



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:08 PM UTC

PDB ID : 9K8W / pdb_00009k8w
Title : Crystal structure of the calcium indicator GCaMP6s-BrUS in calcium-bound state
Authors : Varfolomeeva, L.A.; Simonyan, T.R.; Mamontova, A.V.; Bogdanov, A.M.; Popov, V.O.; Boyko, K.M.
Deposited on : 2024-10-24
Resolution : 2.65 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

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

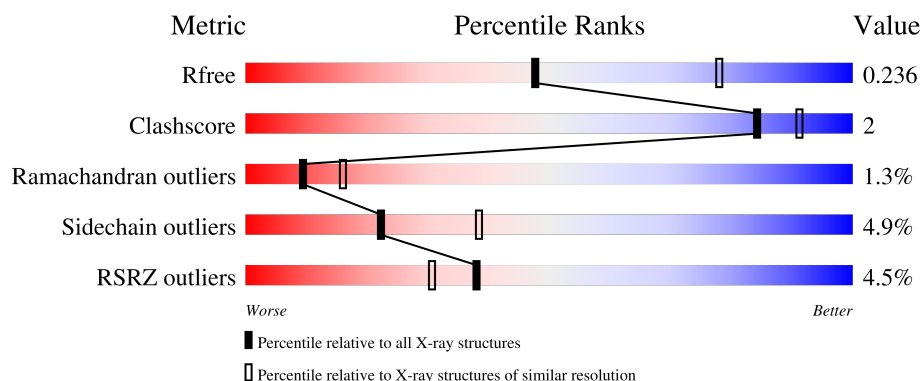
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 ≥ 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	461	4% 61% 25% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3230 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 Calcium indicator GCaMP6s-BrUS,Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3136	1975	524	621	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	PRO	ALA	engineered mutation	UNP P0DP23
A	375	ASP	ASN	engineered mutation	UNP P0DP23
A	393	TYR	ASP	engineered mutation	UNP P0DP23
A	394	ARG	THR	engineered mutation	UNP P0DP23
A	396	THR	SER	engineered mutation	UNP P0DP23
A	405	GLY	ARG	engineered mutation	UNP P0DP23

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	121.54Å 121.54Å 97.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.52 – 2.65 47.52 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.52-2.65) 98.9 (47.52-2.65)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.181 , 0.236 0.181 , 0.236	Depositor DCC
R_{free} test set	1080 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3230	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CR2, CA

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	0.79	0/3174	1.99	117/4286 (2.7%)

There are no bond length outliers.

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	GLN	N-CA-CB	12.21	128.38	110.06
1	A	81	GLN	CB-CA-C	-10.85	92.23	110.68
1	A	242	ARG	CG-CD-NE	-10.10	89.78	112.00
1	A	53	ARG	CA-CB-CG	9.48	133.06	114.10
1	A	397	GLU	CB-CG-CD	8.71	127.41	112.60
1	A	97	ASP	CB-CA-C	8.63	123.56	111.74
1	A	276	LYS	CB-CG-CD	8.11	129.95	111.30
1	A	301	GLU	CB-CG-CD	8.10	126.36	112.60
1	A	312	TYR	CB-CA-C	7.96	126.25	110.42
1	A	130	LYS	CB-CA-C	7.88	122.75	110.14
1	A	276	LYS	CA-CB-CG	7.80	129.69	114.10
1	A	421	ARG	N-CA-CB	7.61	121.04	110.01
1	A	441	ARG	CA-CB-CG	7.55	129.19	114.10
1	A	47	MET	CA-C-N	7.53	131.12	120.42
1	A	47	MET	C-N-CA	7.53	131.12	120.42
1	A	54	LYS	CB-CG-CD	7.52	128.60	111.30
1	A	146	GLU	N-CA-CB	-7.48	98.25	110.81
1	A	442	GLU	N-CA-CB	7.44	121.22	110.06
1	A	246	HIS	CA-CB-CG	7.34	121.14	113.80
1	A	322	GLU	CB-CA-C	7.23	122.94	110.79
1	A	77	LYS	CA-CB-CG	7.21	128.53	114.10
1	A	392	LYS	N-CA-CB	7.20	121.44	110.28
1	A	398	GLU	CB-CG-CD	7.20	124.83	112.60
1	A	244	PRO	CB-CA-C	7.11	120.29	111.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	375	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	52	ARG	CA-C-N	6.93	129.45	120.44
1	A	52	ARG	C-N-CA	6.93	129.45	120.44
1	A	128	GLN	N-CA-CB	6.92	121.44	110.65
1	A	286	ASP	CB-CA-C	6.91	122.14	111.02
1	A	272	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	172	LYS	CB-CA-C	6.83	121.61	110.88
1	A	320	THR	CA-CB-OG1	6.81	119.81	109.60
1	A	441	ARG	CD-NE-CZ	6.78	133.90	124.40
1	A	134	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	333	LEU	N-CA-CB	6.72	120.00	110.12
1	A	436	VAL	CA-C-N	6.68	129.23	120.28
1	A	436	VAL	C-N-CA	6.68	129.23	120.28
1	A	298	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	96	GLU	CA-C-N	-6.61	112.59	122.24
1	A	96	GLU	C-N-CA	-6.61	112.59	122.24
1	A	461	THR	CA-CB-OG1	-6.54	99.79	109.60
1	A	211	LEU	N-CA-CB	-6.53	99.45	111.13
1	A	390	LYS	CB-CG-CD	6.46	126.15	111.30
1	A	83	ASN	CB-CA-C	6.41	120.83	111.73
1	A	448	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	203	GLU	CB-CG-CD	-6.32	101.86	112.60
1	A	371	ASP	CA-C-N	6.26	129.00	120.54
1	A	371	ASP	C-N-CA	6.26	129.00	120.54
1	A	329	GLU	CB-CA-C	6.24	120.68	110.88
1	A	259	GLU	N-CA-CB	6.23	119.93	110.28
1	A	402	GLU	N-CA-CB	6.16	119.30	110.06
1	A	364	GLN	O-C-N	6.09	128.34	122.07
1	A	170	VAL	CA-CB-CG1	6.06	120.70	110.40
1	A	440	ILE	CA-C-N	6.05	128.67	120.38
1	A	440	ILE	C-N-CA	6.05	128.67	120.38
1	A	327	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	80	LYS	CA-C-O	-5.95	114.54	120.90
1	A	114	ASP	CB-CA-C	5.91	122.34	109.99
1	A	52	ARG	CB-CA-C	5.88	120.56	110.79
1	A	435	GLU	CA-C-N	5.82	128.10	120.60
1	A	435	GLU	C-N-CA	5.82	128.10	120.60
1	A	322	GLU	CB-CG-CD	5.80	122.46	112.60
1	A	95	ILE	CA-C-N	5.80	129.52	120.82
1	A	95	ILE	C-N-CA	5.80	129.52	120.82
1	A	417	ALA	CA-C-N	5.77	127.94	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	ALA	C-N-CA	5.77	127.94	120.44
1	A	138	LYS	N-CA-CB	5.76	119.21	110.28
1	A	46	THR	CA-C-N	5.75	128.46	120.29
1	A	46	THR	C-N-CA	5.75	128.46	120.29
1	A	423	VAL	N-CA-CB	5.67	116.80	110.62
1	A	170	VAL	N-CA-CB	5.64	121.10	111.50
1	A	251	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	433	ASP	CA-C-N	5.62	132.28	121.54
1	A	433	ASP	C-N-CA	5.62	132.28	121.54
1	A	86	LYS	CG-CD-CE	5.57	124.12	111.30
1	A	408	ASP	CB-CA-C	5.56	120.73	111.83
1	A	408	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	401	ARG	CB-CA-C	5.50	119.61	110.81
1	A	444	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	282	LYS	CA-CB-CG	5.47	125.05	114.10
1	A	175	GLU	N-CA-CB	5.44	118.12	110.12
1	A	401	ARG	N-CA-CB	5.42	118.02	109.94
1	A	108	GLN	N-CA-CB	-5.39	101.75	110.81
1	A	404	PHE	N-CA-CB	-5.39	101.92	110.22
1	A	97	ASP	N-CA-CB	5.38	116.54	110.35
1	A	392	LYS	CB-CA-C	-5.38	100.34	110.67
1	A	339	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	425	THR	CA-CB-OG1	-5.38	101.54	109.60
1	A	401	ARG	CD-NE-CZ	5.36	131.90	124.40
1	A	240	PHE	N-CA-CB	5.32	118.19	110.47
1	A	392	LYS	CA-CB-CG	5.31	124.72	114.10
1	A	321	GLU	CA-C-N	5.28	129.53	120.71
1	A	321	GLU	C-N-CA	5.28	129.53	120.71
1	A	140	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	369	GLU	CB-CA-C	-5.26	100.91	110.63
1	A	77	LYS	CB-CA-C	5.25	120.08	109.68
1	A	48	VAL	N-CA-C	5.24	116.02	110.72
1	A	57	LYS	N-CA-CB	5.24	118.31	109.78
1	A	393	TYR	CB-CA-C	5.22	118.75	109.72
1	A	156	GLY	CA-C-N	5.20	131.07	121.70
1	A	156	GLY	C-N-CA	5.20	131.07	121.70
1	A	291	ARG	CG-CD-NE	-5.18	100.60	112.00
1	A	345	LYS	CB-CA-C	5.14	119.03	110.81
1	A	351	MET	CA-C-N	5.14	127.48	120.54
1	A	351	MET	C-N-CA	5.14	127.48	120.54
1	A	430	LYS	CA-C-N	5.10	128.09	120.90
1	A	430	LYS	C-N-CA	5.10	128.09	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	GLU	CA-C-N	5.09	127.06	120.44
1	A	455	GLU	C-N-CA	5.09	127.06	120.44
1	A	224	VAL	N-CA-CB	5.08	115.99	111.67
1	A	45	ALA	CB-CA-C	5.07	118.11	110.50
1	A	316	PRO	CB-CA-C	5.07	118.03	111.64
1	A	120	PRO	CB-CA-C	-5.07	103.60	110.60
1	A	379	ASP	CB-CA-C	5.04	119.79	109.76
1	A	280	GLU	CB-CA-C	-5.01	102.07	110.19
1	A	295	LYS	CB-CG-CD	5.00	122.80	111.30

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	3136	0	2977	14	0
2	A	4	0	0	0	0
3	A	90	0	0	0	0
All	All	3230	0	2977	14	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 2.

All (14) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LYS:HE3	1:A:86:LYS:HD2	1.75	0.69
1:A:451:VAL:HG11	1:A:459:MET:HE2	1.84	0.59
1:A:58:THR:HG21	1:A:424:MET:HG2	1.84	0.58
1:A:353:SER:HB2	1:A:426:ASN:HB3	1.87	0.56
1:A:87:ALA:HB3	1:A:107:GLN:HB3	1.90	0.52
1:A:153:ILE:HD12	1:A:247:MET:HE3	1.93	0.49
1:A:380:PHE:HB3	1:A:381:PRO:HD3	1.97	0.47
1:A:400:ILE:HG21	1:A:457:VAL:HG22	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:HB3	1:A:211:LEU:HB3	1.97	0.46
1:A:222:LEU:HD22	1:A:226:TRP:CE2	2.52	0.45
1:A:215:PHE:CZ	1:A:233:LEU:HB3	2.53	0.43
1:A:50:SER:HA	1:A:53:ARG:HB3	2.02	0.41
1:A:225:PRO:HD3	1:A:305:ILE:O	2.20	0.41
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.94	0.41

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	396/461 (86%)	375 (95%)	16 (4%)	5 (1%)	9	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	GLU
1	A	434	GLU
1	A	314	MET
1	A	433	ASP
1	A	315	LEU

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	328/391 (84%)	312 (95%)	16 (5%)	22	38

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	77	LYS
1	A	157	MET
1	A	184	LEU
1	A	186	GLU
1	A	211	LEU
1	A	212	THR
1	A	227	PRO
1	A	276	LYS
1	A	320	THR
1	A	357	ASN
1	A	391	MET
1	A	438	GLU
1	A	448	ASP
1	A	452	ASN
1	A	459	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	274	ASN
1	A	458	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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$
1	CR2	A	235	1	20,20,21	1.06	1 (5%)	25,27,29	2.38	9 (36%)

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
1	CR2	A	235	1	-	1/6/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	CR2	C1-N3	3.46	1.42	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	CR2	C2-N3-C1	-7.71	104.61	108.08
1	A	235	CR2	CA1-C1-N2	-4.67	118.02	124.28
1	A	235	CR2	N3-C1-N2	3.22	115.48	111.75
1	A	235	CR2	C1-CA1-N1	-2.97	106.27	112.85
1	A	235	CR2	CA2-C2-N3	2.95	105.97	103.50
1	A	235	CR2	CA1-C1-N3	2.86	126.35	122.52
1	A	235	CR2	C3-CA3-N3	2.38	117.84	112.43
1	A	235	CR2	O2-C2-CA2	-2.16	129.64	131.02
1	A	235	CR2	CG2-CB2-CA2	2.14	132.41	129.87

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	235	CR2	C3-CA3-N3-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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, 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	402/461 (87%)	-0.42	18 (4%) 38 31	28, 45, 107, 144	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	5.1
1	A	316	PRO	4.8
1	A	49	ASP	4.6
1	A	48	VAL	4.4
1	A	317	ASP	4.1
1	A	157	MET	3.5
1	A	433	ASP	3.4
1	A	170	VAL	3.4
1	A	315	LEU	3.3
1	A	46	THR	3.1
1	A	47	MET	3.1
1	A	314	MET	2.8
1	A	430	LYS	2.6
1	A	318	GLN	2.4
1	A	443	ALA	2.4
1	A	156	GLY	2.1
1	A	461	THR	2.0
1	A	431	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CR2	A	235	19/20	0.97	0.07	29,36,58,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

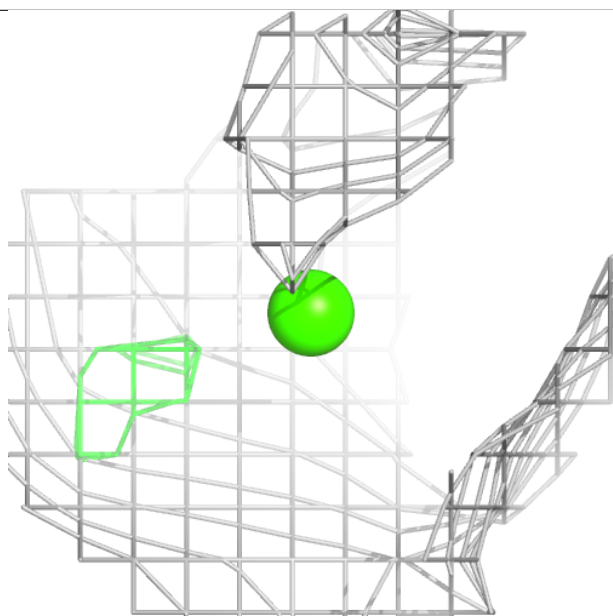
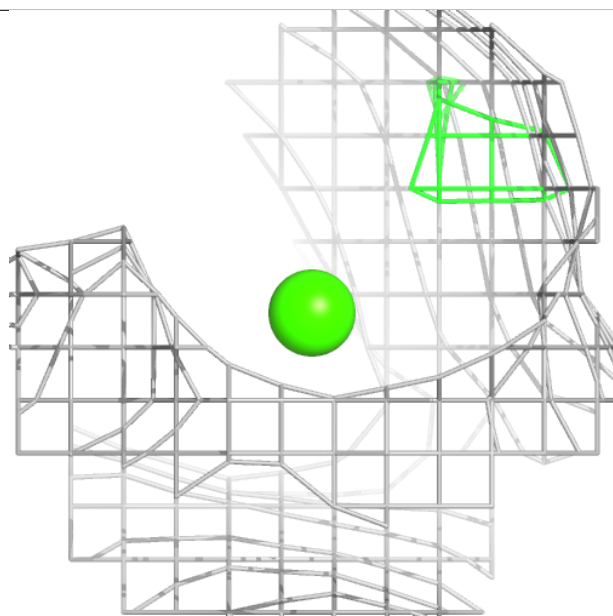
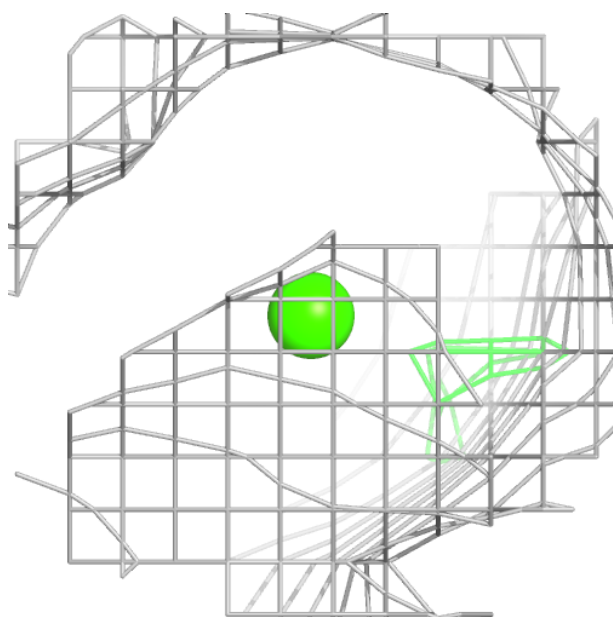
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	503	1/1	0.98	0.07	68,68,68,68	1
2	CA	A	502	1/1	0.99	0.02	37,37,37,37	0
2	CA	A	504	1/1	0.99	0.03	61,61,61,61	1
2	CA	A	501	1/1	1.00	0.01	38,38,38,38	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.

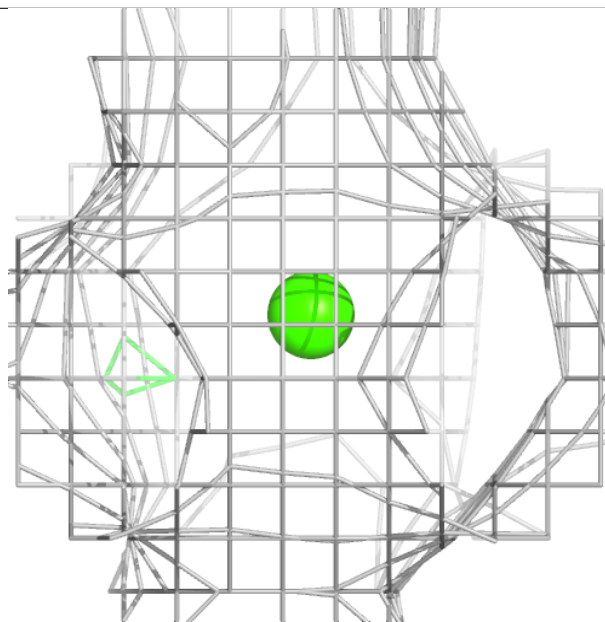
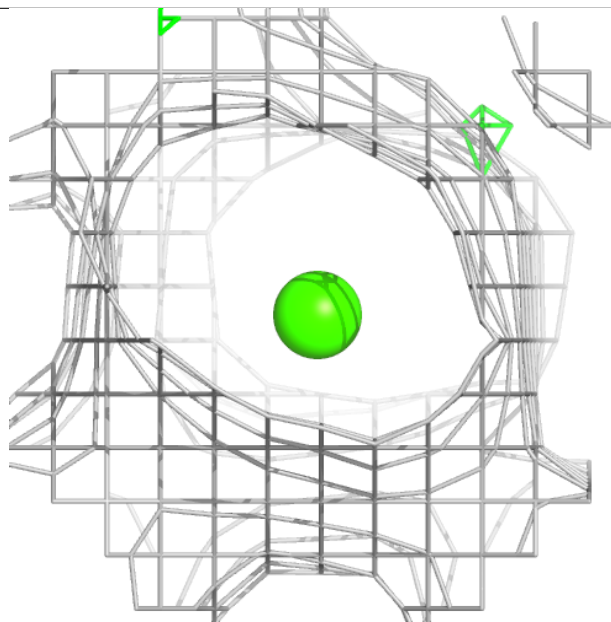
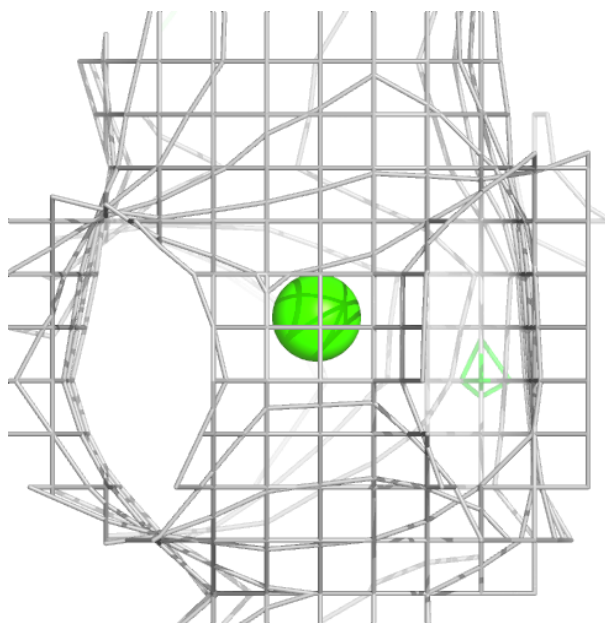
Electron density around CA A 503:

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



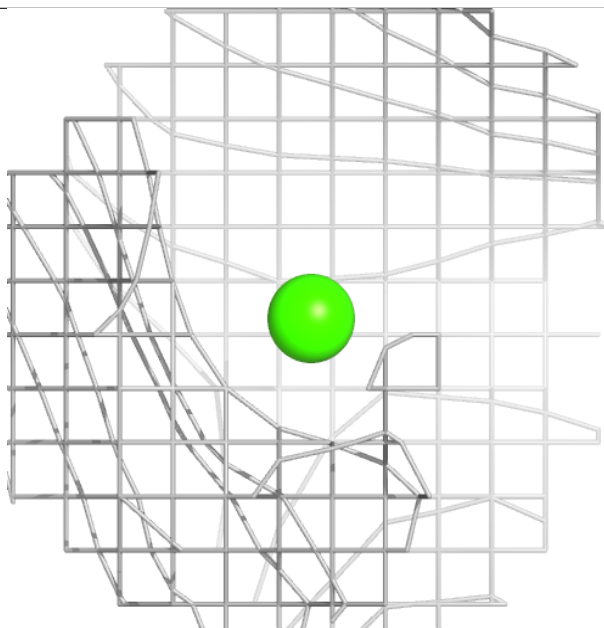
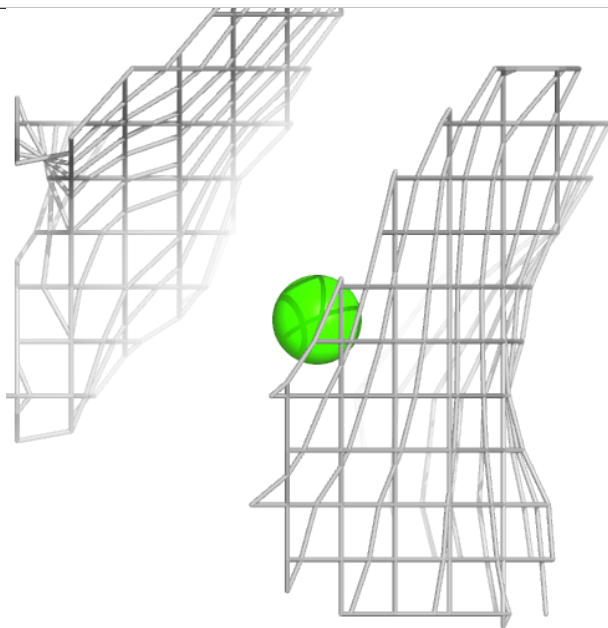
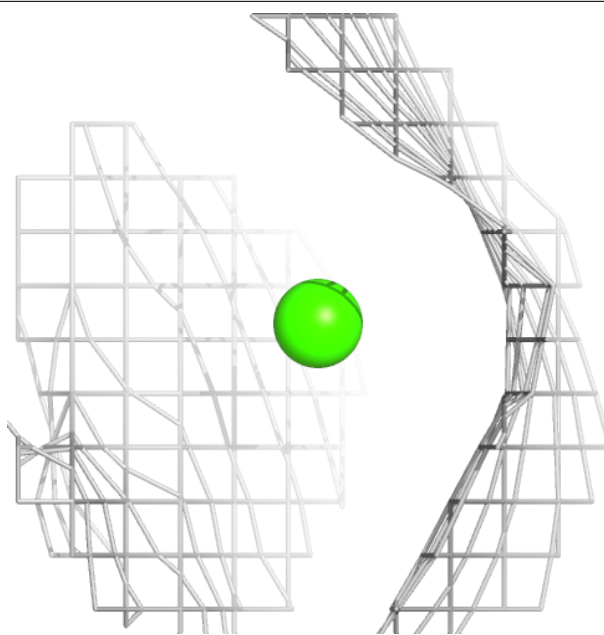
Electron density around CA A 502:

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



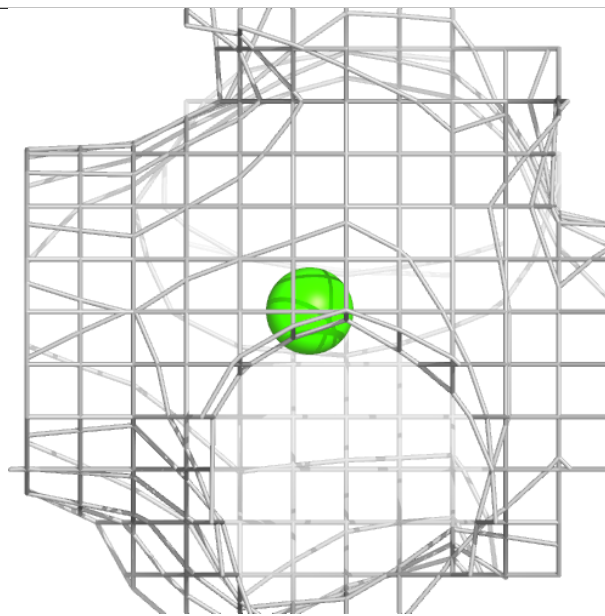
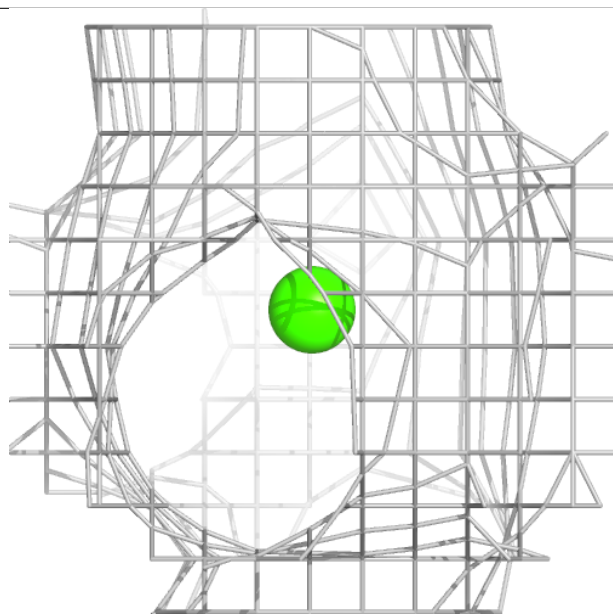
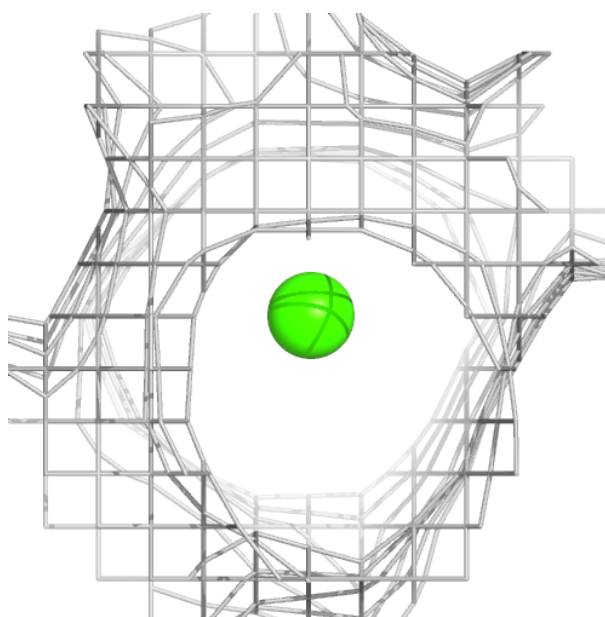
Electron density around CA A 504:

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



Electron density around 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.