Full wwPDB X-ray Structure Validation Report (i)

May 19, 2025 – 04:25 pm BST

PDB ID	:	9FBO / pdb_00009fbo
Title	:	Deletion mutant of chitinase MmChi60
Authors	:	Malecki, P.H.; Rypniewski, W.
Deposited on	:	2024-05-14
Resolution	:	2.69 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 (i) 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 (i)) were used in the production of this report:

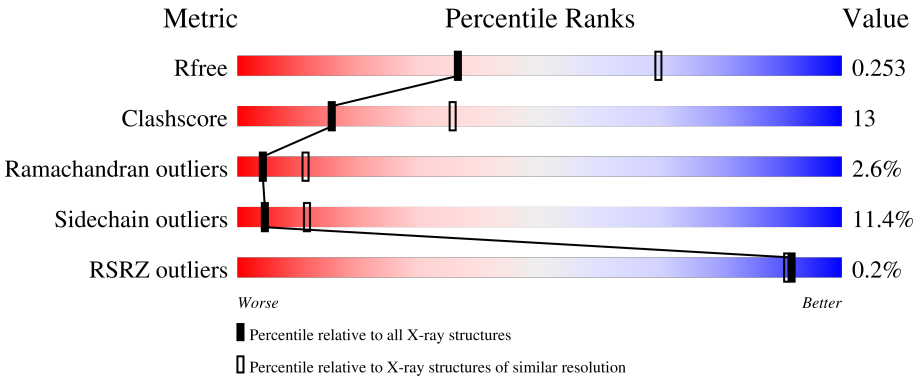
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 <=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	446	64% 31% 5%
2	B	446	64% 29% 6% ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7047 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 Chitinase 60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3513	2226	578	700	9			

- Molecule 2 is a protein called Chitinase 60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	446	Total	C	N	O	S	0	0	0
			3513	2226	579	699	9			

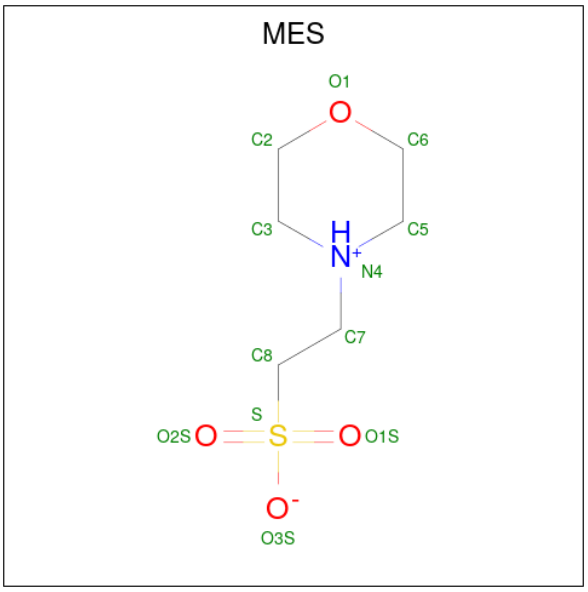
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	153	GLN	GLU	engineered mutation	UNP B1VBB0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 5 is water.

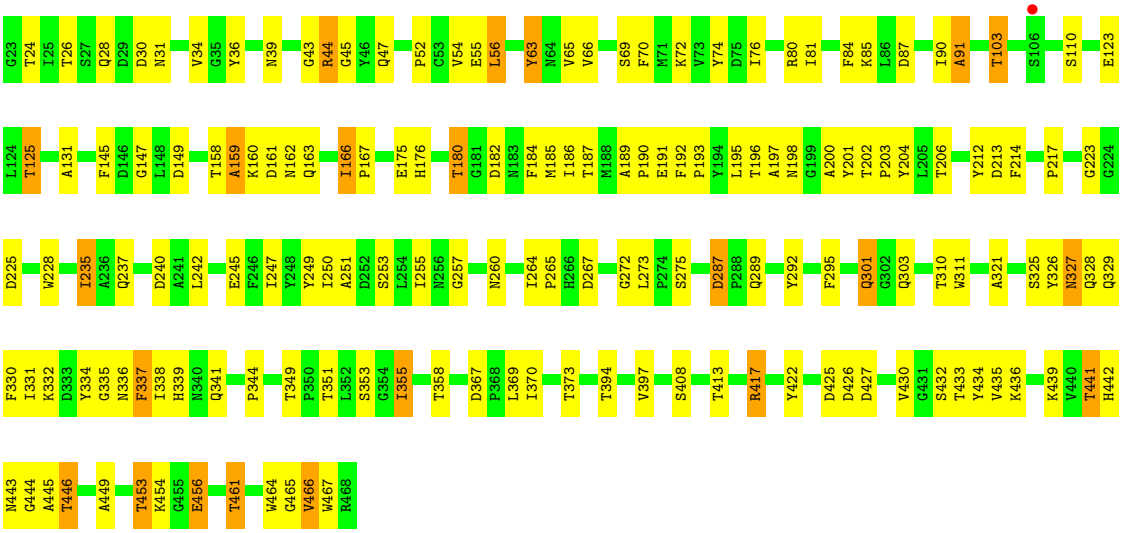
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	4	Total O 4 4	0	0

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.

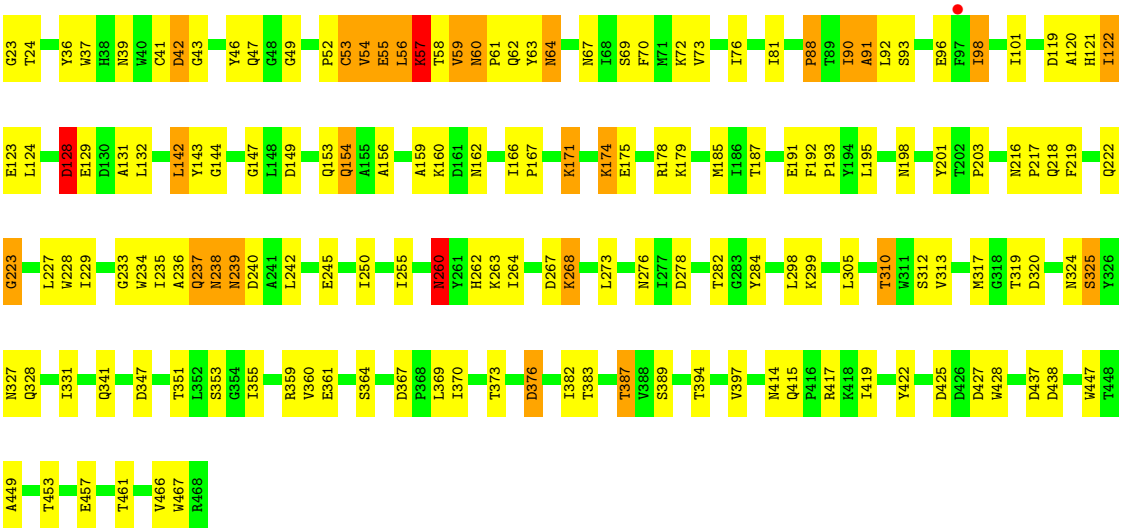
- Molecule 1: Chitinase 60

Chain A:



- Molecule 2: Chitinase 60

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	225.74Å 225.74Å 65.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.17 – 2.69 65.17 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (65.17-2.69) 99.3 (65.17-2.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.194 , 0.252 0.199 , 0.253	Depositor DCC
R_{free} test set	1000 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å^2)	94.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, MES

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	0.63	0/3602	1.27	16/4919 (0.3%)
2	B	0.54	0/3602	1.12	6/4919 (0.1%)
All	All	0.59	0/7204	1.20	22/9838 (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	1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	295	PHE	N-CA-CB	8.03	121.71	110.07
1	A	344	PRO	N-CA-C	-7.22	100.58	111.41
1	A	103	THR	CA-CB-OG1	-6.60	99.70	109.60
2	B	437	ASP	CB-CA-C	6.51	116.27	109.83
1	A	30	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	425	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	413	THR	CA-CB-OG1	-6.03	100.56	109.60
1	A	337	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	422	TYR	CA-CB-CG	5.89	124.50	113.90
1	A	247	ILE	O-C-N	5.65	127.35	121.87
2	B	128	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	52	PRO	N-CA-C	-5.46	102.69	111.38
2	B	376	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	63	TYR	N-CA-CB	-5.37	102.45	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	373	THR	CA-CB-OG1	-5.27	101.69	109.60
1	A	247	ILE	CA-C-O	-5.17	115.57	120.95
1	A	31	ASN	N-CA-C	-5.14	103.75	110.53
2	B	88	PRO	N-CA-CB	-5.10	97.89	103.25
2	B	387	THR	CA-CB-OG1	-5.09	101.96	109.60
1	A	249	TYR	CB-CA-C	5.09	119.26	110.86
2	B	438	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	433	THR	CA-CB-OG1	-5.03	102.06	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	ARG	Sidechain

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	3513	0	3313	95	0
2	B	3513	0	3315	91	0
3	A	1	0	0	0	0
4	A	12	0	13	5	0
5	A	4	0	0	1	0
5	B	4	0	0	0	0
All	All	7047	0	6641	180	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 13.

All (180) 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:B:453:THR:HB	2:B:466:VAL:HG21	1.64	0.79
1:A:449:ALA:HB2	1:A:467:TRP:CZ3	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:TRP:HB3	2:B:198:ASN:HA	1.67	0.77
1:A:44:ARG:O	4:A:502:MES:H81	1.88	0.74
1:A:44:ARG:NH1	1:A:45:GLY:O	2.20	0.73
1:A:326:TYR:O	1:A:327:ASN:C	2.33	0.72
2:B:56:LEU:O	2:B:58:THR:N	2.24	0.70
1:A:39:ASN:ND2	1:A:84:PHE:HE1	1.90	0.70
1:A:158:THR:HA	1:A:163:GLN:HE21	1.56	0.70
1:A:260:ASN:OD1	2:B:260:ASN:HB3	1.94	0.68
2:B:60:ASN:O	2:B:62:GLN:N	2.28	0.67
2:B:298:LEU:HD13	2:B:305:LEU:HD21	1.76	0.67
1:A:166:ILE:HB	1:A:167:PRO:HD3	1.78	0.64
1:A:326:TYR:O	1:A:328:GLN:N	2.30	0.64
1:A:287:ASP:OD2	1:A:289:GLN:HB2	1.97	0.64
1:A:39:ASN:ND2	1:A:84:PHE:CE1	2.67	0.63
2:B:62:GLN:HB2	2:B:331:ILE:HD11	1.81	0.63
2:B:123:GLU:HG3	2:B:159:ALA:HB1	1.80	0.63
1:A:202:THR:N	1:A:203:PRO:HD2	2.15	0.62
1:A:311:TRP:HZ2	4:A:502:MES:H22	1.64	0.62
2:B:23:GLY:HA3	2:B:144:GLY:HA3	1.81	0.62
1:A:161:ASP:HA	5:A:602:HOH:O	1.99	0.61
2:B:59:VAL:O	2:B:60:ASN:C	2.43	0.61
2:B:417:ARG:HD3	2:B:419:ILE:HD11	1.83	0.61
1:A:453:THR:HB	1:A:466:VAL:HG21	1.82	0.60
2:B:236:ALA:HB1	2:B:238:ASN:OD1	2.03	0.59
1:A:235:ILE:HD13	1:A:245:GLU:HB3	1.84	0.58
2:B:219:PHE:C	2:B:237:GLN:HE22	2.10	0.58
2:B:222:GLN:O	2:B:223:GLY:C	2.47	0.58
1:A:432:SER:HB2	1:A:434:TYR:CE1	2.39	0.57
1:A:461:THR:HB	1:A:465:GLY:HA3	1.86	0.57
2:B:123:GLU:CG	2:B:159:ALA:HB1	2.35	0.57
2:B:81:ILE:HD13	2:B:124:LEU:HD22	1.87	0.56
1:A:456:GLU:O	1:A:467:TRP:NE1	2.39	0.56
2:B:229:ILE:O	2:B:233:GLY:N	2.36	0.56
1:A:310:THR:HB	1:A:330:PHE:CZ	2.41	0.56
1:A:180:THR:OG1	1:A:182:ASP:OD1	2.23	0.55
1:A:260:ASN:CG	2:B:260:ASN:HB3	2.31	0.55
1:A:426:ASP:O	1:A:427:ASP:C	2.47	0.55
1:A:34:VAL:HG22	1:A:65:VAL:HB	1.87	0.55
2:B:41:CYS:O	2:B:42:ASP:C	2.49	0.54
1:A:158:THR:HA	1:A:163:GLN:NE2	2.23	0.54
1:A:441:THR:HA	1:A:445:ALA:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:CG	1:A:193:PRO:HD3	2.43	0.54
2:B:238:ASN:OD1	2:B:238:ASN:N	2.38	0.54
2:B:81:ILE:HD11	2:B:128:ASP:HB3	1.90	0.53
2:B:238:ASN:HB3	2:B:282:THR:HG21	1.89	0.53
1:A:275:SER:HA	1:A:330:PHE:CD2	2.44	0.53
2:B:192:PHE:N	2:B:193:PRO:CD	2.72	0.53
1:A:90:ILE:O	1:A:91:ALA:HB3	2.09	0.53
2:B:98:ILE:HG23	2:B:143:TYR:O	2.09	0.53
2:B:276:ASN:OD1	2:B:278:ASP:N	2.43	0.52
2:B:147:GLY:HA3	2:B:185:MET:O	2.09	0.52
2:B:153:GLN:NE2	2:B:154:GLN:OE1	2.42	0.52
1:A:202:THR:N	1:A:203:PRO:CD	2.72	0.52
1:A:237:GLN:O	1:A:237:GLN:HG2	2.09	0.52
1:A:147:GLY:HA2	1:A:184:PHE:CE1	2.44	0.52
1:A:439:LYS:HD2	1:A:446:THR:HG22	1.90	0.52
1:A:192:PHE:O	1:A:195:LEU:HB2	2.10	0.52
1:A:255:ILE:HD12	1:A:303:GLN:HB3	1.92	0.52
1:A:200:ALA:O	1:A:203:PRO:HD2	2.10	0.52
1:A:336:ASN:O	1:A:337:PHE:C	2.52	0.51
2:B:73:VAL:HG11	2:B:121:HIS:O	2.10	0.51
2:B:191:GLU:C	2:B:193:PRO:HD2	2.34	0.51
1:A:186:ILE:HB	1:A:212:TYR:HA	1.92	0.51
2:B:217:PRO:HB2	2:B:219:PHE:CE1	2.45	0.51
2:B:219:PHE:HE2	2:B:250:ILE:HG12	1.76	0.51
2:B:90:ILE:C	2:B:92:LEU:N	2.68	0.51
1:A:301:GLN:HA	2:B:422:TYR:CZ	2.46	0.50
2:B:174:LYS:O	2:B:178:ARG:HG3	2.11	0.50
1:A:228:TRP:CZ3	2:B:203:PRO:HG3	2.47	0.50
1:A:198:ASN:HB3	2:B:227:LEU:HB2	1.95	0.49
1:A:456:GLU:O	1:A:467:TRP:CD1	2.66	0.49
2:B:242:LEU:HD22	2:B:245:GLU:OE1	2.12	0.49
2:B:299:LYS:NZ	2:B:341:GLN:OE1	2.36	0.49
1:A:196:THR:O	1:A:197:ALA:C	2.55	0.49
1:A:289:GLN:HA	1:A:292:TYR:CD2	2.48	0.49
2:B:93:SER:O	2:B:96:GLU:N	2.46	0.48
1:A:81:ILE:HD11	1:A:131:ALA:HB3	1.95	0.48
1:A:329:GLN:O	1:A:330:PHE:C	2.56	0.48
2:B:228:TRP:HE3	2:B:234:TRP:HB2	1.79	0.48
1:A:63:TYR:CD2	1:A:331:ILE:HD13	2.48	0.48
1:A:432:SER:HB2	1:A:434:TYR:CZ	2.48	0.48
2:B:55:GLU:O	2:B:56:LEU:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:O	1:A:310:THR:HA	2.13	0.48
2:B:90:ILE:O	2:B:92:LEU:N	2.47	0.48
1:A:189:ALA:N	1:A:190:PRO:CD	2.77	0.47
1:A:201:TYR:HA	1:A:204:TYR:HD2	1.79	0.47
1:A:251:ALA:O	1:A:255:ILE:HG23	2.12	0.47
2:B:56:LEU:O	2:B:57:LYS:C	2.55	0.47
2:B:359:ARG:HB3	2:B:422:TYR:CD2	2.49	0.47
1:A:255:ILE:HD12	1:A:303:GLN:CB	2.44	0.47
1:A:329:GLN:O	1:A:332:LYS:N	2.46	0.47
1:A:367:ASP:HB3	1:A:370:ILE:HD12	1.97	0.47
2:B:449:ALA:HB2	2:B:467:TRP:CZ3	2.50	0.47
2:B:91:ALA:O	2:B:92:LEU:C	2.58	0.47
2:B:367:ASP:HB3	2:B:370:ILE:CD1	2.45	0.47
1:A:123:GLU:HB3	1:A:160:LYS:HE2	1.95	0.47
2:B:453:THR:CB	2:B:466:VAL:HG21	2.40	0.47
2:B:324:ASN:O	2:B:325:SER:C	2.57	0.46
2:B:166:ILE:HB	2:B:167:PRO:HD3	1.97	0.46
1:A:311:TRP:CZ2	4:A:502:MES:H22	2.47	0.46
2:B:312:SER:O	2:B:313:VAL:C	2.58	0.46
2:B:60:ASN:C	2:B:62:GLN:H	2.23	0.46
1:A:192:PHE:N	1:A:193:PRO:CD	2.78	0.46
2:B:160:LYS:HD2	2:B:160:LYS:HA	1.79	0.46
2:B:428:TRP:CZ2	2:B:457:GLU:HA	2.50	0.46
2:B:376:ASP:HB3	2:B:382:ILE:HD13	1.98	0.46
1:A:26:THR:O	1:A:110:SER:OG	2.34	0.45
2:B:327:ASN:O	2:B:328:GLN:C	2.59	0.45
1:A:147:GLY:HA3	1:A:185:MET:O	2.16	0.45
2:B:228:TRP:CE3	2:B:234:TRP:HB2	2.50	0.45
2:B:298:LEU:HD13	2:B:305:LEU:CD2	2.44	0.45
1:A:125:THR:HA	1:A:161:ASP:OD2	2.16	0.45
1:A:311:TRP:HE1	4:A:502:MES:H21	1.82	0.45
1:A:147:GLY:HA2	1:A:184:PHE:CZ	2.52	0.45
1:A:158:THR:HG22	1:A:163:GLN:NE2	2.31	0.45
1:A:87:ASP:OD1	1:A:87:ASP:C	2.59	0.45
1:A:335:GLY:O	1:A:339:HIS:CD2	2.70	0.44
1:A:149:ASP:OD1	1:A:187:THR:OG1	2.23	0.44
1:A:192:PHE:CD1	1:A:193:PRO:HD3	2.52	0.44
2:B:64:ASN:H	2:B:64:ASN:HD22	1.65	0.44
2:B:153:GLN:O	2:B:154:GLN:C	2.60	0.44
2:B:373:THR:HA	2:B:383:THR:HG23	1.99	0.44
1:A:327:ASN:O	1:A:328:GLN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:ASP:HB3	2:B:370:ILE:HD12	2.00	0.44
2:B:122:ILE:O	2:B:162:ASN:ND2	2.51	0.43
2:B:276:ASN:HA	2:B:284:TYR:CZ	2.53	0.43
1:A:253:SER:O	1:A:257:GLY:N	2.51	0.43
2:B:46:TYR:O	2:B:47:GLN:NE2	2.47	0.43
2:B:239:ASN:ND2	2:B:242:LEU:HB2	2.33	0.43
2:B:361:GLU:O	2:B:364:SER:OG	2.28	0.43
2:B:156:ALA:O	2:B:162:ASN:OD1	2.36	0.43
2:B:195:LEU:O	2:B:262:HIS:HB2	2.19	0.43
1:A:213:ASP:O	1:A:214:PHE:HB3	2.18	0.43
1:A:242:LEU:HA	1:A:245:GLU:OE1	2.19	0.43
1:A:442:HIS:O	1:A:444:GLY:N	2.51	0.43
1:A:74:TYR:CZ	1:A:85:LYS:HG2	2.54	0.42
1:A:355:ILE:CG2	1:A:417:ARG:HB2	2.49	0.42
2:B:228:TRP:HB2	2:B:234:TRP:HD1	1.84	0.42
1:A:36:TYR:HB3	1:A:311:TRP:CZ3	2.55	0.42
1:A:80:ARG:HH11	1:A:80:ARG:HG3	1.84	0.42
1:A:159:ALA:O	1:A:160:LYS:C	2.61	0.42
2:B:191:GLU:OE2	2:B:218:GLN:HB2	2.19	0.42
1:A:69:SER:HA	1:A:70:PHE:HA	1.87	0.42
1:A:217:PRO:O	1:A:272:GLY:HA3	2.20	0.42
1:A:161:ASP:O	1:A:162:ASN:C	2.61	0.42
1:A:334:TYR:O	1:A:338:ILE:HG12	2.20	0.42
2:B:149:ASP:HB2	2:B:187:THR:OG1	2.20	0.42
1:A:325:SER:C	1:A:327:ASN:H	2.27	0.42
2:B:273:LEU:O	2:B:310:THR:HA	2.20	0.42
1:A:47:GLN:O	1:A:321:ALA:HB2	2.20	0.41
2:B:36:TYR:OH	2:B:149:ASP:OD2	2.25	0.41
2:B:427:ASP:O	2:B:428:TRP:C	2.61	0.41
1:A:43:GLY:HA3	4:A:502:MES:H61	2.02	0.41
1:A:267:ASP:OD1	1:A:267:ASP:N	2.52	0.41
2:B:242:LEU:HD23	2:B:242:LEU:HA	1.94	0.41
2:B:267:ASP:OD2	2:B:268:LYS:HD3	2.20	0.41
2:B:238:ASN:O	2:B:240:ASP:N	2.54	0.41
2:B:90:ILE:O	2:B:91:ALA:C	2.62	0.41
1:A:202:THR:O	1:A:206:THR:OG1	2.29	0.41
2:B:53:CYS:HB2	2:B:90:ILE:HG12	2.03	0.41
2:B:60:ASN:HD22	2:B:60:ASN:HA	1.73	0.41
2:B:255:ILE:HA	2:B:264:ILE:O	2.20	0.41
1:A:192:PHE:HA	1:A:195:LEU:HD12	2.02	0.41
2:B:37:TRP:CZ3	2:B:39:ASN:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:O	1:A:56:LEU:C	2.64	0.40
1:A:264:ILE:O	1:A:265:PRO:C	2.62	0.40
1:A:85:LYS:HB3	1:A:85:LYS:HE2	1.88	0.40
1:A:175:GLU:O	1:A:176:HIS:C	2.63	0.40
2:B:37:TRP:N	2:B:67:ASN:O	2.54	0.40
2:B:41:CYS:O	2:B:43:GLY:N	2.54	0.40
2:B:81:ILE:HG13	2:B:131:ALA:HB1	2.02	0.40
2:B:171:LYS:O	2:B:175:GLU:HG2	2.20	0.40
1:A:158:THR:O	1:A:159:ALA:C	2.63	0.40
2:B:123:GLU:HG2	2:B:160:LYS:HB2	2.04	0.40
2:B:52:PRO:C	2:B:54:VAL:H	2.30	0.40
1:A:39:ASN:HD22	1:A:84:PHE:HE1	1.63	0.40
2:B:49:GLY:HA2	2:B:320:ASP:C	2.47	0.40
2:B:355:ILE:HD13	2:B:415:GLN:HB3	2.03	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	444/446 (100%)	385 (87%)	51 (12%)	8 (2%)	7 18
2	B	444/446 (100%)	370 (83%)	59 (13%)	15 (3%)	3 7
All	All	888/892 (100%)	755 (85%)	110 (12%)	23 (3%)	4 11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	443	ASN
1	A	461	THR
2	B	42	ASP

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Mol	Chain	Res	Type
2	B	56	LEU
2	B	57	LYS
2	B	91	ALA
2	B	239	ASN
1	A	159	ALA
1	A	223	GLY
2	B	61	PRO
2	B	120	ALA
2	B	142	LEU
2	B	223	GLY
2	B	325	SER
2	B	63	TYR
2	B	425	ASP
1	A	145	PHE
2	B	119	ASP
2	B	154	GLN
1	A	341	GLN
1	A	91	ALA
2	B	260	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	374/374 (100%)	336 (90%)	38 (10%)	6 15
2	B	374/374 (100%)	327 (87%)	47 (13%)	3 9
All	All	748/748 (100%)	663 (89%)	85 (11%)	4 11

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	28	GLN
1	A	44	ARG
1	A	54	VAL

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Mol	Chain	Res	Type
1	A	56	LEU
1	A	66	VAL
1	A	72	LYS
1	A	76	ILE
1	A	103	THR
1	A	125	THR
1	A	166	ILE
1	A	180	THR
1	A	191	GLU
1	A	225	ASP
1	A	235	ILE
1	A	240	ASP
1	A	250	ILE
1	A	287	ASP
1	A	301	GLN
1	A	349	THR
1	A	351	THR
1	A	353	SER
1	A	355	ILE
1	A	358	THR
1	A	369	LEU
1	A	394	THR
1	A	397	VAL
1	A	408	SER
1	A	430	VAL
1	A	435	VAL
1	A	436	LYS
1	A	441	THR
1	A	446	THR
1	A	453	THR
1	A	454	LYS
1	A	456	GLU
1	A	464	TRP
1	A	466	VAL
2	B	24	THR
2	B	53	CYS
2	B	54	VAL
2	B	55	GLU
2	B	57	LYS
2	B	59	VAL
2	B	60	ASN
2	B	64	ASN

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Mol	Chain	Res	Type
2	B	69	SER
2	B	70	PHE
2	B	72	LYS
2	B	76	ILE
2	B	88	PRO
2	B	90	ILE
2	B	98	ILE
2	B	101	ILE
2	B	122	ILE
2	B	128	ASP
2	B	129	GLU
2	B	132	LEU
2	B	142	LEU
2	B	171	LYS
2	B	174	LYS
2	B	179	LYS
2	B	201	TYR
2	B	216	ASN
2	B	235	ILE
2	B	237	GLN
2	B	238	ASN
2	B	260	ASN
2	B	263	LYS
2	B	268	LYS
2	B	310	THR
2	B	317	MET
2	B	319	THR
2	B	347	ASP
2	B	351	THR
2	B	353	SER
2	B	360	VAL
2	B	369	LEU
2	B	387	THR
2	B	389	SER
2	B	394	THR
2	B	397	VAL
2	B	414	ASN
2	B	447	TRP
2	B	461	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	105	ASN
1	A	163	GLN
1	A	222	GLN
1	A	378	GLN
1	A	395	ASN
1	A	442	HIS
2	B	39	ASN
2	B	60	ASN
2	B	62	GLN
2	B	64	ASN
2	B	67	ASN
2	B	107	GLN
2	B	162	ASN
2	B	218	GLN
2	B	239	ASN
2	B	286	GLN
2	B	336	ASN
2	B	380	ASN
2	B	396	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	MES	A	502	-	12,12,12	0.59	0	14,16,16	1.02	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	502	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	MES	C2-C3-N4	-2.64	106.10	110.10

There are no chirality outliers.

There are no torsion outliers.

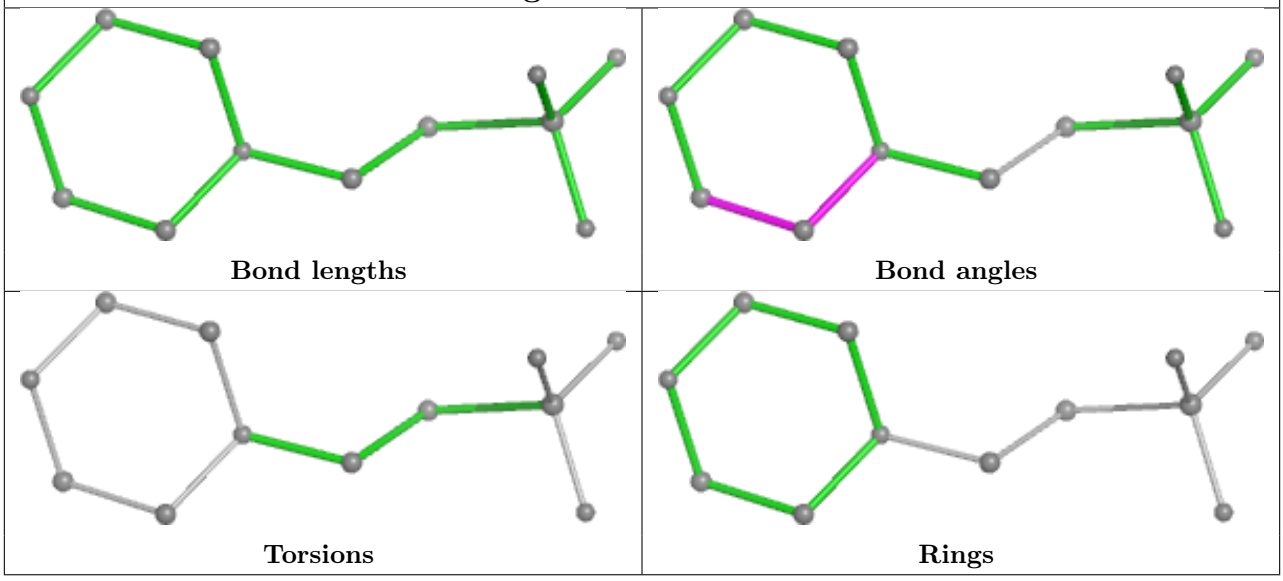
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	MES	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MES A 502



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, 95^{th} 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	446/446 (100%)	-0.49	1 (0%)	92	91	56, 91, 140, 167	1 (0%)
2	B	446/446 (100%)	-0.50	1 (0%)	92	91	63, 134, 207, 267	0
All	All	892/892 (100%)	-0.49	2 (0%)	92	91	56, 108, 194, 267	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	SER	3.3
2	B	97	PHE	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

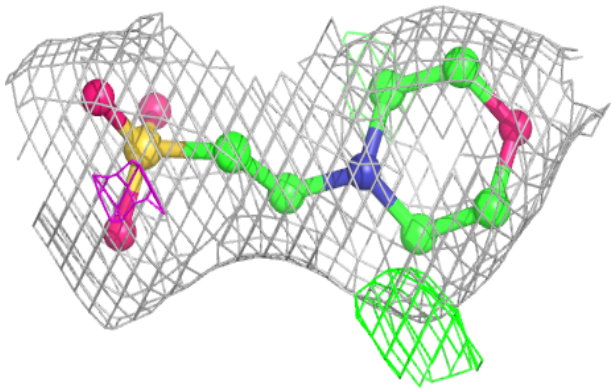
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

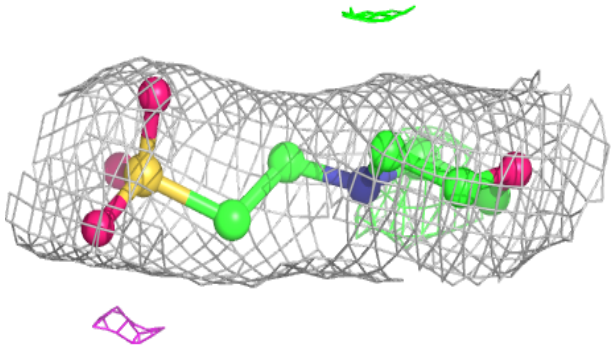
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MES	A	502	12/12	0.86	0.11	92,113,152,192	0
3	NA	A	501	1/1	0.99	0.04	77,77,77,77	0

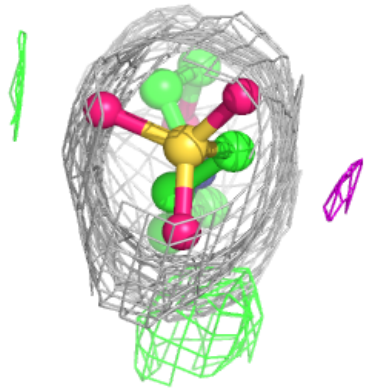
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MES A 502:

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

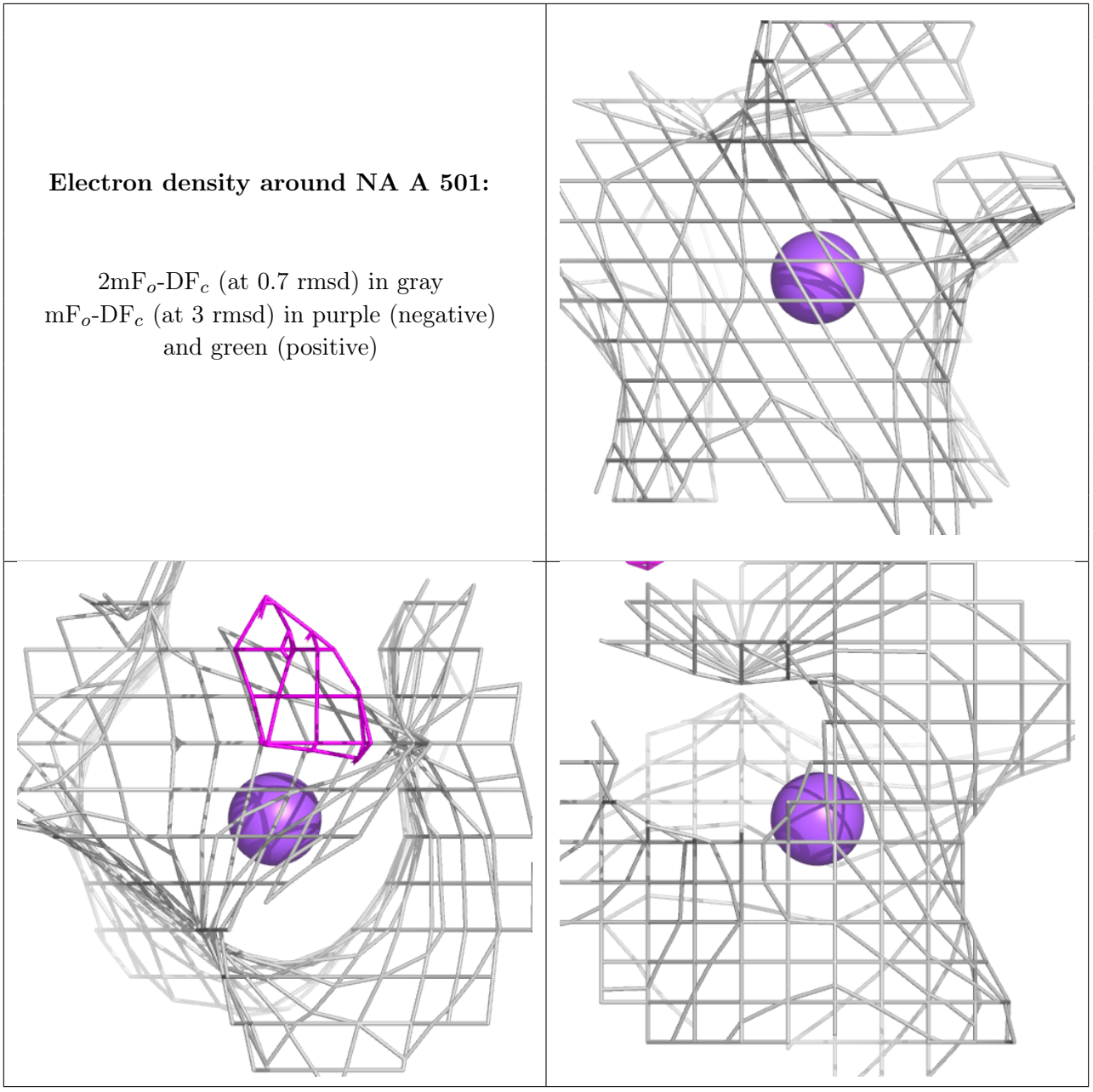






Electron density around NA A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.