:75:PRO:HD2	2.17	0.44
1:G:303:LEU:HD13	1:G:363:GLN:HB3	2.00	0.44
1:C:127:LEU:HA	1:C:131:LEU:HB2	2.00	0.44
1:C:354:THR:O	1:C:358:GLU:HG2	2.18	0.44
2:D:339:GLY:O	2:D:343:ASN:HB2	2.18	0.43
1:E:232:MET:HE2	1:E:241:PRO:HA	1.99	0.43
1:G:73:THR:HG23	1:G:76:VAL:HB	2.00	0.43
1:A:350:GLU:HG3	1:A:351:ASP:N	2.32	0.43
1:E:553:LEU:O	1:E:557:VAL:HG22	2.19	0.43
2:F:497:PHE:HB3	2:F:507:PRO:HG3	2.00	0.43
1:G:5:GLU:HG2	1:G:9:LYS:HE3	1.99	0.43
1:C:390:VAL:HG11	1:C:508:PHE:HB2	1.99	0.43
1:E:21:GLU:O	1:E:25:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:ILE:HD12	1:G:324:LYS:HG2	2.00	0.43
1:G:163:TYR:HA	1:G:166:TYR:HB3	1.99	0.43
1:G:298:PHE:HE1	1:G:391:MET:HG3	1.82	0.43
1:E:368:TYR:O	1:E:376:ARG:HG2	2.18	0.43
1:G:500:THR:HG22	1:G:562:MET:HE1	2.00	0.43
2:H:338:PHE:CD2	2:H:368:LEU:HD11	2.54	0.43
1:C:399:LYS:O	1:C:403:THR:HG23	2.18	0.43
1:A:8:ALA:HB1	1:A:80:LEU:HD11	2.00	0.43
1:E:153:ALA:HA	1:E:157:LYS:HG3	2.00	0.43
2:F:341:VAL:HG11	2:F:397:ALA:HB1	2.01	0.43
1:G:192:THR:HG23	1:G:548:PRO:HB3	2.00	0.43
1:G:212:ILE:HD13	1:G:503:ILE:HG13	2.01	0.43
1:C:167:VAL:HG23	1:C:447:PHE:HD1	1.83	0.43
1:G:82:ILE:HD13	1:G:82:ILE:HA	1.88	0.43
1:G:387:VAL:O	1:G:391:MET:HG2	2.18	0.43
2:H:447:GLY:HA2	2:H:498:GLN:HG3	2.01	0.43
1:A:515:ILE:H	1:A:515:ILE:HG13	1.69	0.43
2:B:518:LEU:HD23	2:B:518:LEU:HA	1.82	0.43
1:C:33:TYR:CE1	1:C:42:VAL:HG22	2.54	0.43
1:C:437:TYR:HB2	1:C:499:TYR:CE2	2.54	0.43
1:E:438:MET:HG2	1:E:468:VAL:CG2	2.48	0.43
1:G:537:LEU:O	1:G:541:LEU:HG	2.18	0.43
2:H:498:GLN:HB2	2:H:501:ASN:ND2	2.34	0.43
1:C:67:PRO:HB2	1:C:70:GLU:HG3	2.00	0.43
1:A:33:TYR:CE1	1:A:37:ILE:HG23	2.53	0.42
1:A:580:GLU:O	1:A:583:ARG:HG3	2.19	0.42
1:C:387:VAL:O	1:C:391:MET:HG2	2.19	0.42
1:C:400:HIS:HB2	1:C:526:ASP:OD2	2.19	0.42
2:D:419:ALA:HA	2:D:423:TYR:O	2.19	0.42
1:E:35:THR:HA	1:E:325:VAL:HG12	2.01	0.42
1:E:441:LYS:O	1:E:445:MET:HG3	2.19	0.42
1:G:61:LYS:HE2	1:G:61:LYS:HB3	1.78	0.42
1:E:438:MET:HE1	1:E:464:LYS:HG2	2.01	0.42
1:C:163:TYR:HA	1:C:166:TYR:HB3	2.00	0.42
1:E:498:TYR:HA	1:E:501:ARG:HG2	2.01	0.42
2:F:431:GLY:HA2	2:F:515:PHE:HD2	1.84	0.42
1:G:6:ASP:HA	1:G:9:LYS:HD2	2.01	0.42
1:G:37:ILE:HB	1:G:324:LYS:HB3	2.01	0.42
1:A:280:MET:HE3	1:A:280:MET:HB2	1.78	0.42
1:A:309:GLY:O	1:A:313:ASN:HB2	2.20	0.42
1:E:439:LEU:HD22	1:E:495:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:ALA:O	1:G:109:ILE:HG13	2.19	0.42
1:G:256:ARG:HD2	1:G:495:PHE:CZ	2.52	0.42
2:H:393:THR:HA	2:H:522:ALA:HA	2.01	0.42
1:A:160:ARG:HB2	1:A:481:CYS:HB2	2.02	0.42
1:A:412:LEU:HG	1:A:413:GLU:H	1.84	0.42
1:C:74:VAL:CG1	1:C:75:PRO:HD3	2.50	0.42
1:E:364:TYR:CG	1:E:541:LEU:HD22	2.55	0.42
2:F:458:LYS:HA	2:F:458:LYS:HD2	1.69	0.42
1:C:471:VAL:HG21	1:C:594:SER:HA	2.02	0.42
2:D:391:CYS:HB2	2:D:525:CYS:HB3	1.93	0.42
2:F:382:VAL:HG21	2:F:387:LEU:HD13	2.01	0.42
1:A:518:HIS:CE1	1:A:525:CYS:HA	2.55	0.42
1:C:357:HIS:CE1	1:C:389:GLU:HG2	2.55	0.42
1:G:40:GLU:O	1:G:44:LYS:HG3	2.20	0.42
1:G:303:LEU:HD23	1:G:303:LEU:HA	1.87	0.42
1:A:37:ILE:HB	1:A:324:LYS:HB2	2.02	0.42
1:C:152:ARG:NH2	5:C:702:HOH:O	2.52	0.42
1:A:118:PRO:HD3	1:A:146:TRP:NE1	2.35	0.42
1:A:498:TYR:HA	1:A:501:ARG:HG2	2.00	0.42
2:F:497:PHE:CG	2:F:507:PRO:HG3	2.55	0.42
1:C:68:LEU:HD11	1:C:80:LEU:HB3	2.02	0.41
1:C:216:ILE:HD13	1:C:433:LEU:HD13	2.02	0.41
1:C:364:TYR:CG	1:C:541:LEU:HD22	2.55	0.41
1:G:216:ILE:HG22	1:G:564:VAL:HG11	2.02	0.41
1:C:295:GLU:O	1:C:299:VAL:HG23	2.20	0.41
1:E:365:ASP:HA	1:E:368:TYR:CZ	2.55	0.41
1:E:414:ASP:O	1:E:418:GLU:HG2	2.21	0.41
2:F:401:VAL:HG22	2:F:509:ARG:HG2	2.02	0.41
1:G:7:ARG:HG2	1:G:66:TYR:HE1	1.85	0.41
1:G:397:THR:HG23	1:G:400:HIS:H	1.85	0.41
1:A:205:LEU:O	1:A:209:VAL:HG23	2.20	0.41
1:A:419:ILE:HD13	1:A:419:ILE:HA	1.90	0.41
2:B:396:TYR:HB2	2:B:514:SER:HB2	2.02	0.41
2:B:411:ALA:HB3	2:B:414:GLN:HG3	2.02	0.41
1:G:15:PHE:CE2	1:G:374:LEU:HD21	2.55	0.41
1:G:128:GLU:HA	1:G:129:PRO:HA	1.80	0.41
1:E:17:ARG:HG2	2:F:453:TYR:OH	2.21	0.41
1:A:583:ARG:HB3	2:F:452:LEU:HD13	2.03	0.41
2:F:350:VAL:HA	2:F:400:PHE:HB2	2.02	0.41
2:H:478:THR:HA	2:H:479:PRO:HD3	1.96	0.41
1:A:128:GLU:HA	1:A:129:PRO:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TRP:CD2	1:A:289:ARG:HG2	2.56	0.41
2:F:338:PHE:HE1	2:F:358:ILE:HD13	1.86	0.41
2:F:379:CYS:HA	2:F:432:CYS:HA	2.03	0.41
2:H:339:GLY:HA2	4:H:601:NAG:O7	2.21	0.41
1:A:501:ARG:HG3	1:A:502:THR:N	2.36	0.41
2:B:347:PHE:CD2	2:B:509:ARG:HG2	2.56	0.41
2:B:395:VAL:HG22	2:B:515:PHE:HD1	1.86	0.41
1:E:5:GLU:HG3	1:E:71:ILE:HG23	2.03	0.41
1:E:515:ILE:HD13	1:E:536:LYS:HG3	2.03	0.41
1:C:91:LEU:HA	1:C:91:LEU:HD23	1.83	0.40
1:E:318:GLU:HG3	1:E:319:PRO:HD2	2.02	0.40
2:H:338:PHE:CE2	2:H:363:ALA:HB1	2.57	0.40
1:A:298:PHE:HD1	1:A:303:LEU:HD12	1.86	0.40
1:C:197:GLY:HA2	5:C:710:HOH:O	2.21	0.40
2:D:363:ALA:O	2:D:527:PRO:HD3	2.21	0.40
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.87	0.40
1:E:8:ALA:HB1	1:E:80:LEU:HD11	2.02	0.40
1:E:372:PRO:HD2	1:E:375:LEU:HD12	2.03	0.40
1:G:51:LYS:HD2	1:G:51:LYS:HA	1.94	0.40
1:A:135:MET:HG3	1:A:253:MET:HG2	2.03	0.40
1:A:407:LEU:HD21	1:A:411:PHE:CD2	2.51	0.40
1:A:482:ASP:N	1:A:483:PRO:HD2	2.36	0.40
1:A:537:LEU:O	1:A:541:LEU:HG	2.21	0.40
1:E:295:GLU:HG3	1:E:306:MET:HG2	2.04	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	594/598 (99%)	584 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	594/598 (99%)	582 (98%)	12 (2%)	0	100	100
1	E	594/598 (99%)	578 (97%)	15 (2%)	1 (0%)	47	76
1	G	594/598 (99%)	581 (98%)	13 (2%)	0	100	100
2	B	193/223 (86%)	185 (96%)	8 (4%)	0	100	100
2	D	193/223 (86%)	190 (98%)	3 (2%)	0	100	100
2	F	193/223 (86%)	185 (96%)	8 (4%)	0	100	100
2	H	193/223 (86%)	185 (96%)	8 (4%)	0	100	100
All	All	3148/3284 (96%)	3070 (98%)	77 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	129	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	532/534 (100%)	528 (99%)	4 (1%)	81	89
1	C	532/534 (100%)	523 (98%)	9 (2%)	60	79
1	E	532/534 (100%)	526 (99%)	6 (1%)	73	85
1	G	532/534 (100%)	528 (99%)	4 (1%)	81	89
2	B	168/196 (86%)	166 (99%)	2 (1%)	71	84
2	D	168/196 (86%)	165 (98%)	3 (2%)	59	79
2	F	168/196 (86%)	166 (99%)	2 (1%)	71	84
2	H	168/196 (86%)	165 (98%)	3 (2%)	59	79
All	All	2800/2920 (96%)	2767 (99%)	33 (1%)	71	84

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	149	GLU
1	A	278	ASP
1	A	364	TYR
2	B	377	PHE
2	B	427	ASP
1	C	61	LYS
1	C	152	ARG
1	C	193	GLU
1	C	364	TYR
1	C	368	TYR
1	C	383	PHE
1	C	414	ASP
1	C	495	PHE
1	C	526	ASP
2	D	377	PHE
2	D	383	SER
2	D	441	LEU
1	E	125	PHE
1	E	149	GLU
1	E	248	HIS
1	E	364	TYR
1	E	481	CYS
1	E	495	PHE
2	F	377	PHE
2	F	389	ASP
1	G	286	ASP
1	G	364	TYR
1	G	384	HIS
1	G	481	CYS
2	H	377	PHE
2	H	389	ASP
2	H	398	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	222	HIS
1	C	380	ASN
1	C	582	ASN
1	E	133	ASN
2	F	414	GLN
2	H	474	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	NAG	F	601	2	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	B	601	2	14,14,15	0.46	0	17,19,21	0.59	0
4	NAG	H	601	2	14,14,15	0.31	0	17,19,21	0.50	0
4	NAG	D	601	2	14,14,15	0.19	0	17,19,21	0.46	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
4	NAG	F	601	2	-	0/6/23/26	0/1/1/1
4	NAG	B	601	2	-	0/6/23/26	0/1/1/1
4	NAG	H	601	2	-	0/6/23/26	0/1/1/1
4	NAG	D	601	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

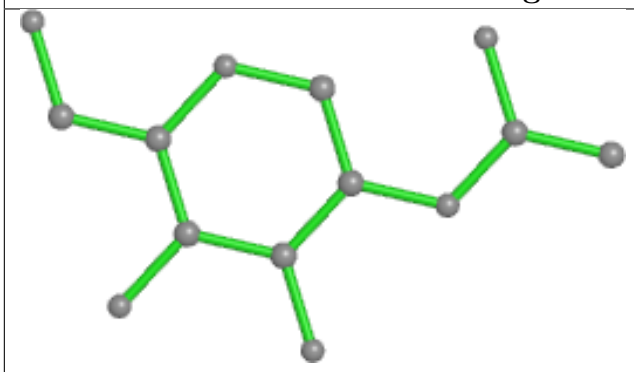
There are no ring outliers.

2 monomers are involved in 3 short contacts:

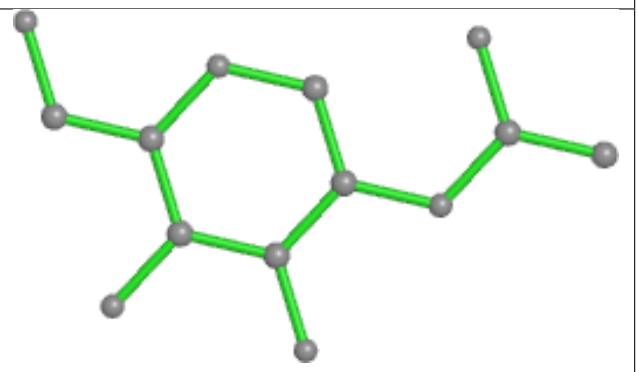
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	NAG	2	0
4	H	601	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

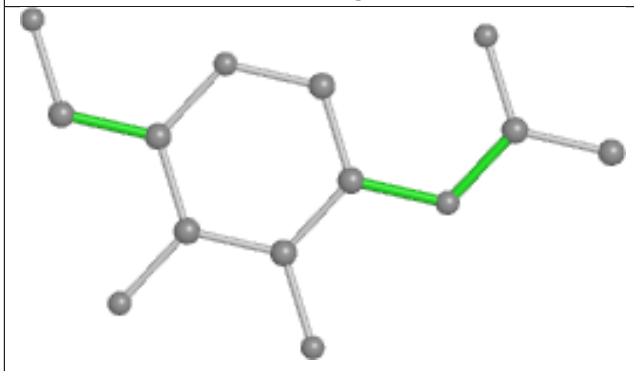
Ligand NAG F 601



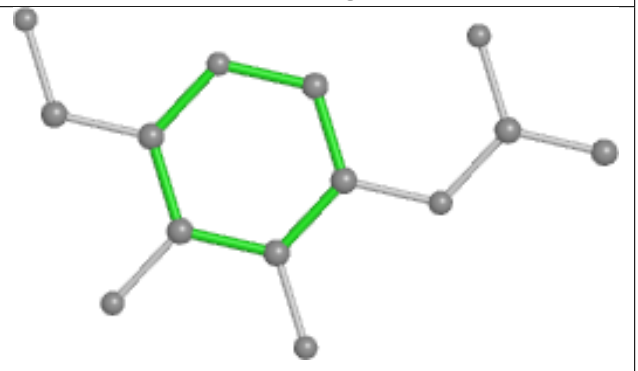
Bond lengths



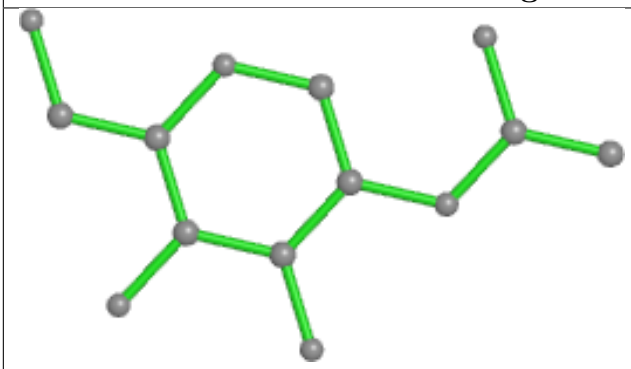
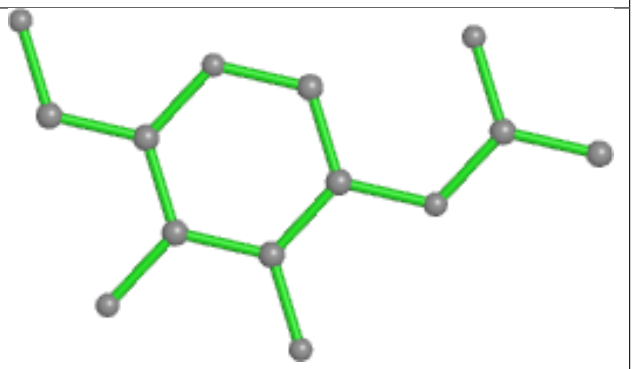
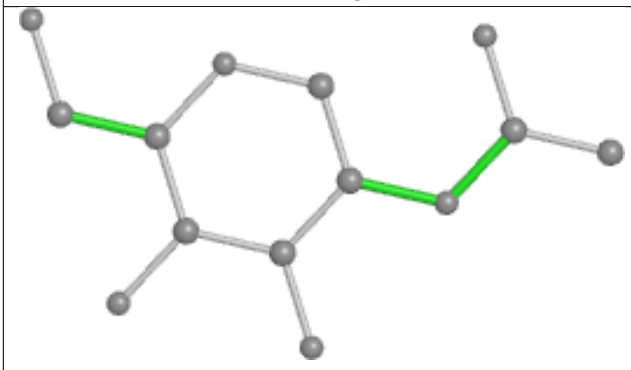
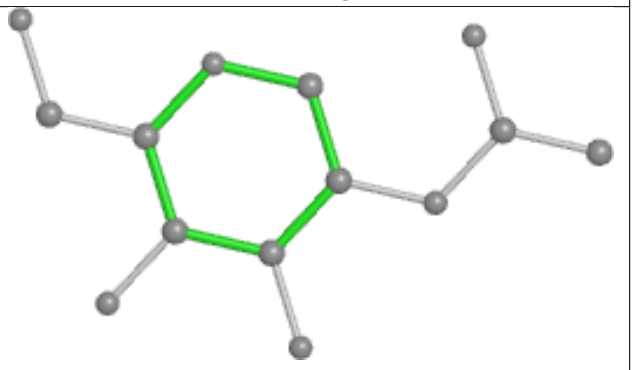
Bond angles

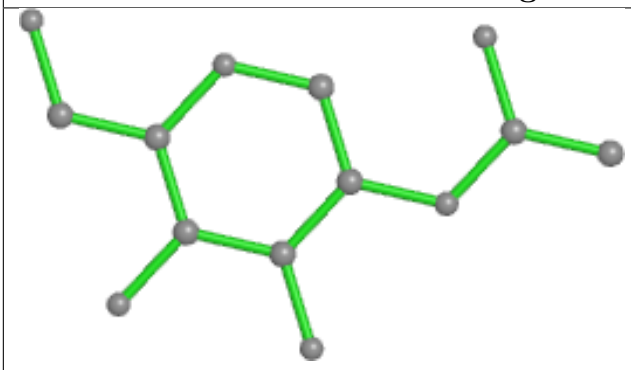
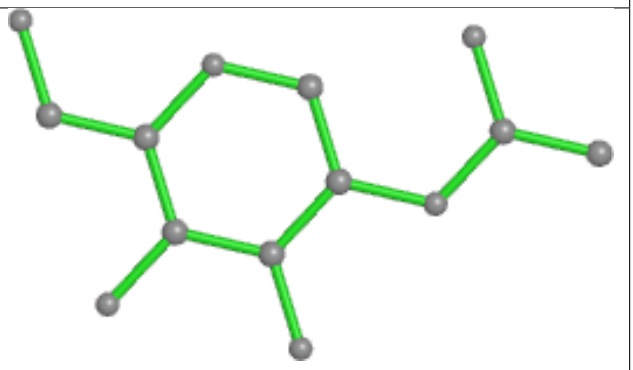
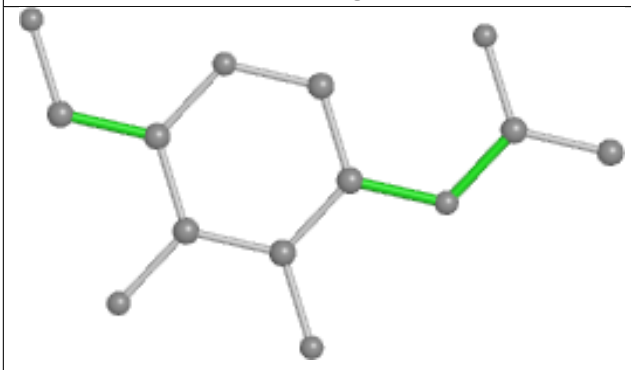
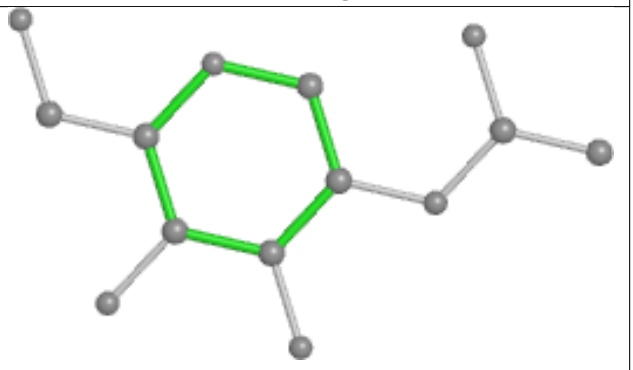


Torsions

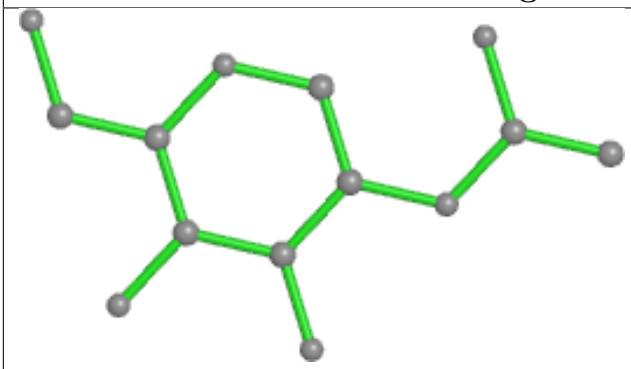


Rings

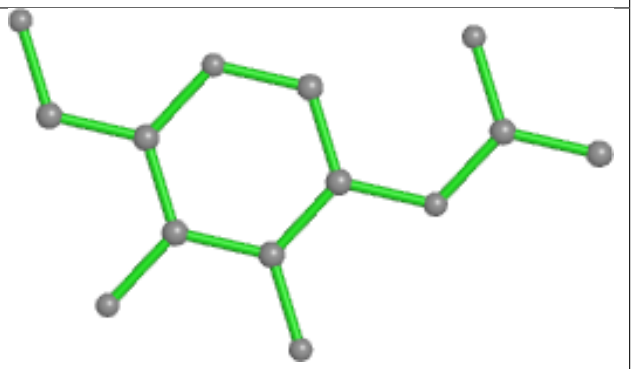
Ligand NAG B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG H 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

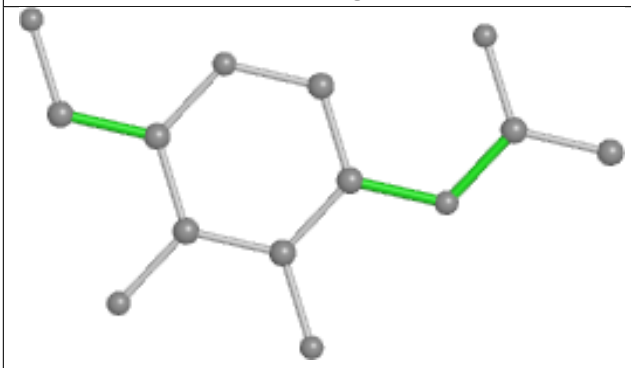
Ligand NAG D 601



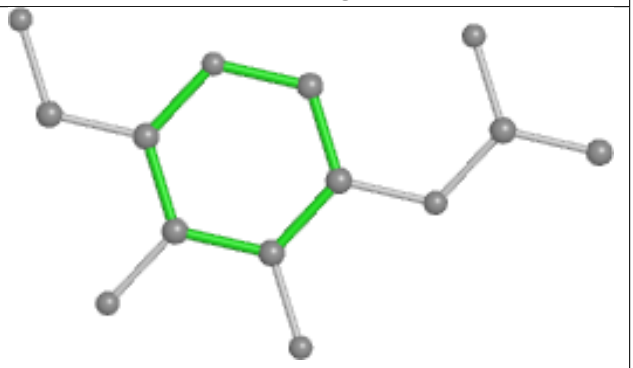
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	596/598 (99%)	0.23	9 (1%) 73 72	58, 81, 106, 134	0
1	C	596/598 (99%)	0.23	15 (2%) 57 55	56, 80, 108, 127	0
1	E	596/598 (99%)	0.32	16 (2%) 54 53	64, 86, 111, 148	0
1	G	596/598 (99%)	0.36	21 (3%) 44 42	67, 97, 122, 155	0
2	B	195/223 (87%)	0.28	10 (5%) 28 27	64, 86, 130, 152	0
2	D	195/223 (87%)	0.83	31 (15%) 1 1	63, 105, 139, 156	0
2	F	195/223 (87%)	0.56	12 (6%) 20 21	58, 86, 134, 144	0
2	H	195/223 (87%)	0.74	25 (12%) 3 3	84, 116, 165, 180	0
All	All	3164/3284 (96%)	0.36	139 (4%) 34 34	56, 88, 127, 180	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	391	CYS	5.5
1	C	194	GLU	5.2
2	D	370	ASN	4.7
1	G	325	VAL	4.5
1	A	198	SER	4.5
2	D	480	CYS	4.2
2	D	479	PRO	4.0
2	D	481	ASN	4.0
2	D	390	LEU	3.9
2	H	522	ALA	3.9
2	F	365	TYR	3.8
2	D	365	TYR	3.8
2	D	522	ALA	3.8
2	H	477	SER	3.6
2	D	392	PHE	3.6
1	E	34	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
2	F	389	ASP	3.5
2	D	523	THR	3.5
1	G	37	ILE	3.5
2	H	527	PRO	3.4
2	D	524	VAL	3.4
1	C	193	GLU	3.3
2	F	391	CYS	3.3
2	H	475	ALA	3.2
2	H	523	THR	3.2
2	B	370	ASN	3.2
2	B	518	LEU	3.1
2	H	368	LEU	3.1
2	D	368	LEU	3.1
2	D	474	GLN	3.1
2	F	517	LEU	3.1
2	F	475	ALA	3.1
1	E	238	HIS	3.0
1	C	4	THR	3.0
2	D	521	PRO	3.0
2	F	390	LEU	3.0
1	A	407	LEU	3.0
2	D	382	VAL	3.0
1	C	321	ASP	2.9
2	D	525	CYS	2.9
2	F	420	ASP	2.9
2	B	517	LEU	2.9
1	A	273	ASN	2.9
2	D	483	VAL	2.9
1	E	141	TYR	2.8
2	H	369	TYR	2.8
1	G	115	VAL	2.8
2	H	373	SER	2.8
1	A	517	GLN	2.8
1	G	324	LYS	2.8
1	A	325	VAL	2.8
2	H	424	LYS	2.8
2	H	363	ALA	2.8
2	B	393	THR	2.8
2	H	478	THR	2.7
2	F	519	HIS	2.7
1	E	115	VAL	2.7
1	E	412	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	36	ASN	2.7
2	D	364	ASP	2.7
2	F	528	LYS	2.6
2	D	377	PHE	2.6
2	H	374	PHE	2.6
2	B	520	ALA	2.6
1	C	2	SER	2.6
1	A	51	LYS	2.6
1	C	412	LEU	2.6
1	G	33	TYR	2.6
2	H	387	LEU	2.6
1	A	66	TYR	2.6
1	G	155	VAL	2.6
1	A	272	PRO	2.6
1	E	146	TRP	2.5
1	C	322	GLY	2.5
1	E	415	ASN	2.5
2	H	486	PHE	2.5
1	G	559	SER	2.5
2	B	479	PRO	2.4
1	G	182	TYR	2.4
1	G	4	THR	2.4
1	G	40	GLU	2.4
1	G	41	ASN	2.4
1	C	456	TRP	2.4
2	H	479	PRO	2.3
1	E	145	LEU	2.3
2	D	425	LEU	2.3
1	G	7	ARG	2.3
2	H	487	ASN	2.3
1	E	406	LEU	2.3
1	E	408	SER	2.3
2	F	521	PRO	2.3
1	E	198	SER	2.3
2	D	374	PHE	2.3
2	D	526	GLY	2.3
2	F	381	GLY	2.3
2	D	389	ASP	2.3
2	H	364	ASP	2.2
1	G	147	ALA	2.2
2	D	387	LEU	2.2
2	D	478	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	387	LEU	2.2
2	D	519	HIS	2.2
1	C	37	ILE	2.2
2	B	365	TYR	2.2
2	D	515	PHE	2.2
1	E	285	TRP	2.2
1	E	147	ALA	2.2
1	A	235	TYR	2.2
2	B	369	TYR	2.2
1	E	41	ASN	2.2
1	G	120	ASN	2.2
1	C	88	SER	2.2
2	H	393	THR	2.2
2	D	373	SER	2.1
2	H	371	SER	2.1
2	D	475	ALA	2.1
1	E	134	ILE	2.1
2	D	476	GLY	2.1
2	B	519	HIS	2.1
1	C	455	GLU	2.1
1	C	72	GLN	2.1
1	G	249	LEU	2.1
2	H	377	PHE	2.1
1	C	238	HIS	2.1
1	G	38	SER	2.1
1	G	178	HIS	2.1
2	H	365	TYR	2.0
2	D	430	THR	2.0
1	E	28	LEU	2.0
2	H	461	LEU	2.0
2	H	362	VAL	2.0
1	C	36	ASN	2.0
2	B	388	ASN	2.0
1	G	146	TRP	2.0
2	H	524	VAL	2.0
1	C	34	ASN	2.0
1	G	35	THR	2.0
2	H	338	PHE	2.0
1	G	193	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

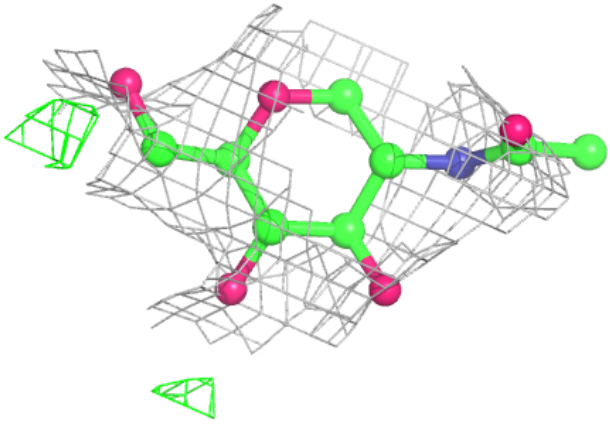
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

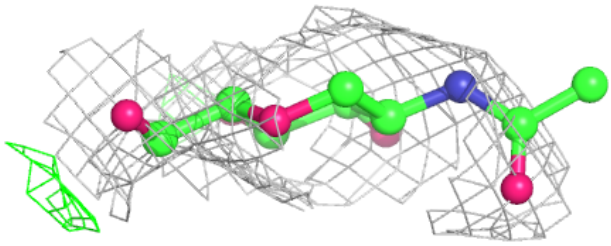
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	601	14/15	0.76	0.32	108,123,137,146	0
4	NAG	F	601	14/15	0.77	0.28	81,120,131,139	0
4	NAG	B	601	14/15	0.86	0.22	84,98,112,115	0
4	NAG	H	601	14/15	0.88	0.17	83,100,114,116	0
3	ZN	E	601	1/1	0.92	0.19	73,73,73,73	0
3	ZN	G	601	1/1	0.96	0.16	72,72,72,72	0
3	ZN	A	601	1/1	0.97	0.24	73,73,73,73	0
3	ZN	C	601	1/1	0.98	0.16	69,69,69,69	0

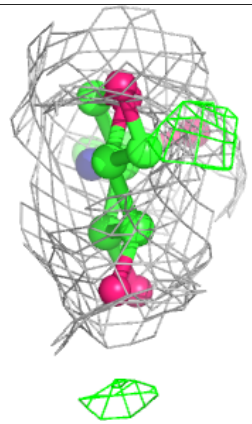
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG 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)

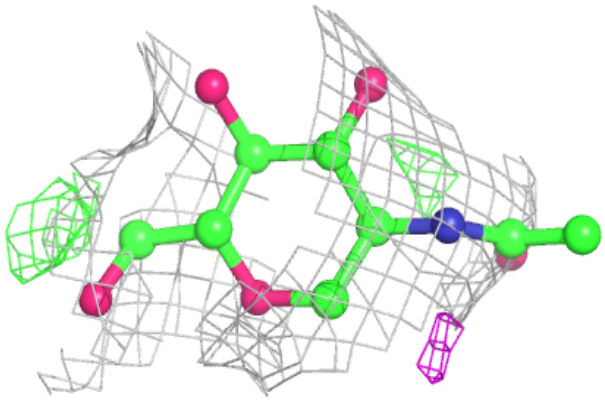


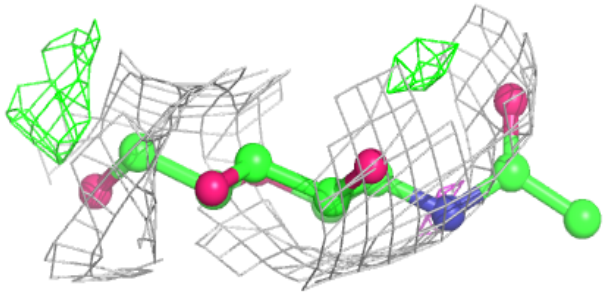


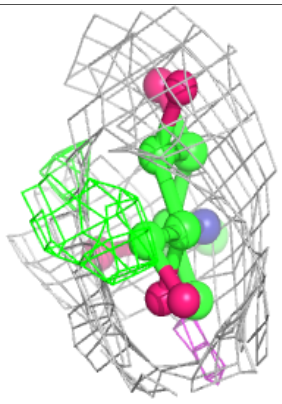


Electron density around NAG F 601:

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

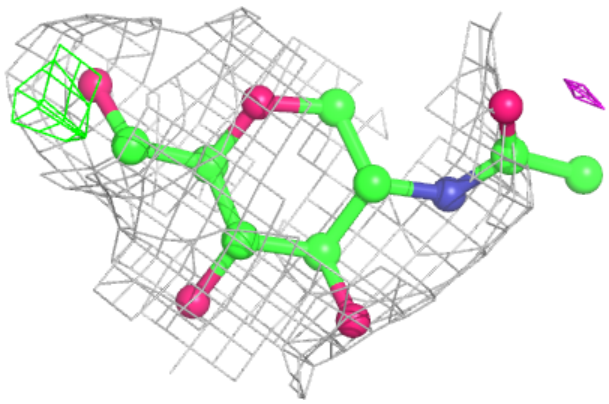


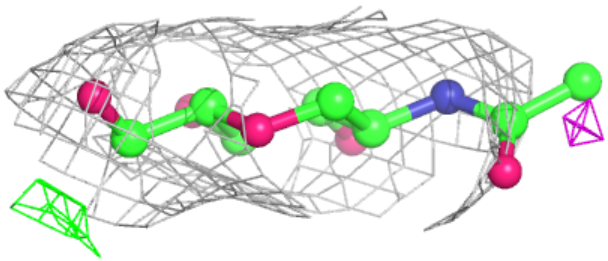


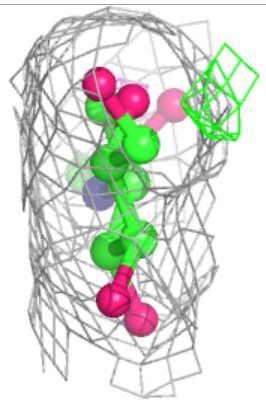


Electron density around NAG B 601:

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

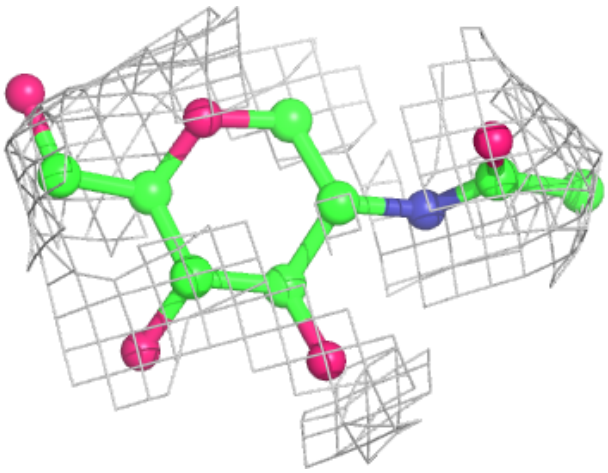


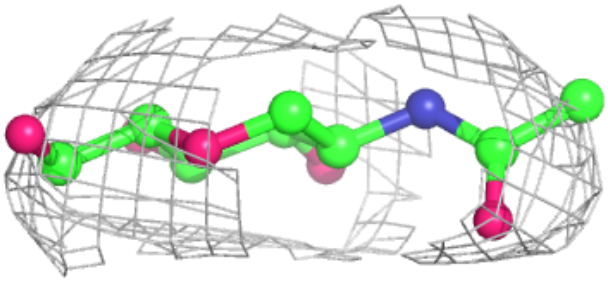


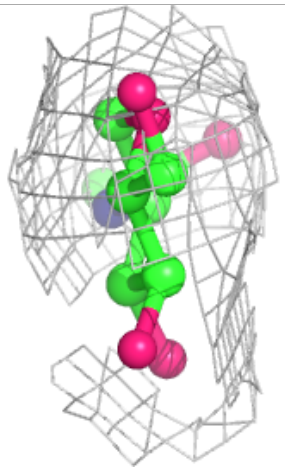


Electron density around NAG H 601:

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

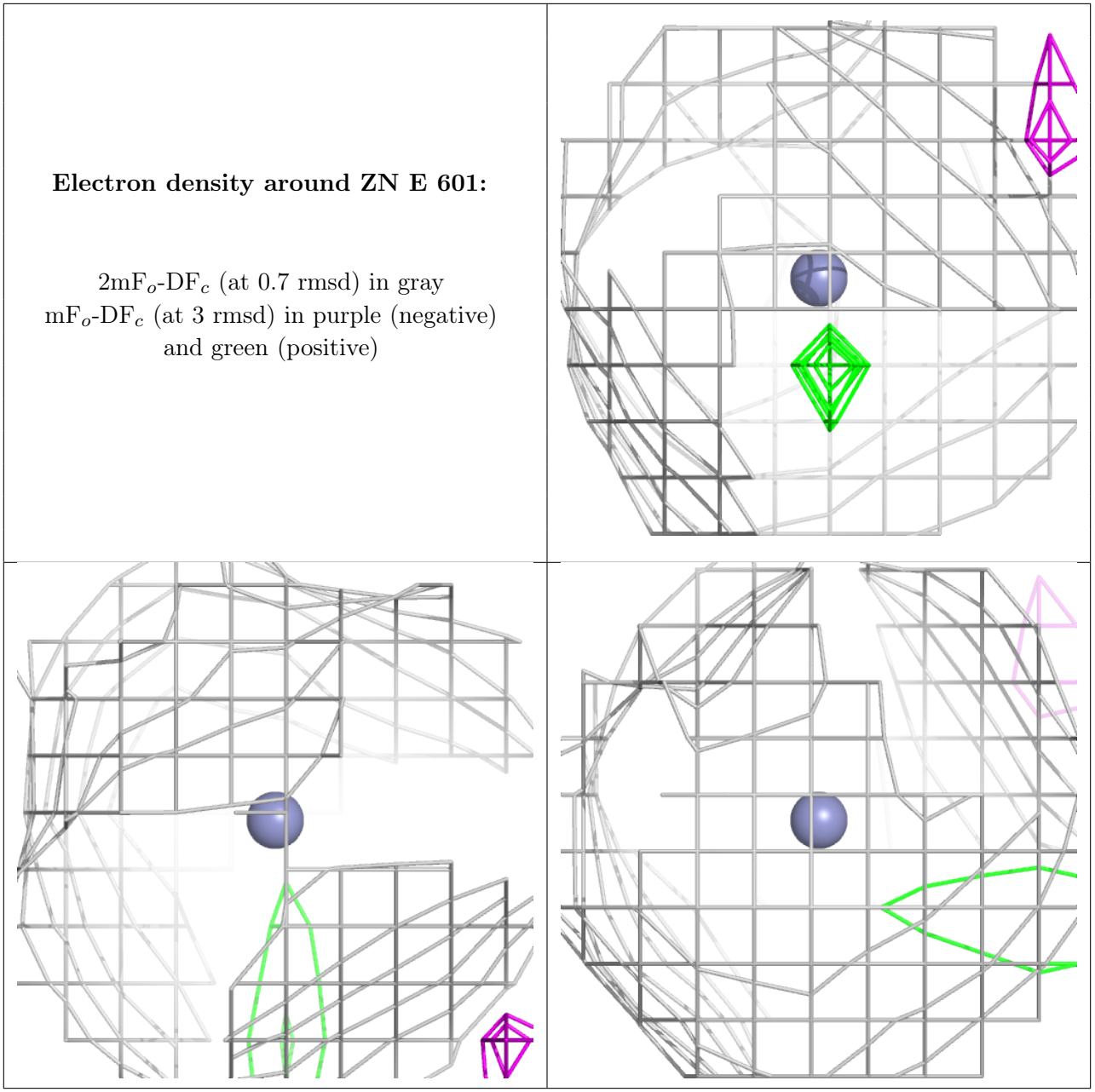






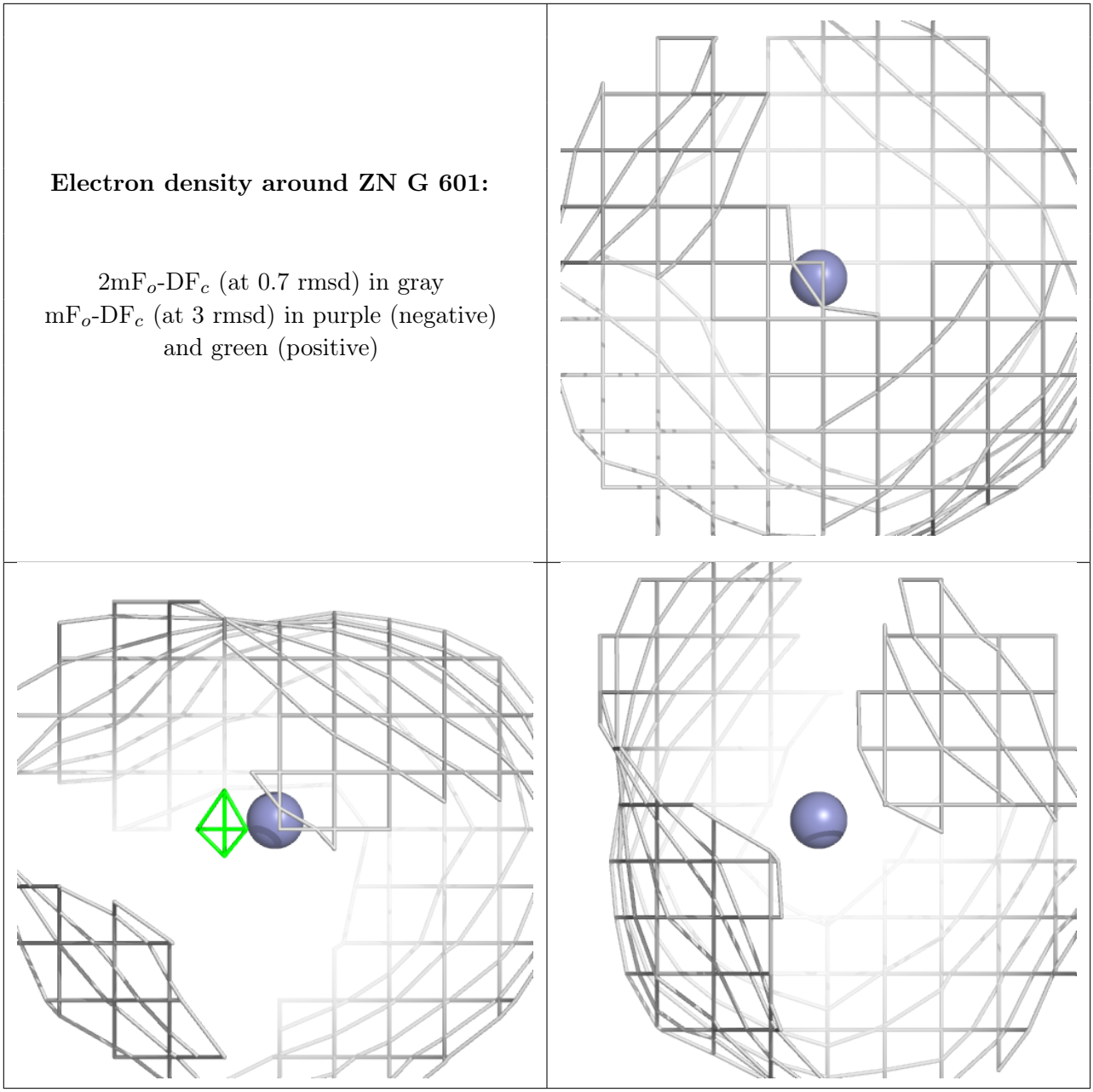
Electron density around ZN E 601:

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



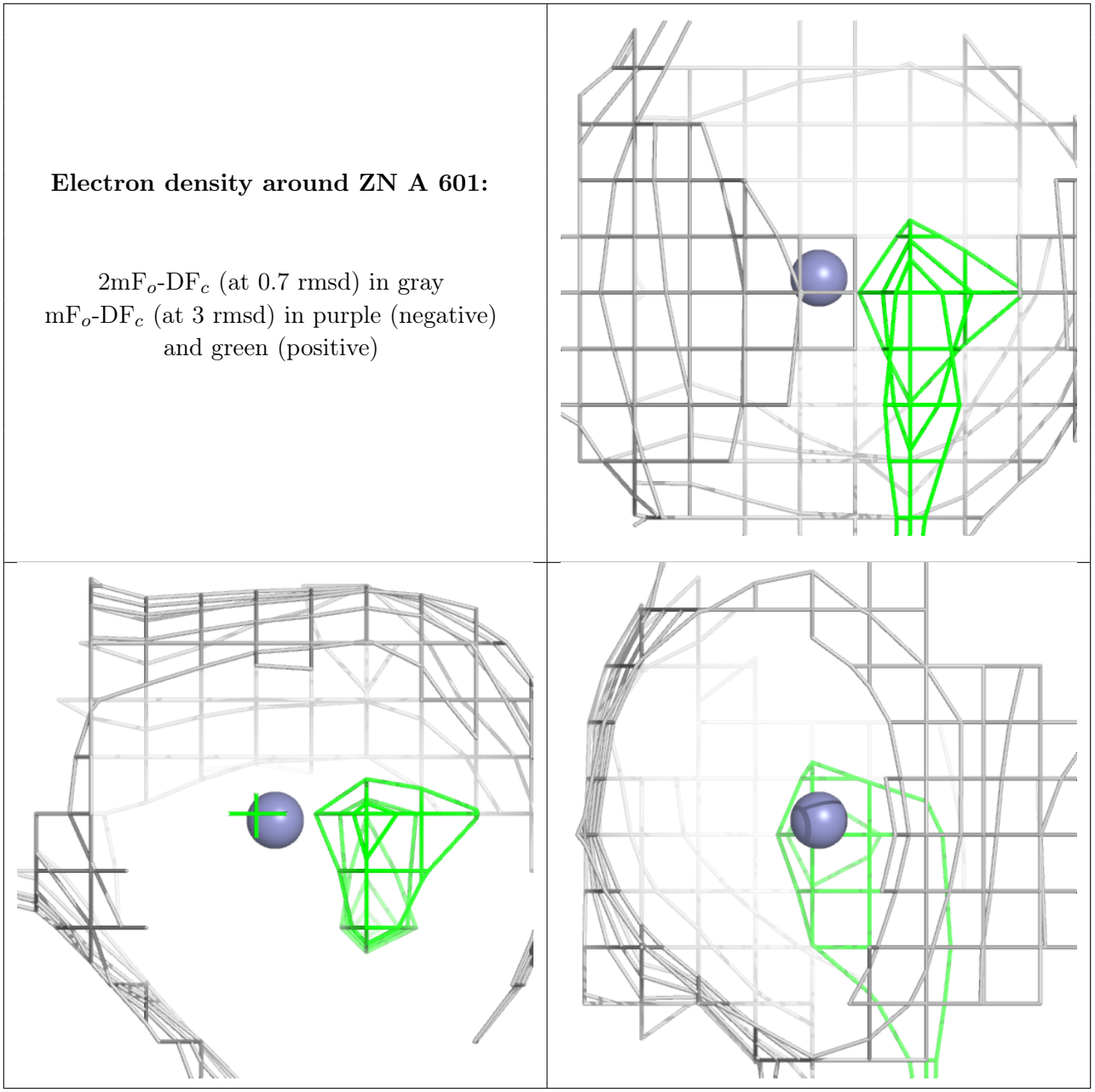
Electron density around ZN G 601:

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



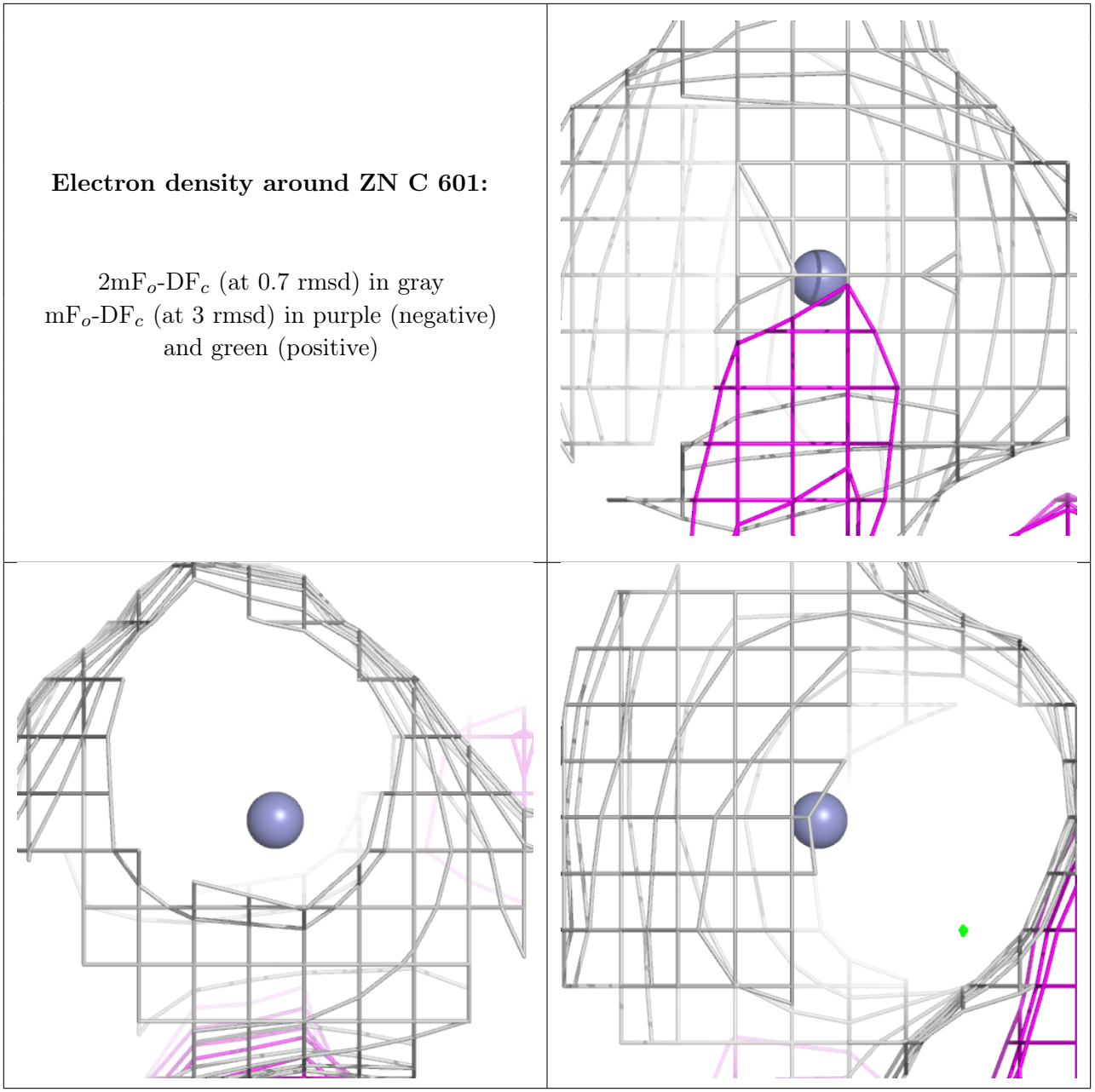
Electron density around ZN A 601:

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



Electron density around ZN 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)



6.5 Other polymers

There are no such residues in this entry.