



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 PM UTC

PDB ID : 8TRI / pdb_00008tri
Title : Crystal Structure of Mouse Cadherin-23 EC25-MAD28 F2894A
Authors : Ashraf, Q.; Sotomayor, M.
Deposited on : 2023-08-09
Resolution : 3.72 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
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

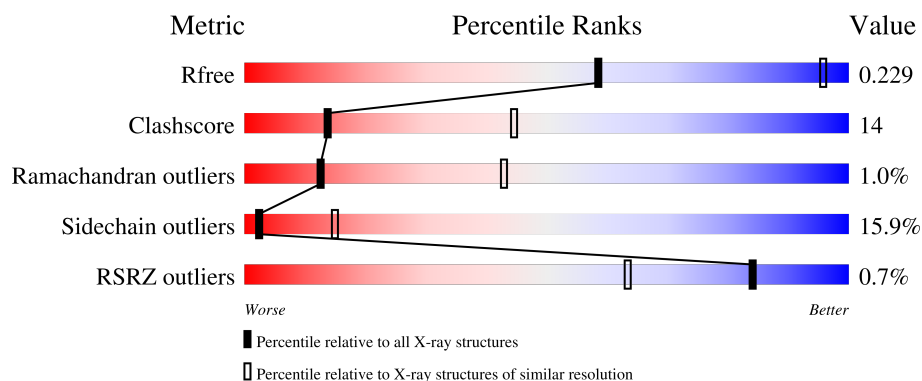
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.72 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	1182 (3.84-3.60)
Clashscore	190562	1222 (3.84-3.60)
Ramachandran outliers	187476	1178 (3.84-3.60)
Sidechain outliers	187428	1174 (3.84-3.60)
RSRZ outliers	180081	1181 (3.84-3.60)

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	474	 58% 30% 7% . .
1	B	474	 53% 36% 7% .
1	C	474	 50% 31% 7% . 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10517 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 Cadherin-23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3584	2266	616	697	5			
1	B	454	Total	C	N	O	S	0	0	0
			3590	2269	617	699	5			
1	C	419	Total	C	N	O	S	0	0	0
			3316	2093	572	647	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2577	MET	-	initiating methionine	UNP Q99PF4
A	2578	ALA	-	expression tag	UNP Q99PF4
A	2579	SER	-	expression tag	UNP Q99PF4
A	2894	ALA	PHE	engineered mutation	UNP Q99PF4
A	3043	LEU	-	expression tag	UNP Q99PF4
A	3044	GLU	-	expression tag	UNP Q99PF4
A	3045	HIS	-	expression tag	UNP Q99PF4
A	3046	HIS	-	expression tag	UNP Q99PF4
A	3047	HIS	-	expression tag	UNP Q99PF4
A	3048	HIS	-	expression tag	UNP Q99PF4
A	3049	HIS	-	expression tag	UNP Q99PF4
A	3050	HIS	-	expression tag	UNP Q99PF4
B	2577	MET	-	initiating methionine	UNP Q99PF4
B	2578	ALA	-	expression tag	UNP Q99PF4
B	2579	SER	-	expression tag	UNP Q99PF4
B	2894	ALA	PHE	engineered mutation	UNP Q99PF4
B	3043	LEU	-	expression tag	UNP Q99PF4
B	3044	GLU	-	expression tag	UNP Q99PF4
B	3045	HIS	-	expression tag	UNP Q99PF4
B	3046	HIS	-	expression tag	UNP Q99PF4
B	3047	HIS	-	expression tag	UNP Q99PF4
B	3048	HIS	-	expression tag	UNP Q99PF4
B	3049	HIS	-	expression tag	UNP Q99PF4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3050	HIS	-	expression tag	UNP Q99PF4
C	2577	MET	-	initiating methionine	UNP Q99PF4
C	2578	ALA	-	expression tag	UNP Q99PF4
C	2579	SER	-	expression tag	UNP Q99PF4
C	2894	ALA	PHE	engineered mutation	UNP Q99PF4
C	3043	LEU	-	expression tag	UNP Q99PF4
C	3044	GLU	-	expression tag	UNP Q99PF4
C	3045	HIS	-	expression tag	UNP Q99PF4
C	3046	HIS	-	expression tag	UNP Q99PF4
C	3047	HIS	-	expression tag	UNP Q99PF4
C	3048	HIS	-	expression tag	UNP Q99PF4
C	3049	HIS	-	expression tag	UNP Q99PF4
C	3050	HIS	-	expression tag	UNP Q99PF4

- 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	6	Total Ca 6 6	0	0
2	B	6	Total Ca 6 6	0	0
2	C	6	Total Ca 6 6	0	0

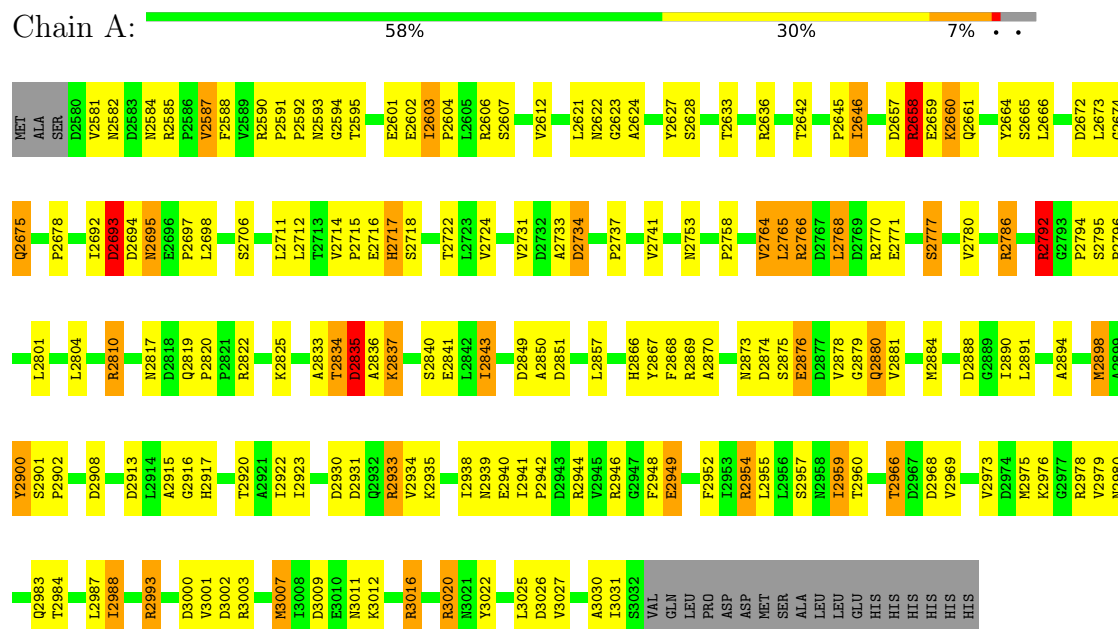
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	2	Total O 2 2	0	0

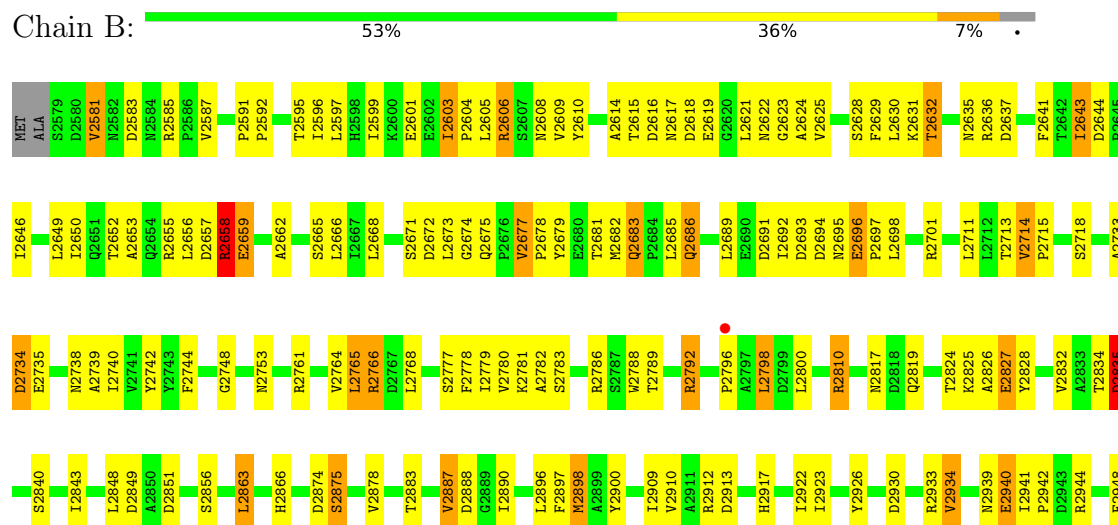
3 Residue-property plots

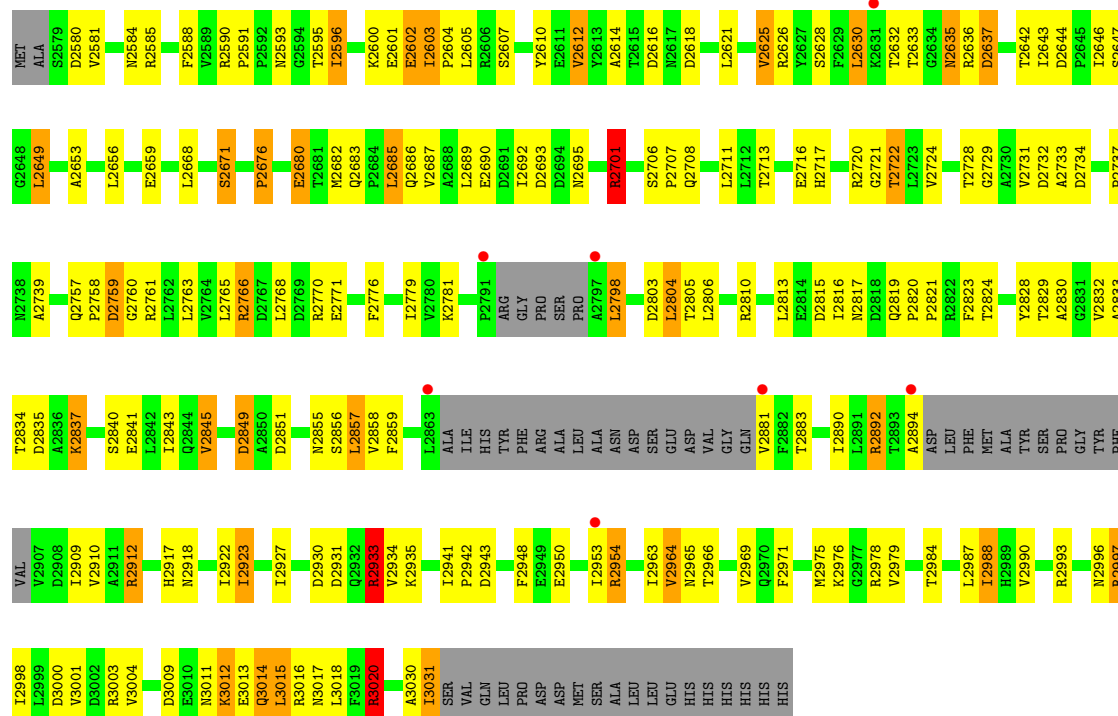
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cadherin-23



• Molecule 1: Cadherin-23





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	146.99Å 164.66Å 183.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 3.72 49.56 – 3.72	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.56-3.72) 98.7 (49.56-3.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.187 , 0.229 0.192 , 0.229	Depositor DCC
R_{free} test set	2329 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	98.8	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 90.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10517	wwPDB-VP
Average B, all atoms (Å ²)	126.0	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 31.10 % 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 1.1709e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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:
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	1.13	4/3654 (0.1%)	1.21	6/4982 (0.1%)
1	B	1.16	6/3660 (0.2%)	1.24	10/4990 (0.2%)
1	C	1.08	3/3373 (0.1%)	1.14	7/4594 (0.2%)
All	All	1.12	13/10687 (0.1%)	1.20	23/14566 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	18
1	B	0	20
1	C	0	17
All	All	0	55

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2628	SER	CA-CB	-6.41	1.43	1.53
1	B	2949	GLU	CD-OE1	6.32	1.37	1.25
1	A	2930	ASP	CG-OD1	6.16	1.37	1.25
1	B	2826	ALA	CA-CB	-6.03	1.45	1.54
1	A	2880	GLN	C-O	-5.81	1.16	1.24
1	C	2646	ILE	CA-C	5.65	1.60	1.52
1	C	2628	SER	CA-CB	-5.64	1.44	1.53
1	B	2887	VAL	CA-CB	-5.56	1.49	1.55
1	C	2680	GLU	CD-OE1	5.38	1.35	1.25
1	B	2866	HIS	CG-CD2	-5.27	1.30	1.35
1	B	2653	ALA	CA-C	5.21	1.55	1.52
1	A	2590	ARG	CA-C	-5.17	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2967	ASP	CG-OD2	5.03	1.34	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2834	THR	CA-CB-OG1	-10.75	93.48	109.60
1	B	2949	GLU	CB-CA-C	-10.52	92.80	110.68
1	C	2635	ASN	CB-CA-C	-8.53	98.74	111.70
1	B	2835	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	2920	THR	CA-CB-OG1	-6.80	99.40	109.60
1	B	2949	GLU	N-CA-CB	6.74	120.17	110.06
1	C	2834	THR	N-CA-C	-6.64	105.05	113.01
1	A	2694	ASP	N-CA-C	-6.09	104.20	111.69
1	B	2835	ASP	N-CA-CB	-6.01	100.33	110.49
1	C	2948	PHE	CA-CB-CG	5.87	119.67	113.80
1	A	2835	ASP	N-CA-CB	-5.75	100.78	110.49
1	A	2737	PRO	CB-CA-C	-5.73	103.72	111.85
1	C	2835	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	2633	THR	CA-CB-OG1	-5.54	101.29	109.60
1	B	2978	ARG	CB-CA-C	5.48	118.44	109.90
1	C	2724	VAL	O-C-N	5.47	127.59	121.90
1	B	2694	ASP	N-CA-C	-5.41	106.81	113.41
1	C	2849	ASP	CB-CA-C	5.39	119.08	109.38
1	A	2841	GLU	CB-CG-CD	5.38	121.74	112.60
1	C	2835	ASP	N-CA-CB	-5.32	104.04	110.53
1	B	2966	THR	CB-CA-C	5.28	118.46	109.80
1	B	2734	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	2615	THR	CA-CB-OG1	-5.08	101.98	109.60

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2585	ARG	Sidechain
1	A	2606	ARG	Sidechain
1	A	2636	ARG	Sidechain
1	A	2658	ARG	Sidechain
1	A	2675	GLN	Peptide
1	A	2766	ARG	Sidechain
1	A	2786	ARG	Sidechain
1	A	2792	ARG	Sidechain
1	A	2810	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2822	ARG	Sidechain
1	A	2835	ASP	Peptide
1	A	2933	ARG	Sidechain
1	A	2944	ARG	Sidechain
1	A	2946	ARG	Sidechain
1	A	2954	ARG	Sidechain
1	A	2978	ARG	Sidechain
1	A	2993	ARG	Sidechain
1	A	3020	ARG	Sidechain
1	B	2585	ARG	Sidechain
1	B	2606	ARG	Sidechain
1	B	2636	ARG	Sidechain
1	B	2655	ARG	Sidechain
1	B	2658	ARG	Sidechain
1	B	2675	GLN	Peptide
1	B	2761	ARG	Sidechain
1	B	2766	ARG	Sidechain
1	B	2786	ARG	Sidechain
1	B	2792	ARG	Sidechain
1	B	2810	ARG	Sidechain
1	B	2835	ASP	Peptide
1	B	2912	ARG	Sidechain
1	B	2933	ARG	Sidechain
1	B	2944	ARG	Sidechain
1	B	2954	ARG	Sidechain
1	B	2993	ARG	Sidechain
1	B	2997	ARG	Sidechain
1	B	3003	ARG	Sidechain
1	B	3016	ARG	Sidechain
1	C	2585	ARG	Sidechain
1	C	2626	ARG	Sidechain
1	C	2636	ARG	Sidechain
1	C	2701	ARG	Sidechain
1	C	2720	ARG	Sidechain
1	C	2761	ARG	Sidechain
1	C	2766	ARG	Sidechain
1	C	2810	ARG	Sidechain
1	C	2892	ARG	Sidechain
1	C	2912	ARG	Sidechain
1	C	2933	ARG	Sidechain
1	C	2954	ARG	Sidechain
1	C	2978	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	2997	ARG	Sidechain
1	C	3003	ARG	Sidechain
1	C	3016	ARG	Sidechain
1	C	3020	ARG	Sidechain

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	3584	0	3527	100	0
1	B	3590	0	3532	103	0
1	C	3316	0	3280	103	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
3	A	7	0	0	1	0
3	B	2	0	0	0	0
All	All	10517	0	10339	302	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 14.

All (302) 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:2657:ASP:OD1	1:B:2659:GLU:HG2	1.66	0.95
1:C:2603:ILE:HB	1:C:2604:PRO:HD2	1.52	0.91
1:C:2857:LEU:C	1:C:2857:LEU:HD13	1.98	0.87
1:C:2817:ASN:ND2	1:C:2855:ASN:HA	1.91	0.86
1:A:2604:PRO:HG2	1:A:2607:SER:HB3	1.59	0.83
1:B:2603:ILE:HD13	1:B:2652:THR:HG21	1.59	0.83
1:A:2888:ASP:OD1	3:A:3201:HOH:O	1.96	0.82
1:C:2716:GLU:HG2	1:C:2816:ILE:HG13	1.63	0.80
1:A:2786:ARG:HG3	1:A:2786:ARG:O	1.79	0.80
1:B:3025:LEU:O	1:B:3026:ASP:HB2	1.83	0.79
1:C:2883:THR:HB	1:C:2892:ARG:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2693:ASP:HA	1:A:2734:ASP:OD2	1.87	0.74
1:A:2939:ASN:HB2	1:A:3025:LEU:HD21	1.67	0.74
1:C:2604:PRO:HG2	1:C:2607:SER:HB3	1.70	0.74
1:B:2677:VAL:HG22	1:B:2678:PRO:HD2	1.69	0.73
1:A:2582:ASN:HD21	1:A:2672:ASP:CG	1.96	0.73
1:B:2608:ASN:HB3	1:B:2649:LEU:HD11	1.71	0.72
1:A:2603:ILE:HB	1:A:2604:PRO:HD2	1.70	0.71
1:C:2644:ASP:HB3	1:C:2647:SER:HB2	1.71	0.71
1:B:2875:SER:O	1:B:2875:SER:OG	2.08	0.71
1:B:2734:ASP:HB3	1:B:2738:ASN:HB2	1.72	0.71
1:A:2817:ASN:HD22	1:A:2915:ALA:HB3	1.55	0.71
1:C:2770:ARG:NH2	1:C:2815:ASP:OD2	2.23	0.70
1:A:2715:PRO:HG2	1:A:2718:SER:OG	1.91	0.70
1:C:2817:ASN:HD22	1:C:2855:ASN:HA	1.57	0.69
1:A:2835:ASP:OD1	1:A:2835:ASP:O	2.11	0.69
1:A:2952:PHE:HD1	1:A:3022:TYR:HD2	1.42	0.67
1:A:2833:ALA:O	1:A:2836:ALA:HB2	1.95	0.67
1:C:2857:LEU:HD13	1:C:2858:VAL:N	2.09	0.67
1:B:2624:ALA:HB3	1:B:2673:LEU:HB2	1.77	0.66
1:C:2656:LEU:HB3	1:C:2689:LEU:HD11	1.78	0.66
1:B:2714:VAL:HG22	1:B:2715:PRO:HD2	1.79	0.65
1:B:2597:LEU:HG	1:B:2685:LEU:HD11	1.78	0.64
1:B:2658:ARG:NH2	1:B:2691:ASP:OD2	2.31	0.64
1:B:2939:ASN:HB2	1:B:3025:LEU:HD11	1.79	0.64
1:B:2715:PRO:HG2	1:B:2718:SER:HB3	1.79	0.64
1:A:2786:ARG:HH12	1:C:2596:ILE:HD11	1.63	0.63
1:A:2881:VAL:C	1:A:2894:ALA:HB3	2.24	0.63
1:A:2792:ARG:HH11	1:A:2794:PRO:HB2	1.63	0.63
1:C:3030:ALA:O	1:C:3031:ILE:C	2.42	0.63
1:B:2753:ASN:HA	1:B:2766:ARG:HG3	1.80	0.62
1:A:2966:THR:HA	1:A:2988:ILE:HG22	1.80	0.62
1:B:2849:ASP:HB3	1:B:2856:SER:HA	1.80	0.62
1:C:2630:LEU:HD13	1:C:2682:MET:HE1	1.80	0.62
1:A:2935:LYS:HE3	1:A:3030:ALA:HA	1.81	0.62
1:A:2879:GLY:O	1:A:2881:VAL:HG23	1.99	0.62
1:B:2656:LEU:HB3	1:B:2689:LEU:HD11	1.82	0.61
1:C:2603:ILE:CB	1:C:2604:PRO:HD2	2.28	0.61
1:B:2953:ILE:HG23	1:B:2964:VAL:HB	1.83	0.61
1:C:2820:PRO:HA	1:C:2917:HIS:HB3	1.82	0.61
1:C:2659:GLU:OE2	1:C:2695:ASN:ND2	2.34	0.60
1:B:2934:VAL:HG23	1:B:3001:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3031:ILE:O	1:B:3031:ILE:HG13	2.01	0.60
1:B:3015:LEU:O	1:B:3016:ARG:C	2.45	0.60
1:C:2857:LEU:C	1:C:2857:LEU:CD1	2.70	0.60
1:A:2869:ARG:HH11	1:A:2876:GLU:HG2	1.66	0.59
1:B:2701:ARG:HG2	1:B:2701:ARG:HH11	1.67	0.59
1:B:2659:GLU:HG3	1:B:2695:ASN:HD21	1.66	0.59
1:A:2819:GLN:HG3	1:A:2850:ALA:HB3	1.84	0.58
1:A:2834:THR:HG23	1:A:2898:MET:HA	1.84	0.58
1:A:3009:ASP:O	1:A:3012:LYS:HB2	2.03	0.58
1:A:3025:LEU:O	1:A:3026:ASP:HB2	2.03	0.58
1:C:2845:VAL:HG12	1:C:2923:ILE:HD11	1.85	0.58
1:B:2614:ALA:HB3	1:B:2625:VAL:HG21	1.84	0.58
1:B:2601:GLU:HG2	1:B:2692:ILE:HG13	1.85	0.58
1:C:2815:ASP:C	1:C:2815:ASP:OD1	2.47	0.57
1:B:2591:PRO:HA	1:B:2610:TYR:OH	2.05	0.57
1:A:2817:ASN:ND2	1:A:2915:ALA:HB3	2.19	0.57
1:A:2870:ALA:HB2	1:A:2902:PRO:HB2	1.87	0.57
1:C:2776:PHE:HE1	1:C:2813:LEU:HD11	1.69	0.57
1:B:2734:ASP:HB3	1:B:2738:ASN:CB	2.35	0.57
1:C:2603:ILE:HB	1:C:2604:PRO:CD	2.31	0.57
1:A:2902:PRO:O	1:A:2902:PRO:HG2	2.05	0.56
1:C:2728:THR:OG1	1:C:2729:GLY:N	2.35	0.56
1:A:2792:ARG:HE	1:A:2794:PRO:HD2	1.70	0.56
1:C:2912:ARG:HG3	1:C:2918:ASN:HD21	1.69	0.56
1:B:3001:VAL:HG11	1:B:3029:PRO:HG3	1.87	0.56
1:B:2888:ASP:HB2	1:B:2890:ILE:HG13	1.86	0.56
1:C:2851:ASP:O	1:C:2856:SER:HB3	2.06	0.56
1:A:3000:ASP:HB2	1:A:3003:ARG:HD3	1.87	0.56
1:B:2972:HIS:HA	1:B:2985:GLU:HG3	1.88	0.56
1:B:2668:LEU:HD11	1:B:2685:LEU:HD23	1.88	0.56
1:A:2849:ASP:OD1	1:A:2851:ASP:HB2	2.06	0.55
1:A:2931:ASP:O	1:A:3001:VAL:HG23	2.07	0.55
1:B:2609:VAL:HB	1:B:2650:ILE:O	2.05	0.55
1:B:2897:PHE:HA	1:B:2900:TYR:CD1	2.41	0.55
1:C:2601:GLU:HG3	1:C:2602:GLU:HG2	1.89	0.55
1:A:2622:ASN:HA	1:A:2674:GLY:CA	2.37	0.55
1:B:3012:LYS:HE2	1:B:3016:ARG:HB2	1.89	0.55
1:A:2868:PHE:CZ	1:A:2875:SER:HB3	2.41	0.54
1:B:2789:THR:HB	1:B:2792:ARG:NH1	2.22	0.54
1:C:2671:SER:HB3	1:C:2680:GLU:HG2	1.89	0.54
1:B:2734:ASP:O	1:B:2739:ALA:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2591:PRO:HG2	1:B:2683:GLN:HE21	1.71	0.54
1:B:2753:ASN:O	1:B:2765:LEU:HB2	2.08	0.54
1:C:2966:THR:HA	1:C:2988:ILE:HG22	1.90	0.54
1:B:2616:ASP:HB3	1:B:2623:GLY:HA2	1.90	0.54
1:A:2697:PRO:HB3	1:A:2741:VAL:HG22	1.90	0.54
1:B:2592:PRO:HG2	1:B:2595:THR:HB	1.88	0.54
1:A:2913:ASP:OD2	1:A:2917:HIS:ND1	2.42	0.53
1:A:2960:THR:HB	1:A:3007:MET:SD	2.49	0.53
1:A:3012:LYS:O	1:A:3016:ARG:N	2.42	0.53
1:A:2952:PHE:HD1	1:A:3022:TYR:CD2	2.25	0.53
1:C:2776:PHE:CE1	1:C:2813:LEU:HD11	2.43	0.53
1:C:2941:ILE:HD12	1:C:2943:ASP:HB3	1.91	0.52
1:A:2878:VAL:HG22	1:A:2879:GLY:N	2.24	0.52
1:A:2582:ASN:ND2	1:A:2672:ASP:OD1	2.42	0.52
1:A:2724:VAL:HG22	1:A:2764:VAL:HG23	1.92	0.52
1:B:2581:VAL:HG13	1:B:2583:ASP:OD1	2.10	0.52
1:C:2616:ASP:OD1	1:C:2618:ASP:HB2	2.09	0.52
1:A:2587:VAL:HG23	1:A:2588:PHE:N	2.25	0.51
1:A:2753:ASN:O	1:A:2765:LEU:HB2	2.09	0.51
1:C:2637:ASP:N	1:C:2637:ASP:OD1	2.42	0.51
1:B:2939:ASN:O	1:B:2940:GLU:HG2	2.11	0.51
1:A:2820:PRO:HA	1:A:2917:HIS:HB3	1.92	0.51
1:C:2857:LEU:HD11	1:C:2859:PHE:CE1	2.46	0.51
1:C:2732:ASP:HB3	1:C:2739:ALA:HB1	1.93	0.50
1:C:2820:PRO:HA	1:C:2917:HIS:CB	2.41	0.50
1:B:2685:LEU:HD12	1:B:2686:GLN:H	1.76	0.50
1:C:2953:ILE:HB	1:C:2964:VAL:HG13	1.94	0.50
1:B:2796:PRO:O	1:B:2798:LEU:HD13	2.11	0.50
1:C:2614:ALA:HB3	1:C:2625:VAL:HG21	1.92	0.50
1:B:2941:ILE:HD13	1:B:2982:ALA:HA	1.94	0.50
1:A:2624:ALA:O	1:A:2673:LEU:HD12	2.12	0.50
1:C:2837:LYS:O	1:C:2840:SER:HB2	2.12	0.50
1:C:2950:GLU:O	1:C:2953:ILE:HG13	2.12	0.50
1:C:3011:ASN:O	1:C:3013:GLU:N	2.37	0.49
1:A:2902:PRO:O	1:A:2902:PRO:CG	2.60	0.49
1:B:2628:SER:HA	1:B:2643:ILE:HD13	1.95	0.49
1:B:2672:ASP:HB3	1:B:2679:TYR:H	1.77	0.49
1:B:2696:GLU:HG2	1:B:2697:PRO:HD2	1.93	0.49
1:B:2939:ASN:HB2	1:B:3025:LEU:HD21	1.94	0.49
1:B:2789:THR:CB	1:B:2792:ARG:NH1	2.76	0.49
1:B:2817:ASN:OD1	1:B:2913:ASP:OD2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2979:VAL:O	1:B:2979:VAL:HG13	2.13	0.48
1:A:2658:ARG:NH1	1:A:2659:GLU:OE2	2.47	0.48
1:B:2617:ASN:O	1:B:2618:ASP:C	2.55	0.48
1:C:2647:SER:HB3	1:C:2649:LEU:HD12	1.95	0.48
1:C:2950:GLU:HB3	1:C:2954:ARG:HH11	1.77	0.48
1:A:2672:ASP:O	1:A:2678:PRO:HB3	2.13	0.48
1:C:2823:PHE:HZ	1:C:2909:ILE:HG22	1.79	0.48
1:A:2621:LEU:HD23	1:A:2621:LEU:H	1.79	0.48
1:C:2819:GLN:HB2	1:C:2849:ASP:OD1	2.13	0.48
1:A:2955:LEU:O	1:A:2959:ILE:HG13	2.13	0.48
1:A:3011:ASN:O	1:A:3012:LYS:C	2.56	0.48
1:B:2963:ILE:HG13	1:B:2991:VAL:O	2.14	0.48
1:C:2935:LYS:HD2	1:C:3030:ALA:HA	1.94	0.48
1:C:3017:ASN:HA	1:C:3020:ARG:CZ	2.44	0.48
1:A:2770:ARG:NH2	1:A:2771:GLU:OE1	2.47	0.48
1:A:2948:PHE:O	1:A:2949:GLU:C	2.57	0.48
1:B:3026:ASP:OD2	1:B:3028:GLN:HG2	2.14	0.48
1:C:2933:ARG:HE	1:C:2933:ARG:HB3	1.46	0.47
1:C:2593:ASN:HA	1:C:2683:GLN:HE22	1.78	0.47
1:C:2851:ASP:C	1:C:2856:SER:HB3	2.40	0.47
1:A:2836:ALA:O	1:A:2837:LYS:C	2.58	0.47
1:B:2595:THR:OG1	1:B:2596:ILE:N	2.48	0.47
1:C:2601:GLU:OE2	1:C:2692:ILE:HG12	2.15	0.47
1:C:2721:GLY:O	1:C:2722:THR:C	2.56	0.47
1:A:2866:HIS:HB3	1:A:2875:SER:HB2	1.97	0.47
1:B:3011:ASN:O	1:B:3015:LEU:HG	2.15	0.47
1:B:2738:ASN:OD1	1:B:2738:ASN:N	2.47	0.47
1:B:2878:VAL:HG11	1:B:2900:TYR:HE2	1.80	0.47
1:C:2695:ASN:CB	1:C:2733:ALA:HB3	2.45	0.47
1:C:3020:ARG:HE	1:C:3020:ARG:HB2	1.46	0.47
1:A:2657:ASP:HB3	1:A:2660:LYS:HG2	1.97	0.46
1:B:2978:ARG:HH22	1:B:2980:ASN:HD22	1.62	0.46
1:C:2942:PRO:HA	1:C:2984:THR:HG21	1.98	0.46
1:A:2868:PHE:CE2	1:A:2875:SER:HB3	2.50	0.46
1:A:2980:ASN:HB3	1:A:2983:GLN:HB2	1.98	0.46
1:A:2645:PRO:HG2	1:A:2646:ILE:HD12	1.97	0.46
1:A:2913:ASP:C	1:A:2915:ALA:H	2.24	0.46
1:C:2593:ASN:HA	1:C:2683:GLN:NE2	2.30	0.46
1:B:2789:THR:CB	1:B:2792:ARG:HH12	2.28	0.46
1:B:2827:GLU:OE2	1:C:2621:LEU:CD1	2.64	0.46
1:B:2827:GLU:OE2	1:C:2621:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2999:LEU:HD23	1:B:2999:LEU:HA	1.74	0.46
1:A:2604:PRO:HG2	1:A:2607:SER:CB	2.39	0.46
1:A:2786:ARG:O	1:A:2786:ARG:CG	2.60	0.46
1:B:2635:ASN:HD21	1:B:2637:ASP:HB2	1.81	0.46
1:B:2742:TYR:HB3	1:B:2744:PHE:CZ	2.51	0.46
1:A:2622:ASN:HA	1:A:2674:GLY:HA3	1.97	0.46
1:C:2881:VAL:C	1:C:2894:ALA:HB3	2.41	0.46
1:A:2898:MET:H	1:A:2898:MET:HG2	1.51	0.46
1:C:2823:PHE:CZ	1:C:2909:ILE:HG22	2.52	0.45
1:C:2963:ILE:O	1:C:2990:VAL:HA	2.16	0.45
1:C:2716:GLU:O	1:C:2816:ILE:HD11	2.16	0.45
1:C:2732:ASP:HB3	1:C:2739:ALA:CB	2.46	0.45
1:A:2716:GLU:O	1:A:2717:HIS:C	2.59	0.45
1:A:2786:ARG:NH1	1:C:2596:ILE:HD11	2.31	0.45
1:A:2916:GLY:O	1:A:2917:HIS:C	2.59	0.45
1:C:2820:PRO:CA	1:C:2917:HIS:HB3	2.47	0.45
1:C:3009:ASP:O	1:C:3012:LYS:HB2	2.17	0.45
1:B:2913:ASP:HB2	1:B:2917:HIS:HB2	1.99	0.45
1:C:2706:SER:O	1:C:2707:PRO:C	2.59	0.45
1:A:2711:LEU:O	1:A:2712:LEU:HD23	2.17	0.44
1:B:2659:GLU:OE1	1:B:2695:ASN:OD1	2.35	0.44
1:B:2863:LEU:HD11	1:B:2910:VAL:HB	1.99	0.44
1:C:2600:LYS:HD2	1:C:2690:GLU:HB2	1.99	0.44
1:A:2627:TYR:O	1:A:2645:PRO:HA	2.18	0.44
1:B:2618:ASP:O	1:B:2623:GLY:HA3	2.17	0.44
1:B:2658:ARG:HG3	1:B:2662:ALA:HB2	1.98	0.44
1:C:2591:PRO:HB3	1:C:2610:TYR:CE2	2.52	0.44
1:C:2935:LYS:HD2	1:C:3030:ALA:CB	2.48	0.44
1:A:2884:MET:HB2	1:A:2884:MET:HE2	1.71	0.44
1:C:2612:VAL:HG11	1:C:2668:LEU:HD13	1.99	0.44
1:C:2642:THR:HG23	1:C:2653:ALA:HB2	1.99	0.44
1:C:2770:ARG:NH2	1:C:2771:GLU:OE1	2.49	0.44
1:C:2701:ARG:NH1	1:C:2806:LEU:O	2.51	0.44
1:A:2741:VAL:O	1:A:2741:VAL:HG12	2.17	0.43
1:C:2832:VAL:O	1:C:2927:ILE:HA	2.17	0.43
1:A:2593:ASN:O	1:A:2594:GLY:C	2.60	0.43
1:C:2693:ASP:HA	1:C:2734:ASP:OD2	2.18	0.43
1:C:3011:ASN:C	1:C:3013:GLU:N	2.76	0.43
1:A:2592:PRO:O	1:A:2595:THR:HG22	2.18	0.43
1:B:2622:ASN:HA	1:B:2674:GLY:CA	2.48	0.43
1:C:2941:ILE:HB	1:C:2942:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2830:ALA:HB2	1:C:2843:ILE:HD13	2.01	0.43
1:A:2591:PRO:HB2	1:A:2595:THR:HG21	2.01	0.43
1:C:2798:LEU:HD23	1:C:2798:LEU:HA	1.82	0.43
1:A:2621:LEU:C	1:A:2623:GLY:H	2.27	0.43
1:B:2951:GLU:OE1	1:B:2955:LEU:HD21	2.19	0.43
1:C:2630:LEU:HD13	1:C:2682:MET:CE	2.46	0.43
1:A:2695:ASN:ND2	1:A:2733:ALA:HB3	2.33	0.43
1:B:2965:ASN:HB2	1:B:2989:HIS:CE1	2.54	0.43
1:C:2803:ASP:OD1	1:C:2805:THR:HG22	2.18	0.43
1:C:3000:ASP:O	1:C:3004:VAL:HG23	2.19	0.43
1:A:2942:PRO:HA	1:A:2984:THR:HG21	2.01	0.43
1:B:2779:ILE:HD12	1:B:2800:LEU:HD11	2.00	0.43
1:B:2951:GLU:O	1:B:2952:PHE:C	2.60	0.43
1:C:2833:ALA:CB	1:C:2933:ARG:NH2	2.82	0.43
1:A:2724:VAL:CG2	1:A:2764:VAL:HG23	2.47	0.43
1:B:2748:GLY:HA3	1:B:2778:PHE:HB3	2.01	0.43
1:C:2781:LYS:HD2	1:C:2806:LEU:CD1	2.48	0.43
1:A:3026:ASP:CG	1:A:3027:VAL:H	2.27	0.43
1:B:2591:PRO:HB2	1:B:2595:THR:HG21	2.00	0.43
1:B:2657:ASP:O	1:B:2658:ARG:C	2.61	0.43
1:B:2777:SER:HB2	1:B:2810:ARG:HG2	2.01	0.43
1:B:2941:ILE:O	1:B:2942:PRO:C	2.61	0.43
1:A:2621:LEU:HG	1:A:2622:ASN:N	2.34	0.42
1:A:2777:SER:HB2	1:A:2810:ARG:HD3	2.01	0.42
1:C:3014:GLN:O	1:C:3015:LEU:C	2.62	0.42
1:A:2601:GLU:HG2	1:A:2692:ILE:HG23	2.01	0.42
1:A:2975:MET:SD	1:A:3031:ILE:HG23	2.59	0.42
1:A:2888:ASP:CB	1:A:2890:ILE:HG13	2.49	0.42
1:A:2969:VAL:O	1:A:2969:VAL:HG12	2.20	0.42
1:B:2599:ILE:O	1:B:2689:LEU:HA	2.20	0.42
1:C:2685:LEU:HG	1:C:2686:GLN:N	2.34	0.42
1:B:2781:LYS:HG2	1:B:2788:TRP:CE2	2.54	0.42
1:B:2963:ILE:O	1:B:2990:VAL:HA	2.20	0.42
1:A:2661:GLN:HB3	1:A:2664:TYR:CZ	2.55	0.42
1:B:2632:THR:OG1	1:B:2635:ASN:HB3	2.20	0.42
1:C:2931:ASP:O	1:C:3001:VAL:HG23	2.19	0.42
1:B:2733:ALA:O	1:B:2734:ASP:C	2.63	0.42
1:B:2898:MET:H	1:B:2898:MET:HG2	1.59	0.42
1:C:2942:PRO:HD3	1:C:2971:PHE:CE1	2.55	0.42
1:A:2624:ALA:O	1:A:2672:ASP:HA	2.19	0.42
1:A:2804:LEU:HA	1:A:2804:LEU:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2828:TYR:O	1:B:2923:ILE:HA	2.20	0.42
1:A:2766:ARG:O	1:A:2768:LEU:HG	2.20	0.42
1:B:2621:LEU:C	1:B:2623:GLY:H	2.27	0.42
1:B:2975:MET:SD	1:B:2975:MET:N	2.88	0.42
1:C:2758:PRO:C	1:C:2760:GLY:H	2.27	0.42
1:B:2603:ILE:CD1	1:B:2652:THR:HG21	2.41	0.41
1:C:2581:VAL:HG13	1:C:2676:PRO:HG3	2.01	0.41
1:C:3011:ASN:C	1:C:3013:GLU:H	2.24	0.41
1:A:2898:MET:HE2	1:A:2898:MET:HB3	1.79	0.41
1:B:2948:PHE:O	1:B:2949:GLU:C	2.63	0.41
1:A:2973:VAL:HG13	1:A:2973:VAL:O	2.20	0.41
1:C:2584:ASN:H	1:C:2618:ASP:CG	2.29	0.41
1:C:2716:GLU:O	1:C:2717:HIS:C	2.63	0.41
1:C:2737:PRO:C	1:C:2739:ALA:H	2.28	0.41
1:C:2757:GLN:C	1:C:2759:ASP:N	2.77	0.41
1:B:2742:TYR:O	1:B:2782:ALA:HA	2.20	0.41
1:A:3012:LYS:HD2	1:A:3012:LYS:HA	1.83	0.41
1:B:2629:PHE:HE2	1:B:2641:PHE:HB2	1.85	0.41
1:C:2721:GLY:O	1:C:2763:LEU:HD22	2.20	0.41
1:A:2843:ILE:HD11	1:A:2923:ILE:HG21	2.03	0.41
1:C:2845:VAL:CG1	1:C:2923:ILE:HD11	2.49	0.41
1:A:2979:VAL:O	1:A:2979:VAL:HG13	2.20	0.41
1:B:2621:LEU:C	1:B:2623:GLY:N	2.77	0.41
1:C:2766:ARG:O	1:C:2768:LEU:HG	2.21	0.41
1:C:2804:LEU:HD23	1:C:2804:LEU:HA	1.87	0.41
1:C:2832:VAL:HG13	1:C:2927:ILE:HD13	2.02	0.41
1:A:2833:ALA:O	1:A:2834:THR:C	2.63	0.41
1:B:2606:ARG:HA	1:B:2652:THR:O	2.21	0.41
1:B:2819:GLN:HB2	1:B:2851:ASP:CG	2.46	0.41
1:B:2832:VAL:O	1:B:2832:VAL:HG13	2.21	0.41
1:A:2698:LEU:HD22	1:A:2804:LEU:HB3	2.03	0.40
1:A:2867:TYR:CZ	1:A:2900:TYR:HB3	2.56	0.40
1:A:2938:ILE:HG22	1:A:2940:GLU:H	1.86	0.40
1:A:2940:GLU:O	1:A:2984:THR:OG1	2.27	0.40
1:B:2897:PHE:O	1:B:2898:MET:C	2.65	0.40
1:B:2973:VAL:O	1:B:2974:ASP:C	2.64	0.40
1:A:2817:ASN:HD22	1:A:2915:ALA:CB	2.26	0.40
1:A:2913:ASP:O	1:A:2915:ALA:N	2.55	0.40
1:B:2668:LEU:HD12	1:B:2668:LEU:N	2.35	0.40
1:B:2596:ILE:O	1:B:2596:ILE:HG22	2.20	0.40
1:B:2998:ILE:HD12	1:B:2999:LEU:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2824:THR:HB	1:C:2828:TYR:OH	2.21	0.40
1:B:2995:THR:O	1:B:2996:ASN:C	2.65	0.40
1:C:2781:LYS:HD2	1:C:2806:LEU:HD12	2.04	0.40
1:C:2817:ASN:ND2	1:C:2855:ASN:CA	2.75	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	451/474 (95%)	405 (90%)	41 (9%)	5 (1%)	11	41
1	B	452/474 (95%)	402 (89%)	47 (10%)	3 (1%)	18	49
1	C	411/474 (87%)	375 (91%)	31 (8%)	5 (1%)	10	39
All	All	1314/1422 (92%)	1182 (90%)	119 (9%)	13 (1%)	12	43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2693	ASP
1	A	2880	GLN
1	B	2835	ASP
1	A	2717	HIS
1	C	2759	ASP
1	A	2734	ASP
1	B	2693	ASP
1	C	3012	LYS
1	C	2633	THR
1	C	2676	PRO
1	B	2604	PRO
1	C	2821	PRO
1	A	2796	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/414 (95%)	335 (85%)	60 (15%)	3	16
1	B	396/414 (96%)	330 (83%)	66 (17%)	2	14
1	C	368/414 (89%)	310 (84%)	58 (16%)	2	15
All	All	1159/1242 (93%)	975 (84%)	184 (16%)	2	15

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2581	VAL
1	A	2584	ASN
1	A	2587	VAL
1	A	2602	GLU
1	A	2603	ILE
1	A	2612	VAL
1	A	2642	THR
1	A	2646	ILE
1	A	2658	ARG
1	A	2660	LYS
1	A	2665	SER
1	A	2666	LEU
1	A	2675	GLN
1	A	2693	ASP
1	A	2695	ASN
1	A	2706	SER
1	A	2714	VAL
1	A	2722	THR
1	A	2731	VAL
1	A	2758	PRO
1	A	2764	VAL
1	A	2765	LEU
1	A	2768	LEU
1	A	2777	SER
1	A	2780	VAL
1	A	2792	ARG

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Mol	Chain	Res	Type
1	A	2795	SER
1	A	2801	LEU
1	A	2825	LYS
1	A	2834	THR
1	A	2837	LYS
1	A	2840	SER
1	A	2843	ILE
1	A	2857	LEU
1	A	2873	ASN
1	A	2874	ASP
1	A	2876	GLU
1	A	2891	LEU
1	A	2898	MET
1	A	2900	TYR
1	A	2901	SER
1	A	2908	ASP
1	A	2922	ILE
1	A	2933	ARG
1	A	2934	VAL
1	A	2941	ILE
1	A	2949	GLU
1	A	2954	ARG
1	A	2957	SER
1	A	2959	ILE
1	A	2966	THR
1	A	2968	ASP
1	A	2976	LYS
1	A	2987	LEU
1	A	2988	ILE
1	A	2993	ARG
1	A	3002	ASP
1	A	3007	MET
1	A	3016	ARG
1	A	3020	ARG
1	B	2581	VAL
1	B	2587	VAL
1	B	2603	ILE
1	B	2605	LEU
1	B	2619	GLU
1	B	2630	LEU
1	B	2631	LYS
1	B	2632	THR

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Mol	Chain	Res	Type
1	B	2643	ILE
1	B	2644	ASP
1	B	2646	ILE
1	B	2658	ARG
1	B	2659	GLU
1	B	2665	SER
1	B	2666	LEU
1	B	2671	SER
1	B	2677	VAL
1	B	2681	THR
1	B	2682	MET
1	B	2683	GLN
1	B	2686	GLN
1	B	2696	GLU
1	B	2698	LEU
1	B	2711	LEU
1	B	2713	THR
1	B	2714	VAL
1	B	2735	GLU
1	B	2740	ILE
1	B	2764	VAL
1	B	2765	LEU
1	B	2768	LEU
1	B	2780	VAL
1	B	2783	SER
1	B	2798	LEU
1	B	2824	THR
1	B	2825	LYS
1	B	2827	GLU
1	B	2840	SER
1	B	2843	ILE
1	B	2848	LEU
1	B	2863	LEU
1	B	2874	ASP
1	B	2875	SER
1	B	2883	THR
1	B	2887	VAL
1	B	2896	LEU
1	B	2898	MET
1	B	2909	ILE
1	B	2922	ILE
1	B	2926	TYR

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Mol	Chain	Res	Type
1	B	2930	ASP
1	B	2934	VAL
1	B	2940	GLU
1	B	2959	ILE
1	B	2963	ILE
1	B	2968	ASP
1	B	2975	MET
1	B	2976	LYS
1	B	2988	ILE
1	B	2990	VAL
1	B	2998	ILE
1	B	3008	ILE
1	B	3012	LYS
1	B	3015	LEU
1	B	3018	LEU
1	B	3023	ASN
1	C	2580	ASP
1	C	2588	PHE
1	C	2590	ARG
1	C	2595	THR
1	C	2596	ILE
1	C	2602	GLU
1	C	2603	ILE
1	C	2605	LEU
1	C	2612	VAL
1	C	2625	VAL
1	C	2630	LEU
1	C	2632	THR
1	C	2635	ASN
1	C	2637	ASP
1	C	2643	ILE
1	C	2649	LEU
1	C	2671	SER
1	C	2685	LEU
1	C	2687	VAL
1	C	2701	ARG
1	C	2708	GLN
1	C	2711	LEU
1	C	2713	THR
1	C	2722	THR
1	C	2731	VAL
1	C	2765	LEU

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Mol	Chain	Res	Type
1	C	2779	ILE
1	C	2798	LEU
1	C	2804	LEU
1	C	2829	THR
1	C	2837	LYS
1	C	2841	GLU
1	C	2845	VAL
1	C	2857	LEU
1	C	2890	ILE
1	C	2910	VAL
1	C	2922	ILE
1	C	2923	ILE
1	C	2930	ASP
1	C	2933	ARG
1	C	2934	VAL
1	C	2964	VAL
1	C	2965	ASN
1	C	2969	VAL
1	C	2975	MET
1	C	2976	LYS
1	C	2979	VAL
1	C	2987	LEU
1	C	2988	ILE
1	C	2993	ARG
1	C	2996	ASN
1	C	2997	ARG
1	C	2998	ILE
1	C	3014	GLN
1	C	3015	LEU
1	C	3018	LEU
1	C	3020	ARG
1	C	3031	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2622	ASN
1	A	2675	GLN
1	A	2683	GLN
1	A	2686	GLN
1	A	2708	GLN
1	A	2880	GLN

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Mol	Chain	Res	Type
1	A	2972	HIS
1	B	2593	ASN
1	B	2683	GLN
1	B	2695	ASN
1	B	2708	GLN
1	B	2817	ASN
1	B	2844	GLN
1	B	2939	ASN
1	B	2965	ASN
1	B	2972	HIS
1	B	2983	GLN
1	C	2635	ASN
1	C	2683	GLN
1	C	2855	ASN
1	C	2918	ASN
1	C	2996	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 18 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	453/474 (95%)	-0.47	0 100 100	64, 106, 171, 212	0
1	B	454/474 (95%)	-0.43	2 (0%) 88 72	68, 113, 166, 234	0
1	C	419/474 (88%)	-0.22	7 (1%) 69 43	73, 147, 222, 269	0
All	All	1326/1422 (93%)	-0.37	9 (0%) 84 63	64, 117, 200, 269	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2797	ALA	3.8
1	C	2791	PRO	3.4
1	C	2894	ALA	3.3
1	C	2881	VAL	3.3
1	B	3031	ILE	2.9
1	C	2631	LYS	2.8
1	C	2863	LEU	2.5
1	B	2796	PRO	2.4
1	C	2953	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

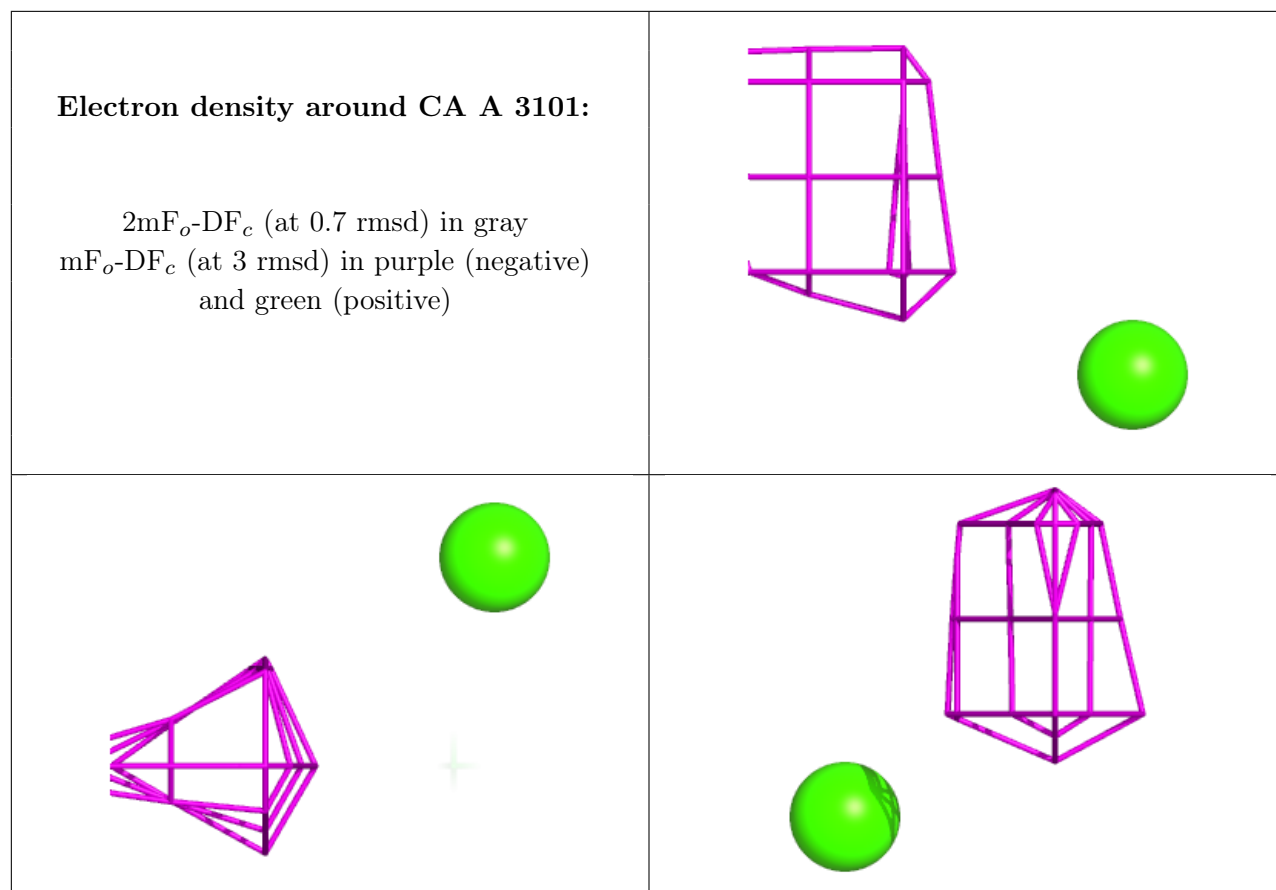
There are no oligosaccharides in this entry.

6.4 Ligands

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.

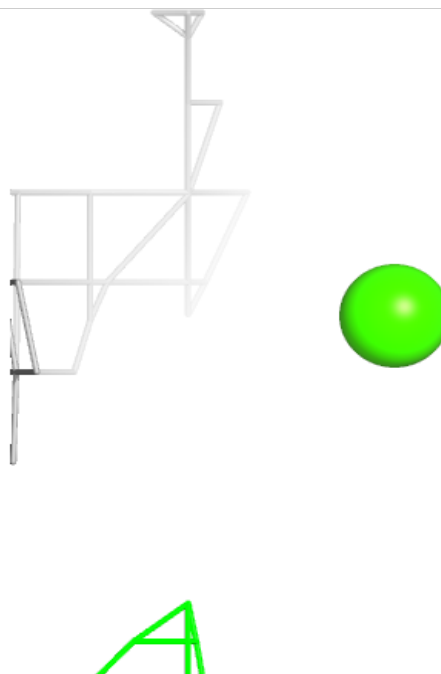
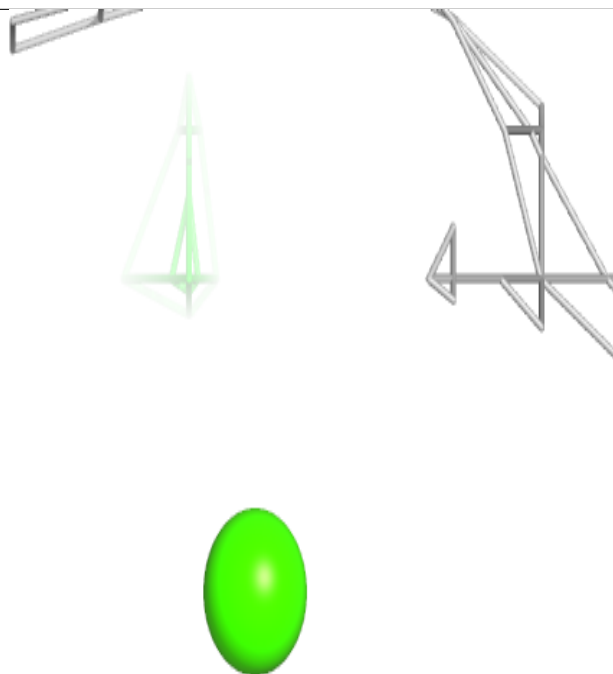
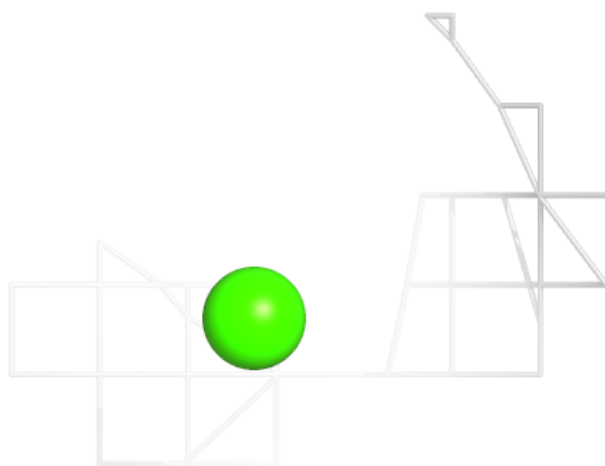
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	3101	1/1	0.99	0.02	82,82,82,82	0
2	CA	B	3101	1/1	0.99	0.03	116,116,116,116	0
2	CA	C	3102	1/1	0.99	0.03	110,110,110,110	0
2	CA	C	3106	1/1	0.99	0.02	154,154,154,154	0
2	CA	A	3105	1/1	1.00	0.02	111,111,111,111	0
2	CA	A	3106	1/1	1.00	0.01	95,95,95,95	0
2	CA	A	3102	1/1	1.00	0.02	103,103,103,103	0
2	CA	B	3102	1/1	1.00	0.02	122,122,122,122	0
2	CA	B	3103	1/1	1.00	0.01	118,118,118,118	0
2	CA	B	3104	1/1	1.00	0.03	102,102,102,102	0
2	CA	B	3105	1/1	1.00	0.03	105,105,105,105	0
2	CA	B	3106	1/1	1.00	0.03	94,94,94,94	0
2	CA	C	3101	1/1	1.00	0.06	70,70,70,70	0
2	CA	A	3103	1/1	1.00	0.02	84,84,84,84	0
2	CA	C	3103	1/1	1.00	0.04	115,115,115,115	0
2	CA	C	3104	1/1	1.00	0.03	96,96,96,96	0
2	CA	C	3105	1/1	1.00	0.03	140,140,140,140	0
2	CA	A	3104	1/1	1.00	0.03	87,87,87,87	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.



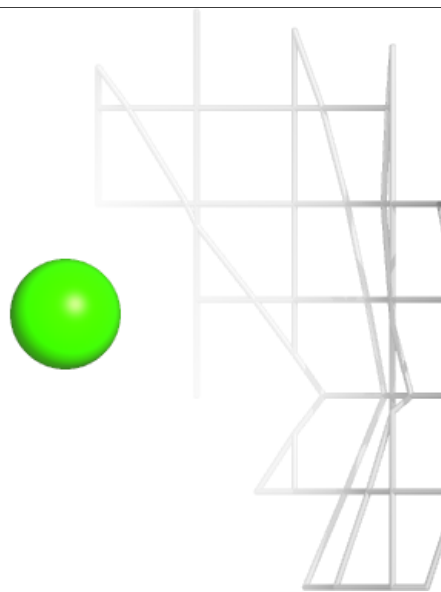
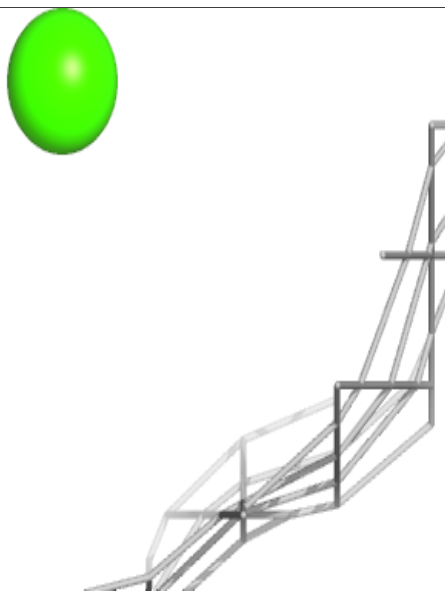
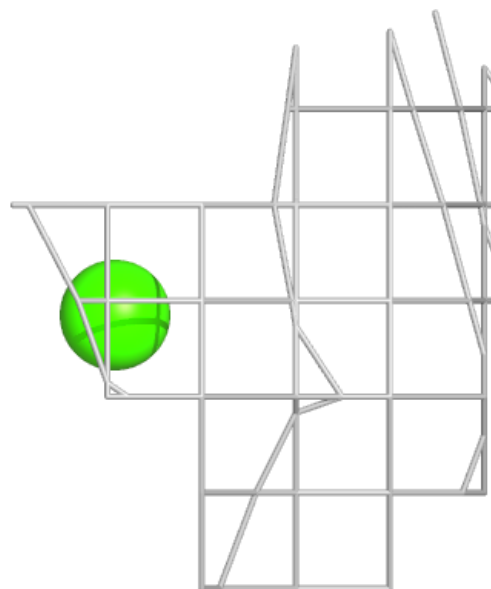
Electron density around CA B 3101:

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



Electron density around CA C 3102:

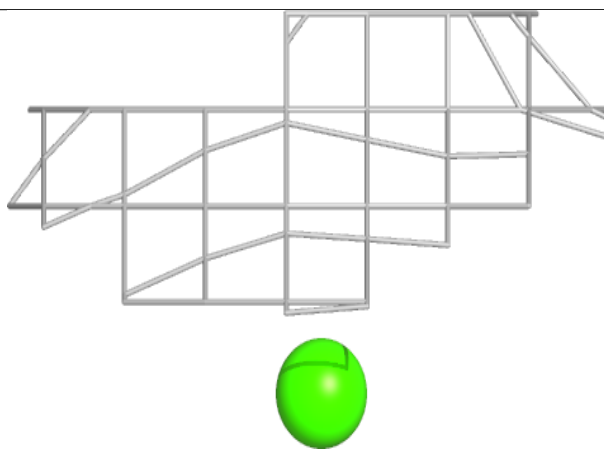
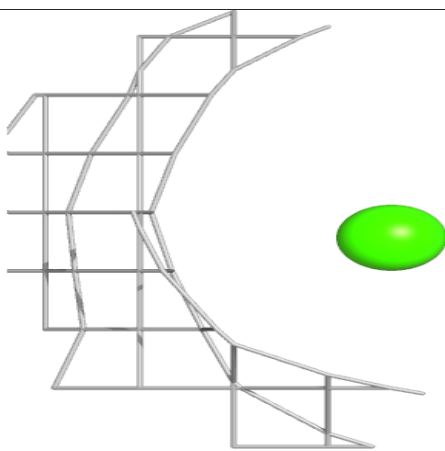
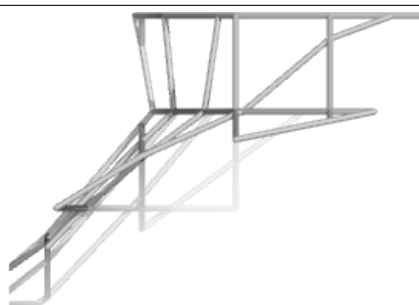
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



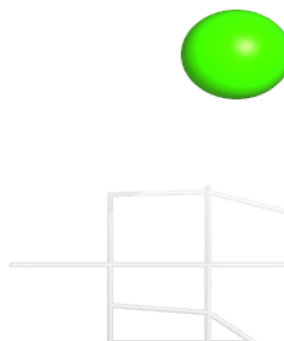
Electron density around CA C 3106: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	
Electron density around CA A 3105: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around CA A 3106:

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

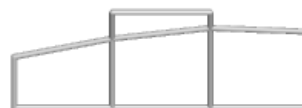
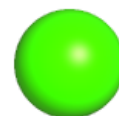
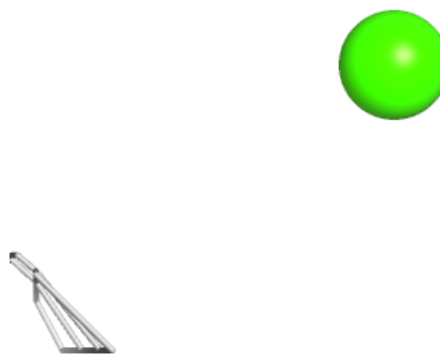
**Electron density around CA A 3102:**

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

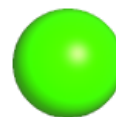
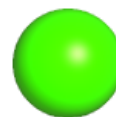


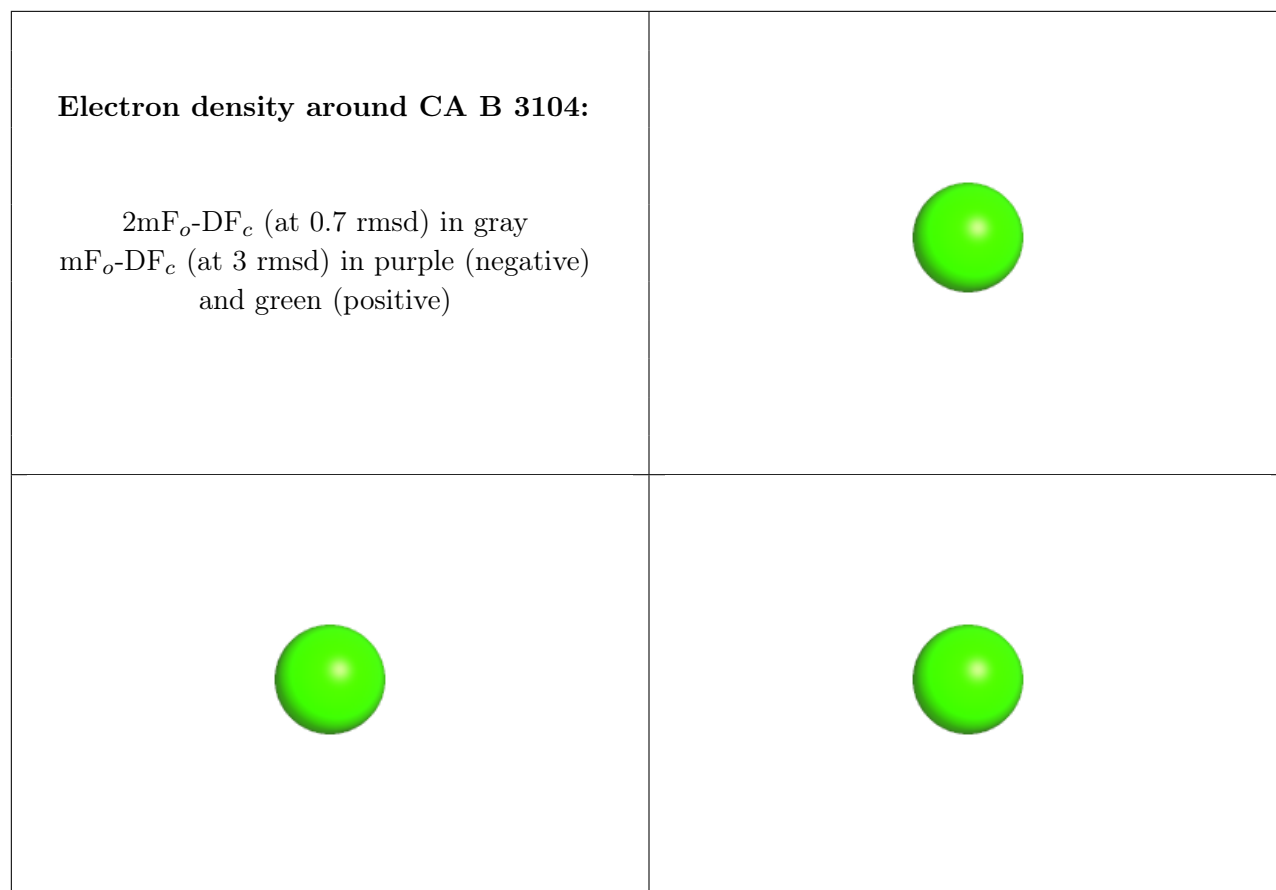
Electron density around CA B 3102:

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

**Electron density around CA B 3103:**

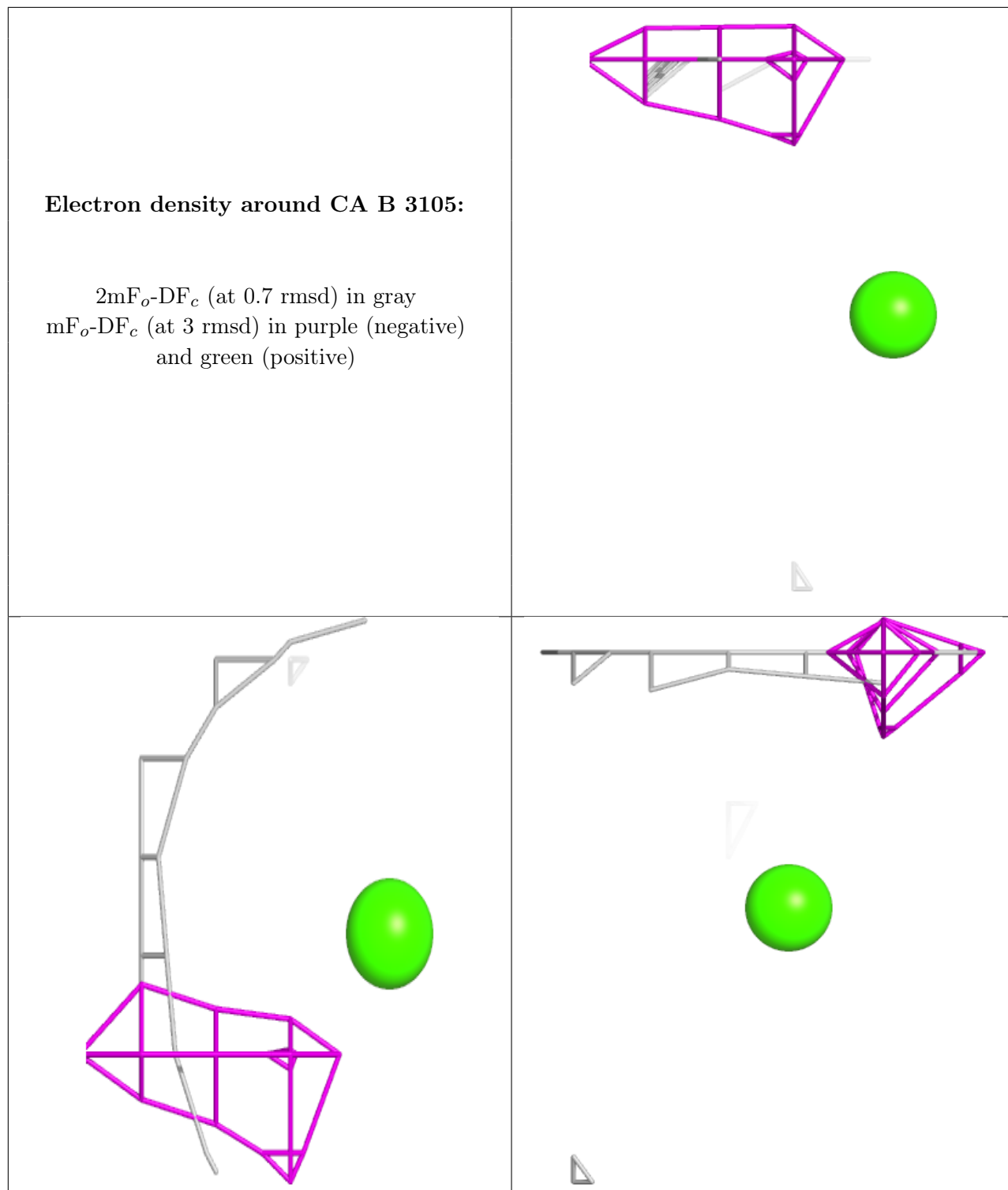
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





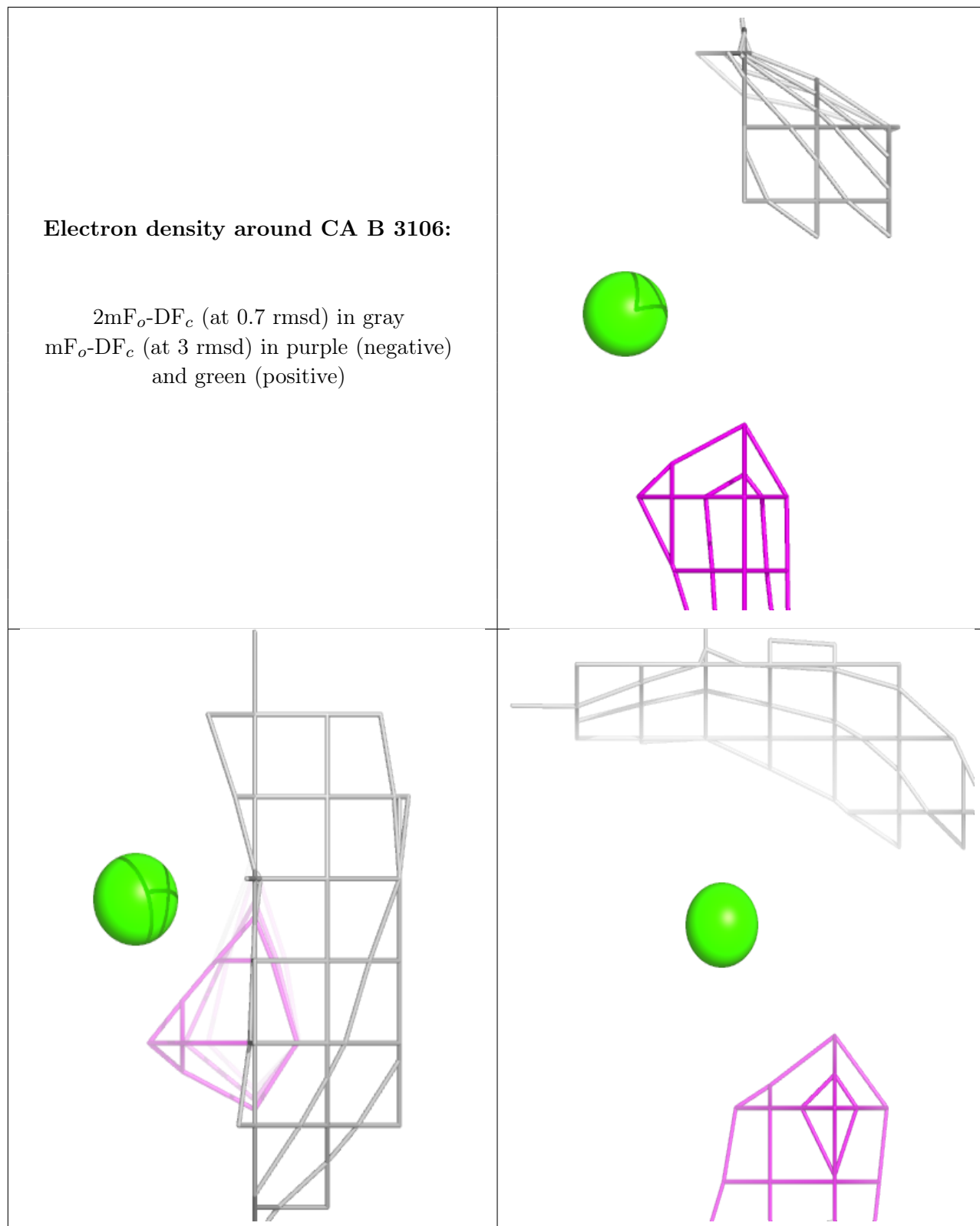
Electron density around CA B 3105:

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and green (positive)



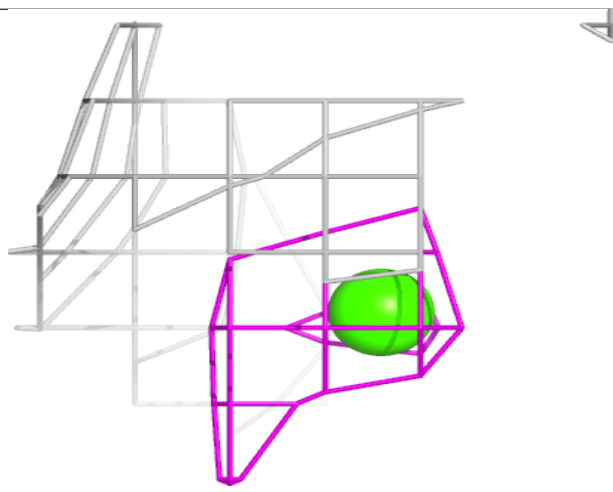
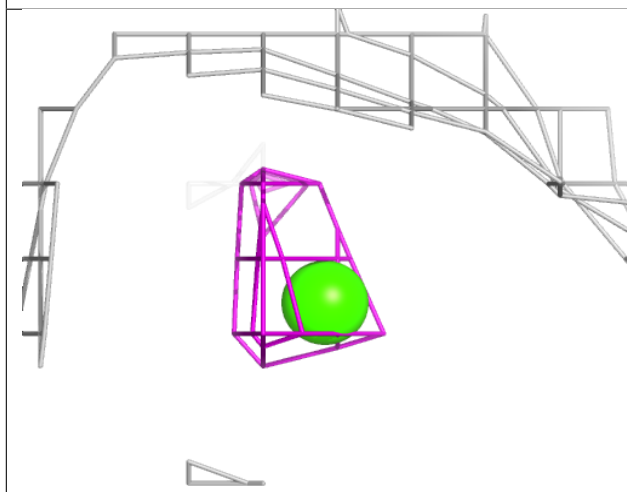
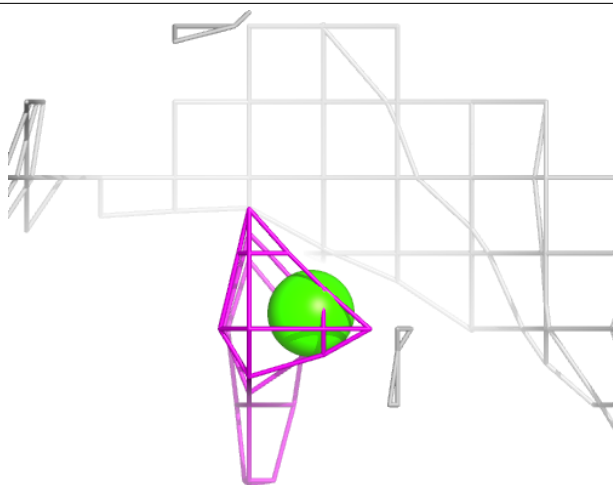
Electron density around CA B 3106:

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



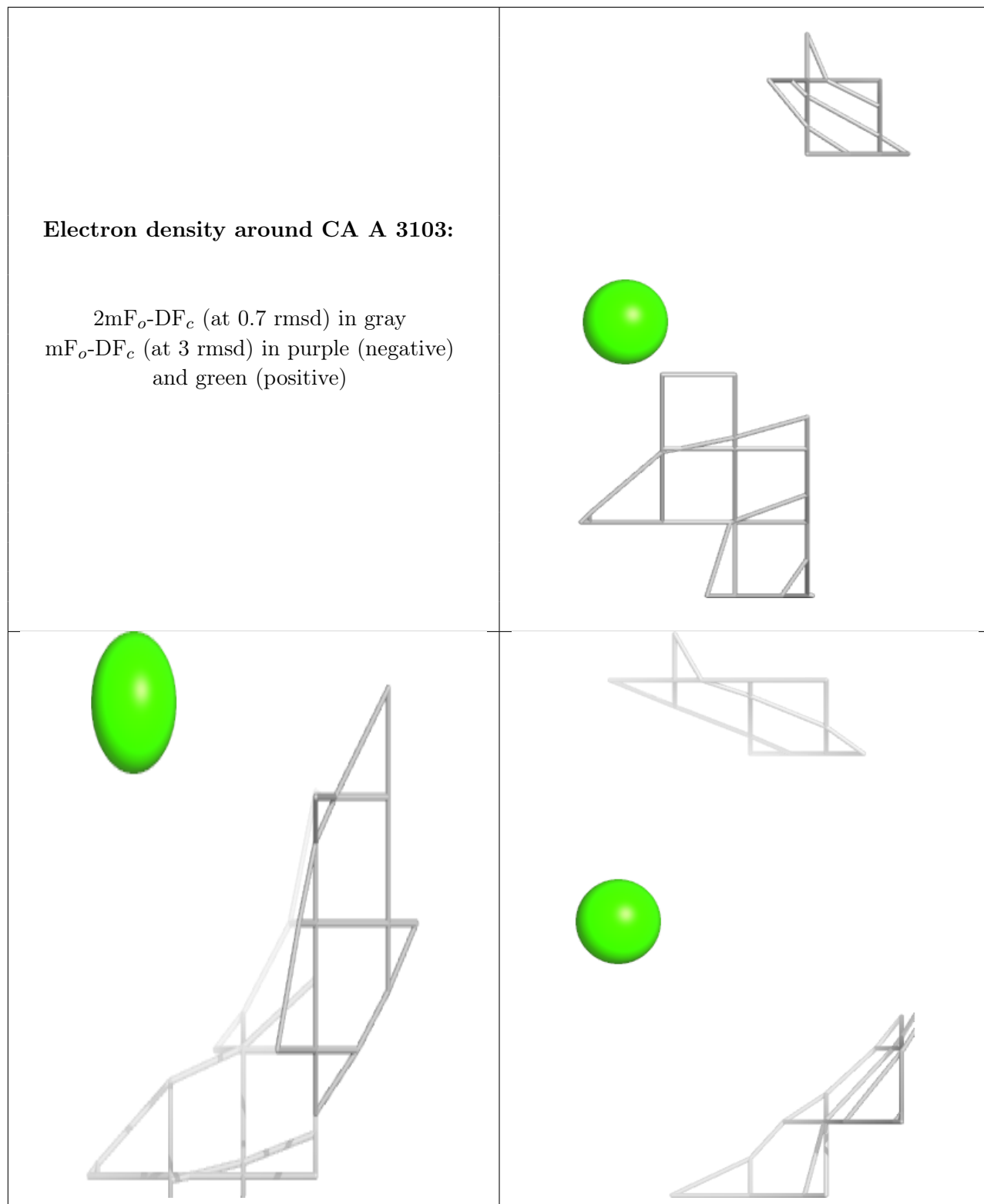
Electron density around CA C 3101:

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



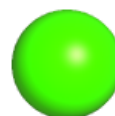
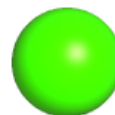
Electron density around CA A 3103:

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and green (positive)

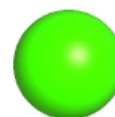
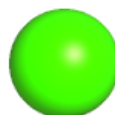


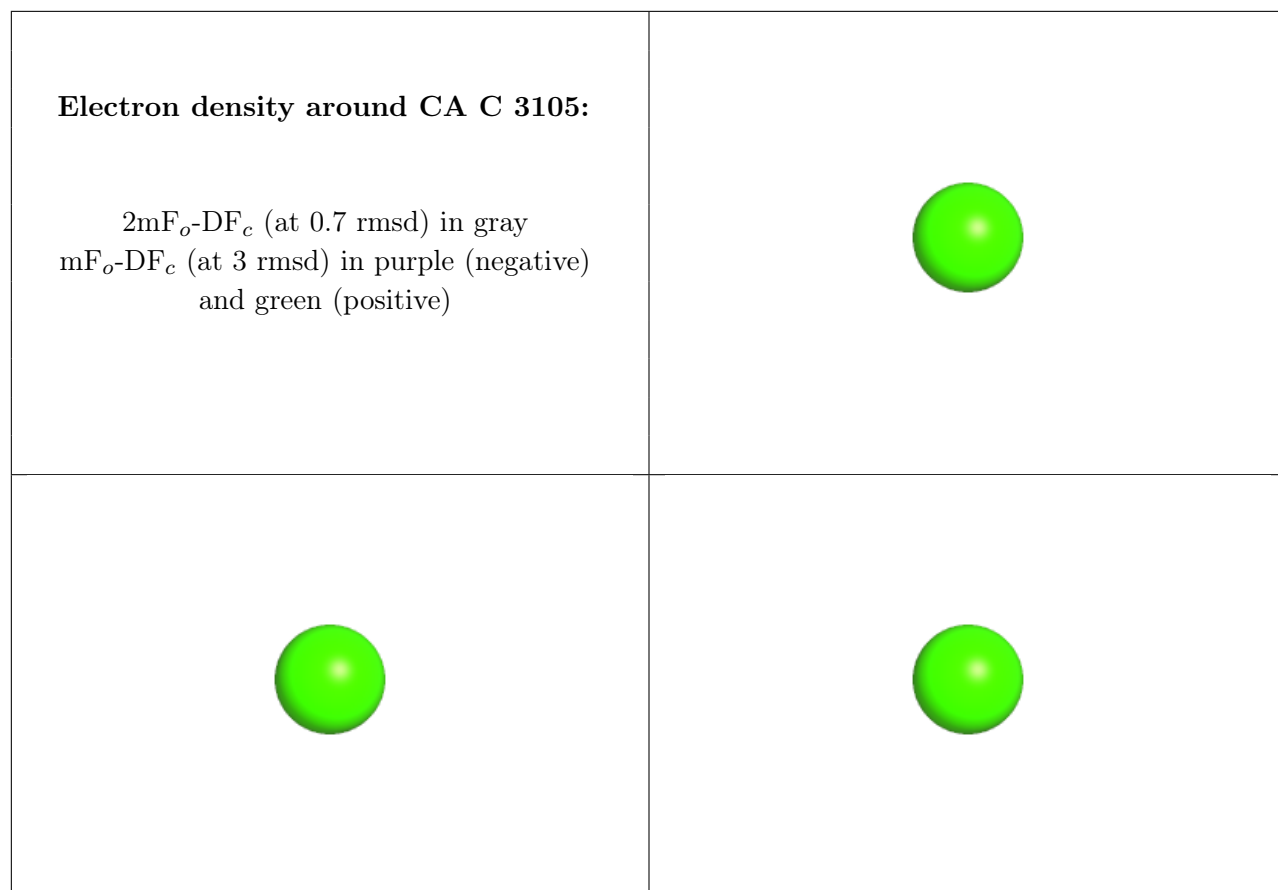
Electron density around CA C 3103:

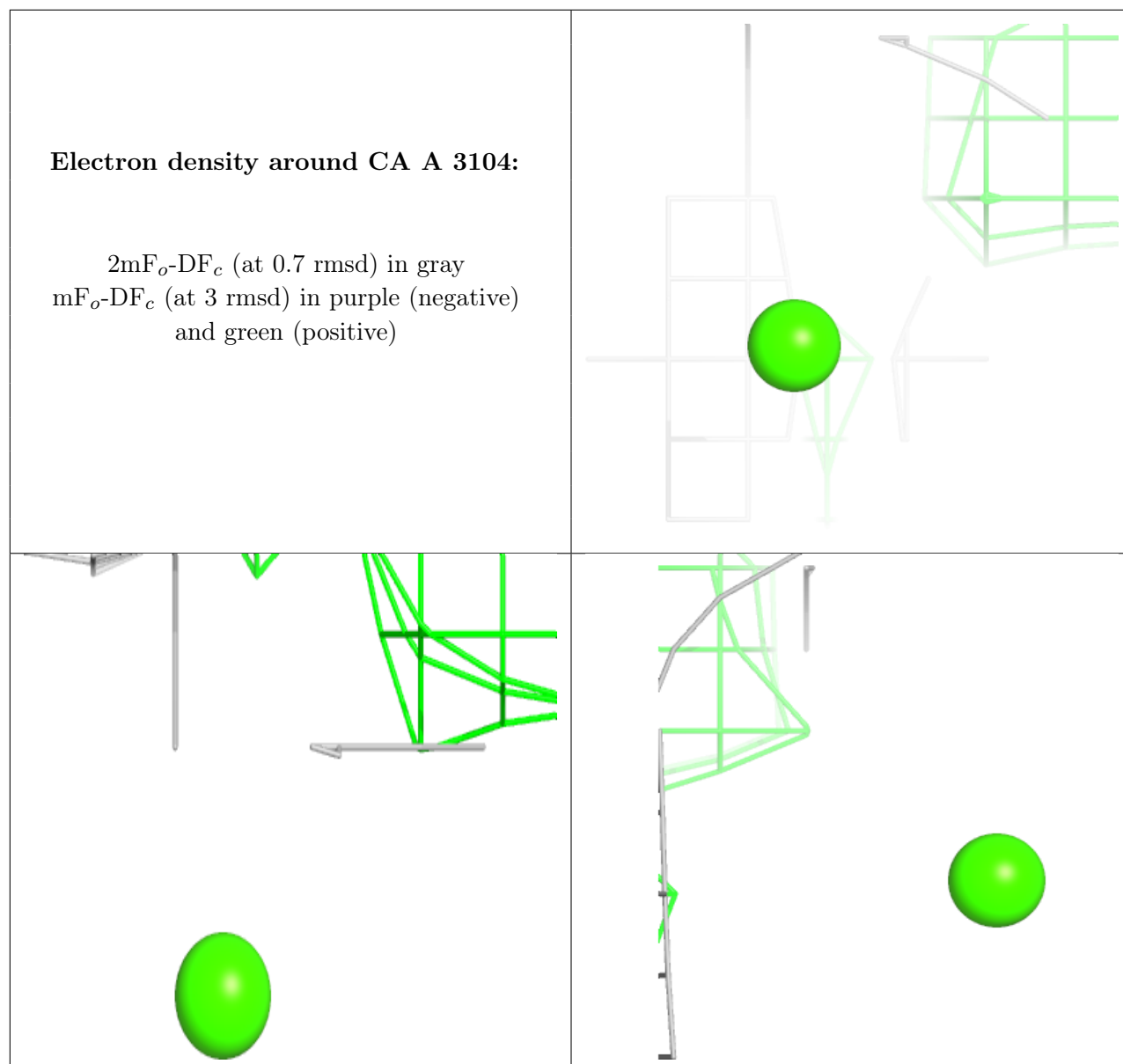
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CA C 3104:**

$2mF_o-DF_c$ (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.