



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 22, 2025 – 10:15 AM EDT

PDB ID : 9O8W / pdb_00009o8w
Title : Crystal structure of an MKP5 mutant, Y435F, in complex with an allosteric inhibitor
Authors : Manjula, R.; Bennett, A.M.; Lolis, E.
Deposited on : 2025-04-16
Resolution : 2.39 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
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	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

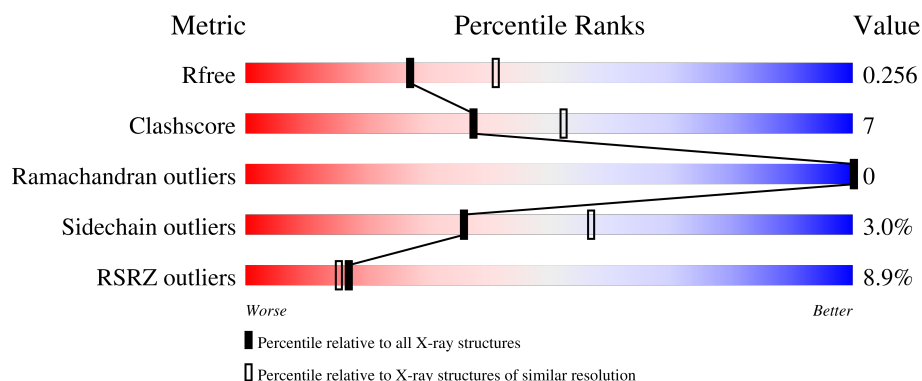
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


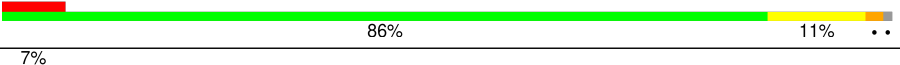
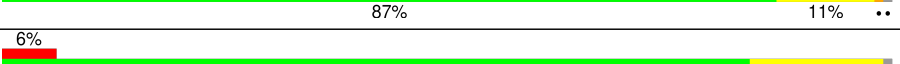
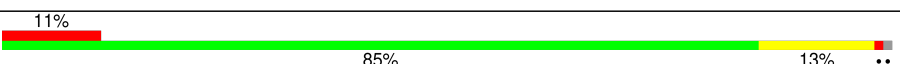

The reported resolution of this entry is 2.39 Å.

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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	149	
1	B	149	
1	C	149	
1	D	149	
1	E	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	149	<div><div></div><div>14%</div><div></div><div>80%</div><div></div><div>17%</div><div>..</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14199 atoms, of which 6939 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.

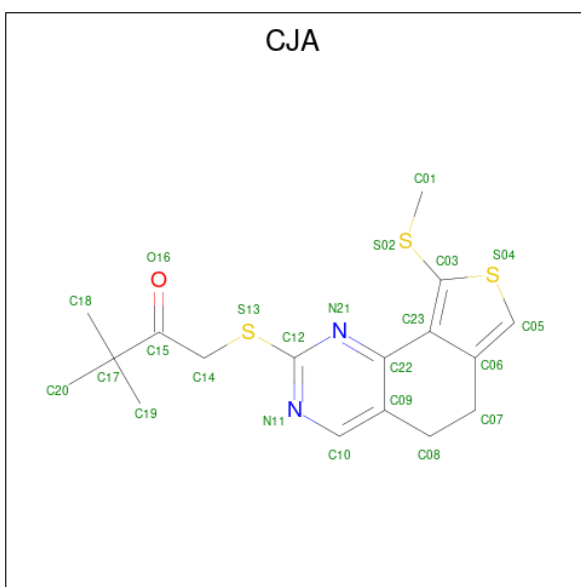
- Molecule 1 is a protein called Dual specificity protein phosphatase 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	148	Total	C	H	N	O	S	0	0	0
			2333	759	1149	199	219	7			
1	B	148	Total	C	H	N	O	S	0	0	0
			2323	756	1144	200	216	7			
1	C	147	Total	C	H	N	O	S	0	0	0
			2312	755	1138	195	217	7			
1	D	147	Total	C	H	N	O	S	0	0	0
			2350	759	1169	201	214	7			
1	E	147	Total	C	H	N	O	S	0	0	0
			2252	738	1106	192	209	7			
1	F	147	Total	C	H	N	O	S	0	0	0
			2276	744	1113	195	217	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	319	MET	-	initiating methionine	UNP Q9Y6W6
A	435	PHE	TYR	engineered mutation	UNP Q9Y6W6
B	319	MET	-	initiating methionine	UNP Q9Y6W6
B	435	PHE	TYR	engineered mutation	UNP Q9Y6W6
C	319	MET	-	initiating methionine	UNP Q9Y6W6
C	435	PHE	TYR	engineered mutation	UNP Q9Y6W6
D	319	MET	-	initiating methionine	UNP Q9Y6W6
D	435	PHE	TYR	engineered mutation	UNP Q9Y6W6
E	319	MET	-	initiating methionine	UNP Q9Y6W6
E	435	PHE	TYR	engineered mutation	UNP Q9Y6W6
F	319	MET	-	initiating methionine	UNP Q9Y6W6
F	435	PHE	TYR	engineered mutation	UNP Q9Y6W6

- Molecule 2 is 3,3-dimethyl-1-{{9-(methylsulfanyl)-5,6-dihydrothieno[3,4-h]quinazolin-2-yl}sulfanyl}butan-2-one (CCD ID: CJA) (formula: C₁₇H₂₀N₂OS₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	B	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	C	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	D	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	E	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	F	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

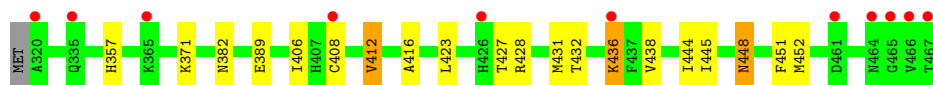
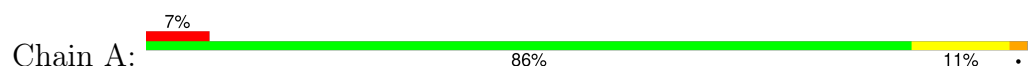
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	15	Total	O	0	0
			15	15		
4	B	13	Total	O	0	0
			13	13		
4	C	23	Total	O	0	0
			23	23		
4	D	14	Total	O	0	0
			14	14		
4	E	8	Total	O	0	0
			8	8		
4	F	12	Total	O	0	0
			12	12		

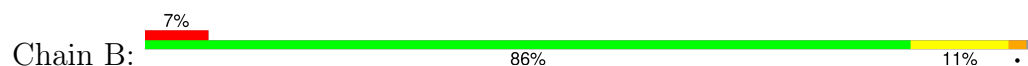
3 Residue-property plots [i](#)

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.

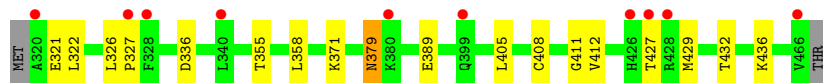
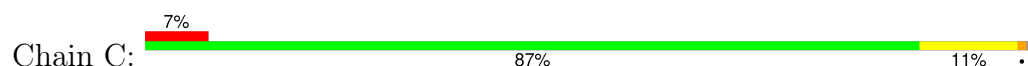
- Molecule 1: Dual specificity protein phosphatase 10



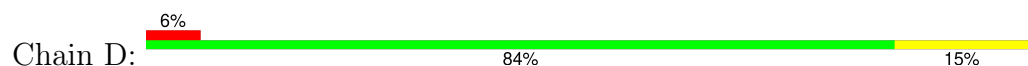
- Molecule 1: Dual specificity protein phosphatase 10



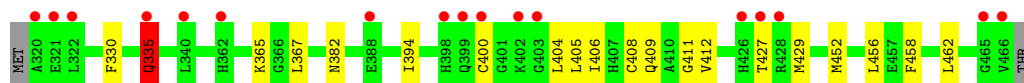
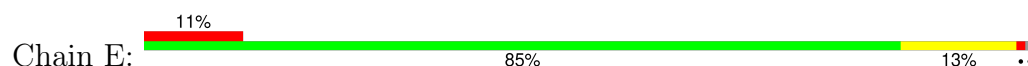
- Molecule 1: Dual specificity protein phosphatase 10



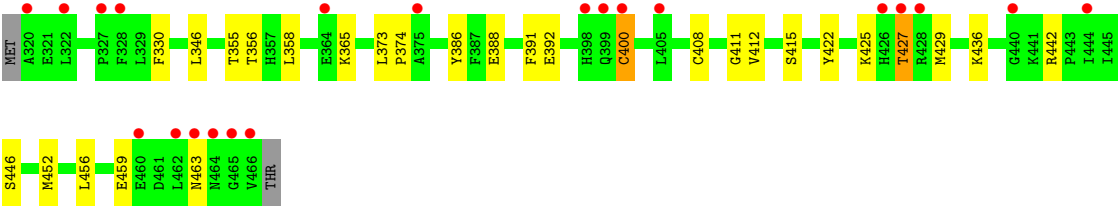
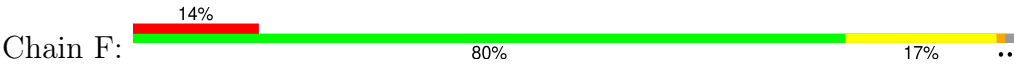
- Molecule 1: Dual specificity protein phosphatase 10



- Molecule 1: Dual specificity protein phosphatase 10



- Molecule 1: Dual specificity protein phosphatase 10



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.13Å 95.77Å 92.81Å 90.00° 117.39° 90.00°	Depositor
Resolution (Å)	33.73 – 2.39 33.73 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.73-2.39) 99.9 (33.73-2.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.18_3845: ???)	Depositor
R, R_{free}	0.217 , 0.251 0.221 , 0.256	Depositor DCC
R_{free} test set	2842 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14199	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: CJA, SO4

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	0.25	0/1210	0.49	0/1638
1	B	0.20	0/1205	0.41	0/1631
1	C	0.23	0/1200	0.50	0/1624
1	D	0.25	0/1207	0.48	0/1631
1	E	0.44	0/1171	0.75	1/1589 (0.1%)
1	F	0.27	0/1189	0.54	0/1610
All	All	0.29	0/7182	0.54	1/9723 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	335	GLN	CA-CB-CG	-8.31	97.47	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1184	1149	1156	18	0
1	B	1179	1144	1149	18	0
1	C	1174	1138	1144	12	0
1	D	1181	1169	1169	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1146	1106	1106	19	0
1	F	1163	1113	1113	18	0
2	A	23	20	0	1	0
2	B	23	20	0	0	0
2	C	23	20	0	0	0
2	D	23	20	0	0	0
2	E	23	20	0	0	0
2	F	23	20	0	1	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
4	A	15	0	0	1	0
4	B	13	0	0	0	0
4	C	23	0	0	0	0
4	D	14	0	0	1	0
4	E	8	0	0	0	0
4	F	12	0	0	1	0
All	All	7260	6939	6837	97	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 7.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:MET:HE1	1:E:452:MET:HE1	1.48	0.93
1:B:466:VAL:HG22	1:D:429:MET:HE3	1.51	0.92
1:E:427:THR:HG21	1:E:429:MET:HE3	1.61	0.81
1:C:355:THR:HG21	1:C:358:LEU:HD12	1.67	0.76
1:B:412:VAL:HG13	1:B:412:VAL:O	1.95	0.67
1:F:355:THR:HG21	1:F:358:LEU:HD12	1.80	0.64
1:E:427:THR:HG22	1:E:429:MET:HG3	1.80	0.62
1:C:427:THR:HG21	1:C:429:MET:HE3	1.83	0.60
1:A:412:VAL:CG1	1:A:412:VAL:O	2.51	0.59
1:A:436:LYS:HE2	1:E:456:LEU:HD11	1.84	0.59
1:E:394:ILE:HA	1:E:404:LEU:HD13	1.85	0.58
1:B:466:VAL:HG22	1:D:429:MET:CE	2.28	0.58
1:C:432:THR:HG22	1:C:436:LYS:HD2	1.86	0.57
1:E:458:PHE:O	1:E:462:LEU:HD12	2.04	0.56
1:D:438:VAL:HG12	1:D:445:ILE:HD11	1.86	0.56
1:F:330:PHE:HE2	1:F:346:LEU:HD13	1.71	0.56
1:A:427:THR:HG22	1:A:427:THR:O	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:THR:O	1:C:427:THR:HG22	2.07	0.55
1:E:427:THR:HG21	1:E:429:MET:CE	2.34	0.55
1:B:331:LEU:HD11	1:B:412:VAL:HG22	1.89	0.55
1:B:412:VAL:HG13	1:B:416:ALA:HB2	1.89	0.54
1:A:427:THR:O	1:A:428:ARG:HG2	2.07	0.53
1:F:459:GLU:O	1:F:463:ASN:N	2.41	0.52
1:C:408:CYS:SG	1:C:412:VAL:HA	2.50	0.51
1:C:379:ASN:OD1	1:C:379:ASN:N	2.42	0.51
1:A:412:VAL:CG1	1:A:416:ALA:HB2	2.41	0.50
1:B:427:THR:HG22	1:B:429:MET:HG3	1.93	0.50
1:E:427:THR:HG22	1:E:427:THR:O	2.10	0.50
1:D:330:PHE:CE2	1:D:346:LEU:HD22	2.47	0.50
1:D:408:CYS:SG	1:D:412:VAL:HA	2.52	0.49
1:A:412:VAL:O	1:A:412:VAL:HG13	2.12	0.49
1:D:431:MET:HE1	1:D:456:LEU:HD13	1.95	0.48
1:F:408:CYS:SG	1:F:412:VAL:HA	2.54	0.48
1:A:357:HIS:HD2	4:A:605:HOH:O	1.97	0.48
1:B:412:VAL:O	1:B:412:VAL:CG1	2.62	0.48
1:F:452:MET:HE3	2:F:501:CJA:C03	2.44	0.48
1:C:322:LEU:HD12	1:C:336:ASP:HB3	1.95	0.48
1:E:408:CYS:SG	1:E:412:VAL:HA	2.54	0.47
1:C:371:LYS:HD3	1:C:389:GLU:HG2	1.96	0.47
1:E:427:THR:O	1:E:427:THR:CG2	2.62	0.47
1:A:408:CYS:SG	1:A:412:VAL:HA	2.55	0.47
1:B:427:THR:CG2	1:B:427:THR:O	2.63	0.47
1:C:411:GLY:C	1:C:412:VAL:HG22	2.40	0.47
1:E:411:GLY:C	1:E:412:VAL:HG22	2.40	0.47
1:B:415:SER:O	1:B:419:VAL:HG23	2.15	0.46
1:A:448:ASN:OD1	1:A:451:PHE:CG	2.69	0.46
1:E:365:LYS:HB2	1:E:367:LEU:HD13	1.98	0.46
1:C:326:LEU:HB3	1:C:327:PRO:HD2	1.97	0.46
1:F:356:THR:HG22	1:F:374:PRO:C	2.41	0.46
1:A:438:VAL:HG12	1:A:445:ILE:HD11	1.97	0.46
1:E:365:LYS:CB	1:E:367:LEU:HD13	2.46	0.46
1:D:428:ARG:O	1:D:428:ARG:HG2	2.15	0.45
1:D:444:ILE:O	1:D:444:ILE:HG22	2.16	0.45
1:A:423:LEU:O	1:A:427:THR:HB	2.17	0.45
1:F:411:GLY:C	1:F:412:VAL:HG22	2.41	0.45
1:F:427:THR:CG2	1:F:429:MET:HE3	2.47	0.45
1:D:352:ILE:HG13	1:D:404:LEU:HD21	2.00	0.44
1:D:428:ARG:O	1:D:428:ARG:CG	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:CYS:SG	1:E:409:GLN:N	2.91	0.44
1:F:400:CYS:O	1:F:400:CYS:SG	2.76	0.44
1:D:367:LEU:N	4:D:603:HOH:O	2.47	0.43
1:F:411:GLY:O	1:F:412:VAL:HG22	2.18	0.43
1:A:371:LYS:HD3	1:A:389:GLU:HG2	2.00	0.43
1:C:322:LEU:HG	1:C:405:LEU:HD13	2.00	0.43
1:F:456:LEU:HD12	1:F:456:LEU:O	2.17	0.43
1:A:382:ASN:OD1	1:A:382:ASN:C	2.61	0.43
1:D:371:LYS:HD3	1:D:389:GLU:CG	2.48	0.43
1:A:448:ASN:OD1	1:A:448:ASN:O	2.35	0.43
1:B:322:LEU:HD23	1:B:405:LEU:HD13	2.01	0.43
1:F:330:PHE:N	1:F:330:PHE:CD1	2.87	0.43
1:A:448:ASN:OD1	1:A:451:PHE:CD1	2.72	0.42
1:B:427:THR:HG22	1:B:427:THR:O	2.17	0.42
1:D:458:PHE:CE1	1:D:462:LEU:HD11	2.54	0.42
1:E:335:GLN:HE21	1:E:335:GLN:HB3	1.63	0.42
1:F:442:ARG:NE	4:F:601:HOH:O	2.47	0.42
1:A:448:ASN:OD1	1:A:451:PHE:HB2	2.20	0.42
1:B:355:THR:HG21	1:B:358:LEU:HD12	2.02	0.42
1:D:342:THR:HG22	1:D:346:LEU:HD12	2.01	0.42
1:E:330:PHE:CD2	1:E:330:PHE:N	2.87	0.42
1:F:373:LEU:HD22	1:F:386:TYR:HB3	2.01	0.42
1:B:339:ASP:OD1	1:B:342:THR:OG1	2.37	0.42
1:B:394:ILE:HA	1:B:404:LEU:HD13	2.01	0.42
1:F:391:PHE:CE2	1:F:422:TYR:HA	2.55	0.42
1:B:408:CYS:SG	1:B:412:VAL:HA	2.60	0.41
1:E:405:LEU:HD12	1:E:406:ILE:N	2.34	0.41
1:F:388:GLU:O	1:F:392:GLU:HG3	2.20	0.41
1:E:382:ASN:OD1	1:E:382:ASN:C	2.63	0.41
1:E:365:LYS:O	1:E:367:LEU:HD12	2.20	0.41
1:A:431:MET:HE3	2:A:501:CJA:S04	2.61	0.41
1:B:461:ASP:C	1:B:467:THR:HG22	2.46	0.41
1:D:412:VAL:O	1:D:412:VAL:HG23	2.20	0.41
1:D:371:LYS:HE3	1:D:393:PHE:CD1	2.56	0.40
1:B:427:THR:CG2	1:B:429:MET:HG3	2.51	0.40
1:F:427:THR:HG21	1:F:429:MET:HE3	2.03	0.40
1:B:404:LEU:C	1:B:404:LEU:HD23	2.45	0.40
1:C:326:LEU:HB3	1:C:327:PRO:CD	2.51	0.40
1:F:436:LYS:HB2	1:F:436:LYS:HE3	1.77	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	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
1	B	146/149 (98%)	140 (96%)	6 (4%)	0	100	100
1	C	145/149 (97%)	139 (96%)	6 (4%)	0	100	100
1	D	145/149 (97%)	139 (96%)	6 (4%)	0	100	100
1	E	145/149 (97%)	138 (95%)	7 (5%)	0	100	100
1	F	145/149 (97%)	137 (94%)	8 (6%)	0	100	100
All	All	872/894 (98%)	832 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	127/131 (97%)	121 (95%)	6 (5%)	22	38
1	B	125/131 (95%)	121 (97%)	4 (3%)	34	54
1	C	125/131 (95%)	123 (98%)	2 (2%)	58	76
1	D	127/131 (97%)	125 (98%)	2 (2%)	58	76
1	E	119/131 (91%)	117 (98%)	2 (2%)	56	75
1	F	122/131 (93%)	116 (95%)	6 (5%)	21	36
All	All	745/786 (95%)	723 (97%)	22 (3%)	36	57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	ILE
1	A	412	VAL
1	A	432	THR
1	A	436	LYS
1	A	444	ILE
1	A	448	ASN
1	B	379	ASN
1	B	412	VAL
1	B	466	VAL
1	B	467	THR
1	C	321	GLU
1	C	379	ASN
1	D	400	CYS
1	D	406	ILE
1	E	335	GLN
1	E	400	CYS
1	F	365	LYS
1	F	400	CYS
1	F	415	SER
1	F	425	LYS
1	F	427	THR
1	F	446	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	GLN
1	B	335	GLN
1	B	379	ASN
1	B	385	GLN
1	B	399	GLN
1	C	335	GLN
1	C	362	HIS
1	C	463	ASN
1	D	369	ASN
1	E	335	GLN
1	E	398	HIS
1	F	357	HIS
1	F	398	HIS

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	CJA	D	501	-	23,25,25	1.42	3 (13%)	24,37,37	3.44	6 (25%)
3	SO4	F	502	-	4,4,4	0.24	0	6,6,6	0.08	0
2	CJA	A	501	-	23,25,25	1.69	4 (17%)	24,37,37	3.10	6 (25%)
2	CJA	B	501	-	23,25,25	1.44	4 (17%)	24,37,37	3.44	6 (25%)
2	CJA	F	501	-	23,25,25	1.46	4 (17%)	24,37,37	3.28	7 (29%)
2	CJA	E	501	-	23,25,25	1.60	4 (17%)	24,37,37	3.12	7 (29%)
3	SO4	D	502	-	4,4,4	0.22	0	6,6,6	0.09	0
2	CJA	C	501	-	23,25,25	1.62	4 (17%)	24,37,37	3.09	6 (25%)

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
2	CJA	D	501	-	-	6/13/22/22	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CJA	A	501	-	-	6/13/22/22	0/3/3/3
2	CJA	B	501	-	-	6/13/22/22	0/3/3/3
2	CJA	F	501	-	-	1/13/22/22	0/3/3/3
2	CJA	E	501	-	-	6/13/22/22	0/3/3/3
2	CJA	C	501	-	-	1/13/22/22	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CJA	C23-C22	-5.75	1.39	1.48
2	E	501	CJA	C23-C22	-5.35	1.39	1.48
2	C	501	CJA	C23-C22	-5.11	1.40	1.48
2	F	501	CJA	C23-C22	-5.06	1.40	1.48
2	D	501	CJA	C23-C22	-4.93	1.40	1.48
2	B	501	CJA	C23-C22	-4.87	1.40	1.48
2	A	501	CJA	C03-S04	-3.91	1.65	1.72
2	C	501	CJA	C03-S04	-3.62	1.66	1.72
2	E	501	CJA	C03-S04	-3.48	1.66	1.72
2	B	501	CJA	C03-S04	-2.86	1.67	1.72
2	F	501	CJA	C03-S04	-2.78	1.67	1.72
2	D	501	CJA	C03-S04	-2.74	1.67	1.72
2	C	501	CJA	C05-S04	-2.72	1.66	1.70
2	C	501	CJA	C23-C06	2.62	1.45	1.40
2	F	501	CJA	C23-C06	2.62	1.45	1.40
2	B	501	CJA	C23-C06	2.61	1.45	1.40
2	D	501	CJA	C23-C06	2.59	1.45	1.40
2	A	501	CJA	C23-C06	2.53	1.45	1.40
2	E	501	CJA	C23-C06	2.52	1.45	1.40
2	A	501	CJA	C05-S04	-2.45	1.66	1.70
2	E	501	CJA	C05-S04	-2.38	1.66	1.70
2	B	501	CJA	C05-S04	-2.21	1.67	1.70
2	F	501	CJA	C05-S04	-2.08	1.67	1.70

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	CJA	C14-S13-C12	15.02	120.94	101.65
2	B	501	CJA	C14-S13-C12	14.93	120.83	101.65
2	F	501	CJA	C14-S13-C12	14.10	119.76	101.65
2	A	501	CJA	C14-S13-C12	13.33	118.77	101.65
2	C	501	CJA	C14-S13-C12	13.20	118.61	101.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	CJA	C14-S13-C12	13.04	118.40	101.65
2	B	501	CJA	C05-C06-C23	3.76	112.21	105.29
2	F	501	CJA	C05-C06-C23	3.67	112.03	105.29
2	D	501	CJA	C05-C06-C23	3.65	112.00	105.29
2	C	501	CJA	C05-C06-C23	3.59	111.90	105.29
2	A	501	CJA	C05-C06-C23	3.31	111.38	105.29
2	E	501	CJA	C05-C06-C23	3.28	111.32	105.29
2	E	501	CJA	C10-N11-C12	3.20	118.01	115.39
2	D	501	CJA	C10-N11-C12	3.20	118.01	115.39
2	C	501	CJA	C10-N11-C12	3.15	117.97	115.39
2	B	501	CJA	C10-N11-C12	3.12	117.95	115.39
2	F	501	CJA	C10-N11-C12	3.07	117.90	115.39
2	E	501	CJA	N11-C12-N21	-2.99	123.87	127.57
2	A	501	CJA	C10-N11-C12	2.98	117.83	115.39
2	C	501	CJA	N11-C12-N21	-2.94	123.93	127.57
2	E	501	CJA	C07-C08-C09	2.85	117.68	110.71
2	A	501	CJA	N11-C12-N21	-2.80	124.10	127.57
2	D	501	CJA	N11-C12-N21	-2.78	124.12	127.57
2	B	501	CJA	N11-C12-N21	-2.77	124.14	127.57
2	F	501	CJA	N11-C12-N21	-2.76	124.15	127.57
2	E	501	CJA	C09-C22-N21	-2.72	119.74	122.70
2	B	501	CJA	C09-C22-N21	-2.63	119.84	122.70
2	D	501	CJA	C09-C22-N21	-2.62	119.85	122.70
2	B	501	CJA	C23-C22-N21	2.61	120.88	118.02
2	F	501	CJA	C09-C22-N21	-2.60	119.88	122.70
2	C	501	CJA	C09-C22-N21	-2.51	119.96	122.70
2	C	501	CJA	C23-C22-N21	2.51	120.77	118.02
2	D	501	CJA	C23-C22-N21	2.48	120.74	118.02
2	F	501	CJA	C23-C22-N21	2.39	120.65	118.02
2	A	501	CJA	C09-C22-N21	-2.28	120.22	122.70
2	E	501	CJA	C23-C22-N21	2.24	120.47	118.02
2	A	501	CJA	C07-C08-C09	2.13	115.91	110.71
2	F	501	CJA	C07-C08-C09	2.09	115.82	110.71

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CJA	C14-C15-C17-C20
2	A	501	CJA	C14-C15-C17-C18
2	A	501	CJA	C14-C15-C17-C19
2	B	501	CJA	C14-C15-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	501	CJA	C14-C15-C17-C19
2	E	501	CJA	C14-C15-C17-C20
2	E	501	CJA	C14-C15-C17-C19
2	A	501	CJA	O16-C15-C17-C20
2	B	501	CJA	O16-C15-C17-C18
2	B	501	CJA	O16-C15-C17-C19
2	E	501	CJA	O16-C15-C17-C20
2	E	501	CJA	O16-C15-C17-C19
2	A	501	CJA	O16-C15-C17-C18
2	A	501	CJA	O16-C15-C17-C19
2	E	501	CJA	O16-C15-C17-C18
2	B	501	CJA	C14-C15-C17-C20
2	C	501	CJA	C14-C15-C17-C19
2	D	501	CJA	C14-C15-C17-C20
2	D	501	CJA	C14-C15-C17-C19
2	E	501	CJA	C14-C15-C17-C18
2	B	501	CJA	O16-C15-C17-C20
2	D	501	CJA	O16-C15-C17-C20
2	D	501	CJA	O16-C15-C17-C19
2	D	501	CJA	O16-C15-C17-C18
2	D	501	CJA	C14-C15-C17-C18
2	F	501	CJA	C14-C15-C17-C18

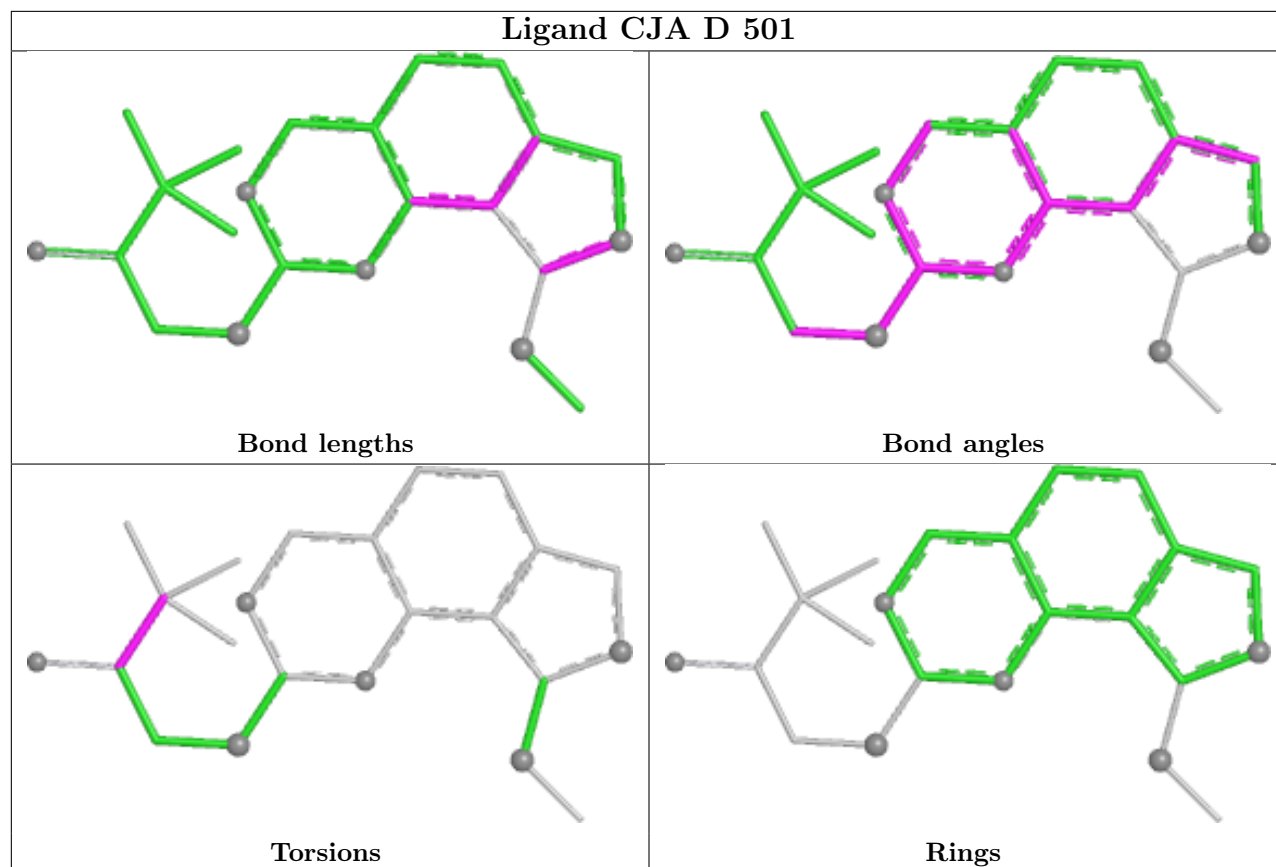
There are no ring outliers.

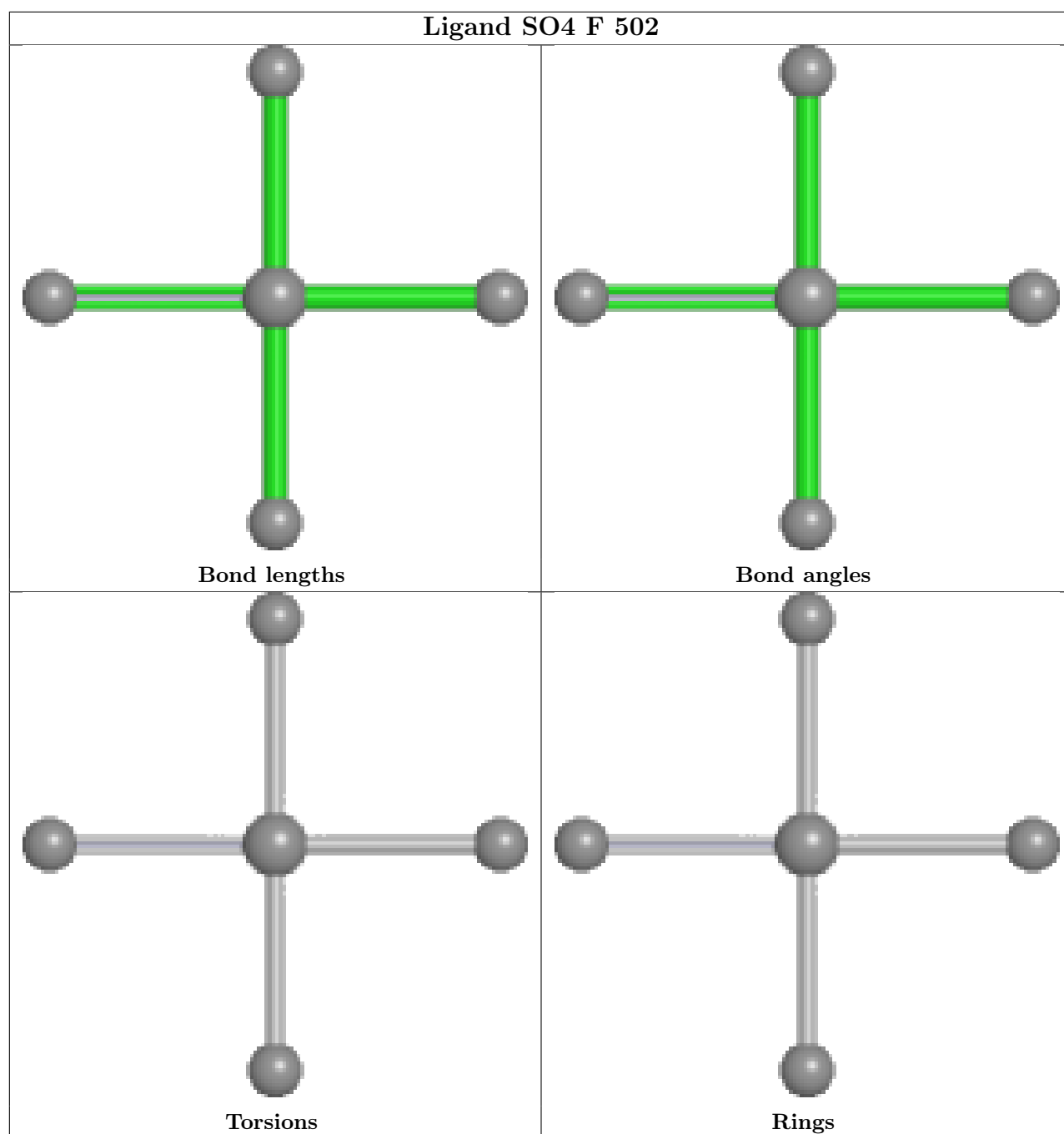
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CJA	1	0
2	F	501	CJA	1	0

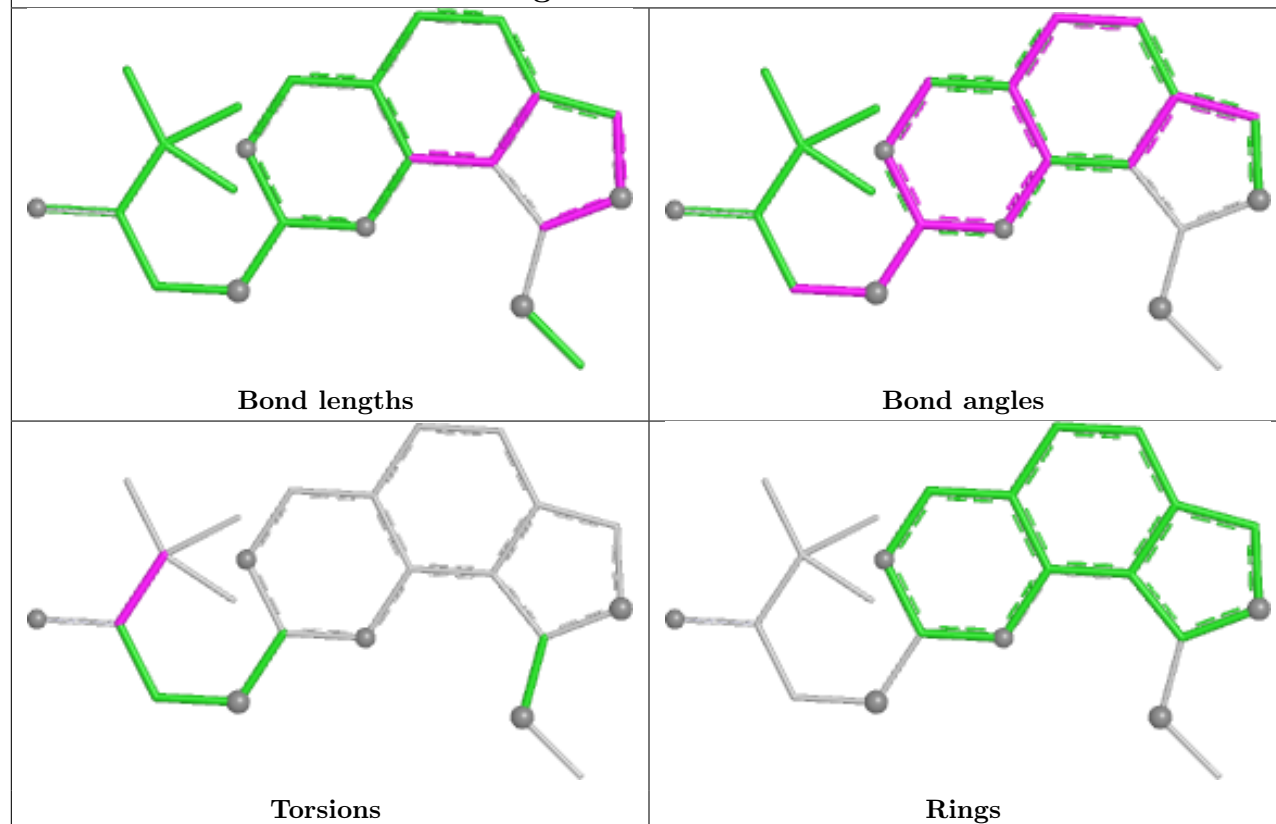
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 CJA D 501

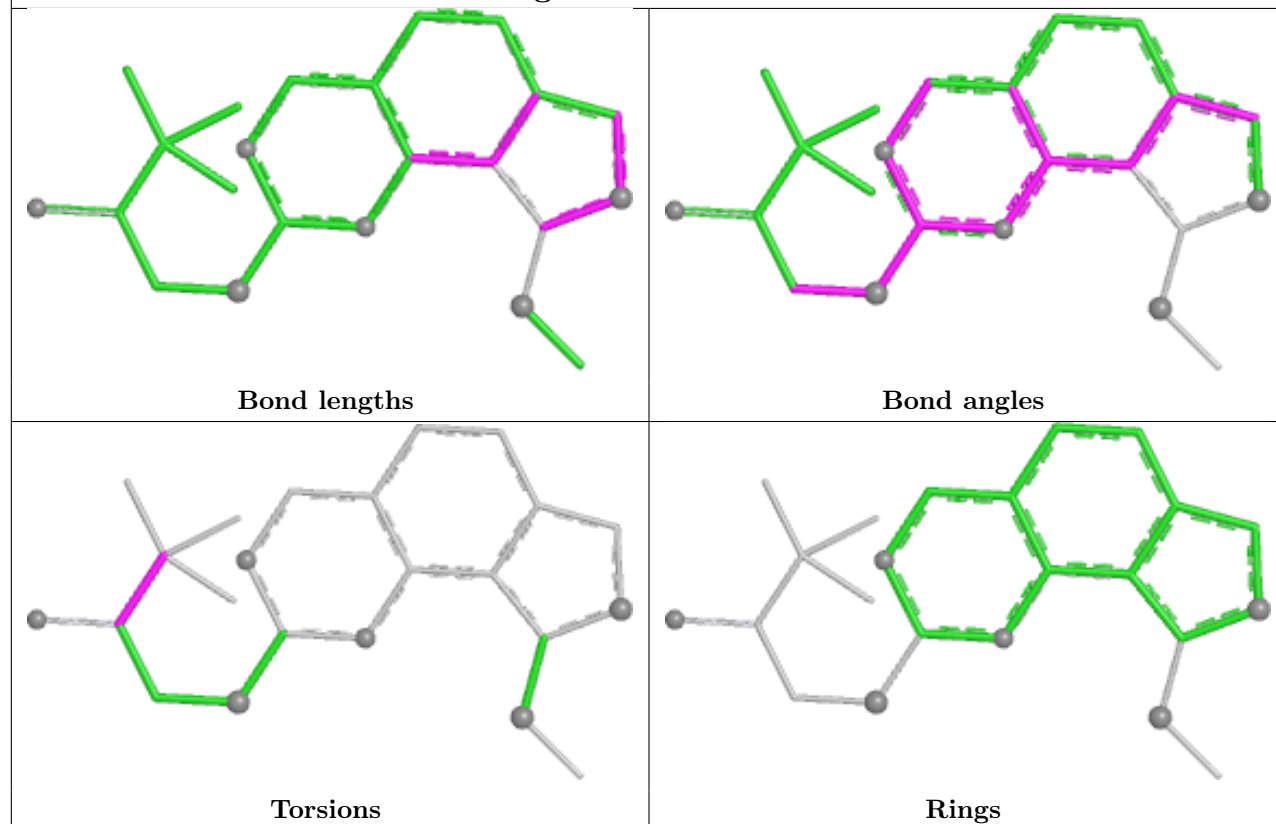




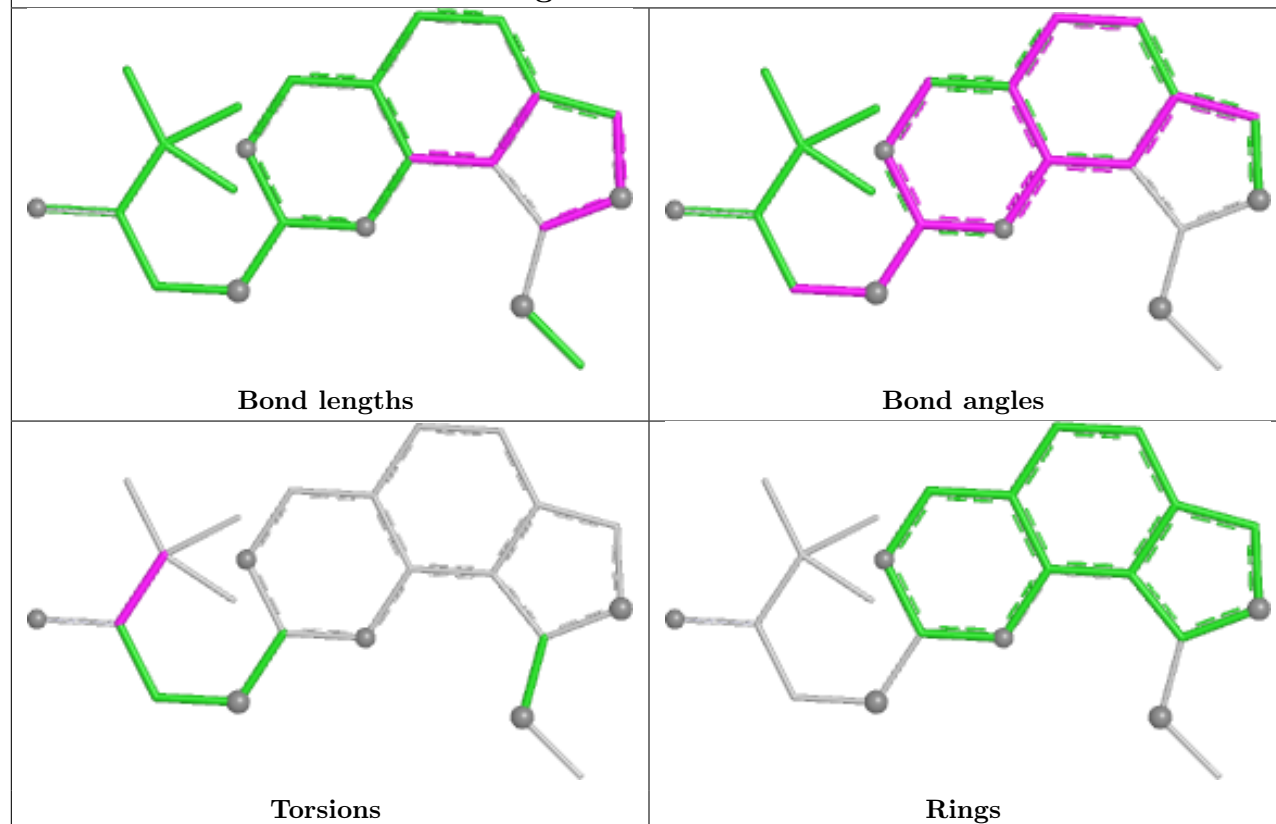
Ligand CJA A 501



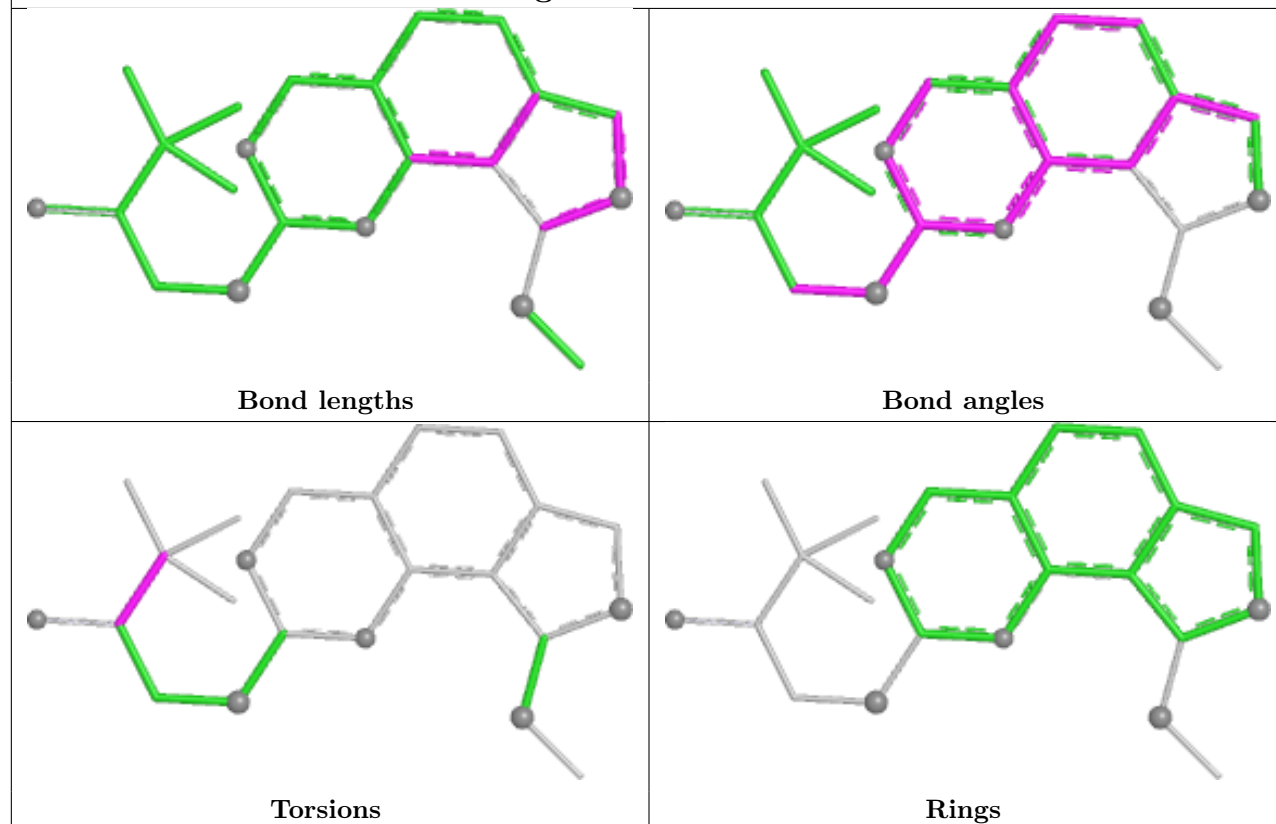
Ligand CJA B 501

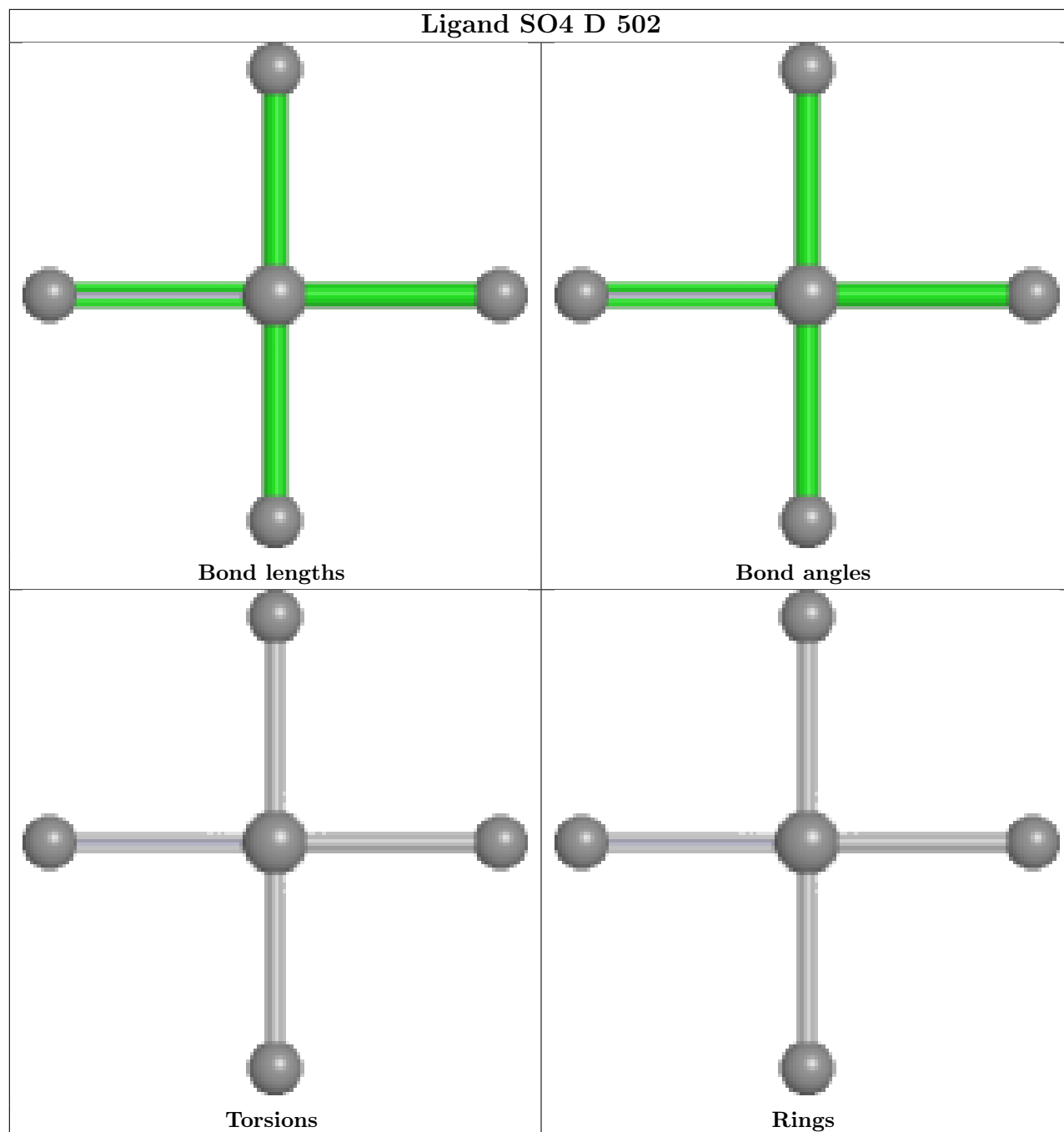


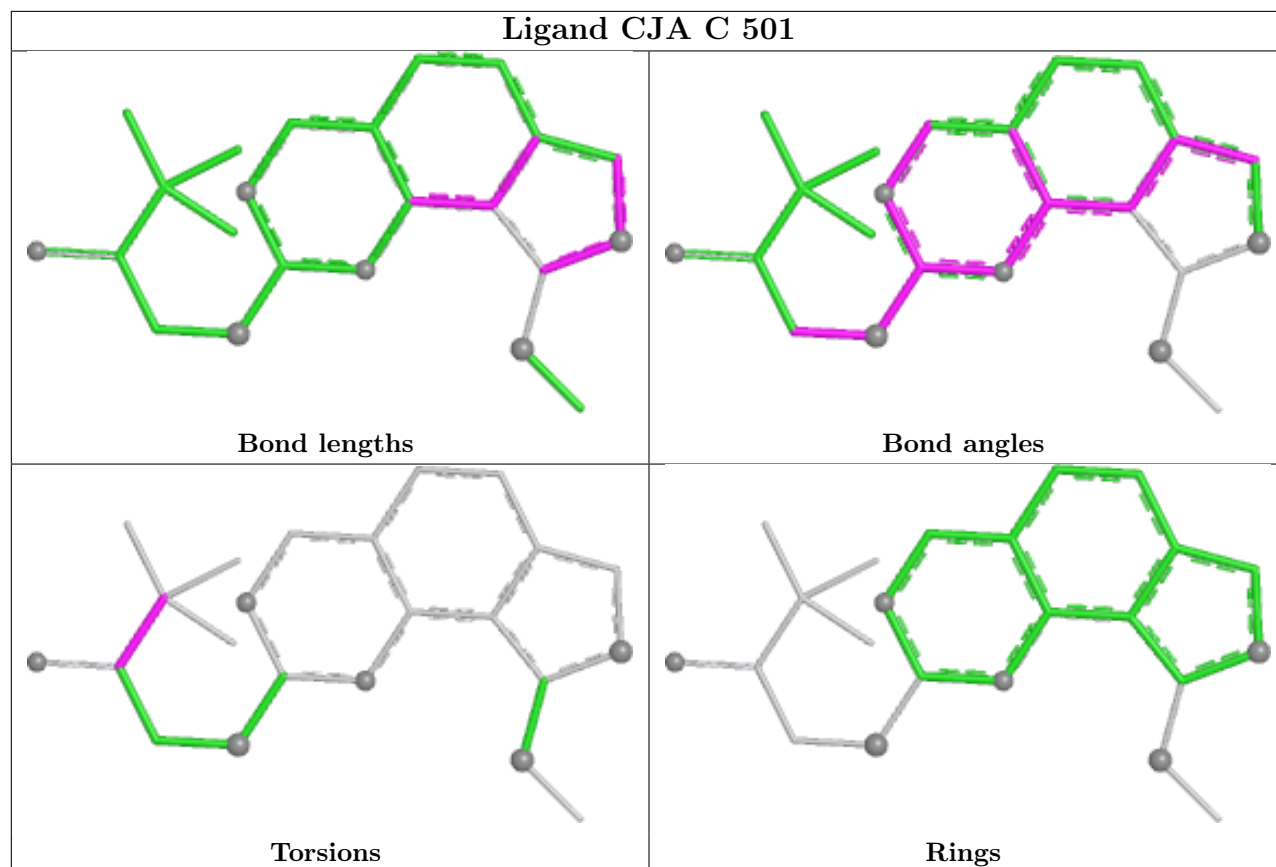
Ligand CJA F 501



Ligand CJA E 501







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	148/149 (99%)	0.68	11 (7%)	22 20	48, 61, 85, 101	0
1	B	148/149 (99%)	0.61	11 (7%)	22 20	44, 61, 88, 105	0
1	C	147/149 (98%)	0.51	10 (6%)	25 22	45, 58, 77, 88	0
1	D	147/149 (98%)	0.55	9 (6%)	28 26	47, 58, 80, 98	0
1	E	147/149 (98%)	0.93	17 (11%)	11 9	47, 65, 94, 106	0
1	F	147/149 (98%)	1.18	21 (14%)	7 6	50, 72, 99, 123	0
All	All	884/894 (98%)	0.74	79 (8%)	17 15	44, 62, 90, 123	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	466	VAL	7.7
1	A	467	THR	6.4
1	F	320	ALA	5.7
1	B	321	GLU	5.7
1	E	466	VAL	5.1
1	A	320	ALA	5.0
1	F	465	GLY	4.8
1	B	467	THR	4.8
1	D	466	VAL	4.6
1	C	320	ALA	4.5
1	E	320	ALA	4.4
1	E	321	GLU	4.2
1	E	427	THR	4.2
1	C	466	VAL	4.1
1	F	462	LEU	4.1
1	A	466	VAL	4.0
1	F	428	ARG	3.9
1	F	322	LEU	3.8
1	F	427	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	427	THR	3.8
1	B	322	LEU	3.7
1	E	428	ARG	3.7
1	F	444	ILE	3.6
1	F	399	GLN	3.6
1	C	426	HIS	3.6
1	E	335	GLN	3.4
1	B	320	ALA	3.4
1	A	408	CYS	3.3
1	E	465	GLY	3.2
1	D	320	ALA	3.2
1	F	463	ASN	3.1
1	E	322	LEU	3.1
1	E	426	HIS	3.0
1	E	403	GLY	3.0
1	F	464	ASN	3.0
1	F	405	LEU	2.9
1	F	364	GLU	2.8
1	F	460	GLU	2.6
1	E	398	HIS	2.6
1	B	365	LYS	2.6
1	B	367	LEU	2.6
1	D	428	ARG	2.6
1	B	340	LEU	2.6
1	E	399	GLN	2.6
1	F	327	PRO	2.5
1	D	457	GLU	2.5
1	A	465	GLY	2.5
1	E	388	GLU	2.5
1	D	400	CYS	2.5
1	C	328	PHE	2.5
1	D	377	ASP	2.4
1	B	400	CYS	2.4
1	E	340	LEU	2.4
1	F	426	HIS	2.4
1	A	464	ASN	2.4
1	D	460	GLU	2.4
1	E	402	LYS	2.4
1	A	426	HIS	2.3
1	E	362	HIS	2.3
1	B	466	VAL	2.3
1	C	427	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	364	GLU	2.3
1	A	461	ASP	2.3
1	A	365	LYS	2.2
1	F	375	ALA	2.2
1	E	400	CYS	2.2
1	C	380	LYS	2.2
1	C	340	LEU	2.2
1	F	398	HIS	2.2
1	C	399	GLN	2.2
1	F	328	PHE	2.2
1	A	335	GLN	2.1
1	C	428	ARG	2.1
1	F	400	CYS	2.1
1	A	436	LYS	2.1
1	B	335	GLN	2.1
1	F	440	GLY	2.1
1	B	368	PHE	2.0
1	C	327	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	F	502	5/5	0.83	0.11	68,78,104,162	0
2	CJA	A	501	23/23	0.90	0.16	53,70,90,99	0
2	CJA	F	501	23/23	0.92	0.14	49,64,82,87	0
2	CJA	C	501	23/23	0.93	0.14	47,58,72,73	0
2	CJA	E	501	23/23	0.93	0.13	46,61,71,86	0

Continued on next page...

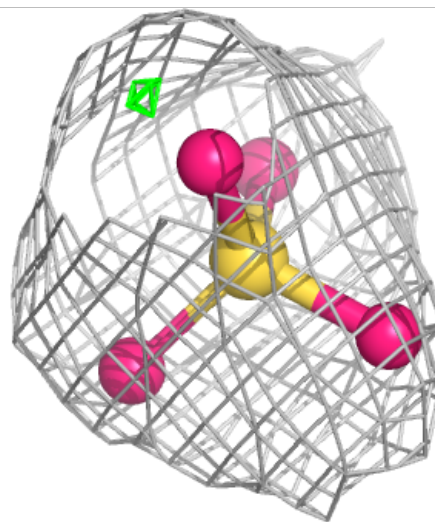
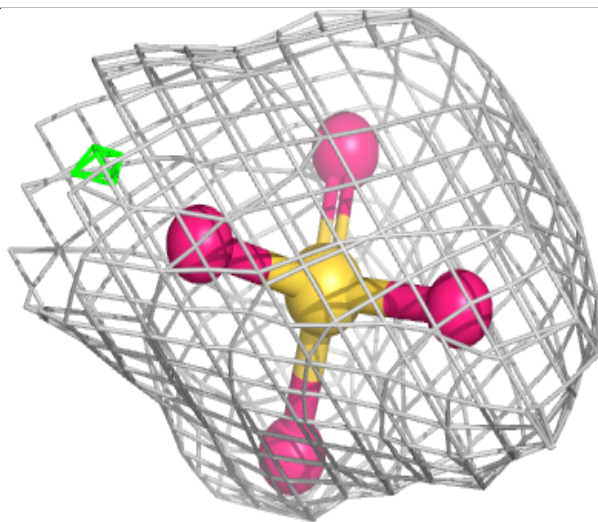
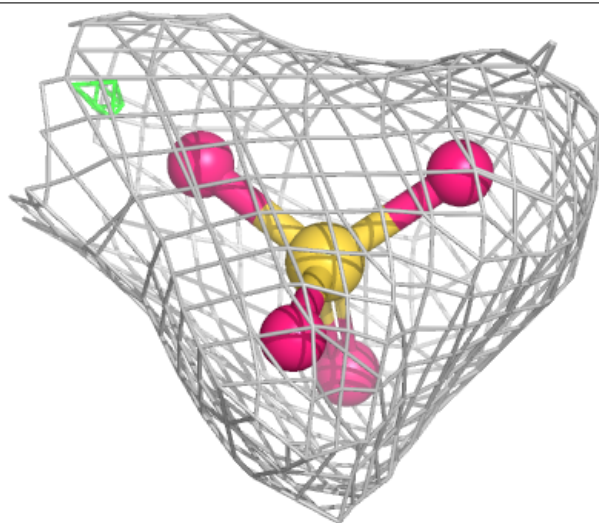
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CJA	B	501	23/23	0.94	0.12	52,63,75,79	0
2	CJA	D	501	23/23	0.95	0.10	47,63,75,77	0
3	SO4	D	502	5/5	0.97	0.12	58,60,68,70	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.

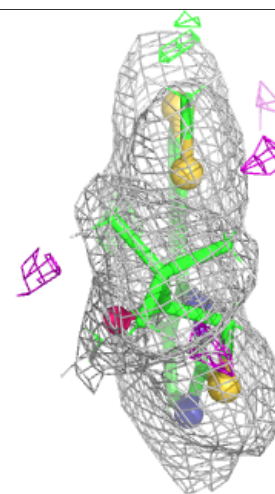
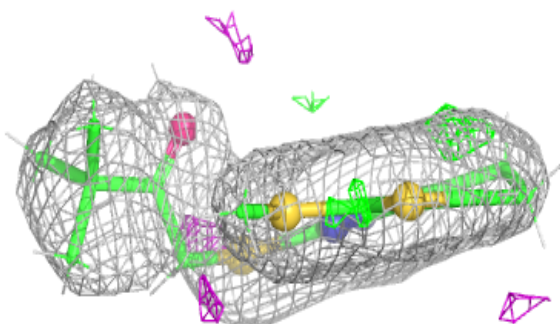
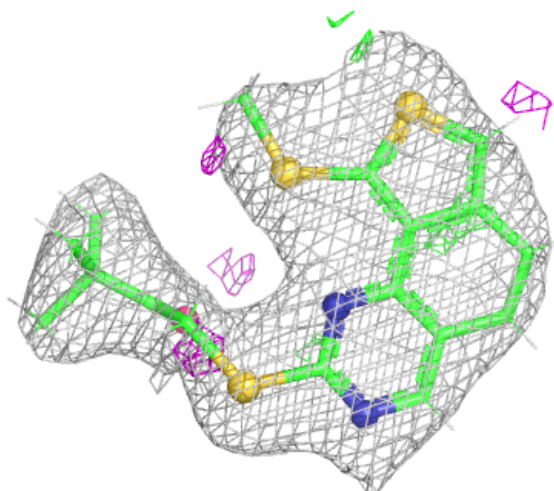
Electron density around SO4 F 502:

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



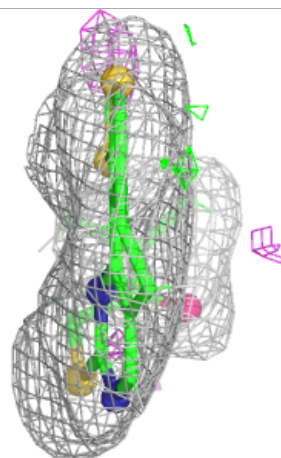
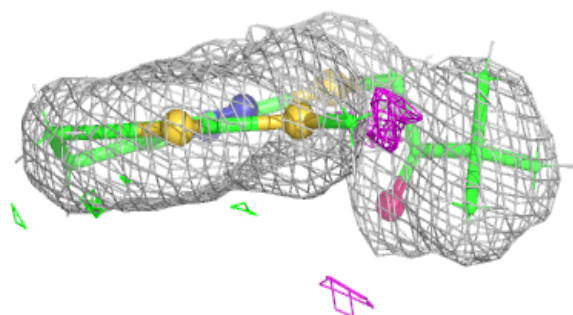
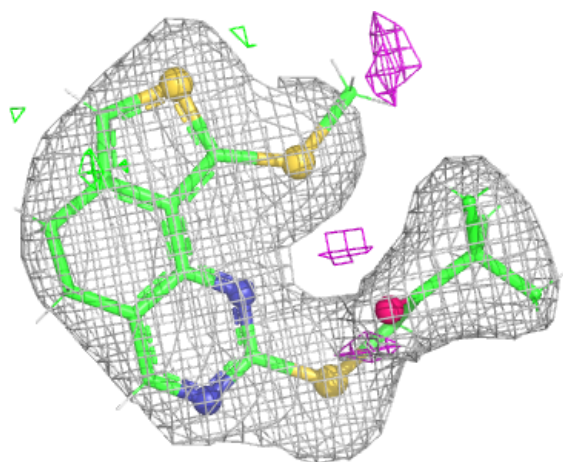
Electron density around CJA A 501:

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



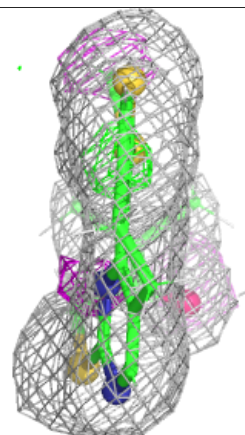
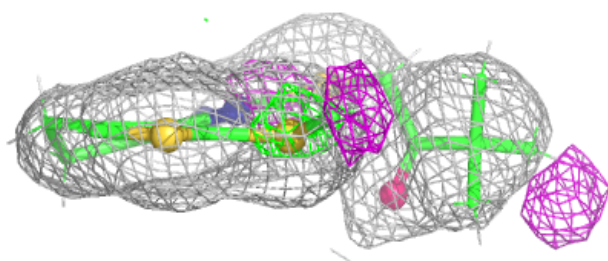
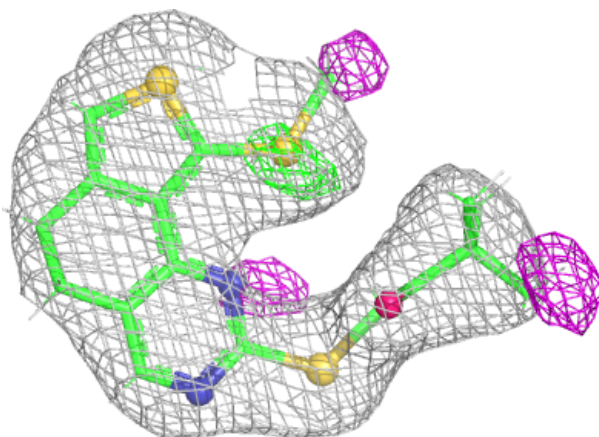
Electron density around CJA F 501:

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



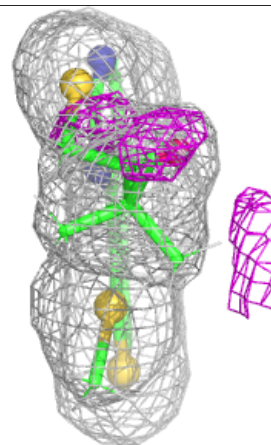
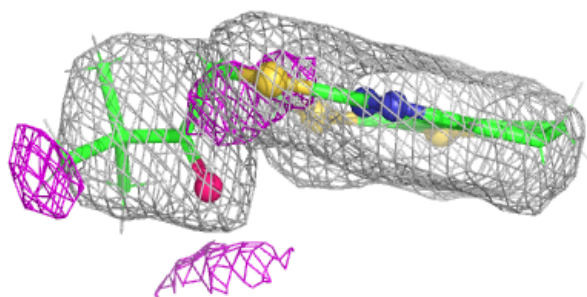
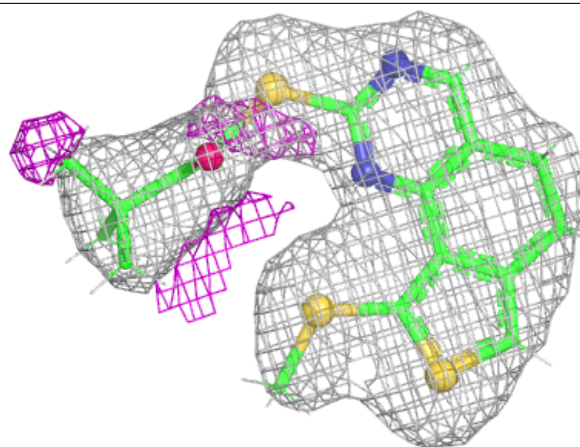
Electron density around CJA C 501:

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



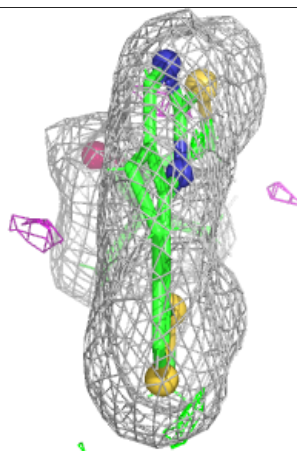
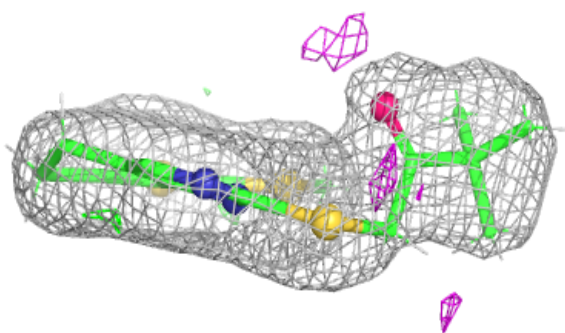
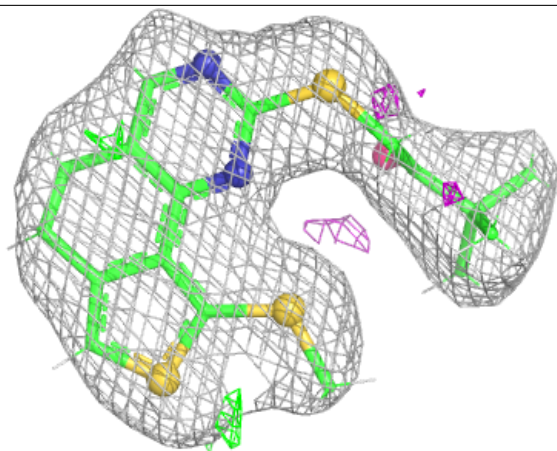
Electron density around CJA E 501:

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



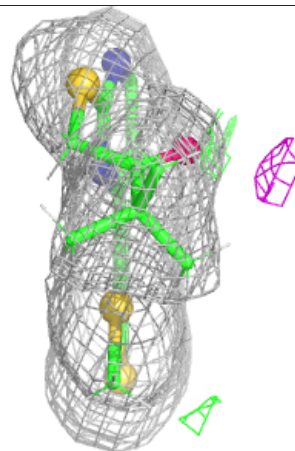
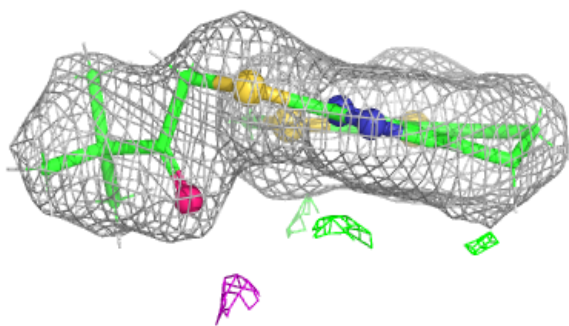
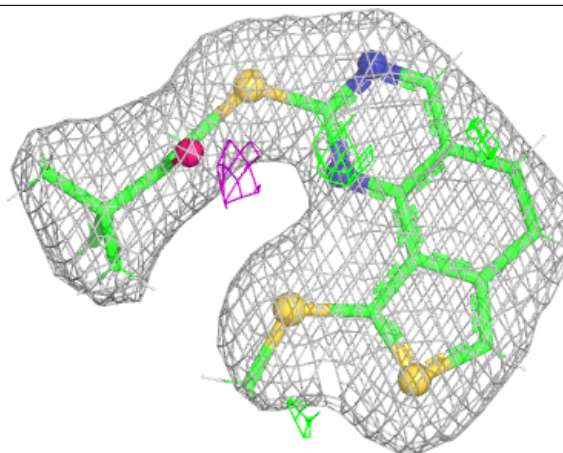
Electron density around CJA B 501:

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



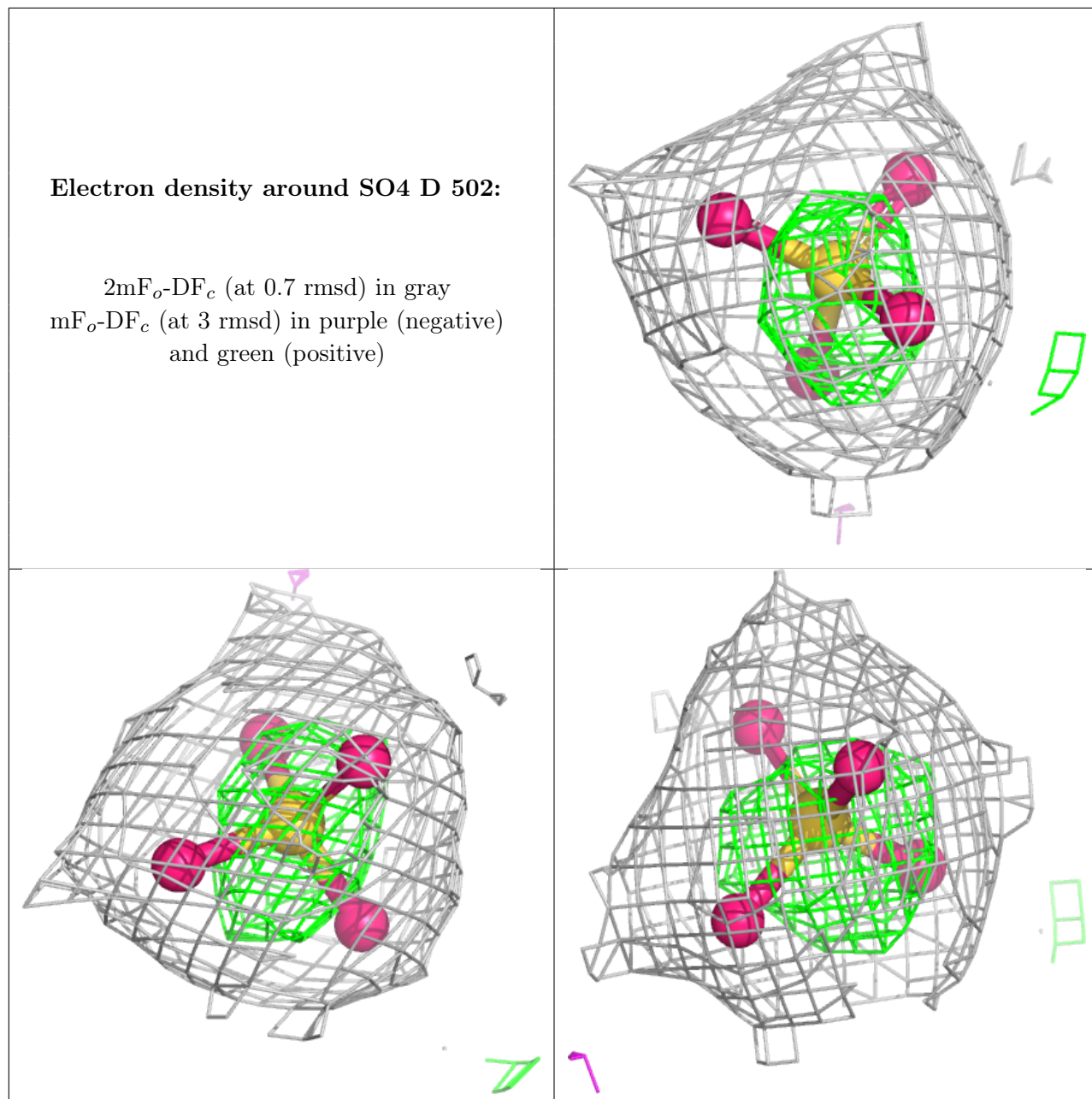
Electron density around CJA D 501:

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



Electron density around SO4 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.