



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 09:10 PM UTC

PDB ID : 7PHW / pdb_00007phw
Title : PfCyRPA bound to monoclonal antibody Cy.004 Fab fragment
Authors : Ragotte, R.J.; Higgins, M.K.
Deposited on : 2021-08-18
Resolution : 2.79 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtrriage (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

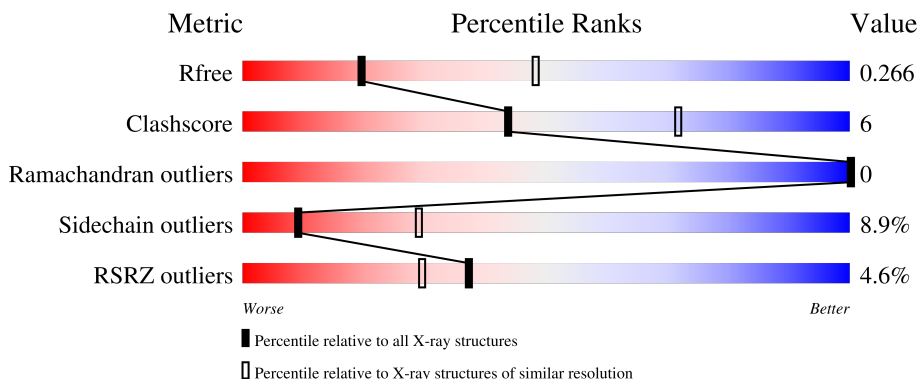
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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.



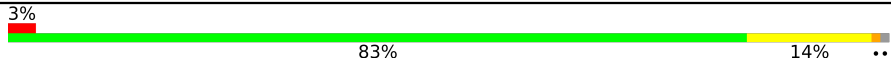
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	343	 5% 70% 20% 8%
1	D	343	 8% 70% 19% 9%
2	B	321	 2% 61% 7% 31%
2	E	321	 2% 60% 8% 30%
3	C	209	 % 83% 15%

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Mol	Chain	Length	Quality of chain
3	F	209	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '3%', a large green segment in the middle labeled '83%', and a small yellow segment on the right labeled '14%'. At the far right end of the bar, there are two small black dots.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11683 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 Cysteine-rich protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2648	1708	424	503	13	0	0	0
1	D	312	2599	1677	415	494	13	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	SER	conflict	UNP Q8IFM8
A	324	ALA	THR	conflict	UNP Q8IFM8
A	340	ALA	THR	conflict	UNP Q8IFM8
A	363	GLY	-	expression tag	UNP Q8IFM8
A	364	GLY	-	expression tag	UNP Q8IFM8
A	365	GLY	-	expression tag	UNP Q8IFM8
A	366	GLY	-	expression tag	UNP Q8IFM8
A	367	SER	-	expression tag	UNP Q8IFM8
A	368	GLU	-	expression tag	UNP Q8IFM8
A	369	PRO	-	expression tag	UNP Q8IFM8
A	370	GLU	-	expression tag	UNP Q8IFM8
A	371	ALA	-	expression tag	UNP Q8IFM8
D	147	ALA	SER	conflict	UNP Q8IFM8
D	324	ALA	THR	conflict	UNP Q8IFM8
D	340	ALA	THR	conflict	UNP Q8IFM8
D	363	GLY	-	expression tag	UNP Q8IFM8
D	364	GLY	-	expression tag	UNP Q8IFM8
D	365	GLY	-	expression tag	UNP Q8IFM8
D	366	GLY	-	expression tag	UNP Q8IFM8
D	367	SER	-	expression tag	UNP Q8IFM8
D	368	GLU	-	expression tag	UNP Q8IFM8
D	369	PRO	-	expression tag	UNP Q8IFM8
D	370	GLU	-	expression tag	UNP Q8IFM8
D	371	ALA	-	expression tag	UNP Q8IFM8

- Molecule 2 is a protein called Monoclonal antibody Cy.004 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	223	Total 1634	C 1023	N 277	O 329	S 5	0	0	0
2	E	226	Total 1655	C 1034	N 280	O 335	S 6	0	1	0

- Molecule 3 is a protein called Monoclonal antibody Cy.004 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	209	Total 1577	C 978	N 265	O 329	S 5	0	0	0
3	F	207	Total 1566	C 972	N 263	O 327	S 4	0	0	0

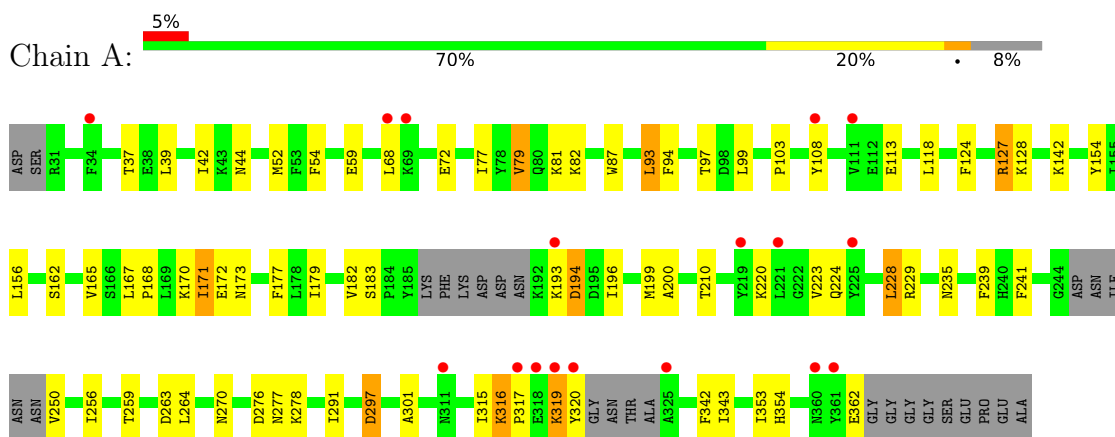
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0

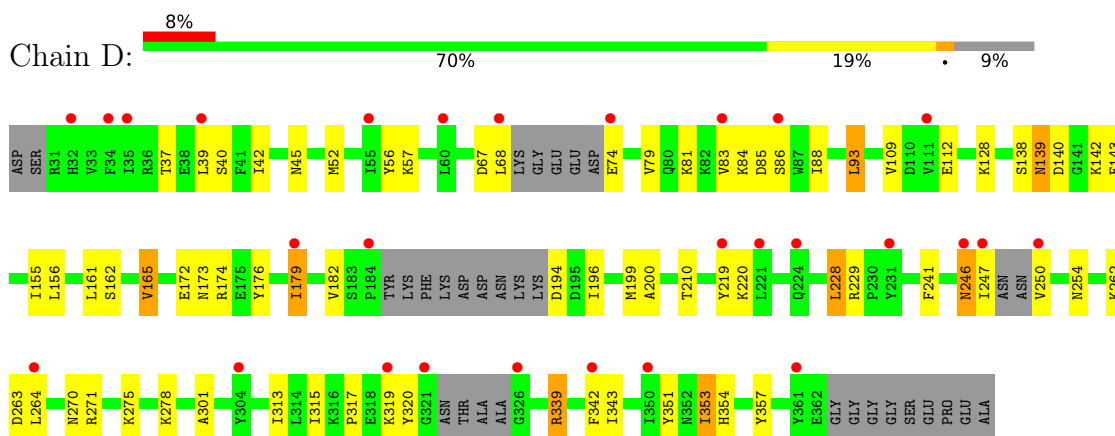
3 Residue-property plots [i](#)

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.

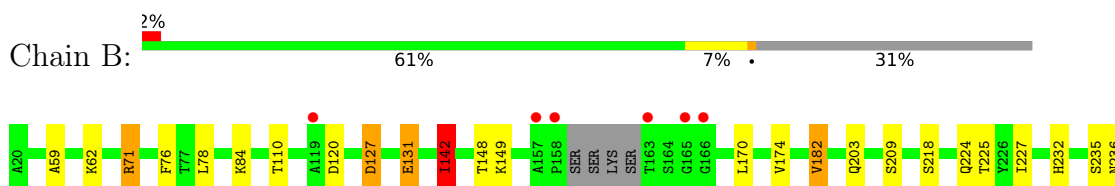
- Molecule 1: Cysteine-rich protective antigen

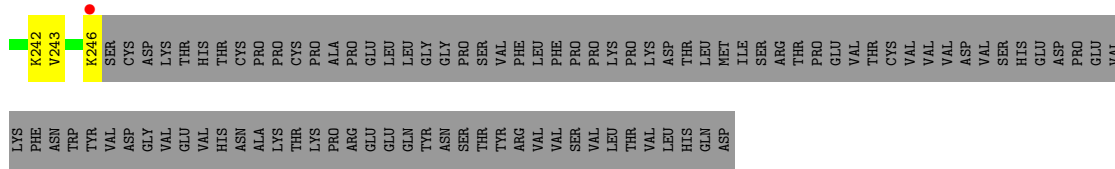


- Molecule 1: Cysteine-rich protective antigen

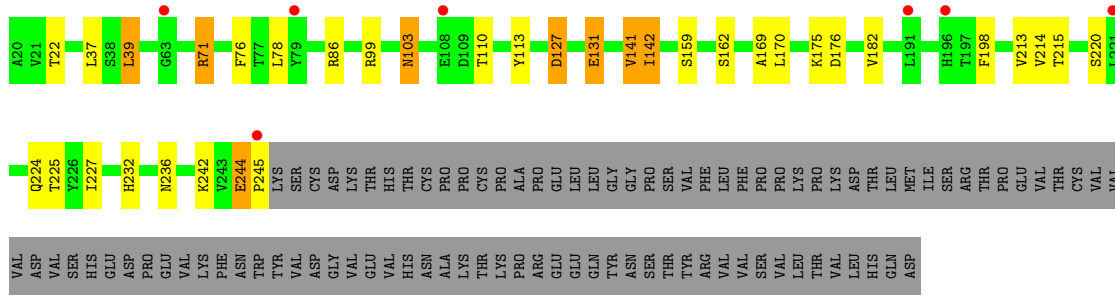


- Molecule 2: Monoclonal antibody Cy.004 heavy chain

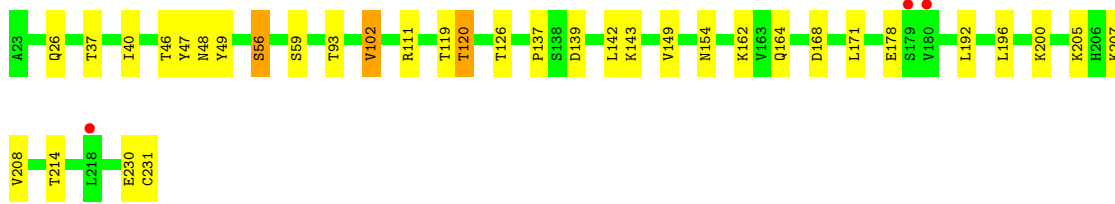
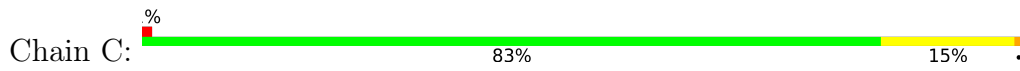




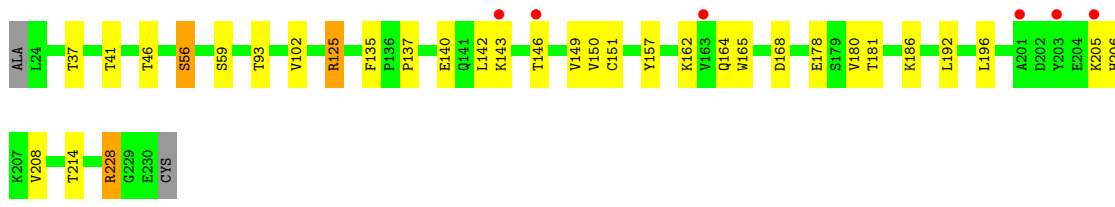
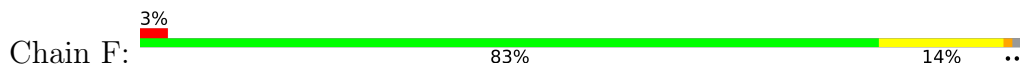
● Molecule 2: Monoclonal antibody Cy.004 heavy chain



● Molecule 3: Monoclonal antibody Cy.004 light chain



● Molecule 3: Monoclonal antibody Cy.004 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.06Å 80.32Å 114.91Å 90.00° 115.23° 90.00°	Depositor
Resolution (Å)	47.11 – 2.79 47.11 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.11-2.79) 99.0 (47.11-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.81Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (24-FEB-2021)	Depositor
R, R_{free}	0.239 , 0.277 0.225 , 0.266	Depositor DCC
R_{free} test set	2164 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtrriage
Anisotropy	0.628	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11683	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.50 % 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 1.5323e-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 [i](#)

5.1 Standard geometry [i](#)

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	0.78	1/2708 (0.0%)	1.08	10/3652 (0.3%)
1	D	0.72	0/2657	1.08	7/3585 (0.2%)
2	B	0.78	1/1670 (0.1%)	1.03	1/2273 (0.0%)
2	E	0.72	0/1695	1.04	3/2308 (0.1%)
3	C	0.73	0/1610	1.05	6/2192 (0.3%)
3	F	0.71	0/1599	1.05	0/2177
All	All	0.74	2/11939 (0.0%)	1.06	27/16187 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	GLU	CA-C	-8.08	1.42	1.52
2	B	142	ILE	CG1-CD1	5.59	1.73	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ASN	CA-CB-CG	8.56	121.16	112.60
2	E	103	ASN	CA-CB-CG	6.72	119.33	112.60
1	A	316	LYS	N-CA-C	-6.52	98.97	109.40
1	A	297	ASP	CA-CB-CG	6.39	118.99	112.60
1	D	86	SER	N-CA-C	6.30	118.65	108.32

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	2648	0	2548	35	0
1	D	2599	0	2494	57	0
2	B	1634	0	1582	11	0
2	E	1655	0	1602	15	0
3	C	1577	0	1513	16	0
3	F	1566	0	1503	13	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	11683	0	11242	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 139 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:D:83:VAL:HG21	1:D:88:ILE:CD1	1.66	1.23
2:E:127:ASP:HA	2:E:131:GLU:HG3	1.29	1.10
2:B:127:ASP:HA	2:B:131:GLU:HG3	1.29	1.10
1:D:83:VAL:HG21	1:D:88:ILE:HD12	1.11	1.09
3:C:40:ILE:HG21	3:C:119:THR:HG21	1.43	1.00

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	309/343 (90%)	288 (93%)	21 (7%)	0	100	100
1	D	302/343 (88%)	283 (94%)	19 (6%)	0	100	100
2	B	219/321 (68%)	210 (96%)	9 (4%)	0	100	100
2	E	225/321 (70%)	214 (95%)	11 (5%)	0	100	100
3	C	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
3	F	205/209 (98%)	197 (96%)	8 (4%)	0	100	100
All	All	1467/1746 (84%)	1392 (95%)	75 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	297/316 (94%)	267 (90%)	30 (10%)	7	23
1	D	292/316 (92%)	264 (90%)	28 (10%)	8	26
2	B	179/272 (66%)	164 (92%)	15 (8%)	10	32
2	E	183/272 (67%)	163 (89%)	20 (11%)	6	21
3	C	180/180 (100%)	170 (94%)	10 (6%)	19	50
3	F	179/180 (99%)	166 (93%)	13 (7%)	13	38
All	All	1310/1536 (85%)	1194 (91%)	116 (9%)	9	29

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	85	ASP
3	F	164	GLN
1	D	250	VAL
3	F	146	THR
2	E	224	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	224	GLN
2	E	236	ASN
1	D	338	ASN
3	F	33	ASN
1	A	348	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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	317/343 (92%)	0.63	17 (5%) 31 24	52, 84, 125, 146	0
1	D	312/343 (90%)	1.04	28 (8%) 15 11	66, 103, 143, 159	0
2	B	223/321 (69%)	0.45	7 (3%) 51 41	53, 79, 102, 109	0
2	E	226/321 (70%)	0.52	7 (3%) 51 41	46, 89, 131, 138	1 (0%)
3	C	209/209 (100%)	0.37	3 (1%) 73 64	58, 77, 107, 115	0
3	F	207/209 (99%)	0.55	6 (2%) 53 43	53, 81, 137, 151	0
All	All	1494/1746 (85%)	0.63	68 (4%) 37 29	46, 85, 132, 159	1 (0%)

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	LEU	5.8
1	D	321	GLY	5.8
1	A	325	ALA	4.5
1	A	320	TYR	4.5
1	A	361	TYR	4.4

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

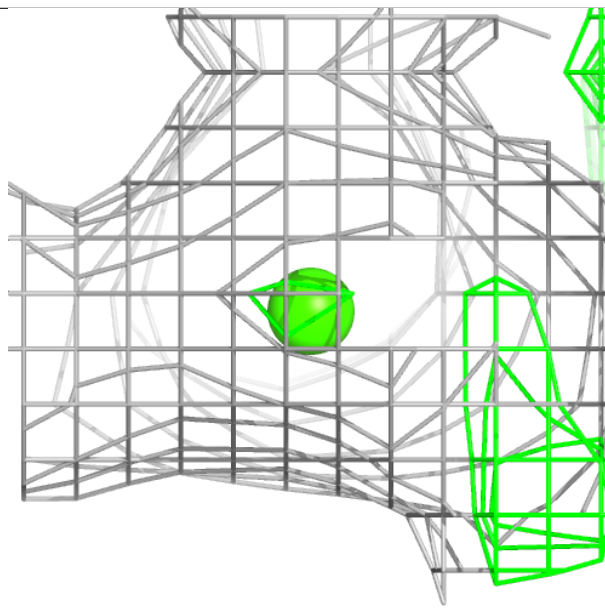
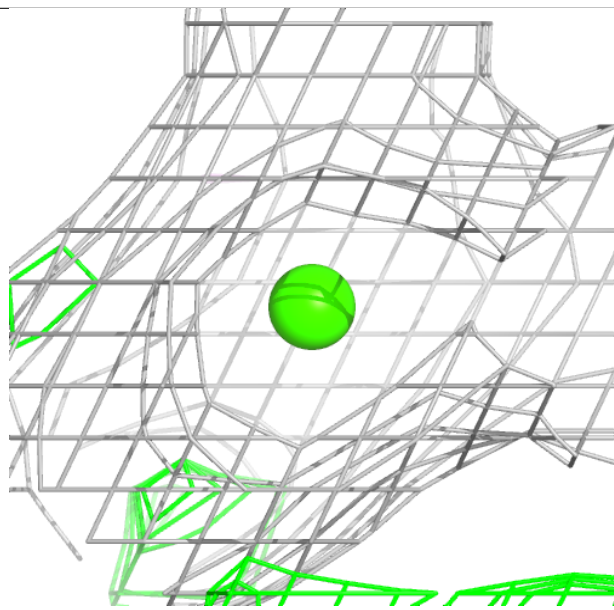
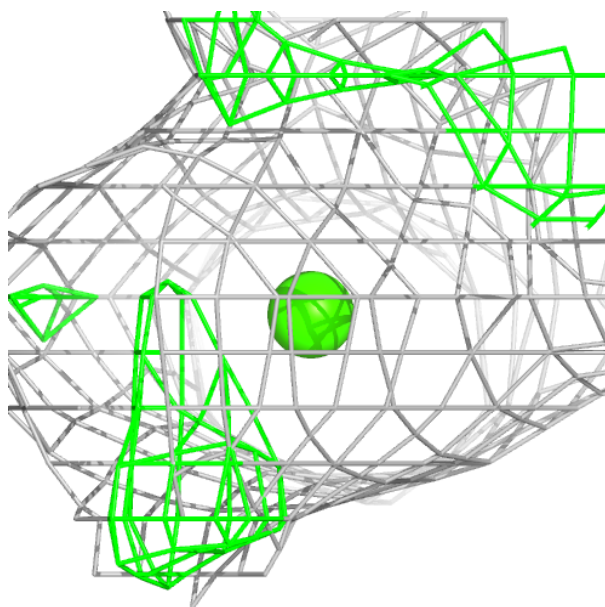
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	B	401	1/1	0.89	0.16	100,100,100,100	0
4	CA	E	401	1/1	0.91	0.14	98,98,98,98	0
4	CA	D	401	1/1	0.96	0.12	67,67,67,67	0
4	CA	A	401	1/1	0.96	0.10	63,63,63,63	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.

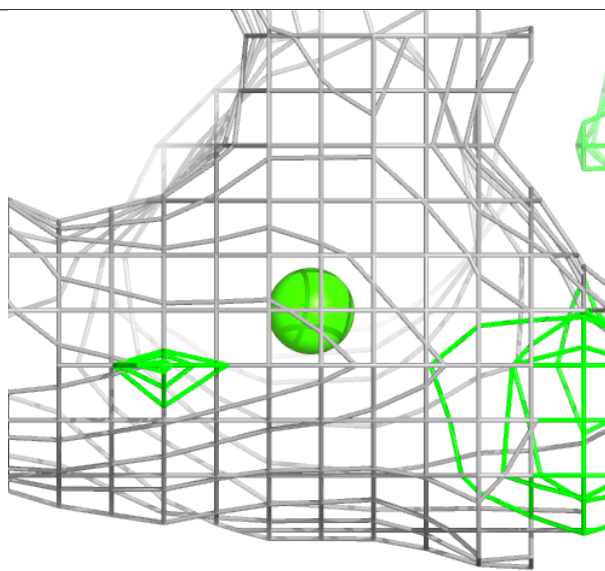
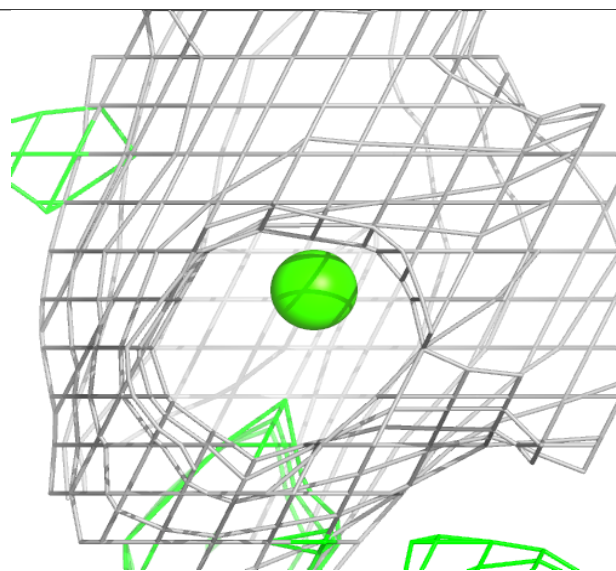
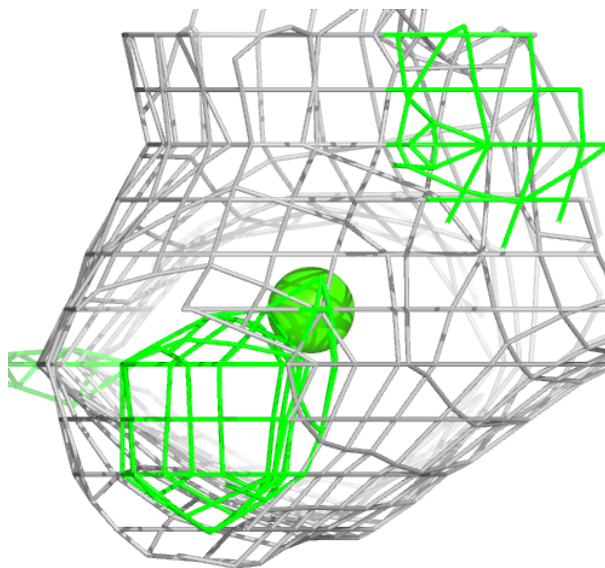
Electron density around CA B 401:

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



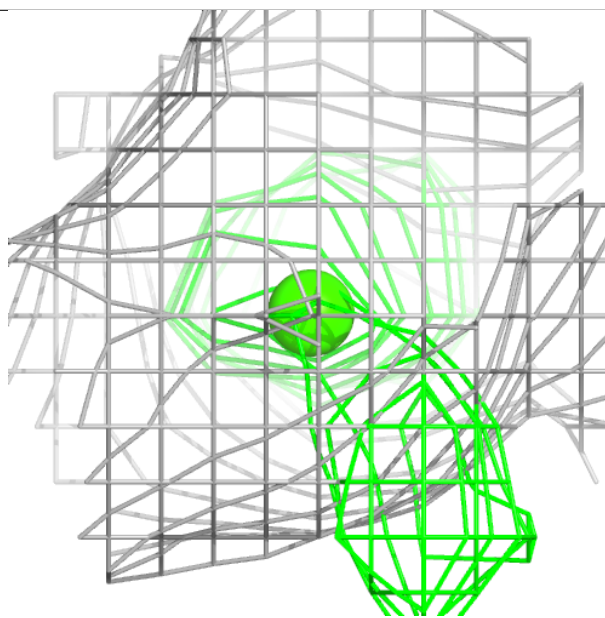
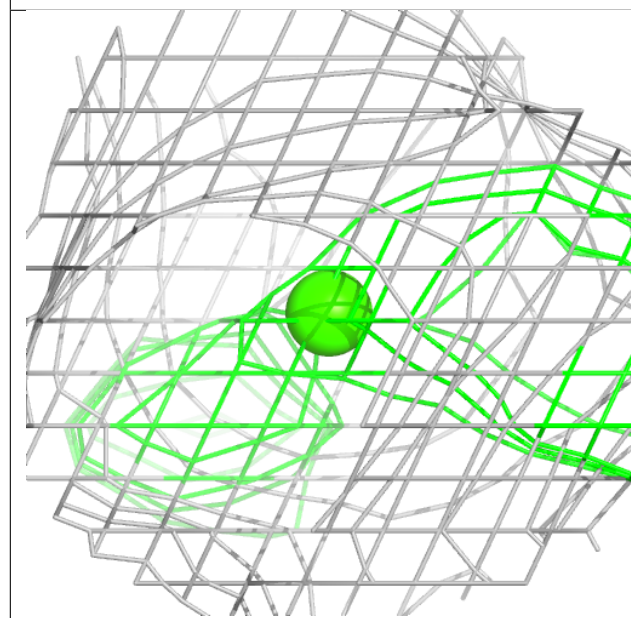
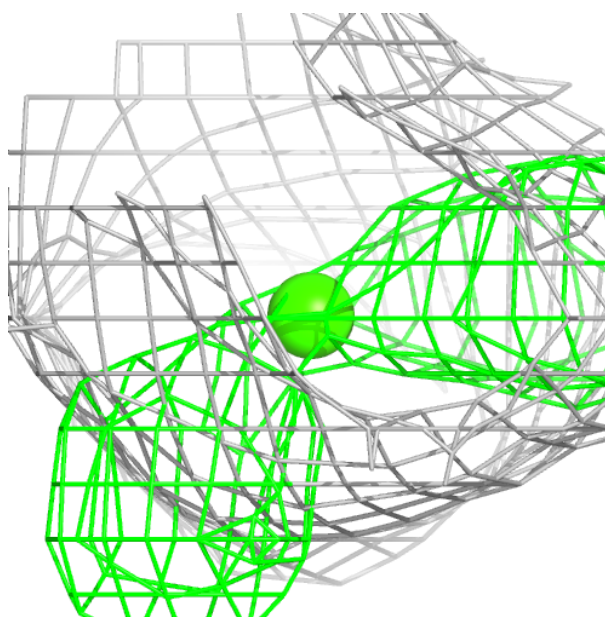
Electron density around CA E 401:

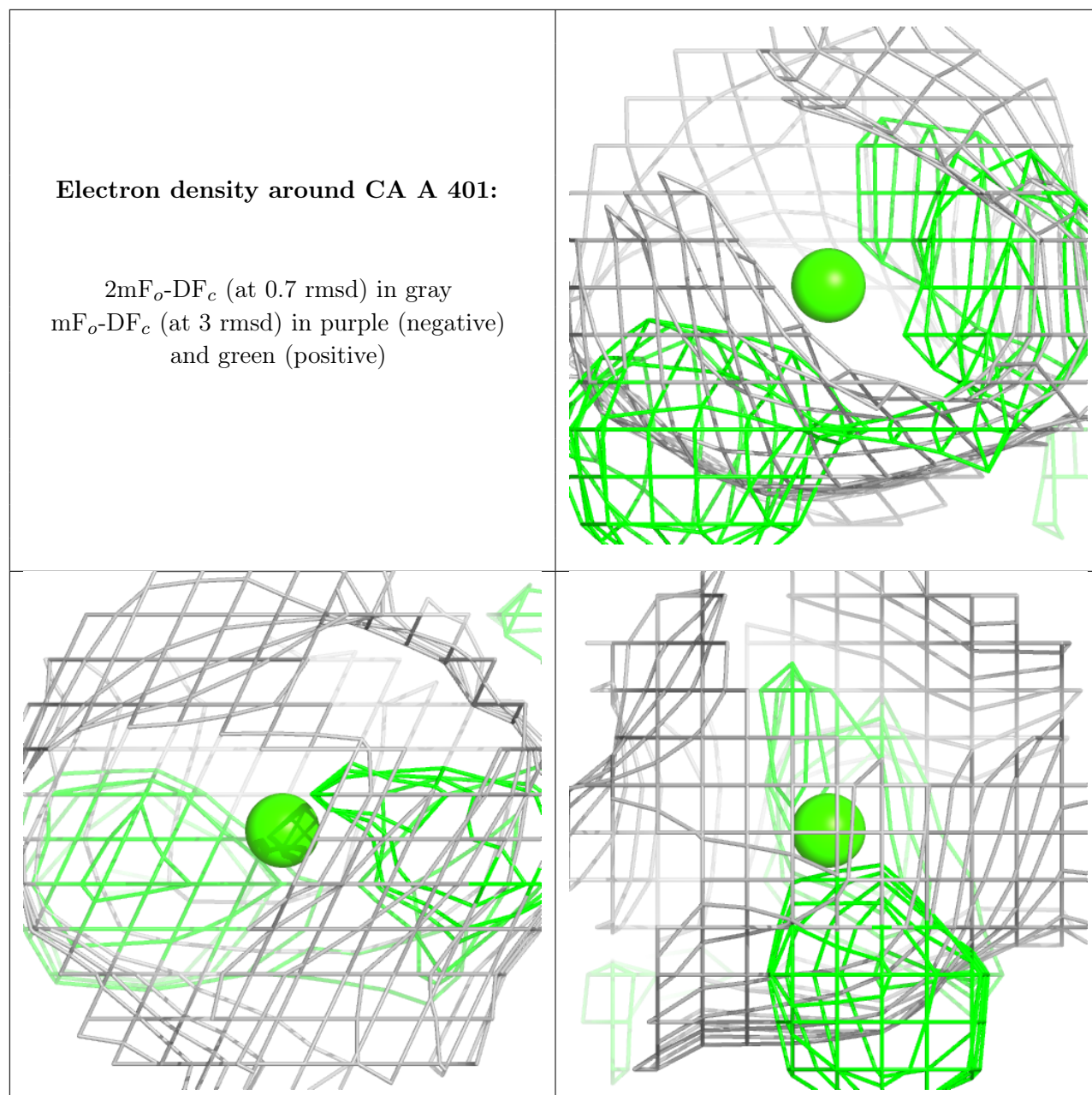
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA D 401:

$2mF_o-DF_c$ (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.