



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 06:09 pm GMT

PDB ID : 8RMX
Title : Transglutaminase 3 in complex with DH patient-derived Fab DH63-A02
Authors : Heggelund, J.E.; Sollid, L.M.
Deposited on : 2024-01-09
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

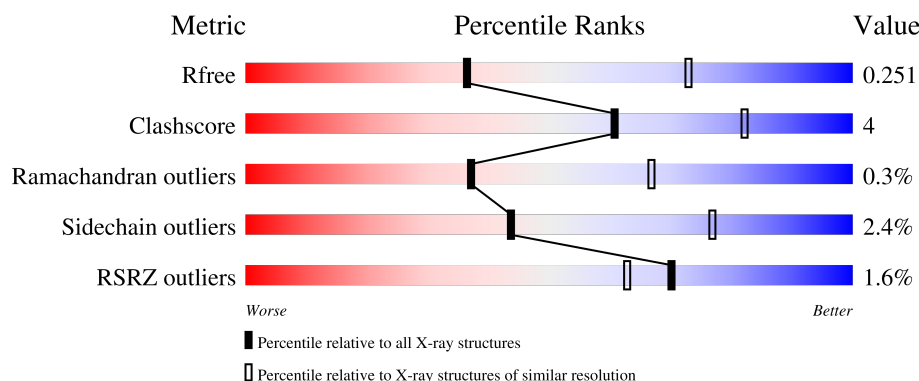
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (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	464	
1	D	464	
2	B	220	
2	E	220	
3	C	219	

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Mol	Chain	Length	Quality of chain
3	F	219	 82%17%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13861 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 Protein-glutamine gamma-glutamyltransferase E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3597	2265	634	685	13			
1	D	462	Total	C	N	O	S	0	0	0
			3605	2270	635	686	14			

- Molecule 2 is a protein called Antibody Fab fragment heavy chain IGHV2-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	220	Total	C	N	O	S	0	0	0
			1654	1049	273	326	6			
2	B	196	Total	C	N	O	S	0	0	0
			1499	957	246	290	6			

- Molecule 3 is a protein called Antibody Fab fragment light chain IGKV4-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	219	Total	C	N	O	S	0	0	0
			1697	1063	283	345	6			
3	C	218	Total	C	N	O	S	0	0	0
			1691	1060	282	344	5			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	D	3	Total	Ca	0	0
			3	3		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	E	13	Total	O	0	0
			13	13		
6	F	19	Total	O	0	0
			19	19		
6	D	16	Total	O	0	0
			16	16		

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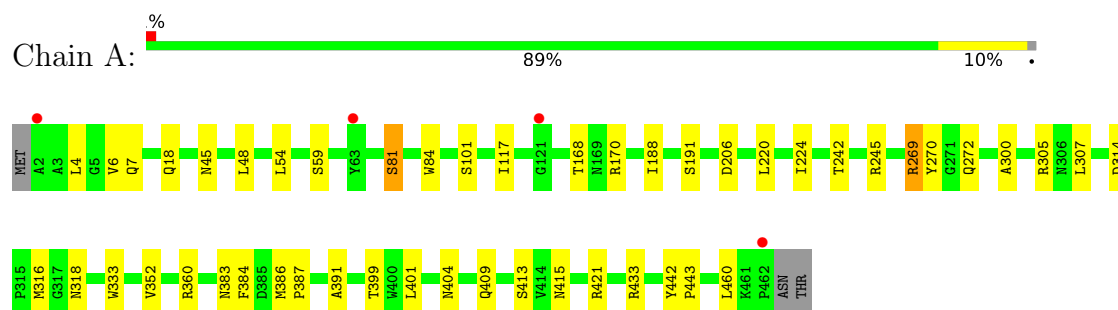
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total	O	0	0
			4	4		
6	C	2	Total	O	0	0
			2	2		

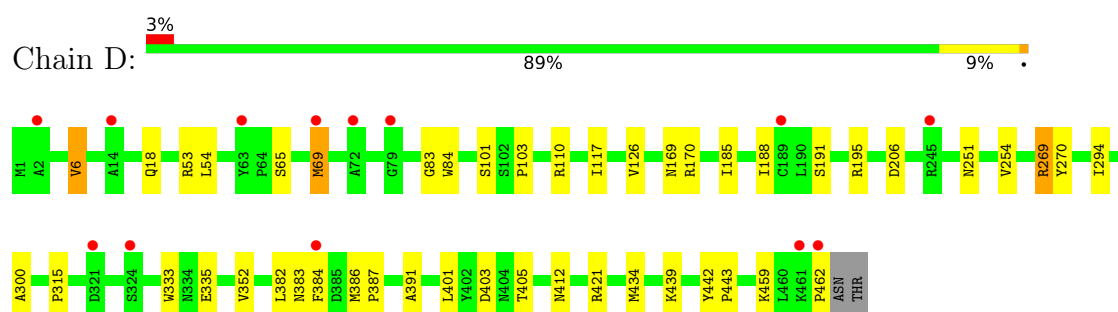
3 Residue-property plots [i](#)

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.

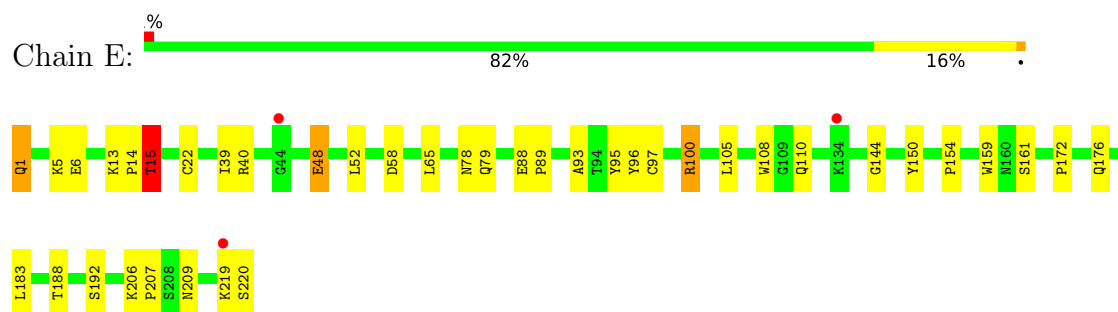
- Molecule 1: Protein-glutamine gamma-glutamyltransferase E



- Molecule 1: Protein-glutamine gamma-glutamyltransferase E



- Molecule 2: Antibody Fab fragment heavy chain IGHV2-5



- Molecule 2: Antibody Fab fragment heavy chain IGHV2-5





4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.03Å 264.00Å 148.70Å 90.00° 106.29° 90.00°	Depositor
Resolution (Å)	132.00 – 2.80 132.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (132.00-2.80) 98.8 (132.00-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.205 , 0.250 0.208 , 0.251	Depositor DCC
R_{free} test set	4245 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.0	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	13861	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: CA, PO4

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	0.65	1/3684 (0.0%)	0.67	0/4999
1	D	0.60	0/3692	0.66	2/5009 (0.0%)
2	B	0.51	0/1535	0.62	0/2097
2	E	0.65	1/1694 (0.1%)	0.69	1/2317 (0.0%)
3	C	0.54	1/1728 (0.1%)	0.60	0/2348
3	F	0.69	2/1734 (0.1%)	0.74	1/2356 (0.0%)
All	All	0.61	5/14067 (0.0%)	0.66	4/19126 (0.0%)

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	7
1	D	0	5
2	B	0	2
2	E	0	2
3	C	0	1
3	F	0	2
All	All	0	19

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	82	SER	CA-CB	-6.71	1.42	1.52
3	C	32	SER	CA-CB	-6.27	1.43	1.52
1	A	59	SER	CA-CB	-5.49	1.44	1.52
3	F	32	SER	CA-CB	-5.36	1.45	1.52
2	E	48	GLU	CD-OE2	5.11	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	94	CYS	CB-CA-C	-10.12	90.17	110.40
2	E	15	THR	CA-CB-OG1	-7.37	93.53	109.00
1	D	434	MET	CG-SD-CE	6.04	109.86	100.20
1	D	69	MET	CG-SD-CE	5.17	108.48	100.20

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	272	GLN	Peptide
1	A	360	ARG	Sidechain
1	A	433	ARG	Sidechain
1	A	81	SER	Peptide
2	B	100	ARG	Sidechain
2	B	215	ARG	Sidechain
3	C	216	ARG	Sidechain
1	D	110	ARG	Sidechain
1	D	195	ARG	Sidechain
1	D	269	ARG	Sidechain
1	D	421	ARG	Sidechain
1	D	53	ARG	Sidechain
2	E	100	ARG	Sidechain
2	E	40	ARG	Sidechain
3	F	216	ARG	Sidechain
3	F	94	CYS	Mainchain

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	3597	0	3466	21	0
1	D	3605	0	3478	23	0
2	B	1499	0	1497	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1654	0	1658	24	0
3	C	1691	0	1637	14	0
3	F	1697	0	1642	24	0
4	A	3	0	0	0	0
4	D	3	0	0	0	0
5	A	15	0	0	0	0
5	D	20	0	0	0	0
5	F	5	0	0	0	0
6	A	18	0	0	0	0
6	B	4	0	0	0	0
6	C	2	0	0	0	0
6	D	16	0	0	0	0
6	E	13	0	0	0	0
6	F	19	0	0	0	0
All	All	13861	0	13378	110	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 4.

All (110) 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)
2:E:100:ARG:NH2	1:D:403:ASP:OD2	2.16	0.77
1:D:401:LEU:HD23	1:D:412:ASN:HB2	1.66	0.76
1:A:307:LEU:HG	1:A:460:LEU:HD11	1.68	0.75
3:F:168:VAL:HG22	3:F:180:LEU:HD12	1.71	0.73
1:D:83:GLY:HA2	1:D:103:PRO:HB3	1.74	0.67
3:C:13:VAL:HG12	3:C:17:GLU:HB2	1.80	0.63
3:C:172:ASP:OD2	3:C:174:LYS:HB2	1.99	0.62
3:F:13:VAL:HG12	3:F:17:GLU:HB2	1.84	0.60
3:C:78:THR:HG22	3:C:80:THR:HG23	1.84	0.60
2:E:88:GLU:HG3	2:E:89:PRO:HD2	1.84	0.60
3:C:56:TRP:O	3:C:57:ALA:HB3	2.02	0.59
1:A:399:THR:OG1	1:A:413:SER:OG	2.20	0.59
2:B:30:ASP:OD1	2:B:75:THR:HG21	2.03	0.59
2:E:5:LYS:HE3	2:E:110:GLN:HE22	1.67	0.58
3:F:15:LEU:HD12	3:F:84:LEU:O	2.03	0.58
1:A:399:THR:HG1	1:A:413:SER:HG	1.47	0.58
2:E:14:PRO:O	2:E:15:THR:CB	2.52	0.57
3:F:56:TRP:O	3:F:57:ALA:HB3	2.04	0.57
3:F:45:LYS:HB3	3:F:46:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:84:LEU:HD23	3:F:111:ILE:HD13	1.86	0.56
2:B:36:VAL:HG21	2:B:80:VAL:HG21	1.88	0.56
2:B:36:VAL:CG2	2:B:80:VAL:HG21	2.36	0.55
1:A:54:LEU:HD22	1:A:117:ILE:HG12	1.88	0.55
2:E:14:PRO:O	2:E:15:THR:HB	2.06	0.55
2:B:131:PRO:HB3	2:B:143:LEU:HB3	1.89	0.54
2:B:88:GLU:HG3	2:B:89:PRO:HD2	1.90	0.54
3:F:65:PRO:HG2	3:F:67:ARG:NH1	2.24	0.53
2:B:173:ALA:HA	2:B:183:LEU:HB3	1.91	0.53
3:F:13:VAL:CG1	3:F:17:GLU:HB2	2.39	0.52
2:E:172:PRO:HD2	3:F:167:SER:OG	2.09	0.52
1:D:84:TRP:HA	1:D:101:SER:O	2.08	0.52
3:F:91:VAL:HG12	3:F:93:TYR:CE1	2.45	0.52
3:F:130:LEU:O	3:F:188:LYS:HD2	2.11	0.51
2:B:206:LYS:N	2:B:207:PRO:CD	2.74	0.50
1:A:188:ILE:O	1:A:191:SER:HB2	2.12	0.50
3:C:113:ARG:HG2	3:C:113:ARG:HH21	1.75	0.50
1:D:54:LEU:CD2	1:D:117:ILE:HG12	2.42	0.50
3:F:37:ASN:O	3:F:56:TRP:HA	2.13	0.49
1:D:54:LEU:HD22	1:D:117:ILE:HG12	1.95	0.49
2:E:219:LYS:O	2:E:220:SER:HB3	2.13	0.49
2:E:183:LEU:HD12	2:E:183:LEU:C	2.32	0.49
2:B:122:LYS:HD2	2:B:149:ASP:O	2.13	0.49
3:C:180:LEU:HD23	3:C:181:SER:N	2.30	0.47
3:C:189:ALA:O	3:C:193:LYS:HD3	2.14	0.47
1:A:300:ALA:HB3	1:A:391:ALA:O	2.15	0.47
2:E:206:LYS:N	2:E:207:PRO:CD	2.77	0.47
2:E:52:LEU:HD22	3:F:101:TRP:CH2	2.50	0.47
1:D:300:ALA:HB3	1:D:391:ALA:O	2.15	0.47
2:E:108:TRP:CZ3	3:F:50:PRO:HG2	2.50	0.47
1:D:6:VAL:CG1	1:D:126:VAL:HG11	2.45	0.46
1:A:401:LEU:O	1:A:409:GLN:HA	2.15	0.46
1:A:386:MET:N	1:A:387:PRO:CD	2.79	0.46
1:D:386:MET:N	1:D:387:PRO:CD	2.79	0.46
1:A:415:ASN:OD1	1:A:415:ASN:C	2.53	0.46
2:E:22:CYS:O	2:E:79:GLN:HA	2.16	0.46
2:E:93:ALA:HB3	2:E:95:TYR:CE1	2.50	0.46
1:D:333:TRP:CD1	1:D:352:VAL:HG13	2.52	0.45
1:A:4:LEU:HD21	1:A:48:LEU:HD22	1.98	0.45
1:A:54:LEU:CD2	1:A:117:ILE:HG12	2.46	0.45
2:E:39:ILE:HD11	2:E:105:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD2	1:A:318:ASN:HB2	2.17	0.45
1:D:382:LEU:O	1:D:386:MET:HG3	2.16	0.45
1:A:84:TRP:HA	1:A:101:SER:O	2.16	0.45
2:B:183:LEU:HD12	2:B:183:LEU:C	2.37	0.45
2:B:52:LEU:HD22	3:C:101:TRP:CH2	2.52	0.45
1:A:220:LEU:O	1:A:224:ILE:HG12	2.17	0.45
2:B:96:TYR:CE1	3:C:49:PRO:HB3	2.52	0.45
1:D:269:ARG:HA	1:D:270:TYR:HA	1.84	0.44
1:D:169:ASN:C	1:D:170:ARG:HG3	2.38	0.44
1:D:294:ILE:HG13	1:D:335:GLU:HG3	1.98	0.44
3:F:151:VAL:HG22	3:F:201:VAL:HG22	2.00	0.44
1:A:7:GLN:NE2	1:A:45:ASN:HA	2.33	0.44
1:D:188:ILE:O	1:D:191:SER:HB2	2.17	0.44
1:D:459:LYS:O	1:D:462:PRO:HD3	2.17	0.44
2:E:108:TRP:CE3	3:F:50:PRO:HD2	2.53	0.44
3:F:34:ASN:CG	3:F:36:LYS:HG3	2.38	0.44
2:E:150:TYR:OH	2:E:183:LEU:HD23	2.19	0.43
2:B:14:PRO:O	2:B:15:THR:CB	2.66	0.43
2:E:144:GLY:HA2	2:E:159:TRP:CZ2	2.53	0.43
2:B:121:THR:CG2	2:B:208:SER:HB3	2.49	0.43
2:B:22:CYS:O	2:B:79:GLN:HA	2.18	0.43
2:B:42:PRO:HB2	2:B:45:LYS:HE2	2.01	0.43
1:A:383:ASN:HB3	1:A:384:PHE:CD1	2.54	0.42
1:D:383:ASN:HB3	1:D:384:PHE:CD1	2.53	0.42
1:D:383:ASN:HA	1:D:384:PHE:HA	1.82	0.42
3:C:37:ASN:O	3:C:56:TRP:HA	2.19	0.42
3:C:191:TYR:O	3:C:197:TYR:OH	2.34	0.42
1:A:316:MET:HG3	2:B:102:VAL:HG13	2.00	0.42
3:F:28:SER:HA	3:F:74:GLY:O	2.20	0.42
1:A:333:TRP:CD1	1:A:352:VAL:HG13	2.55	0.42
1:D:442:TYR:HB3	1:D:443:PRO:CD	2.49	0.42
2:E:176:GLN:HA	3:F:165:GLN:HE22	1.85	0.42
3:F:128:GLU:HG2	2:B:76:SER:HB2	2.00	0.42
2:B:42:PRO:HB2	2:B:45:LYS:CE	2.49	0.42
1:D:315:PRO:HA	1:D:401:LEU:CD1	2.50	0.41
3:C:113:ARG:HG2	3:C:114:THR:N	2.35	0.41
2:E:6:GLU:HG3	2:E:97:CYS:SG	2.60	0.41
3:C:56:TRP:O	3:C:57:ALA:CB	2.67	0.41
2:E:48:GLU:OE1	2:E:65:LEU:HD11	2.20	0.41
1:A:442:TYR:HB3	1:A:443:PRO:CD	2.51	0.41
1:A:421:ARG:HA	2:E:1:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:96:TYR:CE1	3:F:49:PRO:HB3	2.55	0.41
3:F:97:TYR:O	1:D:405:THR:HG23	2.20	0.41
2:E:52:LEU:HD22	3:F:101:TRP:HH2	1.86	0.40
3:C:141:LEU:N	3:C:141:LEU:HD12	2.35	0.40
1:A:269:ARG:HA	1:A:270:TYR:HA	1.81	0.40
3:F:56:TRP:O	3:F:57:ALA:CB	2.70	0.40
1:D:185:ILE:HD11	1:D:254:VAL:HG13	2.04	0.40
2:E:144:GLY:HA2	2:E:159:TRP:CH2	2.56	0.40
1:D:439:LYS:HA	1:D:439:LYS:HD3	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	459/464 (99%)	441 (96%)	18 (4%)	0	100	100
1	D	460/464 (99%)	446 (97%)	14 (3%)	0	100	100
2	B	190/220 (86%)	180 (95%)	9 (5%)	1 (0%)	25	56
2	E	218/220 (99%)	205 (94%)	11 (5%)	2 (1%)	14	42
3	C	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	14	42
3	F	217/219 (99%)	207 (95%)	9 (4%)	1 (0%)	25	56
All	All	1760/1806 (98%)	1684 (96%)	70 (4%)	6 (0%)	37	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	100	LEU
3	F	100	LEU
2	E	15	THR

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Mol	Chain	Res	Type
3	C	57	ALA
2	E	154	PRO
2	B	154	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	388/391 (99%)	380 (98%)	8 (2%)	48	80
1	D	389/391 (100%)	383 (98%)	6 (2%)	60	86
2	B	175/194 (90%)	169 (97%)	6 (3%)	32	66
2	E	194/194 (100%)	186 (96%)	8 (4%)	26	59
3	C	193/194 (100%)	187 (97%)	6 (3%)	35	69
3	F	194/194 (100%)	191 (98%)	3 (2%)	60	86
All	All	1533/1558 (98%)	1496 (98%)	37 (2%)	44	77

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	18	GLN
1	A	81	SER
1	A	168	THR
1	A	206	ASP
1	A	242	THR
1	A	305	ARG
1	A	404	ASN
2	E	1	GLN
2	E	13	LYS
2	E	58	ASP
2	E	78	ASN
2	E	161	SER
2	E	188	THR
2	E	192	SER

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Mol	Chain	Res	Type
2	E	209	ASN
3	F	66	ASP
3	F	76	ASP
3	F	157	ASN
1	D	6	VAL
1	D	18	GLN
1	D	65	SER
1	D	69	MET
1	D	206	ASP
1	D	251	ASN
2	B	36	VAL
2	B	110	GLN
2	B	156	THR
2	B	174	VAL
2	B	177	SER
2	B	198	THR
3	C	20	THR
3	C	69	SER
3	C	113	ARG
3	C	190	ASP
3	C	192	GLU
3	C	193	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	78	ASN
2	E	169	HIS
2	E	197	GLN
3	C	85	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z > 2$
5	PO4	A	506	-	4,4,4	1.76	1 (25%)	6,6,6	0.40	0
5	PO4	D	504	-	4,4,4	0.97	0	6,6,6	0.51	0
5	PO4	D	506	-	4,4,4	1.42	1 (25%)	6,6,6	0.38	0
5	PO4	A	505	-	4,4,4	1.25	1 (25%)	6,6,6	0.42	0
5	PO4	F	301	-	4,4,4	1.90	2 (50%)	6,6,6	0.55	0
5	PO4	A	504	-	4,4,4	1.22	0	6,6,6	0.54	0
5	PO4	D	507	-	4,4,4	0.99	0	6,6,6	0.47	0
5	PO4	D	505	-	4,4,4	0.92	0	6,6,6	0.42	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	506	PO4	P-O1	3.35	1.58	1.50
5	F	301	PO4	P-O4	2.65	1.62	1.54
5	D	506	PO4	P-O1	2.63	1.57	1.50
5	F	301	PO4	P-O1	2.59	1.56	1.50
5	A	505	PO4	P-O1	2.18	1.55	1.50

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	461/464 (99%)	-0.26	4 (0%) 81 75	65, 93, 126, 174	0
1	D	462/464 (99%)	0.05	13 (2%) 55 46	70, 102, 142, 180	0
2	B	196/220 (89%)	0.07	3 (1%) 71 64	88, 135, 183, 224	0
2	E	220/220 (100%)	-0.13	3 (1%) 73 66	71, 96, 138, 169	0
3	C	218/219 (99%)	0.07	5 (2%) 61 52	91, 140, 175, 185	0
3	F	219/219 (100%)	-0.32	1 (0%) 87 83	67, 98, 128, 165	0
All	All	1776/1806 (98%)	-0.09	29 (1%) 70 63	65, 102, 162, 224	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	175	LEU	7.5
1	D	462	PRO	5.1
1	D	321	ASP	3.5
1	A	462	PRO	3.2
2	B	181	TYR	3.2
1	D	245	ARG	3.1
2	B	186	VAL	2.8
1	D	189	CYS	2.8
3	C	123	PHE	2.7
2	E	44	GLY	2.5
1	D	72	ALA	2.5
2	E	134	LYS	2.4
2	E	219	LYS	2.4
3	C	161	SER	2.4
1	D	461	LYS	2.3
1	D	324	SER	2.3
1	D	384	PHE	2.3
1	D	63	TYR	2.3
3	C	12	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	69	MET	2.3
3	C	140	LEU	2.3
1	A	121	GLY	2.2
3	F	32	SER	2.2
1	A	63	TYR	2.1
3	C	210	VAL	2.1
1	D	14	ALA	2.1
1	A	2	ALA	2.1
1	D	2	ALA	2.0
1	D	79	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	PO4	A	505	5/5	0.64	0.08	122,141,194,235	0
5	PO4	D	505	5/5	0.70	0.09	159,160,192,208	0
5	PO4	D	506	5/5	0.72	0.08	119,158,196,248	0
5	PO4	D	504	5/5	0.74	0.07	127,146,152,198	0
5	PO4	A	504	5/5	0.79	0.08	98,120,153,175	0
5	PO4	F	301	5/5	0.80	0.08	101,121,125,176	0
5	PO4	A	506	5/5	0.85	0.08	88,113,174,213	0
5	PO4	D	507	5/5	0.91	0.06	105,108,147,156	0
4	CA	D	502	1/1	0.99	0.04	92,92,92,92	0
4	CA	A	502	1/1	0.99	0.03	81,81,81,81	0
4	CA	A	503	1/1	0.99	0.03	91,91,91,91	0
4	CA	D	503	1/1	1.00	0.01	96,96,96,96	0
4	CA	D	501	1/1	1.00	0.02	85,85,85,85	0

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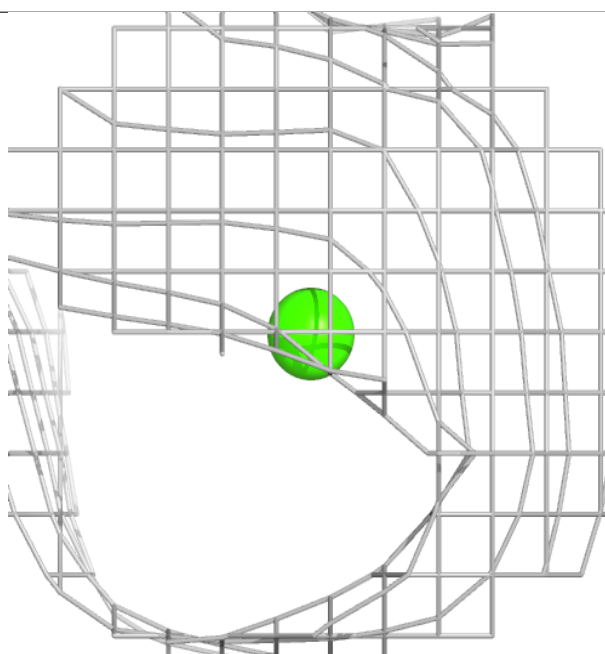
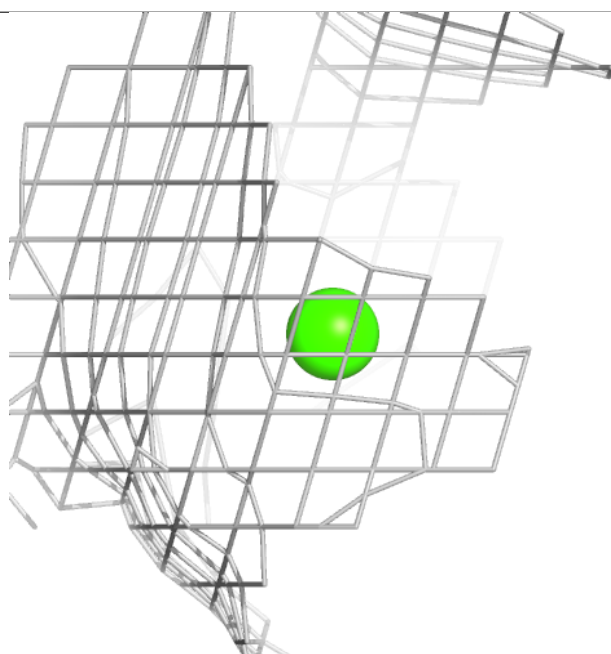
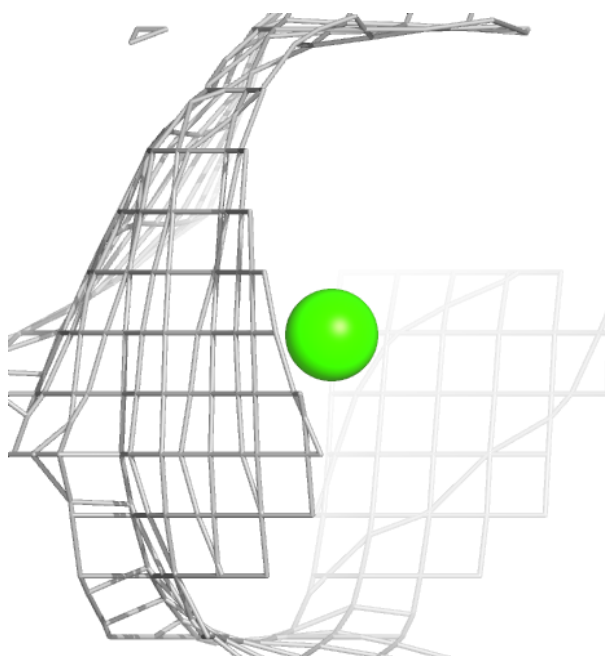
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	A	501	1/1	1.00	0.05	93,93,93,93	0

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.

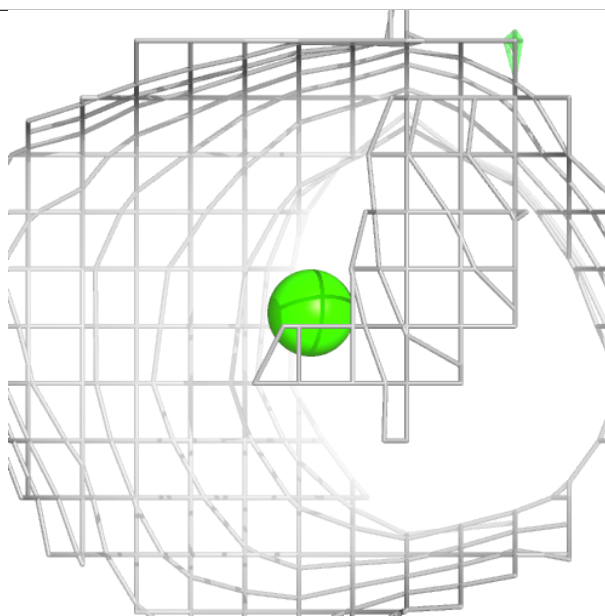
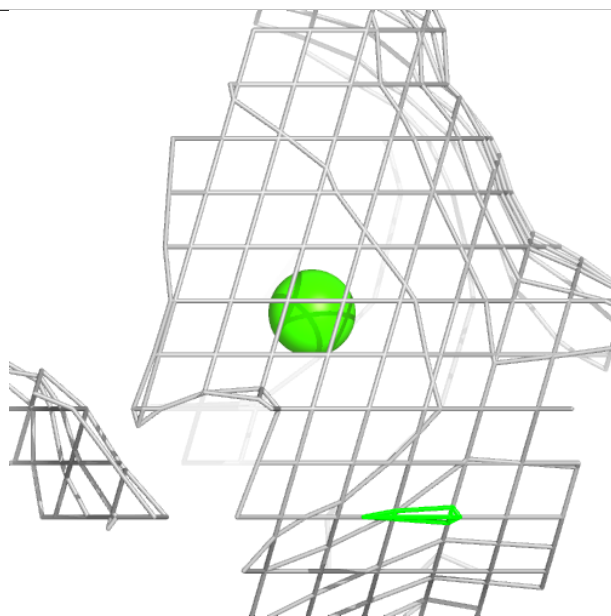
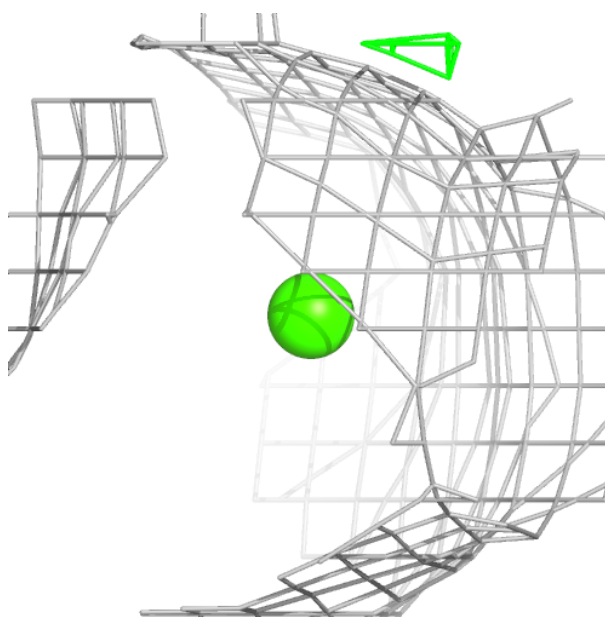
Electron density around CA D 502:

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



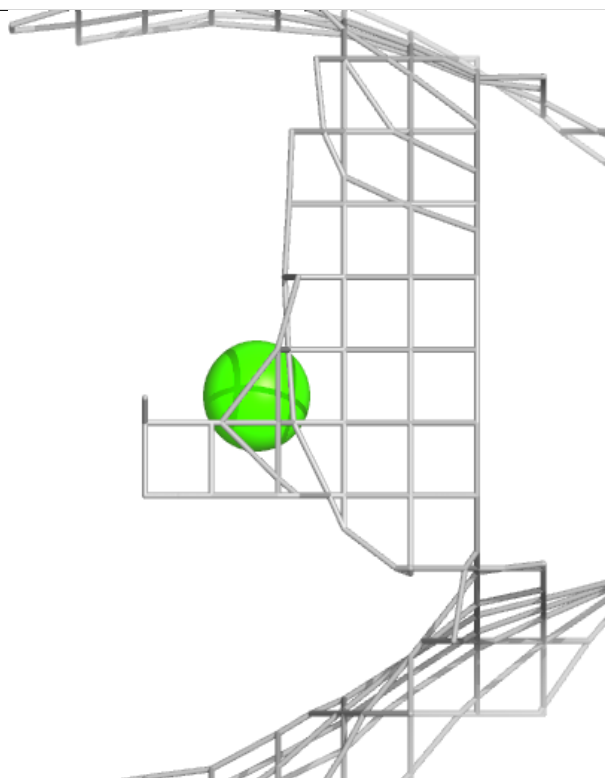
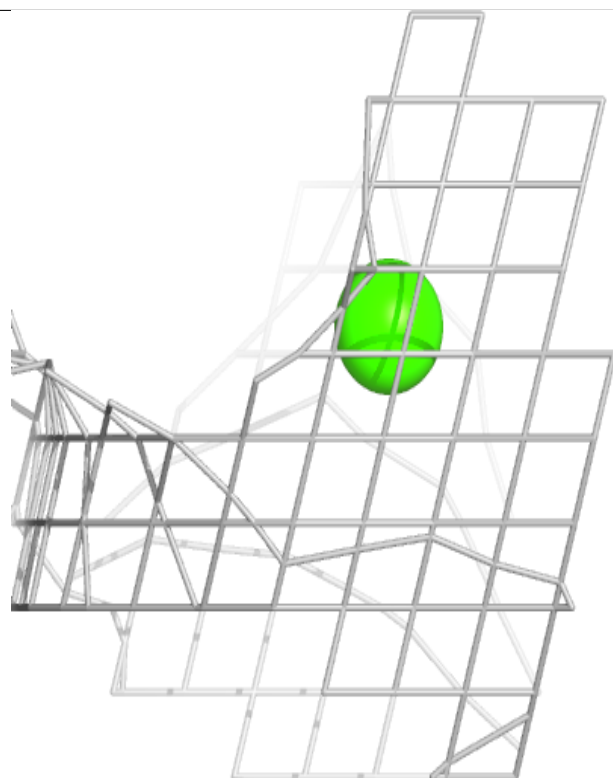
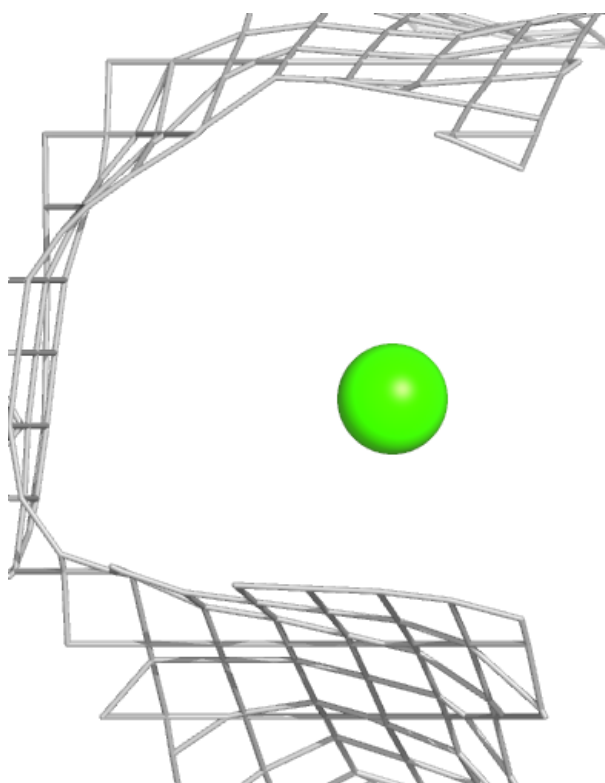
Electron density around CA A 502:

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and green (positive)



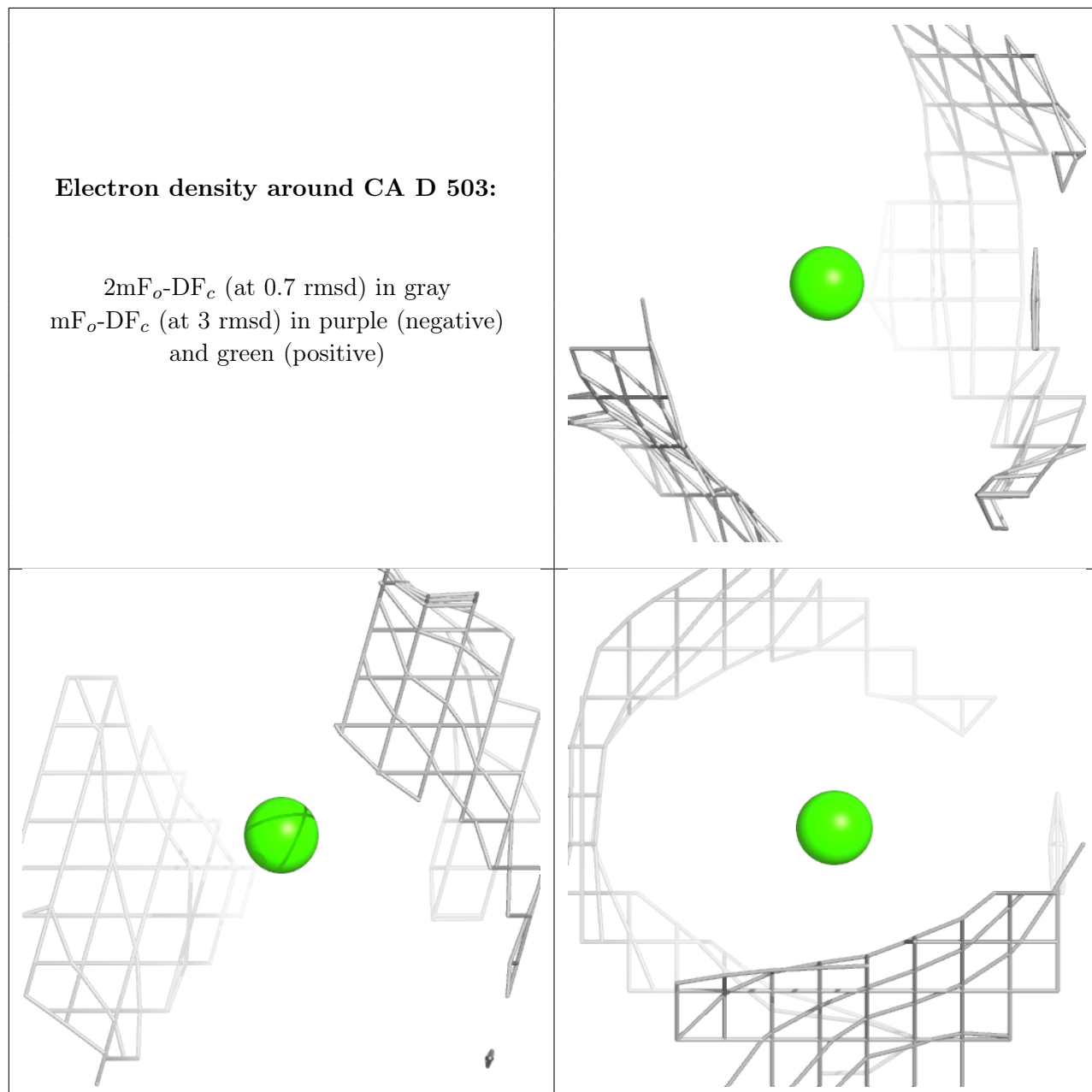
Electron density around CA A 503:

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and green (positive)



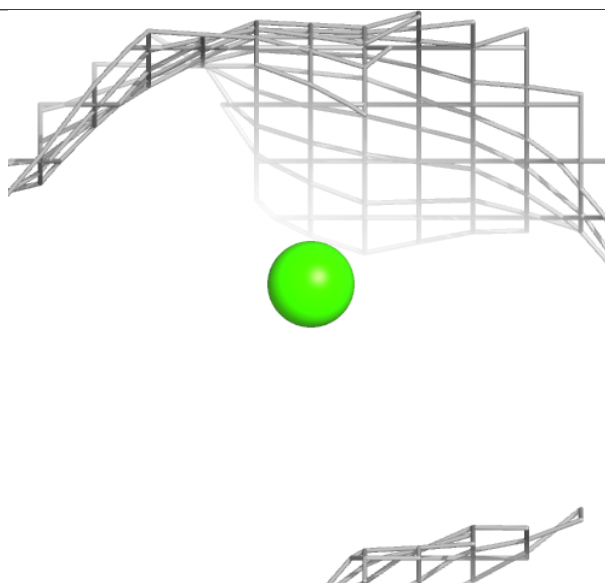
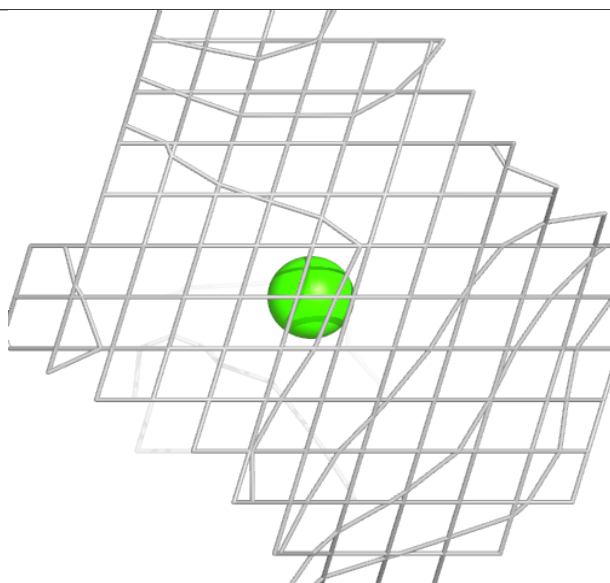
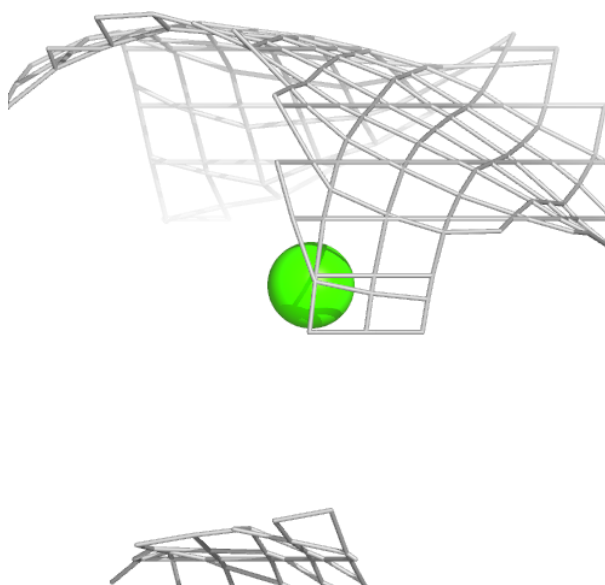
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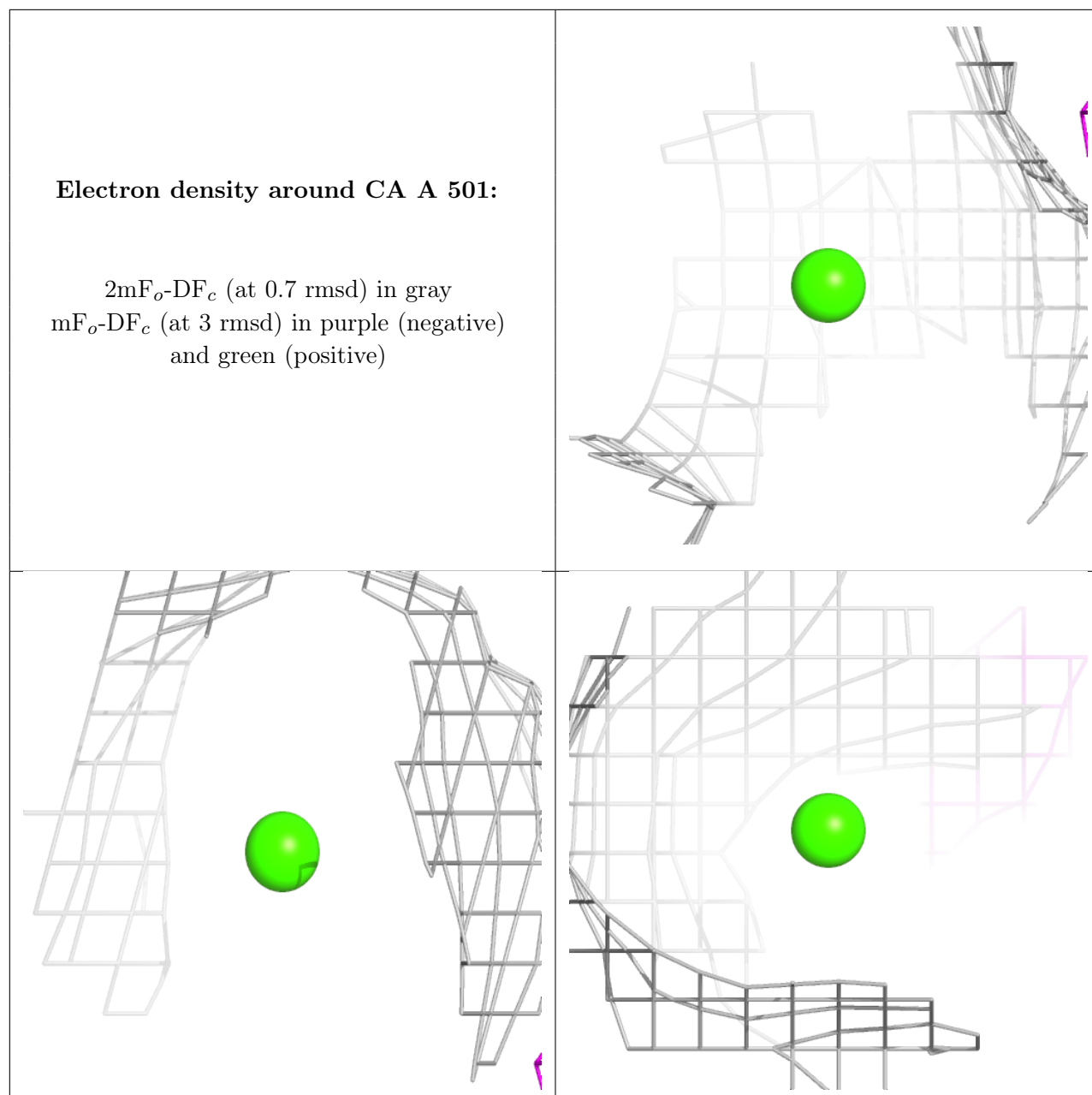
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA D 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 ⓘ

There are no such residues in this entry.