



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 03:03 PM EDT

PDB ID : 7SMH  
Title : Structure of SASG A-domain (residues 163-419) from Staphylococcus aureus  
Authors : Atkin, K.E.; Whelan, F.; Brentnall, A.S.; Dodson, E.J.; Turkenburg, J.P.; Potts, J.R.  
Deposited on : 2021-10-25  
Resolution : 1.65 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

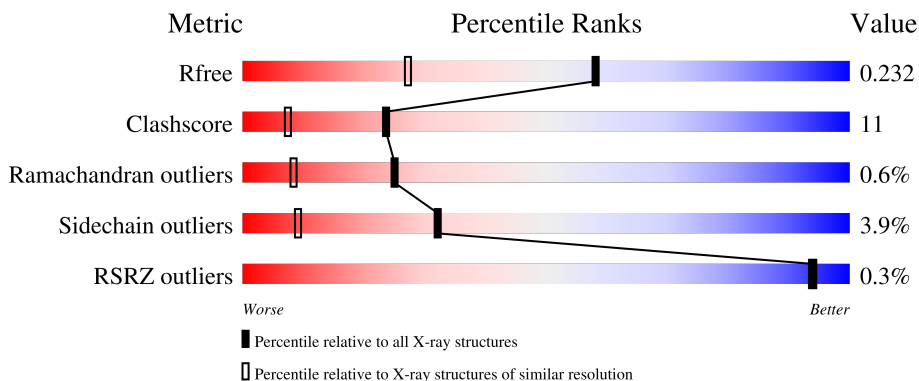
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	
1	B	280	
1	C	280	
1	D	280	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8288 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 Surface protein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	257	1995	1245	345	401	4	0	2	0
1	B	255	1984	1237	342	400	5	0	3	0
1	C	256	1975	1231	342	398	4	0	0	0
1	D	254	1964	1225	339	396	4	0	1	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

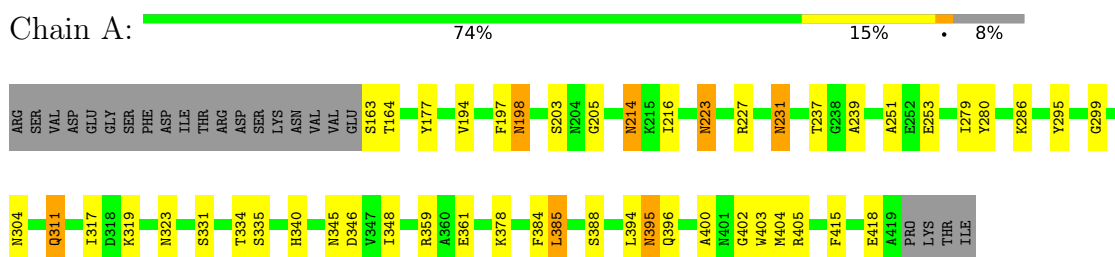
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	86	Total O 89 89	0	3
4	B	84	Total O 85 85	0	1
4	C	97	Total O 98 98	0	1
4	D	80	Total O 82 82	0	2

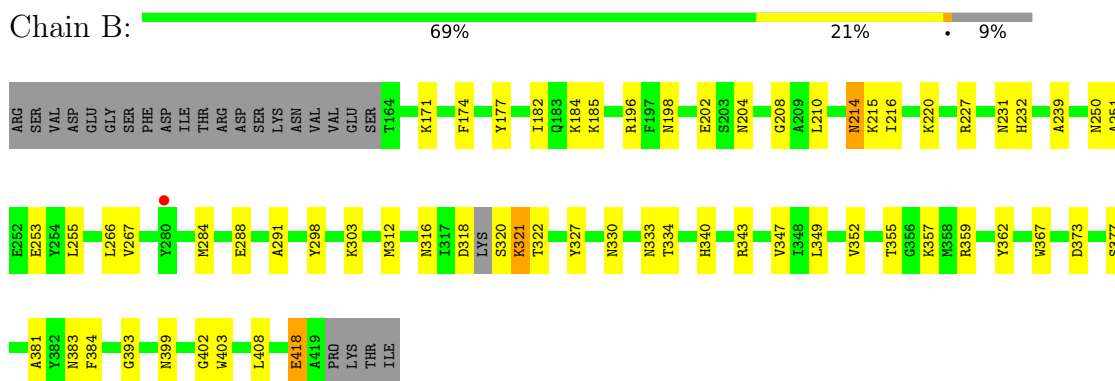
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

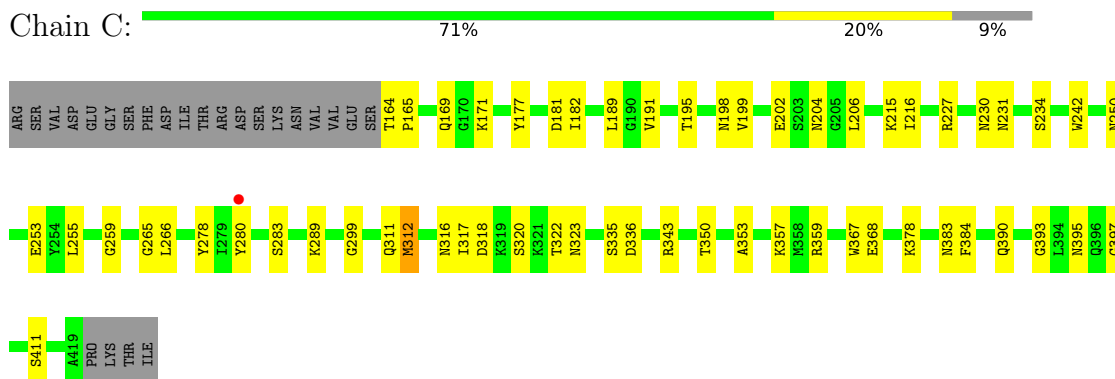
- Molecule 1: Surface protein G



- Molecule 1: Surface protein G

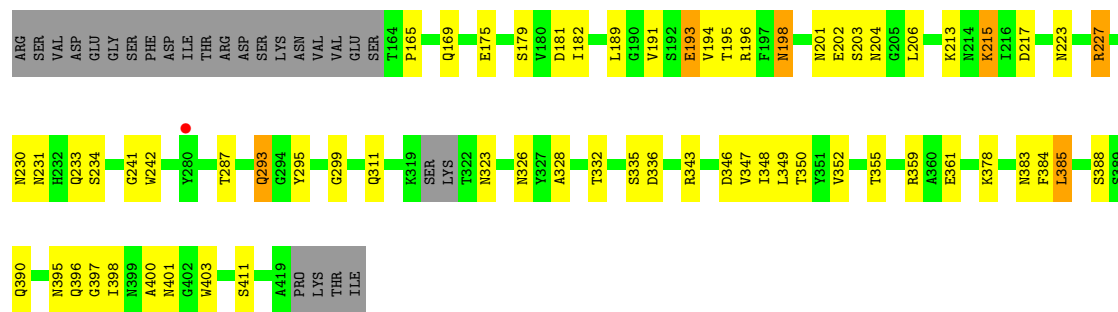


- Molecule 1: Surface protein G



- Molecule 1: Surface protein G

Chain D:  68% 21% 9%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.21Å 63.21Å 273.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.37 – 1.65 57.37 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.1 (57.37-1.65) 99.1 (57.37-1.65)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.185 , 0.226 0.194 , 0.232	Depositor DCC
$R_{free}$ test set	6365 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 16.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
Reported twinning fraction	0.506 for H, K, L 0.494 for K, H, -L	Depositor
Outliers	0 of 126731 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3298e-06.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.89	3/2035 (0.1%)	1.01	0/2740
1	B	0.90	1/2023 (0.0%)	1.02	1/2724 (0.0%)
1	C	0.91	0/2012	1.06	4/2710 (0.1%)
1	D	0.89	0/2000	1.04	3/2695 (0.1%)
All	All	0.90	4/8070 (0.0%)	1.03	8/10869 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	GLY	C-O	5.95	1.33	1.23
1	A	253	GLU	CD-OE1	5.20	1.31	1.25
1	A	205	GLY	C-O	5.09	1.31	1.23
1	A	418	GLU	CD-OE2	-5.09	1.20	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	227	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	C	227	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	343	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	C	353	ALA	CB-CA-C	5.71	118.67	110.10
1	D	217	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	C	171	LYS	CB-CA-C	-5.09	100.22	110.40
1	B	327	TYR	CB-CG-CD1	5.04	124.02	121.00
1	C	227	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	1995	0	1917	35	0
1	B	1984	0	1896	54	0
1	C	1975	0	1889	37	0
1	D	1964	0	1869	53	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
3	A	4	0	6	1	0
3	C	8	0	12	3	0
4	A	89	0	0	8	0
4	B	85	0	0	8	0
4	C	98	0	0	4	0
4	D	82	0	0	6	0
All	All	8288	0	7589	174	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 11.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:MET:SD	1:B:312[B]:MET:HG3	2.01	1.00
1:B:352[A]:VAL:HG13	1:B:355:THR:OG1	1.67	0.92
1:D:202:GLU:O	1:D:397:GLY:HA2	1.71	0.88
1:C:204:ASN:HD21	1:C:393:GLY:HA2	1.38	0.87
1:D:203:SER:O	1:D:395:ASN:C	2.13	0.86
1:D:203:SER:O	1:D:396:GLN:N	2.09	0.84
1:A:216[A]:ILE:HD13	1:A:415:PHE:CD2	2.12	0.83
1:B:298:TYR:CE2	1:B:312[B]:MET:CE	2.62	0.83
1:A:378:LYS:HG2	4:A:673:HOH:O	1.79	0.79
1:B:231:ASN:HD21	1:B:239:ALA:H	1.30	0.79
1:A:280:TYR:HE2	1:A:396:GLN:HE22	1.27	0.78
1:A:384:PHE:C	1:A:385:LEU:HD22	2.08	0.74
1:B:177:TYR:HB3	1:B:255:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352[A]:VAL:HG13	1:B:355:THR:HG1	1.55	0.71
1:D:352:VAL:HG13	1:D:355:THR:OG1	1.89	0.71
1:A:280:TYR:HE2	1:A:396:GLN:NE2	1.88	0.70
1:B:231:ASN:HD22	1:B:402:GLY:HA2	1.55	0.70
1:A:203:SER:O	1:A:395:ASN:HA	1.91	0.70
1:B:291:ALA:HA	4:B:660:HOH:O	1.94	0.67
1:B:298:TYR:HE2	1:B:312[B]:MET:CE	2.08	0.66
1:B:357:LYS:NZ	4:B:603:HOH:O	2.28	0.66
1:C:316:ASN:HD21	1:C:318:ASP:HB2	1.60	0.65
1:A:304:ASN:O	4:A:601:HOH:O	2.13	0.65
1:C:289:LYS:O	1:C:289:LYS:HG3	1.96	0.65
1:D:384:PHE:C	1:D:385:LEU:HD12	2.17	0.65
1:C:204:ASN:ND2	1:C:393:GLY:HA2	2.10	0.64
1:B:352[A]:VAL:CG1	1:B:355:THR:OG1	2.42	0.64
1:C:311:GLN:NE2	4:C:603:HOH:O	2.30	0.63
1:B:316:ASN:HD21	1:B:318:ASP:HB2	1.61	0.63
1:B:298:TYR:HE2	1:B:312[B]:MET:HE2	1.62	0.63
1:B:210:LEU:HD13	1:B:408:LEU:HD11	1.79	0.63
1:B:298:TYR:CD2	1:B:312[B]:MET:HE1	2.34	0.62
1:D:202:GLU:O	1:D:397:GLY:CA	2.45	0.61
1:A:385:LEU:N	1:A:385:LEU:CD2	2.64	0.61
1:D:201:ASN:OD1	1:D:398:ILE:N	2.25	0.61
1:D:326:ASN:ND2	4:D:601:HOH:O	2.34	0.61
1:D:352:VAL:CG1	1:D:355:THR:OG1	2.48	0.61
1:D:204:ASN:HA	1:D:395:ASN:HA	1.82	0.60
1:B:210:LEU:CD1	1:B:408:LEU:HD11	2.31	0.59
1:A:335:SER:OG	1:B:343:ARG:NH2	2.34	0.59
1:A:385:LEU:HD22	1:A:385:LEU:N	2.16	0.59
1:D:206:LEU:HG	1:D:398:ILE:HD11	1.85	0.59
1:B:381:ALA:CB	1:B:418:GLU:HB2	2.34	0.58
1:B:381:ALA:HB2	1:B:418:GLU:HB2	1.86	0.58
1:C:216:ILE:HD11	1:C:384:PHE:HB2	1.86	0.58
1:D:195:THR:HG23	4:D:622:HOH:O	2.04	0.58
1:A:280:TYR:CE2	1:A:396:GLN:NE2	2.70	0.57
1:C:189:LEU:O	1:D:335:SER:HB2	2.05	0.57
1:A:227:ARG:HD3	1:A:346:ASP:OD1	2.05	0.57
1:C:191:VAL:HG12	1:D:336:ASP:HA	1.86	0.56
1:D:347:VAL:HG12	1:D:349:LEU:CD1	2.36	0.56
1:D:233:GLN:NE2	1:D:233:GLN:HA	2.21	0.55
1:C:253:GLU:HB2	1:C:266:LEU:HD21	1.89	0.55
1:C:216:ILE:CD1	1:C:384:PHE:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LYS:HD2	1:B:182:ILE:HD11	1.89	0.54
1:B:298:TYR:CE2	1:B:312[B]:MET:HE1	2.42	0.54
1:C:164:THR:HG22	1:C:165:PRO:O	2.07	0.54
1:B:320:SER:HB3	1:B:322:THR:HG22	1.90	0.54
1:D:202:GLU:C	1:D:397:GLY:HA2	2.29	0.53
1:D:299:GLY:O	1:D:323:ASN:HB3	2.08	0.53
1:D:215:LYS:HE2	1:D:383:ASN:HD21	1.74	0.53
3:C:502:EDO:H21	4:C:690:HOH:O	2.09	0.53
1:B:216:ILE:CD1	1:B:384:PHE:HB2	2.39	0.52
1:D:227:ARG:HD3	1:D:346:ASP:OD1	2.09	0.52
1:D:206:LEU:HG	1:D:398:ILE:CD1	2.39	0.52
1:A:214:ASN:N	1:A:214:ASN:OD1	2.43	0.52
1:D:215:LYS:HD2	4:D:640:HOH:O	2.11	0.51
1:C:317:ILE:HD13	1:C:368:GLU:HB2	1.92	0.51
1:D:195:THR:CG2	4:D:622:HOH:O	2.59	0.51
1:A:311:GLN:HB2	4:A:678:HOH:O	2.11	0.50
1:D:385:LEU:CD1	1:D:385:LEU:N	2.75	0.50
1:B:196:ARG:NH2	3:C:503:EDO:O2	2.45	0.50
1:D:233:GLN:HE21	1:D:234:SER:H	1.59	0.50
1:D:223:ASN:ND2	1:D:350:THR:HG22	2.26	0.50
1:C:182:ILE:HD13	1:C:195:THR:HA	1.94	0.50
1:A:223:ASN:C	1:A:223:ASN:HD22	2.14	0.49
1:B:284:MET:HE2	4:B:659:HOH:O	2.13	0.49
1:D:350:THR:OG1	1:D:359:ARG:HB3	2.13	0.49
1:B:231:ASN:ND2	1:B:239:ALA:H	2.07	0.49
1:C:350:THR:OG1	1:C:359:ARG:HB3	2.13	0.49
1:D:385:LEU:HD12	1:D:385:LEU:N	2.28	0.49
1:B:196:ARG:NH2	3:C:503:EDO:C2	2.76	0.48
1:B:214:ASN:HD22	1:B:214:ASN:N	2.11	0.48
1:B:202:GLU:OE1	1:B:202:GLU:HA	2.13	0.48
1:C:343:ARG:NH2	1:D:335:SER:OG	2.47	0.48
1:B:267:VAL:HG23	4:B:682:HOH:O	2.14	0.48
1:A:331:SER:HA	4:A:638:HOH:O	2.14	0.47
1:D:348:ILE:HB	1:D:361:GLU:HB2	1.96	0.47
1:A:198:ASN:O	4:A:602:HOH:O	2.20	0.47
1:C:215:LYS:HE2	1:C:383:ASN:HD21	1.80	0.47
1:D:182[A]:ILE:HD13	1:D:195:THR:HA	1.96	0.47
1:C:204:ASN:OD1	1:C:395:ASN:N	2.40	0.47
1:A:394:LEU:O	1:A:395:ASN:C	2.53	0.46
1:A:317:ILE:HD11	1:A:359:ARG:CZ	2.46	0.46
1:A:299:GLY:O	1:A:323:ASN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LYS:HD3	1:B:357:LYS:HA	1.80	0.46
1:D:169:GLN:HB3	1:D:411:SER:O	2.16	0.46
1:B:334:THR:HA	1:B:340:HIS:CD2	2.51	0.46
1:D:383:ASN:HA	4:D:626:HOH:O	2.15	0.45
1:C:299:GLY:O	1:C:323:ASN:HB3	2.15	0.45
3:A:502:EDO:H11	4:A:685:HOH:O	2.15	0.45
1:B:359:ARG:HA	1:B:367:TRP:O	2.16	0.45
1:A:237:THR:HB	1:A:400:ALA:HB3	1.99	0.45
1:A:394:LEU:HB3	1:A:396:GLN:NE2	2.32	0.45
1:C:230:ASN:ND2	1:C:242:TRP:HE1	2.15	0.45
1:C:390:GLN:OE1	4:C:601:HOH:O	2.21	0.45
1:A:335:SER:HA	4:B:673:HOH:O	2.17	0.45
1:C:181:ASP:CG	1:C:199:VAL:HG11	2.37	0.45
1:D:175:GLU:HG2	1:D:213:LYS:HE3	1.99	0.45
1:D:193:GLU:HG3	1:D:194:VAL:N	2.31	0.45
1:A:197:PHE:HB3	1:A:388:SER:HB3	1.98	0.44
1:B:216:ILE:HD11	1:B:384:PHE:HB2	1.99	0.44
1:D:201:ASN:HA	1:D:398:ILE:HB	1.98	0.44
1:D:401:ASN:ND2	1:D:403:TRP:CD2	2.84	0.44
1:D:182[A]:ILE:HD12	1:D:193:GLU:OE2	2.17	0.44
1:B:231:ASN:HB3	1:B:403:TRP:O	2.18	0.44
1:B:303:LYS:HD3	1:B:373:ASP:O	2.17	0.44
1:B:316:ASN:HD22	1:B:321:LYS:HA	1.82	0.44
1:A:394:LEU:O	1:A:396:GLN:N	2.51	0.44
1:B:253:GLU:HB2	1:B:266:LEU:HD21	2.00	0.44
1:B:267:VAL:CG2	4:B:682:HOH:O	2.64	0.44
1:A:239:ALA:CB	1:A:404:MET:CG	2.95	0.44
1:D:233:GLN:OE1	1:D:400:ALA:HB1	2.18	0.44
1:B:251:ALA:O	1:B:255:LEU:HG	2.18	0.43
1:D:295:TYR:CD2	1:D:328:ALA:HB3	2.53	0.43
1:C:202:GLU:O	1:C:397:GLY:HA2	2.17	0.43
1:A:348:ILE:HB	1:A:361:GLU:HB2	1.99	0.43
1:D:352:VAL:HG13	1:D:352:VAL:O	2.18	0.43
1:A:334:THR:HA	1:A:340:HIS:CD2	2.52	0.43
1:B:215:LYS:HG2	1:B:383:ASN:ND2	2.34	0.42
1:D:204:ASN:OD1	1:D:395:ASN:N	2.50	0.42
1:C:181:ASP:OD2	1:C:199:VAL:HG11	2.19	0.42
1:D:165:PRO:HB3	4:D:677:HOH:O	2.19	0.42
1:A:231:ASN:HB3	1:A:403:TRP:O	2.20	0.42
1:B:204:ASN:OD1	1:B:393:GLY:O	2.38	0.42
1:B:232:HIS:CE1	1:B:330:ASN:HD22	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLU:HG3	1:B:312[B]:MET:CE	2.50	0.42
1:B:298:TYR:CE2	1:B:312[B]:MET:HE2	2.41	0.42
1:D:206:LEU:HD12	1:D:390:GLN:OE1	2.19	0.42
1:A:197:PHE:CB	1:A:388:SER:HB3	2.50	0.42
4:A:672:HOH:O	1:B:333:ASN:HB3	2.19	0.42
1:D:241:GLY:O	1:D:388:SER:OG	2.26	0.42
1:B:174:PHE:HB3	1:B:210:LEU:HD22	2.01	0.42
1:D:230:ASN:ND2	1:D:242:TRP:HE1	2.18	0.42
1:A:194:VAL:HG21	1:A:405:ARG:HD2	2.02	0.41
1:A:345:ASN:HB3	4:A:647:HOH:O	2.20	0.41
1:C:335:SER:HB2	1:D:189:LEU:O	2.20	0.41
1:C:177:TYR:HB3	1:C:255:LEU:HD11	2.01	0.41
1:C:312:MET:HE2	1:C:312:MET:HB2	1.97	0.41
1:B:232:HIS:HE1	1:B:330:ASN:HD22	1.69	0.41
1:B:284:MET:HG2	1:B:312[B]:MET:HE3	2.01	0.41
1:D:203:SER:O	1:D:395:ASN:CA	2.69	0.41
1:B:347:VAL:HG22	1:B:362:TYR:CD1	2.56	0.41
1:B:373:ASP:CG	4:B:608:HOH:O	2.59	0.41
1:C:169:GLN:HB2	1:C:411:SER:O	2.21	0.41
1:C:357:LYS:HA	1:C:357:LYS:HD3	1.85	0.41
1:B:250:ASN:OD1	1:B:253:GLU:HG3	2.21	0.41
1:D:179:SER:OG	1:D:198:ASN:HA	2.21	0.41
1:C:250:ASN:OD1	1:C:253:GLU:HG3	2.21	0.41
1:C:336:ASP:HA	1:D:191:VAL:HG12	2.02	0.41
1:C:206:LEU:HA	4:C:642:HOH:O	2.21	0.40
1:A:177:TYR:CD2	1:A:251:ALA:CB	3.04	0.40
1:A:394:LEU:O	1:A:396:GLN:HG3	2.21	0.40
1:B:220:LYS:HA	1:B:220:LYS:HD3	1.88	0.40
1:C:320:SER:HB2	1:C:322:THR:HG22	2.03	0.40
1:D:293:GLN:H	1:D:293:GLN:HG3	1.64	0.40
1:A:231:ASN:OD1	1:A:402:GLY:HA2	2.21	0.40
1:B:330:ASN:HB2	4:B:645:HOH:O	2.22	0.40
1:C:259:GLY:O	1:C:265:GLY:HA3	2.21	0.40
1:C:278:TYR:CZ	1:C:280:TYR:HA	2.56	0.40
1:C:323:ASN:HD22	1:C:367:TRP:HE1	1.69	0.40
1:C:169:GLN:CB	1:C:411:SER:O	2.69	0.40
1:D:181:ASP:OD1	1:D:196:ARG:HB3	2.22	0.40
1:C:191:VAL:CG1	1:D:336:ASP:HA	2.51	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	257/280 (92%)	244 (95%)	10 (4%)	3 (1%)	13	2
1	B	254/280 (91%)	244 (96%)	9 (4%)	1 (0%)	34	16
1	C	254/280 (91%)	246 (97%)	7 (3%)	1 (0%)	34	16
1	D	251/280 (90%)	243 (97%)	7 (3%)	1 (0%)	34	16
All	All	1016/1120 (91%)	977 (96%)	33 (3%)	6 (1%)	25	8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	295	TYR
1	A	395	ASN
1	B	198	ASN
1	C	198	ASN
1	D	198	ASN

### 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	213/233 (91%)	203 (95%)	10 (5%)	26	6
1	B	212/233 (91%)	202 (95%)	10 (5%)	26	6
1	C	210/233 (90%)	205 (98%)	5 (2%)	49	23
1	D	208/233 (89%)	199 (96%)	9 (4%)	29	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	843/932 (90%)	809 (96%)	34 (4%)	32 9

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	SER
1	A	164	THR
1	A	214	ASN
1	A	223	ASN
1	A	231	ASN
1	A	279	ILE
1	A	286	LYS
1	A	311	GLN
1	A	319	LYS
1	A	385	LEU
1	B	184	LYS
1	B	185	LYS
1	B	214	ASN
1	B	227	ARG
1	B	321	LYS
1	B	349	LEU
1	B	377[A]	SER
1	B	377[B]	SER
1	B	399	ASN
1	B	418	GLU
1	C	231	ASN
1	C	234	SER
1	C	283	SER
1	C	312	MET
1	C	378	LYS
1	D	193	GLU
1	D	215	LYS
1	D	231	ASN
1	D	287	THR
1	D	293	GLN
1	D	311	GLN
1	D	332	THR
1	D	378	LYS
1	D	385	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	230	ASN
1	A	233	GLN
1	A	316	ASN
1	A	383	ASN
1	A	396	GLN
1	B	169	GLN
1	B	183	GLN
1	B	214	ASN
1	B	230	ASN
1	B	231	ASN
1	B	232	HIS
1	B	316	ASN
1	B	330	ASN
1	B	383	ASN
1	C	230	ASN
1	C	316	ASN
1	C	383	ASN
1	D	198	ASN
1	D	230	ASN
1	D	232	HIS
1	D	233	GLN
1	D	309	ASN
1	D	330	ASN
1	D	333	ASN
1	D	383	ASN

### 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

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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
3	EDO	C	502	-	3,3,3	0.76	0	2,2,2	0.30	0
3	EDO	A	502	-	3,3,3	0.64	0	2,2,2	0.34	0
3	EDO	C	503	-	3,3,3	0.43	0	2,2,2	0.35	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	C	503	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	EDO	O1-C1-C2-O2
3	C	502	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	EDO	1	0
3	A	502	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	EDO	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	257/280 (91%)	-0.25	0 <b>100</b>   <b>100</b>	5, 17, 31, 47	0
1	B	255/280 (91%)	-0.21	1 (0%) <b>92</b>   <b>93</b>	9, 17, 29, 41	0
1	C	256/280 (91%)	-0.32	1 (0%) <b>92</b>   <b>93</b>	7, 16, 27, 44	0
1	D	254/280 (90%)	-0.20	1 (0%) <b>92</b>   <b>93</b>	8, 18, 31, 50	0
All	All	1022/1120 (91%)	-0.25	3 (0%) <b>94</b>   <b>94</b>	5, 17, 30, 50	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	TYR	3.1
1	D	280	TYR	2.6
1	B	280	TYR	2.3

### 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](#)

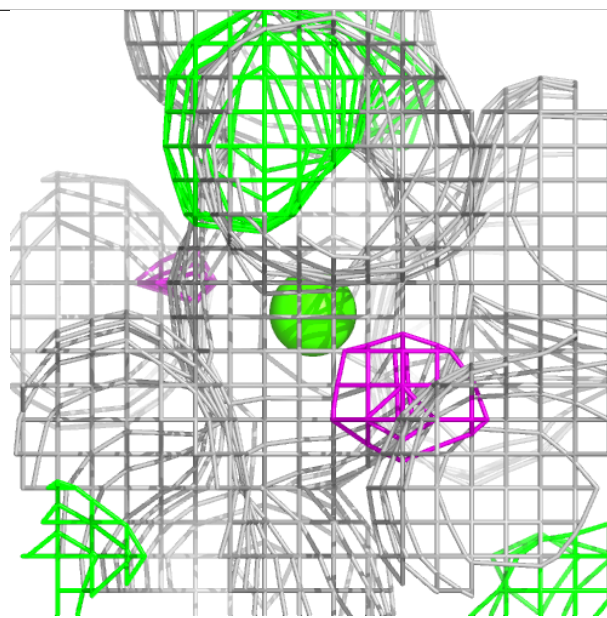
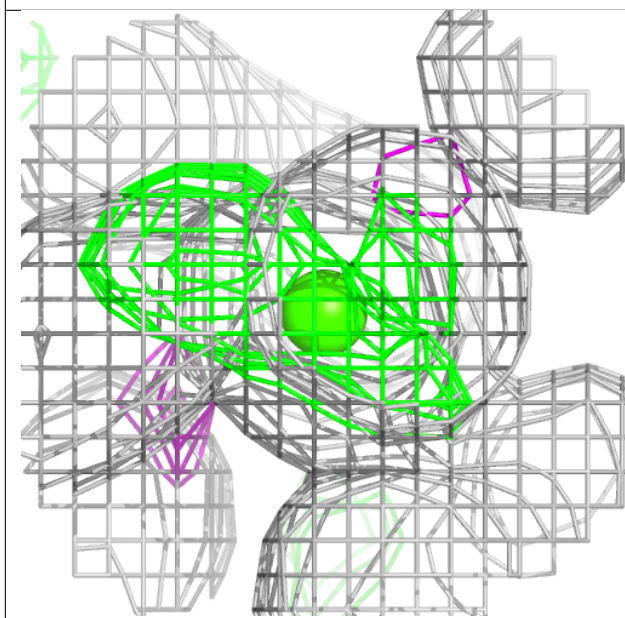
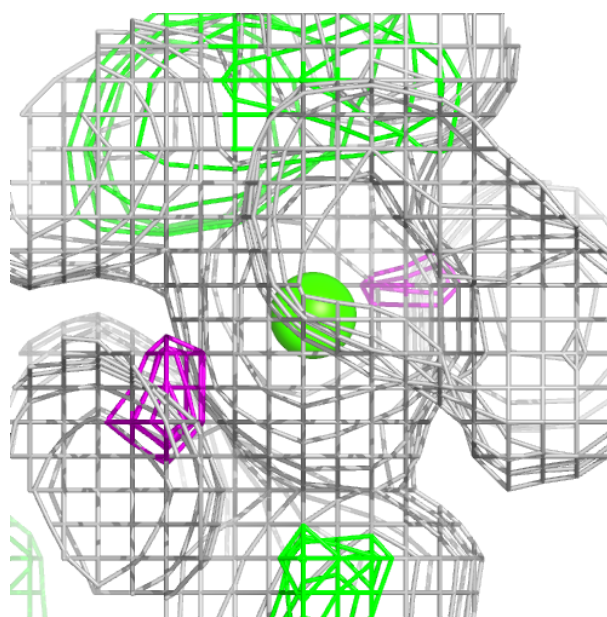
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	C	503	4/4	0.91	0.15	25,28,29,31	0
3	EDO	A	502	4/4	0.92	0.12	18,21,22,31	0
3	EDO	C	502	4/4	0.96	0.10	11,14,14,18	0
2	CA	D	500	1/1	0.98	0.04	20,20,20,20	0
2	CA	B	500	1/1	0.98	0.05	20,20,20,20	0
2	CA	A	501	1/1	0.99	0.04	19,19,19,19	0
2	CA	C	501	1/1	1.00	0.04	16,16,16,16	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.

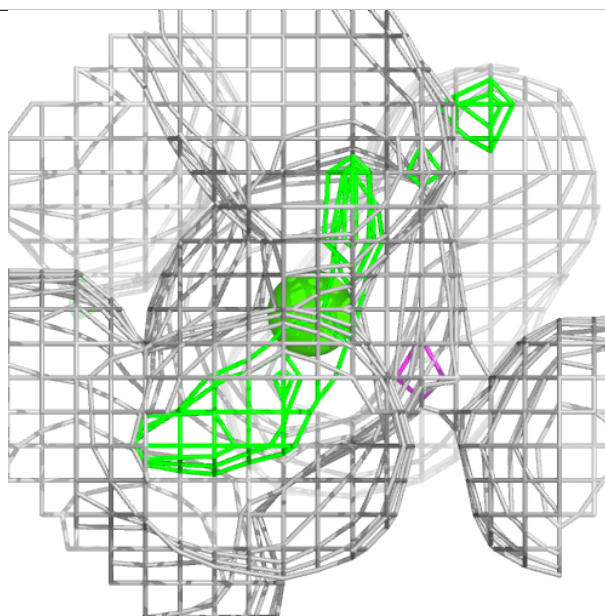
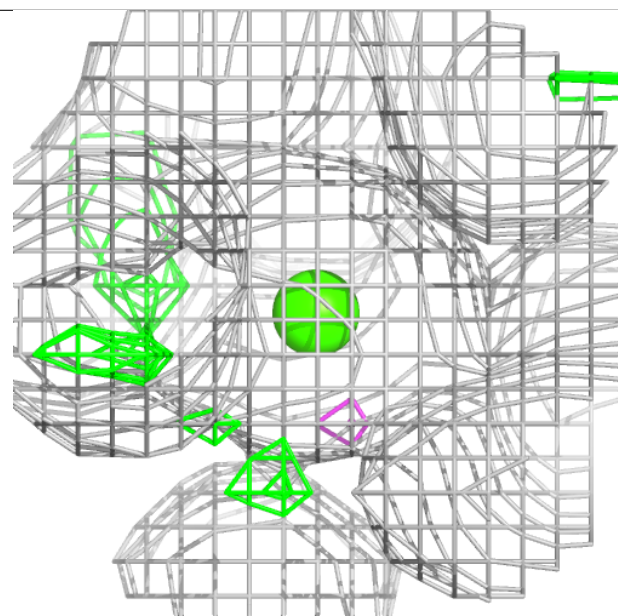
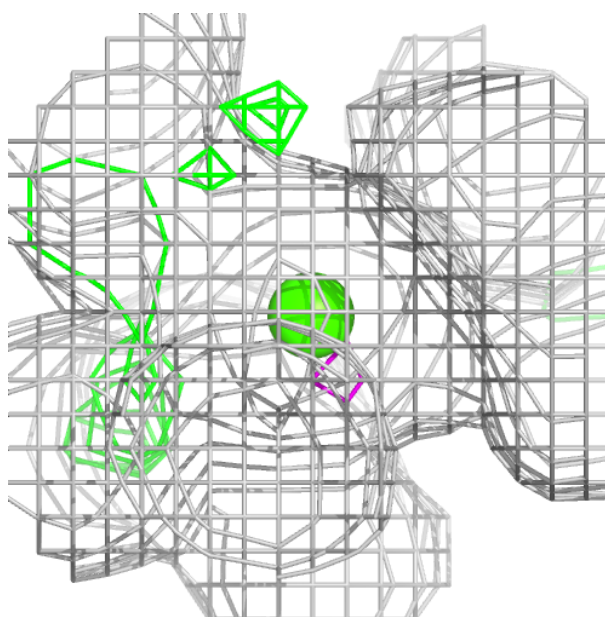
**Electron density around CA D 500:**

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



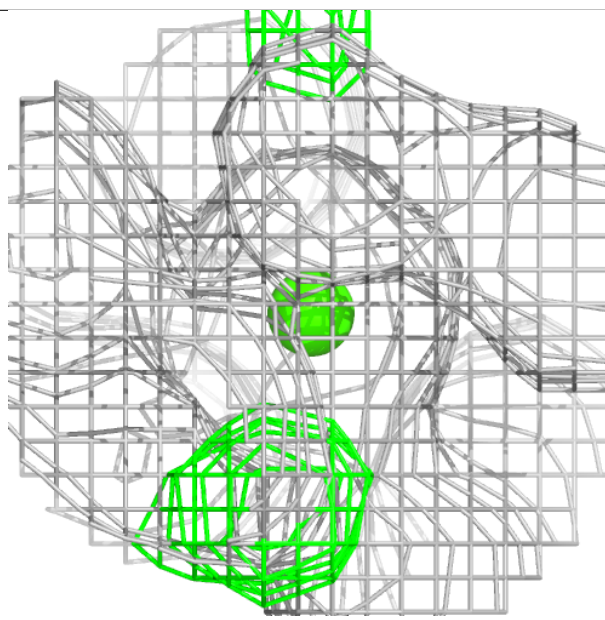
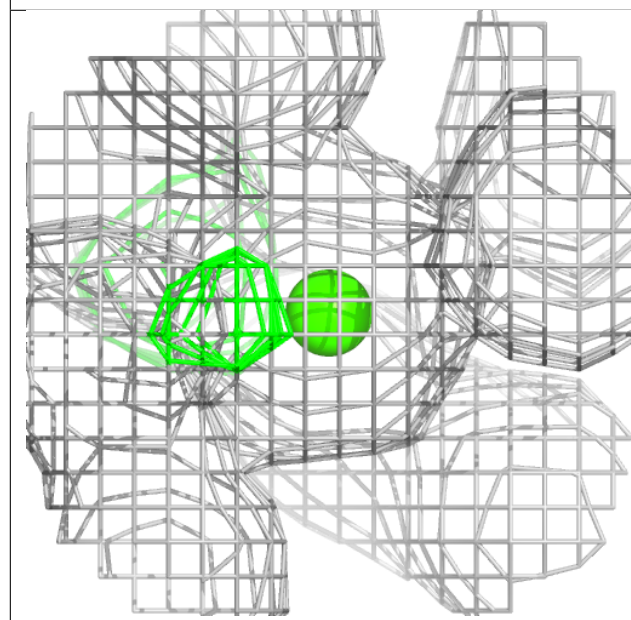
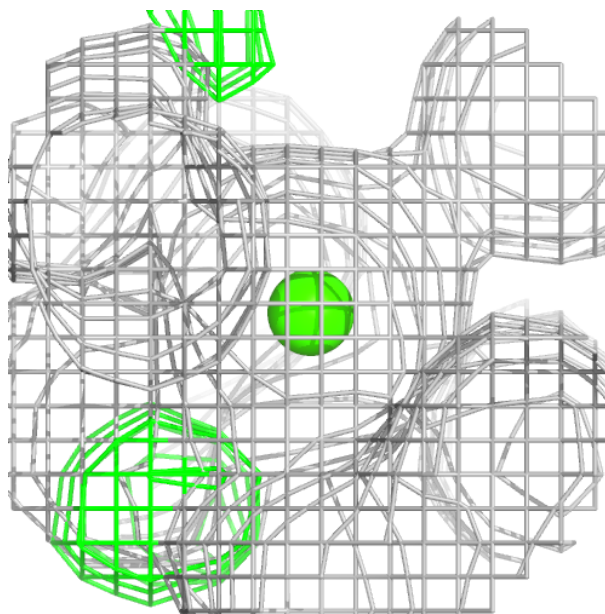
**Electron density around CA B 500:**

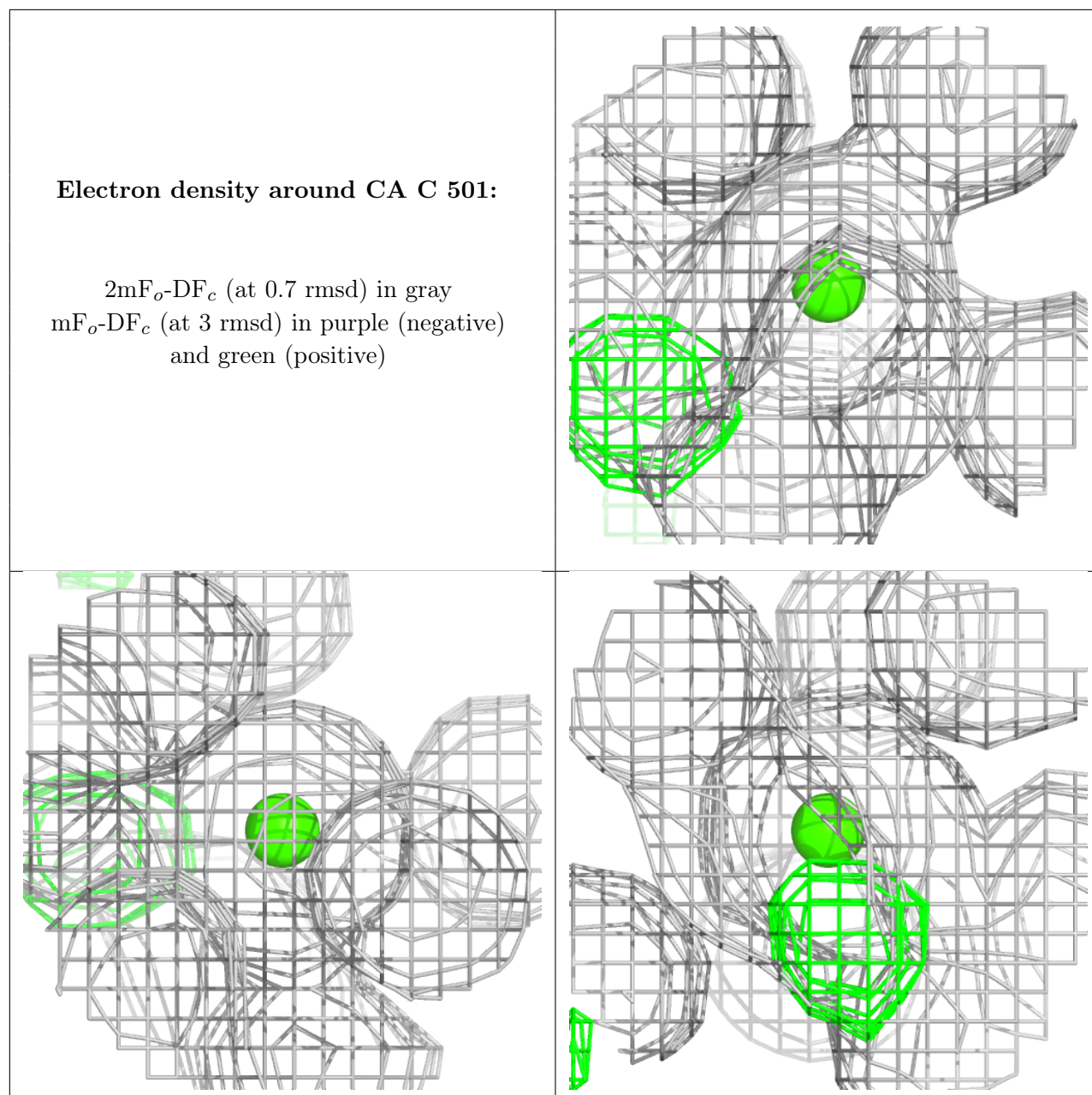
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CA A 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.