



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 22, 2025 – 10:13 AM EDT

PDB ID : 9NSB / pdb_00009nsb
Title : Crystal structure of an MKP5 allosteric loop mutant, S446G, in complex with an allosteric inhibitor
Authors : Manjula, R.; Bennett, A.M.; Lolis, E.
Deposited on : 2025-03-16
Resolution : 2.50 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

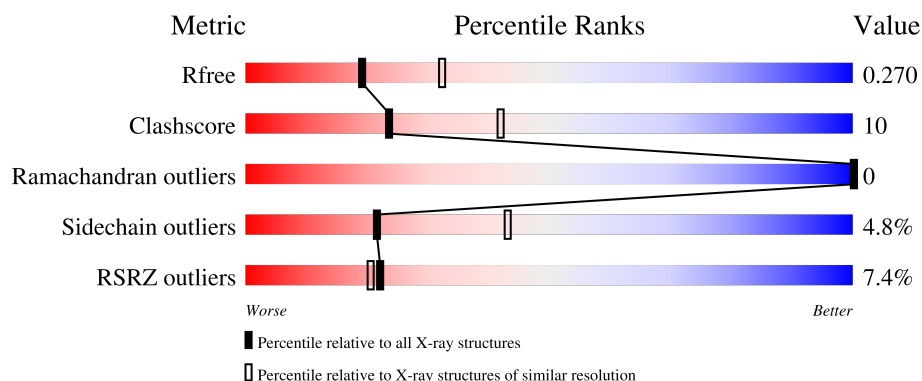
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>..</div> </div> </div>
1	B	149	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	149	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>..</div> </div> </div>
1	D	149	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>
1	E	149	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	149	<div><div></div><div>13%</div><div>77%</div><div>22%</div><div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13922 atoms, of which 6821 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
			2260	744	1102	194	212	8			
1	B	148	Total	C	H	N	O	S	0	0	0
			2310	753	1135	198	217	7			
1	C	148	Total	C	H	N	O	S	0	0	0
			2291	750	1124	196	214	7			
1	D	147	Total	C	H	N	O	S	0	0	0
			2286	747	1125	194	213	7			
1	E	145	Total	C	H	N	O	S	0	0	0
			2212	729	1080	189	208	6			
1	F	148	Total	C	H	N	O	S	0	0	0
			2305	753	1135	197	212	8			

There are 18 discrepancies between the modelled and reference sequences:

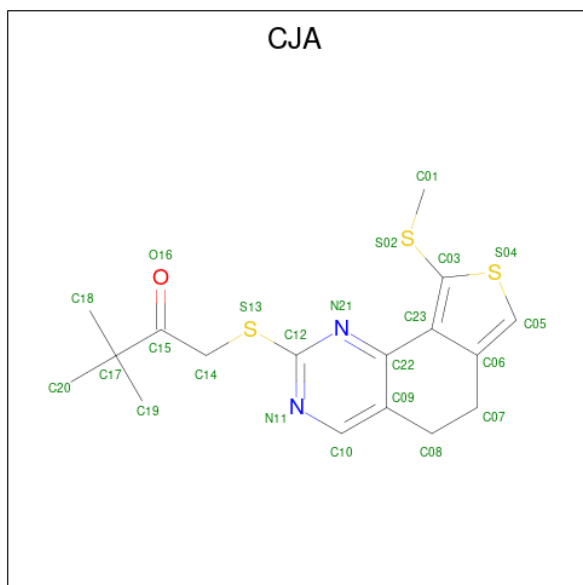
Chain	Residue	Modelled	Actual	Comment	Reference
A	319	MET	-	initiating methionine	UNP Q9Y6W6
A	446	GLY	SER	engineered mutation	UNP Q9Y6W6
A	467	ALA	-	expression tag	UNP Q9Y6W6
B	319	MET	-	initiating methionine	UNP Q9Y6W6
B	446	GLY	SER	engineered mutation	UNP Q9Y6W6
B	467	ALA	-	expression tag	UNP Q9Y6W6
C	319	MET	-	initiating methionine	UNP Q9Y6W6
C	446	GLY	SER	engineered mutation	UNP Q9Y6W6
C	467	ALA	-	expression tag	UNP Q9Y6W6
D	319	MET	-	initiating methionine	UNP Q9Y6W6
D	446	GLY	SER	engineered mutation	UNP Q9Y6W6
D	467	ALA	-	expression tag	UNP Q9Y6W6
E	319	MET	-	initiating methionine	UNP Q9Y6W6
E	446	GLY	SER	engineered mutation	UNP Q9Y6W6
E	467	ALA	-	expression tag	UNP Q9Y6W6
F	319	MET	-	initiating methionine	UNP Q9Y6W6
F	446	GLY	SER	engineered mutation	UNP Q9Y6W6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	467	ALA	-	expression tag	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).

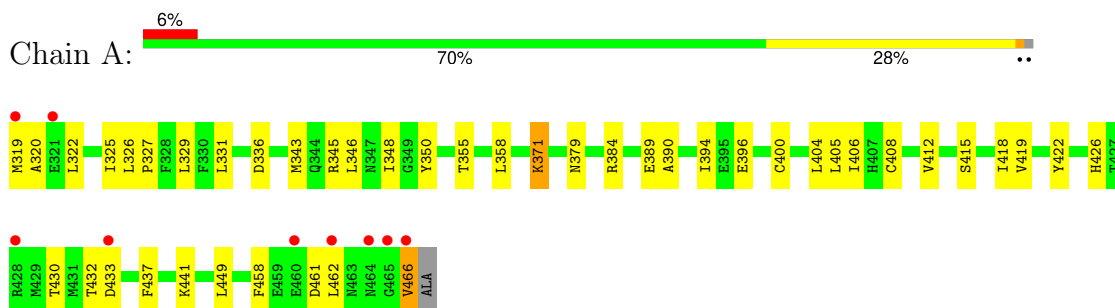


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	B	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	C	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	D	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	E	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0
2	F	1	Total 43	C 17	H 20	N 2	O 1	S 3	0	0

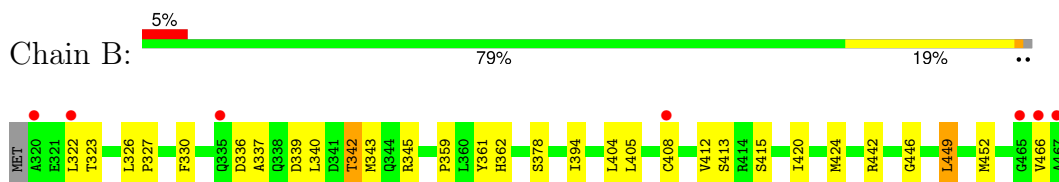
3 Residue-property plots [i](#)

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.

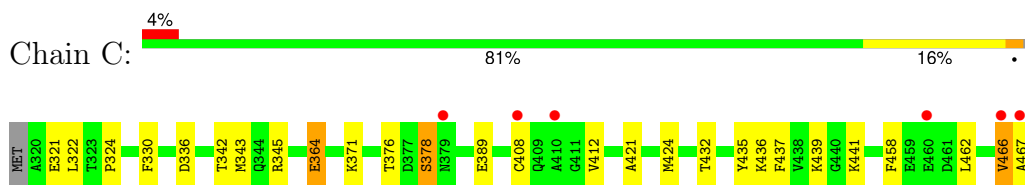
- Molecule 1: Dual specificity protein phosphatase 10



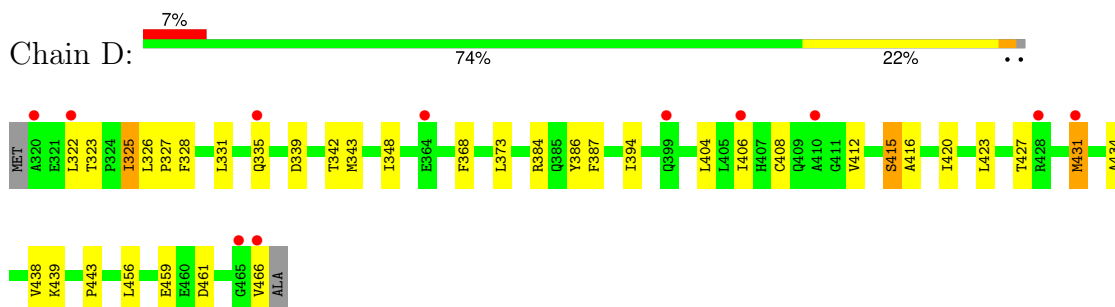
- Molecule 1: Dual specificity protein phosphatase 10



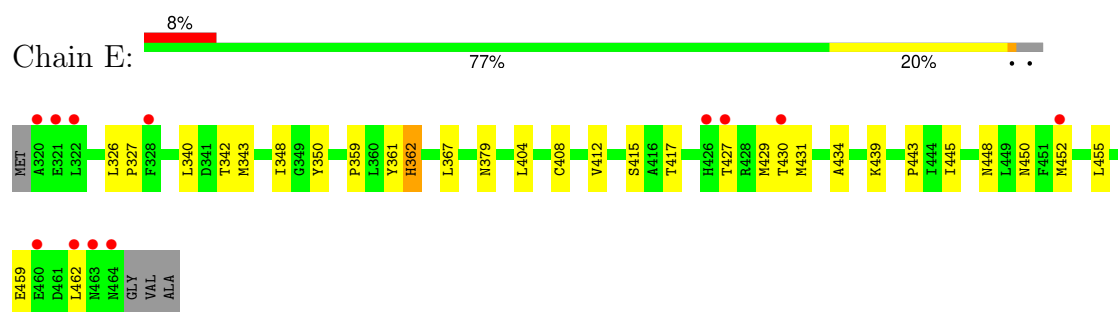
- Molecule 1: Dual specificity protein phosphatase 10



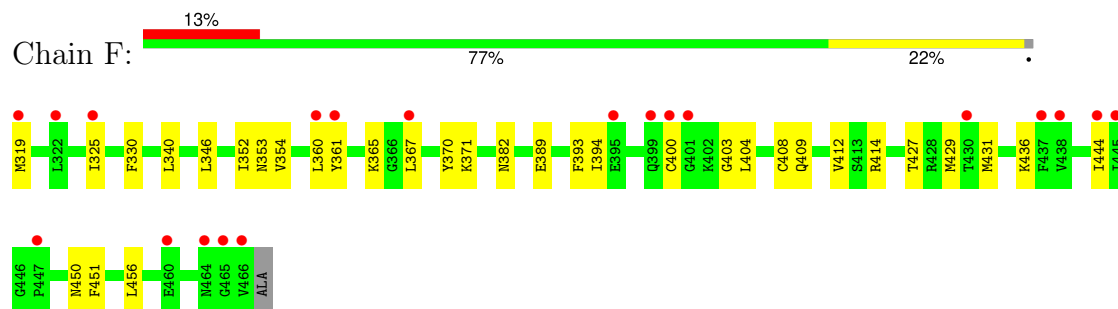
- Molecule 1: Dual specificity protein phosphatase 10



- 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.70Å 99.56Å 135.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.50 34.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.50-2.50) 99.9 (34.50-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.18_3845: ???)	Depositor
R, R_{free}	0.211 , 0.264 0.221 , 0.270	Depositor DCC
R_{free} test set	2370 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13922	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CJA

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	0.64	0/1184	0.88	0/1606
1	B	0.71	0/1201	0.93	1/1628 (0.1%)
1	C	0.71	0/1193	0.96	0/1617
1	D	0.64	0/1187	0.92	0/1609
1	E	0.63	0/1158	0.91	0/1571
1	F	0.76	0/1196	1.21	3/1619 (0.2%)
All	All	0.68	0/7119	0.97	4/9650 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	VAL	N-CA-C	-6.85	106.55	113.47
1	F	361	TYR	N-CA-C	5.31	117.48	111.11
1	F	451	PHE	CA-CB-CG	5.31	119.11	113.80
1	F	403	GLY	CA-C-O	-5.16	115.65	121.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1158	1102	1108	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1175	1135	1136	20	0
1	C	1167	1124	1133	20	0
1	D	1161	1125	1123	31	0
1	E	1132	1080	1078	18	0
1	F	1170	1135	1144	16	0
2	A	23	20	0	0	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	0	0
All	All	7101	6821	6722	138	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 10.

All (138) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:MET:HE1	1:D:456:LEU:HA	1.44	0.97
1:D:322:LEU:HD23	1:D:322:LEU:H	1.33	0.92
1:A:355:THR:HG21	1:A:358:LEU:HD12	1.67	0.77
1:C:371:LYS:HE3	1:C:389:GLU:HG2	1.67	0.76
1:D:431:MET:HE1	1:D:456:LEU:CA	2.21	0.71
1:D:339:ASP:O	1:D:343:MET:HG3	1.95	0.67
1:A:326:LEU:HB3	1:A:327:PRO:HD2	1.76	0.66
1:A:371:LYS:NZ	1:A:389:GLU:OE1	2.28	0.66
1:D:416:ALA:O	1:D:420:ILE:HG13	1.96	0.65
1:E:350:TYR:HB3	1:E:404:LEU:HD12	1.79	0.64
1:F:408:CYS:SG	1:F:412:VAL:HA	2.37	0.64
1:D:408:CYS:SG	1:D:412:VAL:HA	2.38	0.64
1:E:439:LYS:HD2	1:E:445:ILE:HD12	1.79	0.64
1:A:404:LEU:HD23	1:A:405:LEU:N	2.15	0.62
1:D:406:ILE:HG12	1:D:415:SER:HB3	1.80	0.61
1:A:404:LEU:HD23	1:A:404:LEU:C	2.25	0.61
1:B:342:THR:HG23	1:B:345:ARG:HH21	1.66	0.61
1:E:439:LYS:HE3	1:E:443:PRO:O	2.01	0.61
1:A:390:ALA:O	1:A:394:ILE:HG13	2.02	0.60
1:E:429:MET:CE	1:E:434:ALA:HA	2.31	0.59
1:A:331:LEU:HD13	1:A:419:VAL:HG21	1.83	0.58
1:C:432:THR:HG22	1:C:436:LYS:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:LEU:H	1:D:322:LEU:CD2	2.10	0.58
1:B:449:LEU:HD23	1:B:452:MET:HE3	1.86	0.58
1:E:431:MET:HE1	1:E:452:MET:O	2.03	0.57
1:A:322:LEU:H	1:A:322:LEU:HD23	1.70	0.57
1:E:408:CYS:SG	1:E:412:VAL:HA	2.45	0.57
1:A:371:LYS:HE3	1:A:389:GLU:HG3	1.86	0.57
1:C:371:LYS:HE3	1:C:389:GLU:CG	2.34	0.56
1:F:365:LYS:O	1:F:367:LEU:HD22	2.06	0.56
1:E:326:LEU:HB3	1:E:327:PRO:HD2	1.86	0.56
1:F:427:THR:HG22	1:F:427:THR:O	2.04	0.56
1:B:339:ASP:CG	1:B:342:THR:HG1	2.13	0.55
1:B:339:ASP:CG	1:B:342:THR:OG1	2.50	0.55
1:B:342:THR:HG23	1:B:345:ARG:NH2	2.22	0.54
1:A:384:ARG:HG2	1:A:384:ARG:HH11	1.72	0.54
1:F:371:LYS:HD3	1:F:389:GLU:HG2	1.89	0.54
1:F:409:GLN:OE1	1:F:414:ARG:NH2	2.39	0.53
1:D:427:THR:HG22	1:D:427:THR:O	2.07	0.53
1:A:405:LEU:HD12	1:A:406:ILE:N	2.23	0.53
1:C:437:PHE:CZ	1:C:441:LYS:HE3	2.44	0.53
1:C:458:PHE:CE1	1:C:462:LEU:HD11	2.44	0.53
1:E:343:MET:CE	1:E:348:ILE:HG21	2.39	0.53
1:A:325:ILE:O	1:A:326:LEU:HD23	2.09	0.53
1:B:343:MET:HE3	1:B:405:LEU:HD23	1.90	0.53
1:E:417:THR:HG23	1:E:455:LEU:HD11	1.92	0.52
1:C:371:LYS:NZ	1:C:389:GLU:OE1	2.24	0.52
1:F:427:THR:HB	1:F:429:MET:HG3	1.91	0.52
1:D:331:LEU:CD1	1:D:415:SER:HB2	2.40	0.51
1:B:326:LEU:HB3	1:B:327:PRO:HD2	1.91	0.51
1:B:420:ILE:O	1:B:424:MET:HG3	2.11	0.51
1:F:330:PHE:CE1	1:F:346:LEU:HD13	2.46	0.51
1:F:394:ILE:HA	1:F:404:LEU:HD13	1.93	0.50
1:C:364:GLU:H	1:C:364:GLU:CD	2.20	0.50
1:D:373:LEU:HD22	1:D:386:TYR:HB3	1.93	0.50
1:D:322:LEU:HD21	1:D:342:THR:HG22	1.93	0.50
1:E:431:MET:HE3	1:E:455:LEU:CB	2.42	0.50
1:A:345:ARG:CZ	1:A:346:LEU:HD11	2.42	0.49
1:B:413:SER:OG	1:B:446:GLY:O	2.27	0.49
1:C:324:PRO:HB3	1:C:330:PHE:CE1	2.47	0.49
1:D:434:ALA:O	1:D:438:VAL:HG23	2.12	0.49
1:E:359:PRO:HG2	1:E:361:TYR:CE2	2.47	0.49
1:D:325:ILE:O	1:D:326:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:HG2	1:A:384:ARG:NH1	2.28	0.49
1:F:352:ILE:HG13	1:F:404:LEU:HD21	1.94	0.49
1:D:423:LEU:O	1:D:427:THR:HB	2.12	0.49
1:C:466:VAL:HG23	1:C:467:ALA:N	2.26	0.48
1:D:439:LYS:HE3	1:D:443:PRO:O	2.13	0.48
1:A:350:TYR:CE1	1:A:396:GLU:HG2	2.49	0.48
1:E:429:MET:HE3	1:E:434:ALA:HA	1.94	0.48
1:C:324:PRO:HB3	1:C:330:PHE:HE1	1.79	0.47
1:A:408:CYS:SG	1:A:412:VAL:HA	2.54	0.47
1:C:342:THR:HG23	1:C:345:ARG:NH1	2.29	0.47
1:D:394:ILE:HA	1:D:404:LEU:HD13	1.97	0.47
1:B:359:PRO:HG2	1:B:361:TYR:CE2	2.50	0.47
1:A:345:ARG:NH2	1:A:346:LEU:HD11	2.30	0.47
1:A:404:LEU:HD23	1:A:405:LEU:C	2.39	0.47
1:F:382:ASN:OD1	1:F:382:ASN:C	2.58	0.47
1:A:322:LEU:O	1:A:322:LEU:HG	2.14	0.47
1:C:321:GLU:N	1:C:336:ASP:OD1	2.48	0.47
1:D:456:LEU:HD23	1:D:456:LEU:O	2.15	0.46
1:F:431:MET:HE2	1:F:456:LEU:HA	1.97	0.46
1:A:412:VAL:O	1:A:412:VAL:HG23	2.16	0.46
1:E:431:MET:HE3	1:E:455:LEU:HB3	1.97	0.46
1:A:343:MET:HE3	1:A:348:ILE:HG21	1.96	0.46
1:B:404:LEU:HD23	1:B:404:LEU:C	2.40	0.45
1:E:350:TYR:CB	1:E:404:LEU:HD12	2.47	0.45
1:D:420:ILE:HG23	1:D:434:ALA:HB3	1.99	0.45
1:C:421:ALA:HA	1:C:424:MET:HE3	1.98	0.45
1:F:360:LEU:HD22	1:F:370:TYR:CD2	2.51	0.45
1:A:320:ALA:HB3	1:A:336:ASP:OD1	2.17	0.45
1:B:330:PHE:N	1:B:330:PHE:CD1	2.86	0.44
1:C:408:CYS:SG	1:C:412:VAL:HA	2.57	0.44
1:D:323:THR:HG22	1:D:325:ILE:HD13	1.99	0.44
1:D:461:ASP:HB3	1:D:466:VAL:HG22	1.99	0.44
1:A:371:LYS:HE3	1:A:389:GLU:CG	2.48	0.44
1:B:394:ILE:HA	1:B:404:LEU:HD13	2.00	0.44
1:D:322:LEU:HD23	1:D:322:LEU:N	2.16	0.44
1:D:427:THR:O	1:D:427:THR:CG2	2.65	0.44
1:D:326:LEU:HB3	1:D:327:PRO:HD2	1.99	0.44
1:E:379:ASN:O	1:E:450:ASN:ND2	2.50	0.44
1:A:379:ASN:HD22	1:A:379:ASN:C	2.22	0.44
1:A:430:THR:OG1	1:A:433:ASP:HB2	2.18	0.44
1:A:319:MET:HE2	1:A:320:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ALA:O	1:B:362:HIS:HE1	2.02	0.43
1:B:449:LEU:CD2	1:B:452:MET:HE3	2.48	0.43
1:A:329:LEU:HD13	1:A:394:ILE:HD13	2.01	0.43
1:F:340:LEU:HD12	1:F:340:LEU:O	2.18	0.43
1:A:319:MET:CE	1:A:320:ALA:HB2	2.49	0.43
1:A:461:ASP:C	1:A:466:VAL:HG23	2.44	0.43
1:C:376:THR:OG1	1:C:378:SER:HB3	2.19	0.43
1:C:342:THR:HG23	1:C:345:ARG:HH12	1.83	0.42
1:A:422:TYR:HE2	1:A:426:HIS:CD2	2.37	0.42
1:A:458:PHE:CZ	1:A:462:LEU:HD11	2.54	0.42
1:D:420:ILE:HG23	1:D:434:ALA:CB	2.49	0.42
1:F:354:VAL:HG12	1:F:354:VAL:O	2.19	0.42
1:D:404:LEU:C	1:D:404:LEU:HD23	2.44	0.42
1:C:435:TYR:OH	1:C:439:LYS:HD3	2.19	0.42
1:A:329:LEU:CD1	1:A:394:ILE:HD13	2.50	0.42
1:A:449:LEU:HD21	1:B:452:MET:HE1	2.00	0.42
1:F:353:ASN:OD1	1:F:353:ASN:C	2.62	0.42
1:B:408:CYS:SG	1:B:412:VAL:HA	2.60	0.42
1:D:348:ILE:O	1:D:368:PHE:HE1	2.03	0.42
1:F:330:PHE:CD2	1:F:330:PHE:N	2.88	0.41
1:C:322:LEU:HD12	1:C:336:ASP:HB3	2.01	0.41
1:E:379:ASN:OD1	1:E:379:ASN:N	2.49	0.41
1:D:431:MET:HE3	1:D:459:GLU:HB2	2.01	0.41
1:D:328:PHE:CD2	1:D:328:PHE:N	2.89	0.41
1:E:448:ASN:OD1	1:E:450:ASN:HB3	2.20	0.41
1:C:324:PRO:HA	1:C:330:PHE:CD1	2.56	0.41
1:D:322:LEU:HD21	1:D:342:THR:CG2	2.50	0.41
1:D:384:ARG:HD2	1:D:387:PHE:CD1	2.56	0.41
1:B:339:ASP:OD1	1:B:342:THR:OG1	2.39	0.41
1:B:340:LEU:HD12	1:B:362:HIS:CD2	2.55	0.41
1:B:323:THR:OG1	1:B:442:ARG:HD2	2.21	0.40
1:E:340:LEU:HD13	1:E:362:HIS:CG	2.56	0.40
1:A:437:PHE:CZ	1:A:441:LYS:HE3	2.57	0.40
1:C:371:LYS:CE	1:C:389:GLU:CG	3.00	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	146/149 (98%)	141 (97%)	5 (3%)	0	100	100
1	D	145/149 (97%)	138 (95%)	7 (5%)	0	100	100
1	E	143/149 (96%)	139 (97%)	4 (3%)	0	100	100
1	F	146/149 (98%)	141 (97%)	5 (3%)	0	100	100
All	All	872/894 (98%)	838 (96%)	34 (4%)	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	119/129 (92%)	113 (95%)	6 (5%)	20	41
1	B	123/129 (95%)	117 (95%)	6 (5%)	21	42
1	C	122/129 (95%)	118 (97%)	4 (3%)	33	59
1	D	121/129 (94%)	117 (97%)	4 (3%)	33	59
1	E	115/129 (89%)	107 (93%)	8 (7%)	12	26
1	F	123/129 (95%)	116 (94%)	7 (6%)	17	35
All	All	723/774 (93%)	688 (95%)	35 (5%)	21	43

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	LYS
1	A	400	CYS
1	A	415	SER
1	A	418	ILE
1	A	432	THR
1	A	466	VAL
1	B	322	LEU
1	B	336	ASP
1	B	342	THR
1	B	378	SER
1	B	415	SER
1	B	449	LEU
1	C	343	MET
1	C	364	GLU
1	C	378	SER
1	C	466	VAL
1	D	325	ILE
1	D	335	GLN
1	D	415	SER
1	D	431	MET
1	E	342	THR
1	E	362	HIS
1	E	367	LEU
1	E	415	SER
1	E	427	THR
1	E	430	THR
1	E	459	GLU
1	E	462	LEU
1	F	319	MET
1	F	325	ILE
1	F	393	PHE
1	F	400	CYS
1	F	436	LYS
1	F	444	ILE
1	F	450	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	GLN
1	A	357	HIS

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Mol	Chain	Res	Type
1	A	362	HIS
1	A	385	GLN
1	B	338	GLN
1	B	362	HIS
1	C	353	ASN
1	C	426	HIS
1	C	463	ASN
1	D	335	GLN
1	E	369	ASN
1	E	450	ASN
1	F	398	HIS
1	F	407	HIS
1	F	426	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](#)

6 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	F	501	-	23,25,25	1.63	4 (17%)	24,37,37	3.22	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CJA	B	501	-	23,25,25	1.66	4 (17%)	24,37,37	2.54	6 (25%)
2	CJA	E	501	-	23,25,25	1.67	4 (17%)	24,37,37	3.51	6 (25%)
2	CJA	C	501	-	23,25,25	1.70	5 (21%)	24,37,37	2.38	5 (20%)
2	CJA	D	501	-	23,25,25	1.64	4 (17%)	24,37,37	2.79	6 (25%)
2	CJA	A	501	-	23,25,25	1.59	4 (17%)	24,37,37	2.43	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	F	501	-	-	0/13/22/22	0/3/3/3
2	CJA	B	501	-	-	0/13/22/22	0/3/3/3
2	CJA	E	501	-	-	0/13/22/22	0/3/3/3
2	CJA	C	501	-	-	0/13/22/22	0/3/3/3
2	CJA	D	501	-	-	0/13/22/22	0/3/3/3
2	CJA	A	501	-	-	1/13/22/22	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	CJA	C23-C22	-5.65	1.39	1.48
2	E	501	CJA	C23-C22	-5.58	1.39	1.48
2	D	501	CJA	C23-C22	-5.25	1.40	1.48
2	F	501	CJA	C23-C22	-5.25	1.40	1.48
2	A	501	CJA	C23-C22	-5.24	1.40	1.48
2	C	501	CJA	C23-C22	-5.02	1.40	1.48
2	E	501	CJA	C03-S04	-4.05	1.65	1.72
2	B	501	CJA	C03-S04	-3.95	1.65	1.72
2	D	501	CJA	C03-S04	-3.94	1.65	1.72
2	F	501	CJA	C03-S04	-3.68	1.65	1.72
2	A	501	CJA	C03-S04	-3.52	1.66	1.72
2	C	501	CJA	C05-C06	-3.49	1.34	1.37
2	C	501	CJA	C03-S04	-2.86	1.67	1.72
2	F	501	CJA	C05-S04	-2.80	1.66	1.70
2	D	501	CJA	C05-S04	-2.75	1.66	1.70
2	A	501	CJA	C05-S04	-2.49	1.66	1.70
2	F	501	CJA	C23-C06	2.49	1.45	1.40
2	E	501	CJA	C23-C06	2.49	1.45	1.40
2	B	501	CJA	C23-C06	2.46	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CJA	C23-C06	2.45	1.45	1.40
2	B	501	CJA	C05-S04	-2.41	1.66	1.70
2	D	501	CJA	C23-C06	2.41	1.45	1.40
2	E	501	CJA	C05-S04	-2.38	1.66	1.70
2	C	501	CJA	C05-S04	-2.29	1.67	1.70
2	C	501	CJA	C23-C06	2.06	1.44	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	CJA	C14-S13-C12	15.66	121.77	101.65
2	F	501	CJA	C14-S13-C12	13.95	119.57	101.65
2	D	501	CJA	C14-S13-C12	11.77	116.77	101.65
2	B	501	CJA	C14-S13-C12	10.17	114.71	101.65
2	A	501	CJA	C14-S13-C12	9.33	113.63	101.65
2	C	501	CJA	C14-S13-C12	7.62	111.44	101.65
2	C	501	CJA	C05-C06-C23	4.51	113.58	105.29
2	C	501	CJA	C07-C08-C09	3.82	120.05	110.71
2	A	501	CJA	C05-C06-C23	3.56	111.83	105.29
2	D	501	CJA	C05-C06-C23	3.55	111.83	105.29
2	F	501	CJA	C05-C06-C23	3.54	111.80	105.29
2	E	501	CJA	C05-C06-C23	3.47	111.66	105.29
2	B	501	CJA	C05-C06-C23	3.31	111.37	105.29
2	F	501	CJA	C10-N11-C12	3.19	118.00	115.39
2	C	501	CJA	C07-C06-C05	-3.16	123.37	130.92
2	E	501	CJA	C10-N11-C12	3.12	117.94	115.39
2	C	501	CJA	C09-C22-N21	-3.01	119.43	122.70
2	A	501	CJA	C10-N11-C12	2.95	117.81	115.39
2	B	501	CJA	C10-N11-C12	2.94	117.80	115.39
2	D	501	CJA	C10-N11-C12	2.91	117.77	115.39
2	B	501	CJA	N11-C12-N21	-2.83	124.06	127.57
2	A	501	CJA	C23-C22-N21	2.78	121.07	118.02
2	F	501	CJA	N11-C12-N21	-2.77	124.14	127.57
2	A	501	CJA	N11-C12-N21	-2.76	124.14	127.57
2	E	501	CJA	N11-C12-N21	-2.71	124.21	127.57
2	A	501	CJA	C09-C22-N21	-2.68	119.78	122.70
2	F	501	CJA	C23-C22-N21	2.59	120.87	118.02
2	D	501	CJA	N11-C12-N21	-2.56	124.40	127.57
2	F	501	CJA	C09-C22-N21	-2.53	119.94	122.70
2	D	501	CJA	C23-C22-N21	2.50	120.76	118.02
2	D	501	CJA	C09-C22-N21	-2.46	120.03	122.70
2	B	501	CJA	C09-C22-N21	-2.42	120.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	CJA	C23-C22-N21	2.18	120.42	118.02
2	E	501	CJA	C09-C22-N21	-2.17	120.34	122.70
2	B	501	CJA	C07-C08-C09	2.04	115.69	110.71

There are no chirality outliers.

All (1) torsion outliers are listed below:

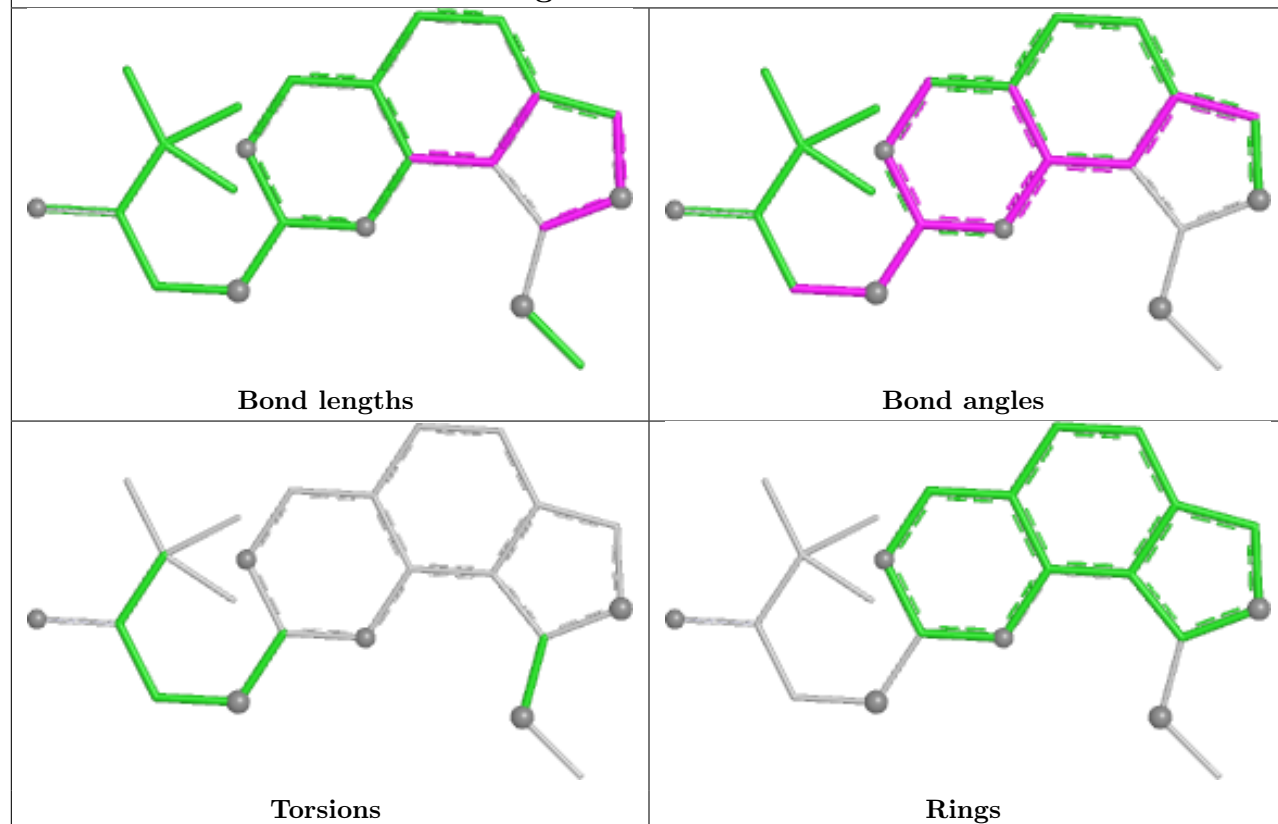
Mol	Chain	Res	Type	Atoms
2	A	501	CJA	C14-C15-C17-C19

There are no ring outliers.

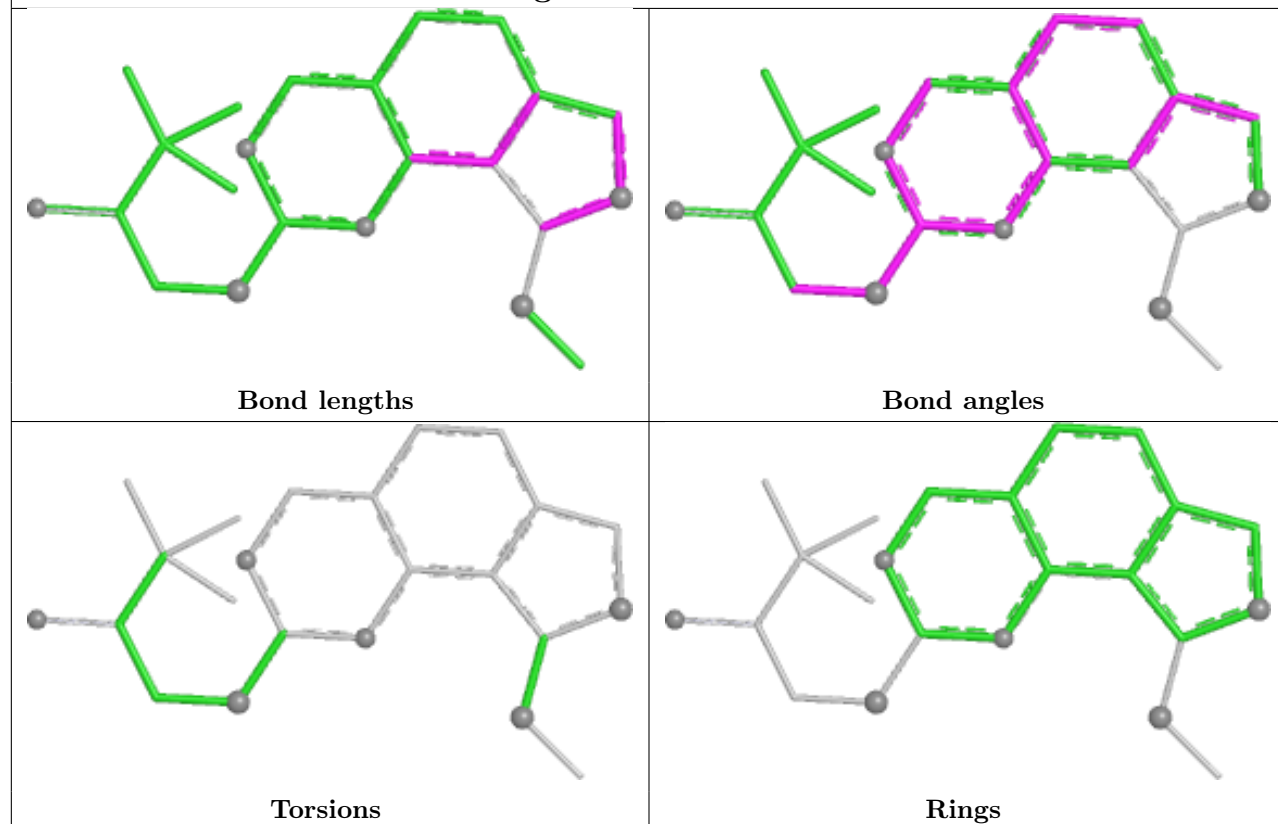
No monomer is involved in short contacts.

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.

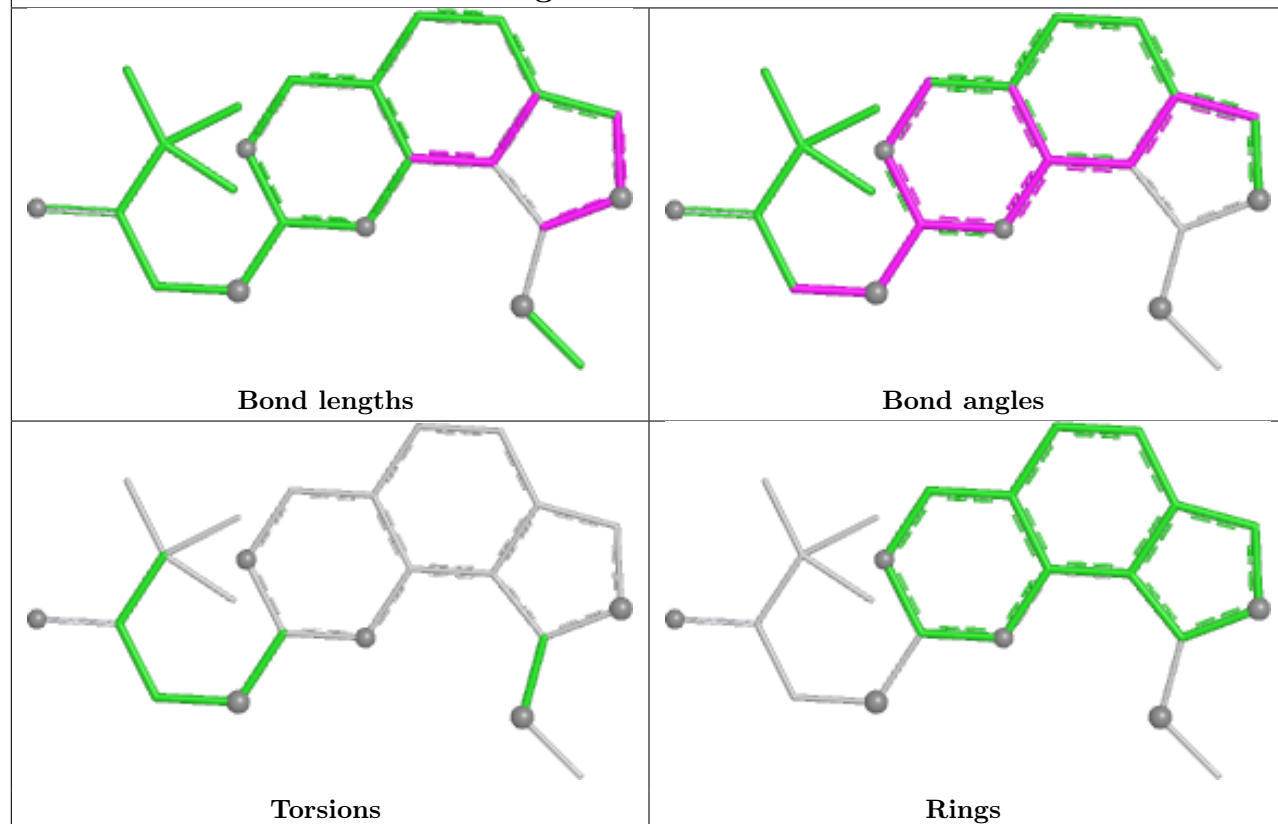
Ligand CJA F 501



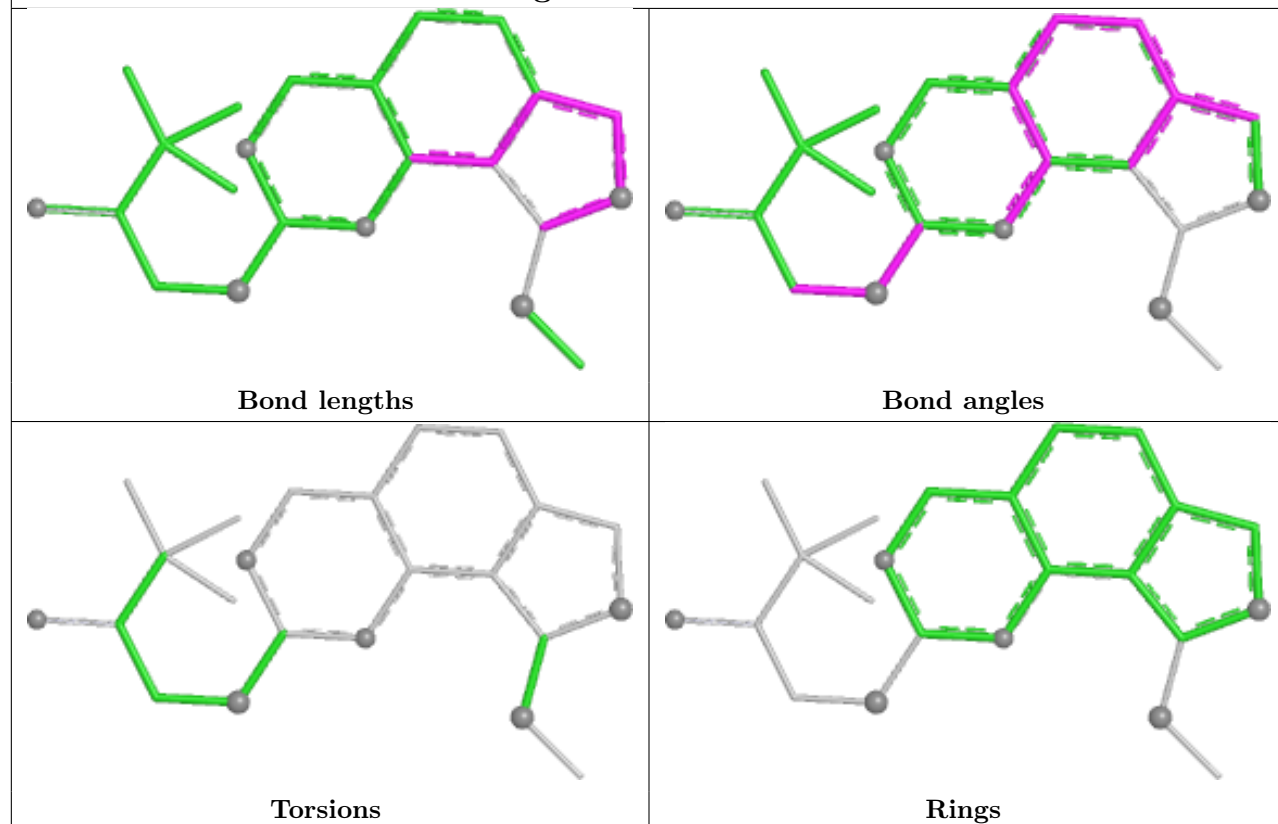
Ligand CJA B 501



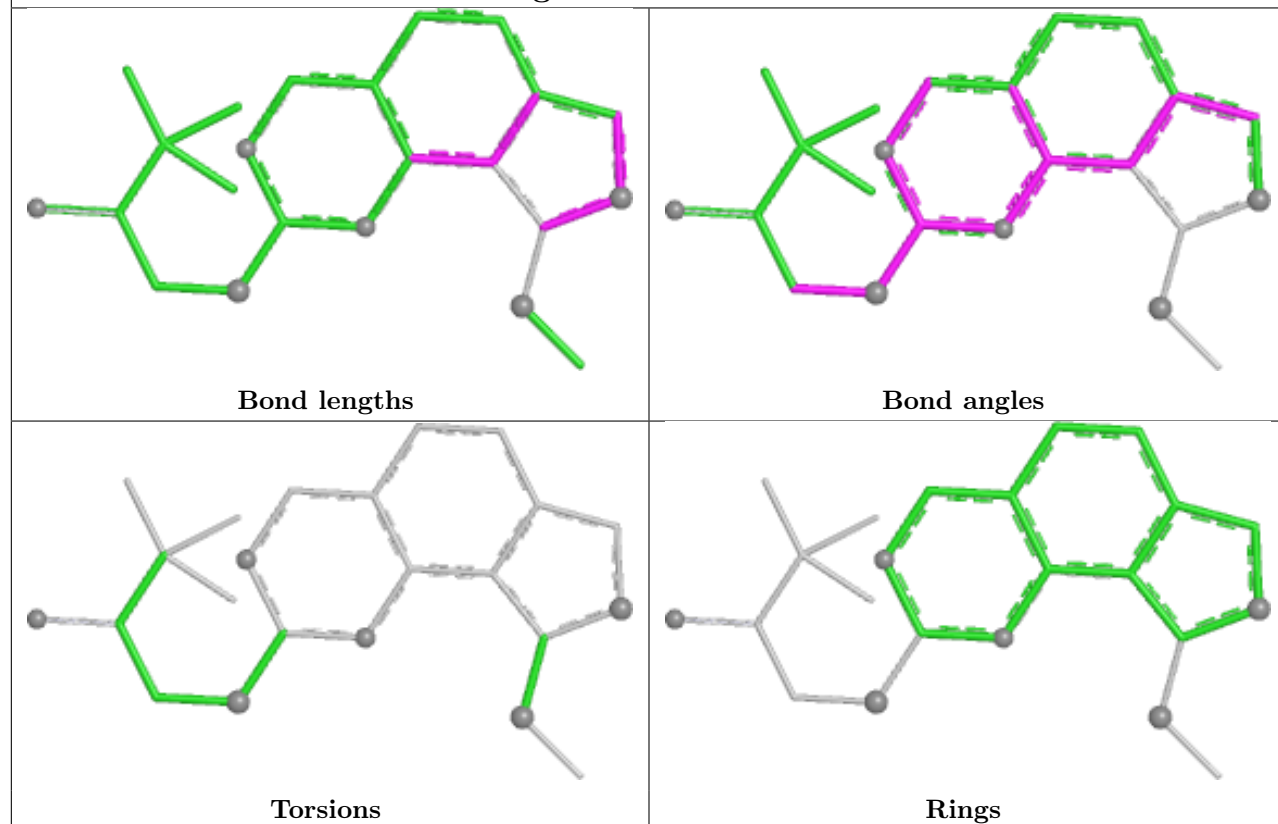
Ligand CJA E 501



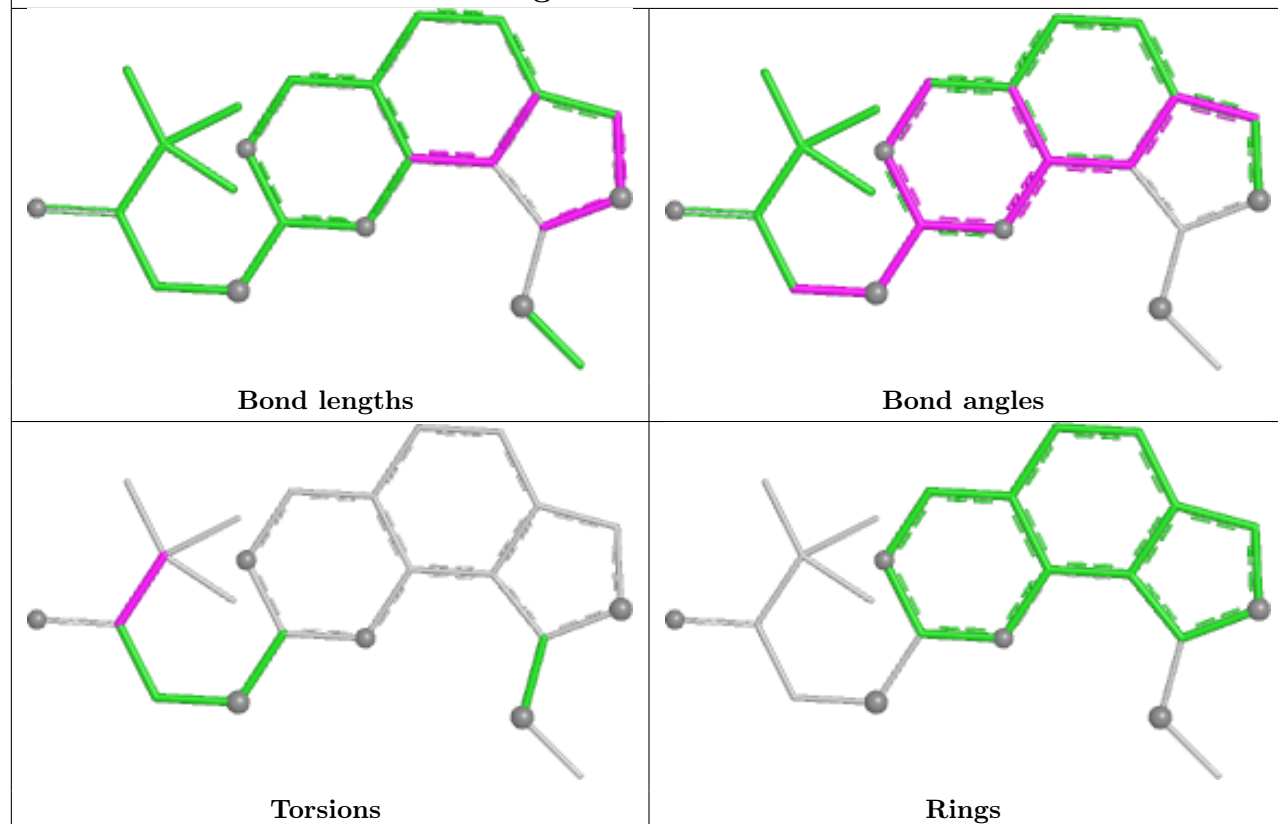
Ligand CJA C 501



Ligand CJA D 501



Ligand CJA A 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%)	0.54	9 (6%)	28 26	51, 73, 100, 125	0
1	B	148/149 (99%)	0.29	7 (4%)	37 34	50, 67, 95, 114	0
1	C	148/149 (99%)	0.21	6 (4%)	42 39	48, 65, 93, 159	0
1	D	147/149 (98%)	0.37	11 (7%)	22 20	53, 70, 97, 123	0
1	E	145/149 (97%)	0.63	12 (8%)	19 18	57, 80, 104, 136	0
1	F	148/149 (99%)	0.96	20 (13%)	8 7	60, 85, 109, 135	0
All	All	884/894 (98%)	0.50	65 (7%)	22 20	48, 72, 102, 159	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	467	ALA	7.3
1	C	408	CYS	7.3
1	B	467	ALA	6.4
1	E	320	ALA	4.4
1	A	466	VAL	4.2
1	F	466	VAL	4.1
1	D	320	ALA	3.8
1	B	465	GLY	3.6
1	D	466	VAL	3.6
1	A	319	MET	3.5
1	F	444	ILE	3.4
1	C	460	GLU	3.4
1	F	319	MET	3.3
1	D	322	LEU	3.2
1	E	464	ASN	3.1
1	F	400	CYS	3.1
1	A	460	GLU	3.1
1	F	399	GLN	3.1
1	F	401	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	460	GLU	3.0
1	D	364	GLU	2.9
1	B	466	VAL	2.9
1	A	465	GLY	2.8
1	F	464	ASN	2.8
1	E	426	HIS	2.8
1	B	408	CYS	2.8
1	F	367	LEU	2.7
1	A	464	ASN	2.7
1	B	322	LEU	2.7
1	E	322	LEU	2.6
1	E	321	GLU	2.6
1	D	335	GLN	2.5
1	A	462	LEU	2.5
1	B	335	GLN	2.5
1	A	321	GLU	2.5
1	D	406	ILE	2.5
1	E	328	PHE	2.5
1	F	460	GLU	2.4
1	D	399	GLN	2.4
1	F	438	VAL	2.3
1	F	437	PHE	2.3
1	C	466	VAL	2.3
1	F	445	ILE	2.3
1	A	433	ASP	2.3
1	C	379	ASN	2.3
1	B	320	ALA	2.3
1	F	465	GLY	2.2
1	E	427	THR	2.2
1	F	325	ILE	2.2
1	F	361	TYR	2.2
1	F	447	PRO	2.2
1	F	395	GLU	2.2
1	E	430	THR	2.2
1	C	410	ALA	2.2
1	A	428	ARG	2.2
1	D	428	ARG	2.2
1	D	465	GLY	2.1
1	E	463	ASN	2.1
1	E	452	MET	2.1
1	D	431	MET	2.1
1	E	462	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	322	LEU	2.0
1	F	360	LEU	2.0
1	D	410	ALA	2.0
1	F	430	THR	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](#)

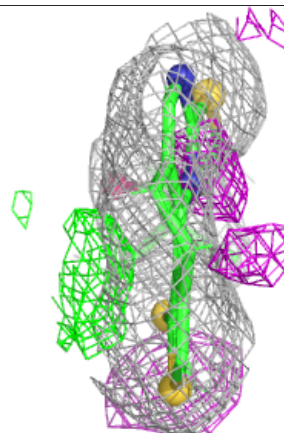
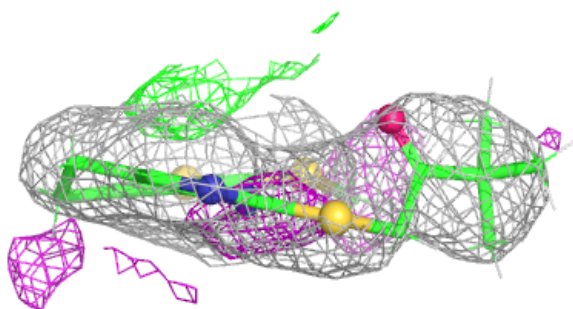
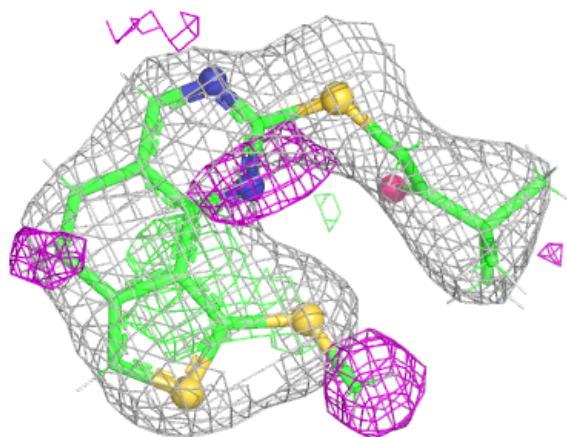
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CJA	E	501	23/23	0.81	0.19	58,81,91,102	0
2	CJA	D	501	23/23	0.88	0.16	45,67,93,113	0
2	CJA	F	501	23/23	0.88	0.15	55,72,87,93	0
2	CJA	A	501	23/23	0.90	0.14	49,63,77,84	0
2	CJA	B	501	23/23	0.92	0.12	50,64,86,90	0
2	CJA	C	501	23/23	0.95	0.09	51,64,73,88	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.

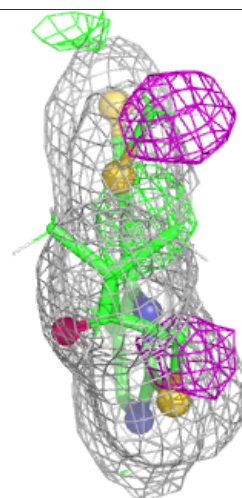
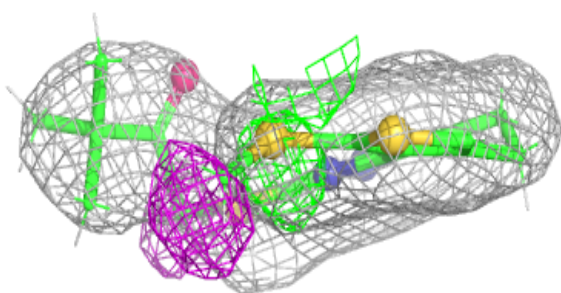
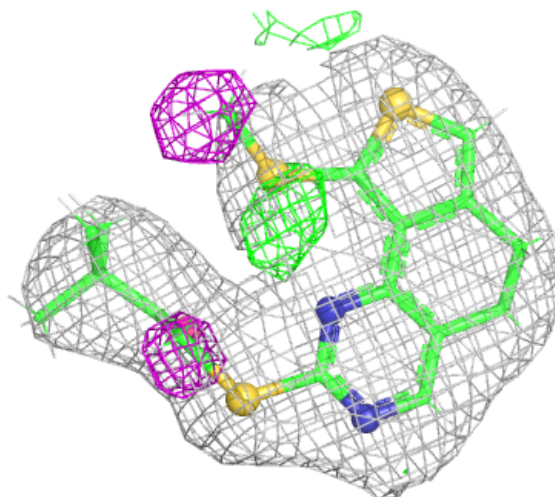
Electron density around CJA E 501:

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



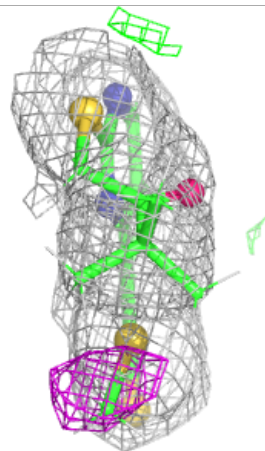
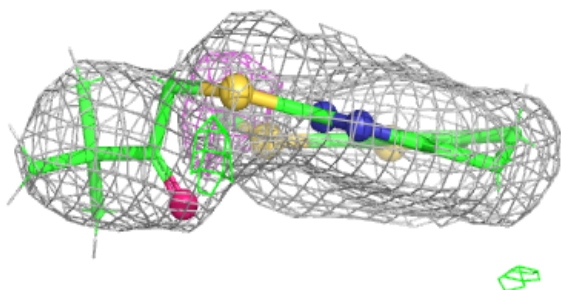
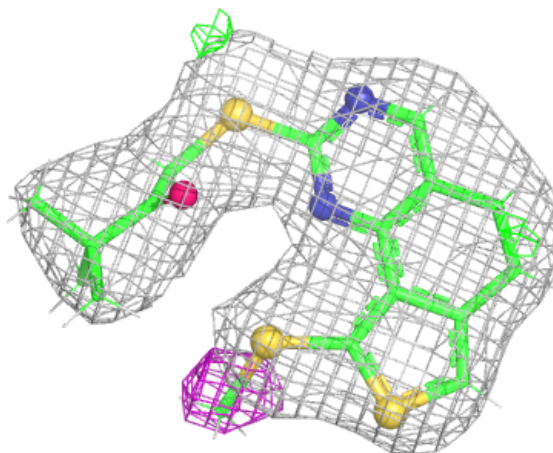
Electron density around CJA D 501:

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



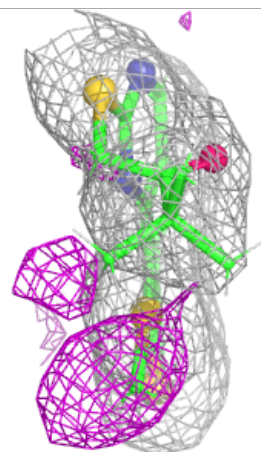
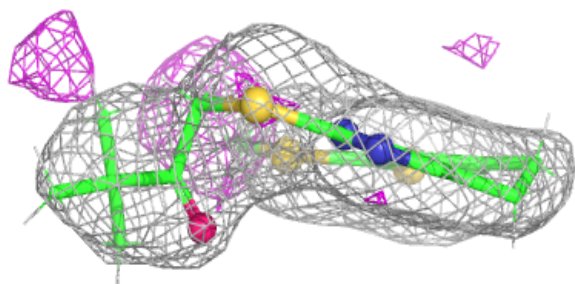
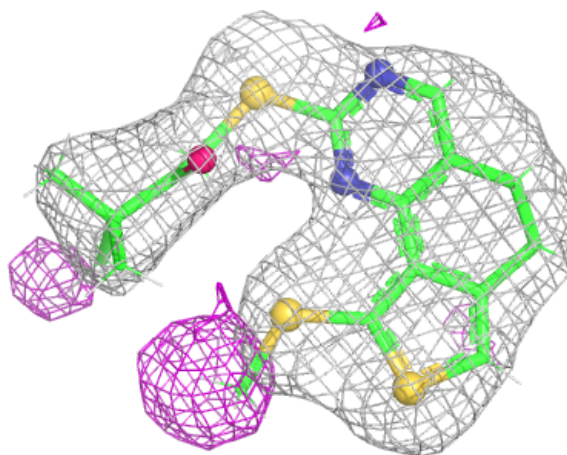
Electron density around CJA F 501:

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



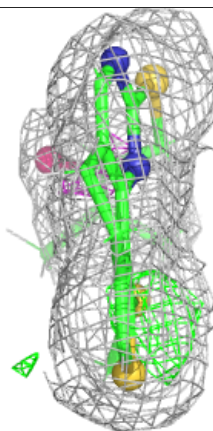
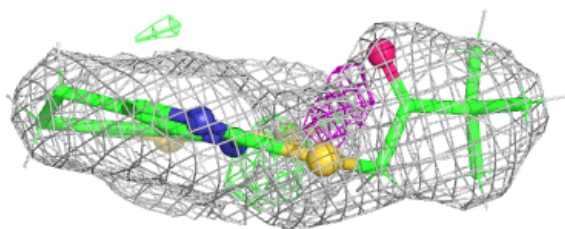
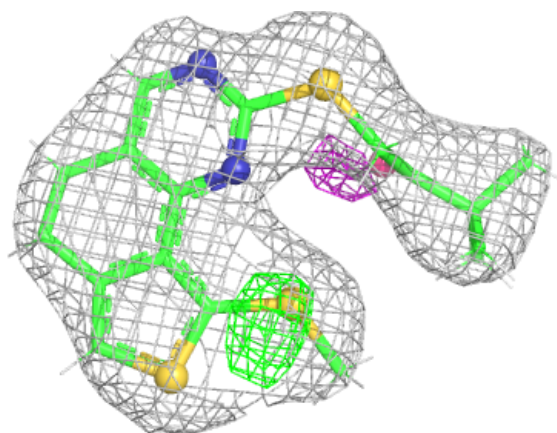
Electron density around CJA A 501:

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



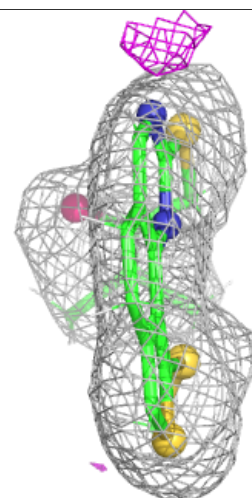
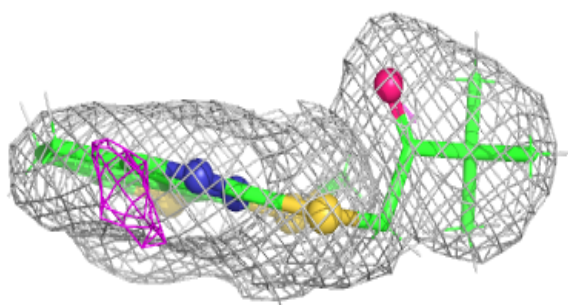
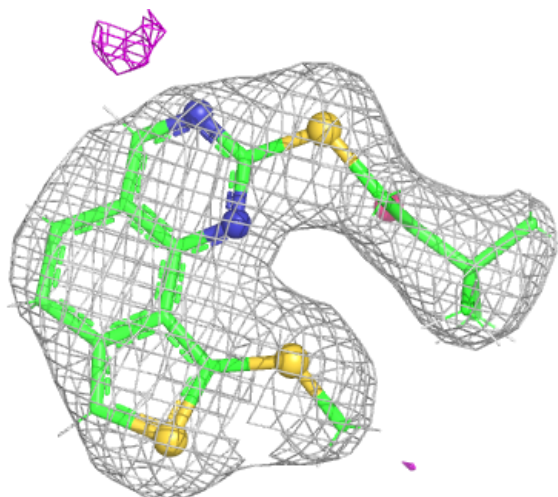
Electron density around CJA B 501:

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



Electron density around CJA 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.