Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2025 – 01:17 PM EDT

PDB ID	:	9BU4 / pdb_00009bu4
Title	:	Crystal structure of an MKP5 mutant, Y435W, in complex with an allosteric inhibitor
Authors	:	Manjula, R.; Bennett, A.M.; Lolis, E.
Deposited on	:	2024-05-16
Resolution	:	2.90 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:

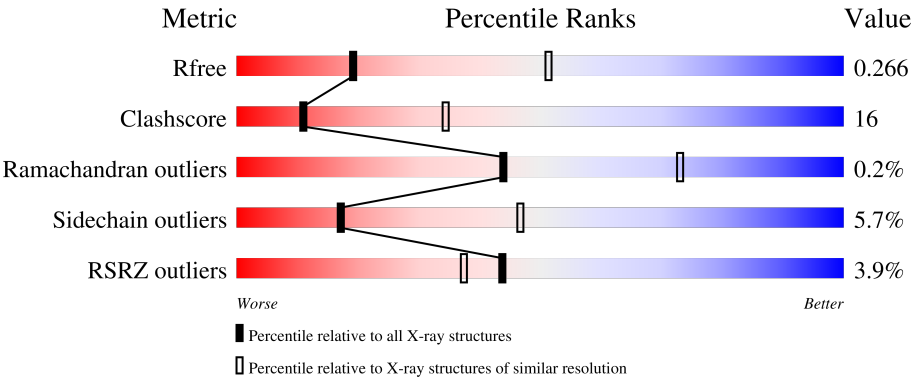
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.90 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	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	148	3% 75% 23%
1	B	148	% 70% 28%
1	C	148	% 68% 30%
1	D	148	% 72% 28%
1	E	148	4% 67% 30%

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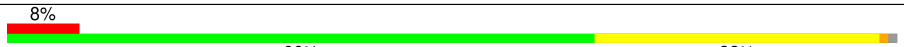
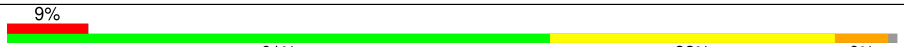
Mol	Chain	Length	Quality of chain
1	F	148	
1	G	148	
1	H	148	
1	I	148	
1	J	148	
1	K	148	
1	L	148	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27622 atoms, of which 13514 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
			2340	761	1155	200	217	7			
1	B	147	Total	C	H	N	O	S	0	0	0
			2337	758	1157	200	215	7			
1	C	147	Total	C	H	N	O	S	0	0	0
			2328	756	1150	200	215	7			
1	D	147	Total	C	H	N	O	S	0	0	0
			2266	744	1109	193	213	7			
1	E	147	Total	C	H	N	O	S	0	0	0
			2296	749	1132	198	210	7			
1	F	146	Total	C	H	N	O	S	0	0	0
			2268	742	1116	194	209	7			
1	G	147	Total	C	H	N	O	S	0	0	0
			2297	750	1131	196	213	7			
1	H	147	Total	C	H	N	O	S	0	0	0
			2317	753	1144	200	213	7			
1	I	147	Total	C	H	N	O	S	0	0	0
			2225	736	1087	190	206	6			
1	J	146	Total	C	H	N	O	S	0	0	0
			2142	715	1035	181	204	7			
1	K	146	Total	C	H	N	O	S	0	0	0
			2146	716	1033	185	205	7			
1	L	143	Total	C	H	N	O	S	0	0	0
			2123	708	1025	184	200	6			

There are 24 discrepancies between the modelled and reference sequences:

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

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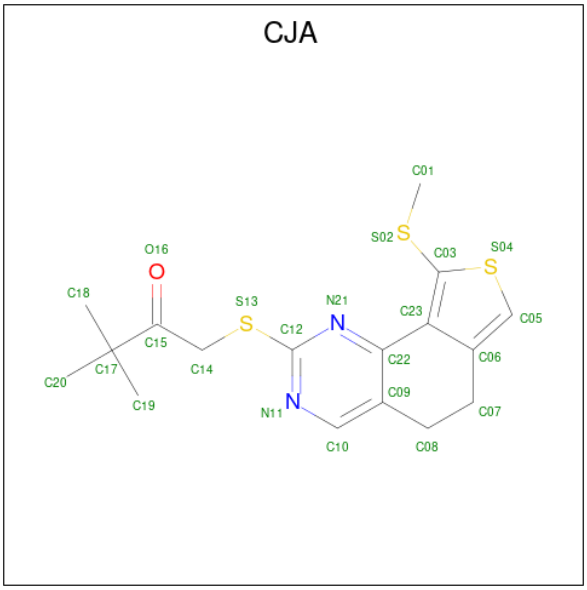
Chain	Residue	Modelled	Actual	Comment	Reference
C	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
D	319	MET	-	initiating methionine	UNP Q9Y6W6
D	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
E	319	MET	-	initiating methionine	UNP Q9Y6W6
E	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
F	319	MET	-	initiating methionine	UNP Q9Y6W6
F	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
G	319	MET	-	initiating methionine	UNP Q9Y6W6
G	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
H	319	MET	-	initiating methionine	UNP Q9Y6W6
H	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
I	319	MET	-	initiating methionine	UNP Q9Y6W6
I	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
J	319	MET	-	initiating methionine	UNP Q9Y6W6
J	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
K	319	MET	-	initiating methionine	UNP Q9Y6W6
K	435	TRP	TYR	engineered mutation	UNP Q9Y6W6
L	319	MET	-	initiating methionine	UNP Q9Y6W6
L	435	TRP	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: $C_{17}H_{20}N_2OS_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	C	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	D	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	E	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	F	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	G	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	H	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	I	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	J	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	K	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		
2	L	1	Total	C	H	N	O	S	0	0
			43	17	20	2	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	1	Total	O	0	0
			1	1		
3	C	2	Total	O	0	0
			2	2		
3	D	2	Total	O	0	0
			2	2		
3	E	3	Total	O	0	0
			3	3		
3	F	3	Total	O	0	0
			3	3		
3	G	3	Total	O	0	0
			3	3		
3	H	2	Total	O	0	0
			2	2		

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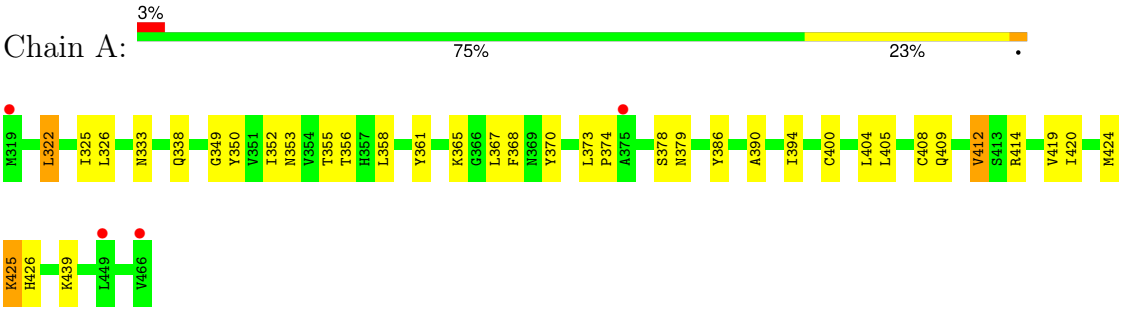
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total O 1 1	0	0
3	J	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

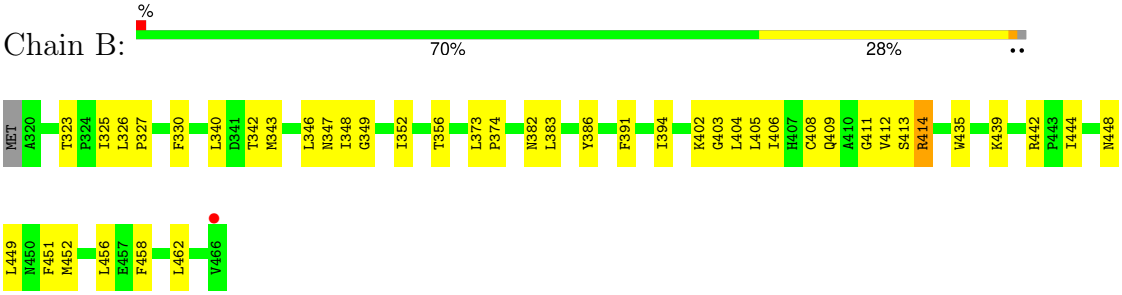
• Molecule 1: Dual specificity protein phosphatase 10

Chain A:



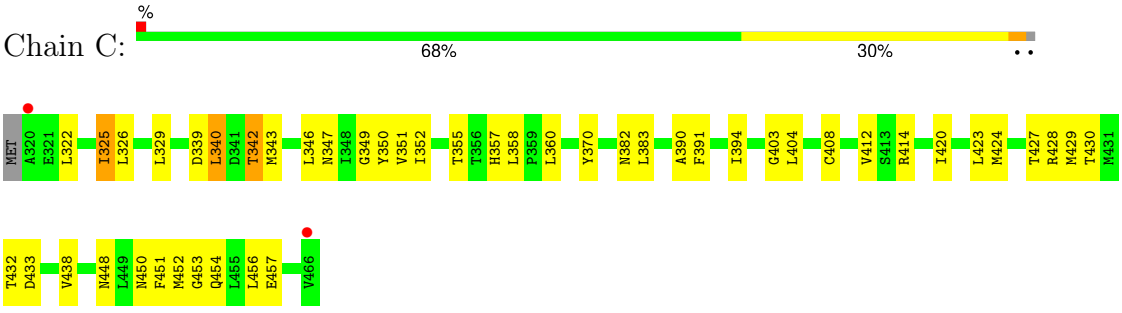
• Molecule 1: Dual specificity protein phosphatase 10

Chain B:



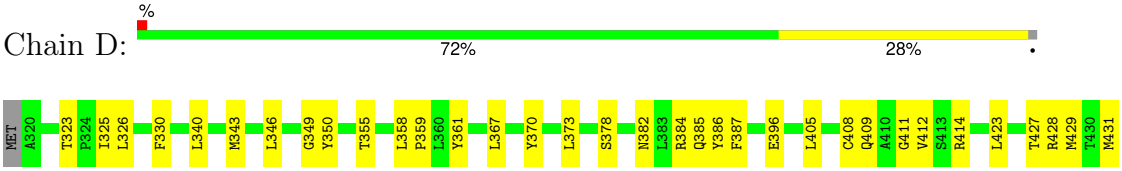
• Molecule 1: Dual specificity protein phosphatase 10

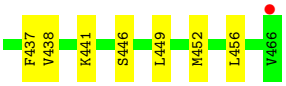
Chain C:



• Molecule 1: Dual specificity protein phosphatase 10

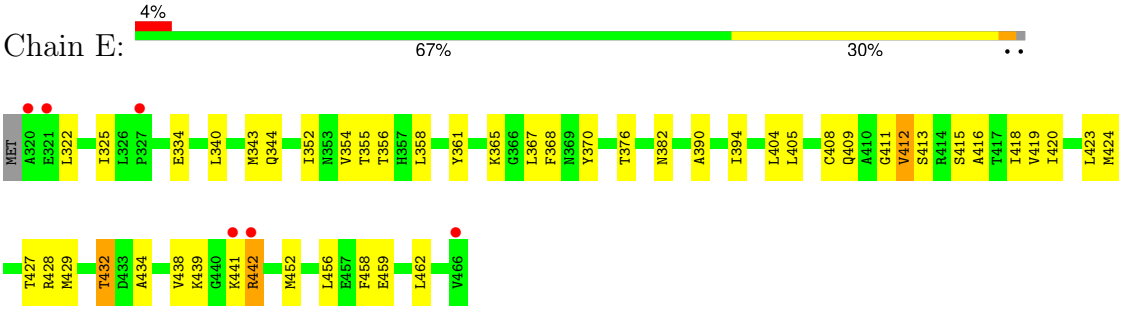
Chain D:





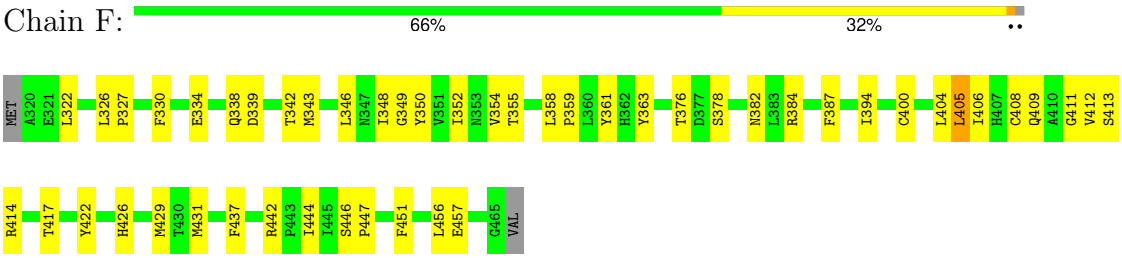
• Molecule 1: Dual specificity protein phosphatase 10

Chain E:



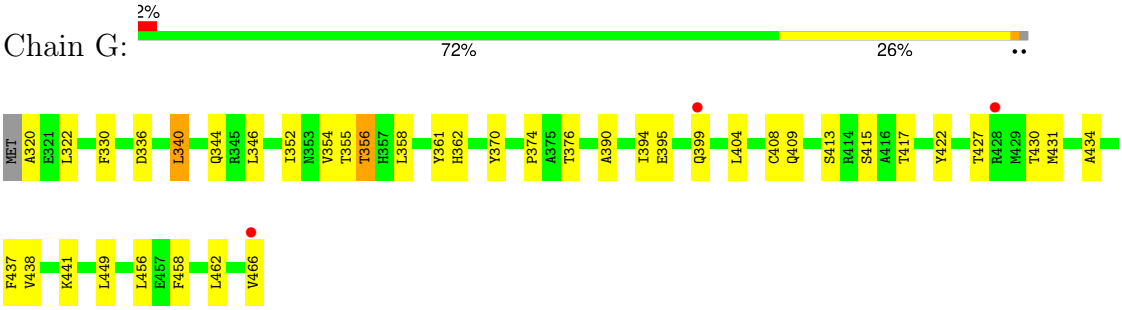
• Molecule 1: Dual specificity protein phosphatase 10

Chain F:



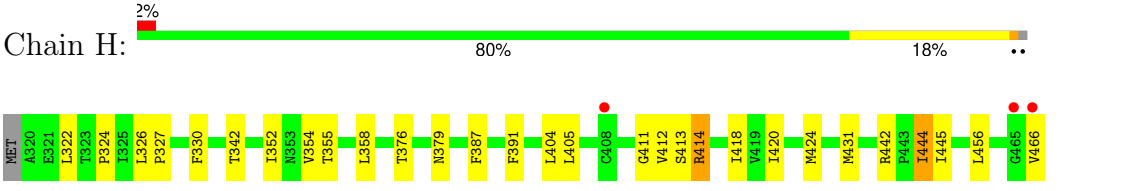
• Molecule 1: Dual specificity protein phosphatase 10

Chain G:



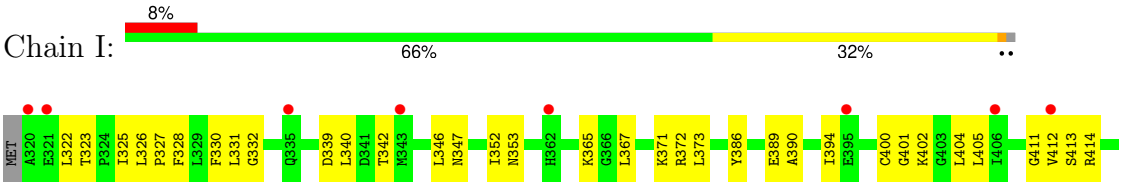
• Molecule 1: Dual specificity protein phosphatase 10

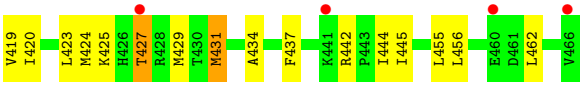
Chain H:



• Molecule 1: Dual specificity protein phosphatase 10

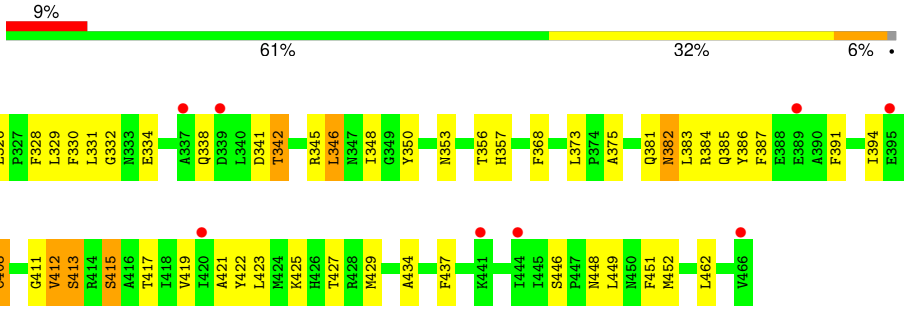
Chain I:





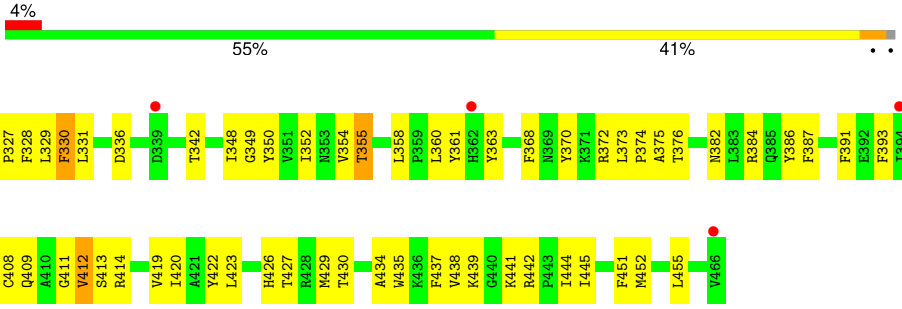
• Molecule 1: Dual specificity protein phosphatase 10

Chain J:



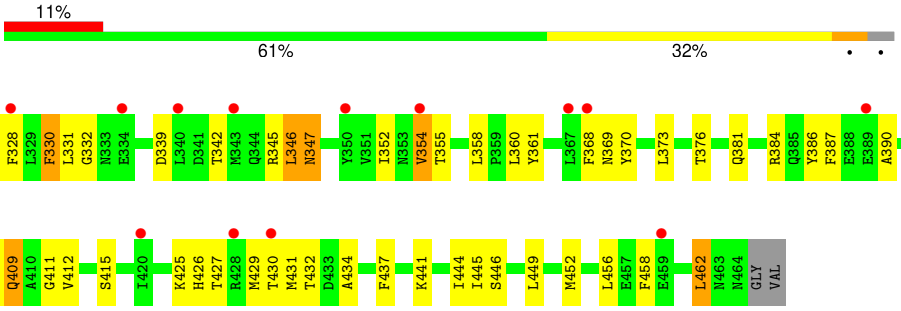
• Molecule 1: Dual specificity protein phosphatase 10

Chain K:



• Molecule 1: Dual specificity protein phosphatase 10

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.71Å 55.80Å 275.91Å 90.36° 93.82° 106.88°	Depositor
Resolution (Å)	42.73 – 2.90 42.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.73-2.90) 98.6 (42.73-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.18_3845: ???)	Depositor
R, R_{free}	0.215 , 0.266 0.217 , 0.266	Depositor DCC
R_{free} test set	3472 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.049 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	27622	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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: 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	0.56	1/1212 (0.1%)	0.59	0/1641
1	B	0.39	0/1207	0.56	0/1634
1	C	0.37	0/1205	0.57	0/1631
1	D	0.45	0/1184	0.66	0/1607
1	E	0.32	0/1191	0.57	1/1615 (0.1%)
1	F	0.34	0/1179	0.59	1/1599 (0.1%)
1	G	0.39	0/1193	0.59	0/1618
1	H	0.45	0/1200	0.67	1/1625 (0.1%)
1	I	0.39	0/1165	0.60	0/1585
1	J	0.37	0/1132	0.60	0/1542
1	K	0.38	0/1139	0.57	1/1553 (0.1%)
1	L	0.35	0/1125	0.55	0/1533
All	All	0.40	1/14132 (0.0%)	0.60	4/19183 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	H	0	1
1	I	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	LEU	N-CA	-12.31	1.37	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	359	PRO	N-CA-CB	-6.87	96.49	103.15
1	K	355	THR	CA-CB-OG1	-6.41	99.99	109.60
1	H	391	PHE	CA-CB-CG	5.57	119.37	113.80
1	E	439	LYS	N-CA-CB	-5.44	101.07	110.32

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	ARG	Sidechain
1	B	414	ARG	Sidechain
1	C	414	ARG	Sidechain
1	D	414	ARG	Sidechain
1	E	442	ARG	Sidechain
1	H	414	ARG	Sidechain
1	I	414	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	1185	1155	1157	18	0
1	B	1180	1157	1157	33	0
1	C	1178	1150	1150	38	0
1	D	1157	1109	1107	26	0
1	E	1164	1132	1132	36	0
1	F	1152	1116	1114	44	0
1	G	1166	1131	1131	27	0
1	H	1173	1144	1144	19	0
1	I	1138	1087	1083	39	0
1	J	1107	1035	1034	53	0
1	K	1113	1033	1032	65	0
1	L	1098	1025	1024	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	0
2	E	23	20	0	0	0
2	F	23	20	0	1	0
2	G	23	20	0	0	0
2	H	23	20	0	0	0
2	I	23	20	0	0	0
2	J	23	20	0	0	0
2	K	23	20	0	0	0
2	L	23	20	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	1	0
3	G	3	0	0	0	0
3	H	2	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
All	All	14108	13514	13265	444	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 16.

All (444) 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:I:339:ASP:OD1	1:I:342:THR:OG1	1.71	1.04
1:C:430:THR:OG1	1:C:433:ASP:OD1	1.81	0.98
1:K:373:LEU:HD13	1:K:386:TYR:HB3	1.52	0.90
1:L:358:LEU:HD11	1:L:409:GLN:HG2	1.57	0.86
1:J:342:THR:O	1:J:346:LEU:HD12	1.76	0.86
1:I:394:ILE:HD13	1:I:404:LEU:HD13	1.57	0.86
1:J:342:THR:HG22	1:J:346:LEU:HD11	1.55	0.85
1:I:429:MET:HE1	1:I:437:PHE:HD1	1.42	0.85
1:L:330:PHE:CE2	1:L:346:LEU:HD23	2.10	0.84
1:K:409:GLN:OE1	1:K:414:ARG:NH2	2.11	0.83
1:I:429:MET:HE1	1:I:437:PHE:CD1	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:408:CYS:SG	1:J:415:SER:OG	2.33	0.82
1:E:358:LEU:HD22	1:E:361:TYR:OH	1.81	0.80
1:C:339:ASP:OD1	1:C:342:THR:OG1	2.02	0.77
1:G:355:THR:HG21	1:G:358:LEU:HD12	1.68	0.75
1:B:342:THR:O	1:B:346:LEU:HD12	1.86	0.75
1:L:373:LEU:HD22	1:L:386:TYR:HB3	1.68	0.75
1:B:330:PHE:CE1	1:B:346:LEU:HD23	2.24	0.71
1:G:408:CYS:SG	1:G:409:GLN:N	2.63	0.71
1:I:404:LEU:HD23	1:I:405:LEU:N	2.06	0.70
1:J:346:LEU:HD12	1:J:346:LEU:H	1.56	0.70
1:K:355:THR:HG21	1:K:358:LEU:HD12	1.74	0.69
1:H:352:ILE:HG13	1:H:404:LEU:HD21	1.75	0.69
1:B:458:PHE:CE1	1:B:462:LEU:HD21	2.27	0.69
1:K:422:TYR:CE1	1:K:426:HIS:CD2	2.81	0.68
1:H:322:LEU:HD12	1:H:322:LEU:O	1.92	0.68
1:K:350:TYR:CD2	1:K:397:ALA:HB2	2.28	0.68
1:J:425:LYS:HA	1:J:462:LEU:HD11	1.76	0.68
1:E:459:GLU:HA	1:E:462:LEU:HD12	1.76	0.68
1:F:400:CYS:SG	3:F:603:HOH:O	2.51	0.68
1:J:353:ASN:OD1	1:J:407:HIS:NE2	2.28	0.67
1:L:360:LEU:HB3	1:L:370:TYR:CE2	2.29	0.67
1:K:420:ILE:HA	1:K:423:LEU:HD23	1.76	0.67
1:F:354:VAL:O	1:F:354:VAL:HG12	1.94	0.67
1:K:361:TYR:O	1:K:370:TYR:OH	2.04	0.66
1:K:375:ALA:O	1:K:414:ARG:NH1	2.29	0.66
1:K:451:PHE:O	1:K:455:LEU:HD12	1.95	0.66
1:E:408:CYS:SG	1:E:409:GLN:N	2.69	0.65
1:J:397:ALA:HB1	1:J:402:LYS:O	1.96	0.65
1:I:331:LEU:HD12	1:I:332:GLY:N	2.12	0.65
1:I:423:LEU:HA	1:I:427:THR:OG1	1.95	0.65
1:K:368:PHE:HB2	1:K:370:TYR:HE2	1.62	0.65
1:K:322:LEU:CD2	1:K:336:ASP:HB3	2.27	0.65
1:K:384:ARG:HH11	1:K:384:ARG:HG2	1.62	0.64
1:K:429:MET:HE1	1:K:437:PHE:CD2	2.32	0.64
1:I:404:LEU:HD23	1:I:405:LEU:C	2.23	0.64
1:L:360:LEU:HB3	1:L:370:TYR:CD2	2.33	0.64
1:K:434:ALA:O	1:K:438:VAL:HG23	1.99	0.63
1:B:342:THR:O	1:B:346:LEU:CD1	2.47	0.63
1:H:355:THR:HG21	1:H:358:LEU:HD12	1.81	0.62
1:A:355:THR:HG21	1:A:358:LEU:HD12	1.81	0.62
1:F:358:LEU:HD11	1:F:409:GLN:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:360:LEU:HD23	1:K:370:TYR:HD1	1.64	0.62
1:L:331:LEU:HD23	1:L:332:GLY:N	2.14	0.62
1:K:382:ASN:OD1	1:K:384:ARG:N	2.33	0.62
1:F:413:SER:O	1:F:417:THR:OG1	2.18	0.61
1:G:352:ILE:HG13	1:G:404:LEU:HD21	1.81	0.61
1:L:449:LEU:HD12	1:L:452:MET:HE3	1.83	0.61
1:G:394:ILE:HD13	1:G:404:LEU:HD13	1.81	0.61
1:F:342:THR:O	1:F:346:LEU:HD13	2.01	0.60
1:G:458:PHE:CZ	1:G:462:LEU:HD11	2.36	0.60
1:L:361:TYR:O	1:L:370:TYR:OH	2.16	0.60
1:B:342:THR:HG22	1:B:346:LEU:HD13	1.84	0.60
1:K:419:VAL:O	1:K:423:LEU:HD22	2.02	0.60
1:L:347:ASN:CG	1:L:347:ASN:O	2.45	0.60
1:L:449:LEU:HD12	1:L:452:MET:CE	2.32	0.59
1:D:343:MET:HE3	1:D:405:LEU:HD13	1.83	0.59
1:F:355:THR:HG21	1:F:358:LEU:HD12	1.84	0.59
1:J:350:TYR:HD1	1:J:397:ALA:HB2	1.65	0.59
1:F:431:MET:CE	1:F:456:LEU:HD12	2.32	0.59
1:K:408:CYS:SG	1:K:409:GLN:N	2.75	0.59
1:A:352:ILE:HG13	1:A:404:LEU:HD21	1.84	0.59
1:C:429:MET:HB3	1:C:433:ASP:HB2	1.84	0.59
1:D:330:PHE:CE1	1:D:346:LEU:HD13	2.37	0.59
1:L:425:LYS:HG3	1:L:426:HIS:CD2	2.38	0.59
1:E:340:LEU:HD23	1:E:340:LEU:O	2.03	0.58
1:G:355:THR:HG21	1:G:358:LEU:CD1	2.33	0.58
1:J:413:SER:O	1:J:417:THR:OG1	2.21	0.58
1:D:373:LEU:HD22	1:D:386:TYR:HB3	1.85	0.58
1:I:394:ILE:CD1	1:I:404:LEU:HD13	2.31	0.58
1:L:369:ASN:C	1:L:370:TYR:HD1	2.12	0.58
1:J:404:LEU:HD23	1:J:405:LEU:N	2.19	0.58
1:K:352:ILE:HG13	1:K:404:LEU:HD21	1.86	0.58
1:B:404:LEU:HD23	1:B:405:LEU:N	2.19	0.57
1:D:423:LEU:O	1:D:427:THR:HB	2.04	0.57
1:L:360:LEU:HD22	1:L:370:TYR:HD2	1.69	0.57
1:L:355:THR:HG21	1:L:358:LEU:HD12	1.87	0.57
1:K:331:LEU:HD12	1:K:419:VAL:HG21	1.87	0.57
1:L:330:PHE:HE2	1:L:346:LEU:HD23	1.68	0.57
1:L:339:ASP:OD2	1:L:342:THR:OG1	2.22	0.57
1:L:369:ASN:C	1:L:370:TYR:CD1	2.82	0.57
1:E:361:TYR:O	1:E:370:TYR:OH	2.14	0.57
1:G:427:THR:HG22	1:G:427:THR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:331:LEU:HD12	1:I:332:GLY:H	1.69	0.56
1:L:425:LYS:HA	1:L:462:LEU:HD11	1.87	0.56
1:D:355:THR:HG21	1:D:358:LEU:HD12	1.87	0.56
1:D:408:CYS:SG	1:D:409:GLN:N	2.78	0.56
1:E:458:PHE:CZ	1:E:462:LEU:HD21	2.41	0.56
1:G:356:THR:HG23	1:G:374:PRO:HB2	1.86	0.56
1:J:373:LEU:HD22	1:J:386:TYR:CG	2.40	0.56
1:J:373:LEU:HD22	1:J:386:TYR:HB3	1.88	0.55
1:F:384:ARG:HD2	1:F:387:PHE:CD2	2.41	0.55
1:I:404:LEU:HD23	1:I:404:LEU:C	2.31	0.55
1:G:340:LEU:HD23	1:G:362:HIS:CG	2.42	0.55
1:G:431:MET:HE2	1:G:456:LEU:HA	1.89	0.55
1:I:420:ILE:HG22	1:I:424:MET:SD	2.47	0.55
1:L:384:ARG:CZ	1:L:458:PHE:HD1	2.19	0.55
1:E:420:ILE:O	1:E:424:MET:HG3	2.07	0.55
1:B:383:LEU:HD12	1:B:451:PHE:CE2	2.42	0.54
1:F:334:GLU:O	1:F:338:GLN:HG3	2.07	0.54
1:F:431:MET:HE1	1:F:456:LEU:CD1	2.37	0.54
1:C:452:MET:HE1	1:E:452:MET:HE1	1.89	0.54
1:B:456:LEU:HD12	1:B:456:LEU:O	2.07	0.54
1:B:408:CYS:SG	1:B:409:GLN:N	2.79	0.54
1:E:334:GLU:OE1	1:E:358:LEU:HD21	2.07	0.54
1:A:404:LEU:HD23	1:A:405:LEU:N	2.23	0.53
1:L:384:ARG:HA	1:L:387:PHE:CD2	2.43	0.53
1:B:342:THR:HG22	1:B:346:LEU:CD1	2.39	0.53
1:I:352:ILE:HG13	1:I:404:LEU:HD21	1.89	0.53
1:E:394:ILE:HG12	1:E:404:LEU:HD13	1.89	0.53
1:B:356:THR:HG22	1:B:374:PRO:HB2	1.91	0.53
1:L:330:PHE:CD2	1:L:346:LEU:HD23	2.43	0.53
1:L:346:LEU:HD12	1:L:346:LEU:N	2.24	0.53
1:D:431:MET:HE3	2:D:501:CJA:S04	2.49	0.53
1:K:326:LEU:HB3	1:K:327:PRO:CD	2.39	0.53
1:E:427:THR:HG21	1:E:429:MET:SD	2.49	0.53
1:H:354:VAL:HG12	1:H:354:VAL:O	2.08	0.53
1:K:322:LEU:HD21	1:K:336:ASP:HB3	1.91	0.53
1:C:322:LEU:HD12	1:C:322:LEU:H	1.73	0.53
1:D:437:PHE:CE2	1:D:441:LYS:HD2	2.45	0.52
1:G:390:ALA:O	1:G:394:ILE:HG12	2.09	0.52
1:C:346:LEU:HD23	1:C:346:LEU:N	2.24	0.52
1:G:356:THR:HG23	1:G:374:PRO:CB	2.39	0.52
1:I:425:LYS:HD3	1:I:462:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:THR:HG21	1:D:429:MET:HE3	1.92	0.52
1:B:326:LEU:HB3	1:B:327:PRO:HD2	1.92	0.52
1:F:339:ASP:O	1:F:343:MET:HG3	2.10	0.52
1:E:343:MET:HE3	1:E:368:PHE:CZ	2.45	0.51
1:B:435:TRP:CZ2	1:B:439:LYS:HD3	2.46	0.51
1:L:339:ASP:OD2	1:L:342:THR:N	2.35	0.51
1:E:434:ALA:O	1:E:438:VAL:HG23	2.11	0.51
1:J:394:ILE:HD13	1:J:404:LEU:HD13	1.92	0.51
1:L:390:ALA:O	1:L:394:ILE:HG13	2.11	0.51
1:B:352:ILE:HB	1:B:406:ILE:HG13	1.93	0.51
1:F:429:MET:HE1	1:F:437:PHE:CD2	2.46	0.51
1:F:408:CYS:SG	1:F:412:VAL:HA	2.51	0.51
1:H:444:ILE:HD12	1:H:444:ILE:H	1.75	0.51
1:I:431:MET:HE2	1:I:456:LEU:HA	1.93	0.51
1:J:382:ASN:C	1:J:382:ASN:OD1	2.53	0.51
1:C:390:ALA:O	1:C:394:ILE:HG13	2.11	0.51
1:E:352:ILE:HG13	1:E:404:LEU:HD21	1.92	0.51
1:E:404:LEU:HD23	1:E:405:LEU:N	2.26	0.51
1:J:427:THR:HG21	1:J:429:MET:HE3	1.93	0.51
1:C:325:ILE:HD12	1:C:438:VAL:HG22	1.93	0.50
1:J:326:LEU:HB2	1:J:329:LEU:HB3	1.94	0.50
1:L:411:GLY:HA3	1:L:446:SER:HB3	1.94	0.50
1:C:448:ASN:OD1	1:C:451:PHE:N	2.33	0.50
1:E:325:ILE:HG13	1:E:419:VAL:HG11	1.93	0.50
1:J:427:THR:O	1:J:427:THR:HG22	2.11	0.50
1:A:390:ALA:O	1:A:394:ILE:HG13	2.11	0.50
1:C:427:THR:CG2	1:C:429:MET:HG3	2.42	0.50
1:A:322:LEU:HG	1:A:405:LEU:HD13	1.92	0.50
1:K:322:LEU:HD23	1:K:336:ASP:OD1	2.11	0.50
1:L:345:ARG:HB2	1:L:346:LEU:HD12	1.94	0.50
1:K:368:PHE:HB2	1:K:370:TYR:CE2	2.46	0.50
1:G:458:PHE:CE2	1:G:462:LEU:HD11	2.46	0.50
1:J:384:ARG:HA	1:J:387:PHE:CD2	2.47	0.50
1:K:325:ILE:HD11	1:K:438:VAL:HG13	1.94	0.50
1:A:408:CYS:SG	1:A:412:VAL:HA	2.52	0.49
1:C:355:THR:HG21	1:C:358:LEU:HD12	1.93	0.49
1:B:349:GLY:HA3	1:B:402:LYS:HE3	1.93	0.49
1:L:368:PHE:HB2	1:L:370:TYR:HE1	1.77	0.49
1:B:340:LEU:HD23	1:B:340:LEU:C	2.36	0.49
1:D:411:GLY:O	1:D:412:VAL:C	2.54	0.49
1:E:416:ALA:O	1:E:420:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:375:ALA:HB1	1:J:381:GLN:HG2	1.93	0.49
1:G:358:LEU:HD11	1:G:409:GLN:HG3	1.94	0.49
1:C:428:ARG:HA	1:C:428:ARG:CZ	2.42	0.49
1:J:425:LYS:CA	1:J:462:LEU:HD11	2.41	0.49
1:F:346:LEU:N	1:F:346:LEU:HD12	2.28	0.49
1:K:404:LEU:HD23	1:K:404:LEU:C	2.37	0.49
1:A:325:ILE:HG13	1:A:419:VAL:HG11	1.95	0.49
1:E:365:LYS:HB2	1:E:367:LEU:HD23	1.94	0.49
1:H:404:LEU:HD23	1:H:405:LEU:N	2.28	0.49
1:K:423:LEU:HD22	1:K:423:LEU:H	1.78	0.49
1:J:415:SER:O	1:J:419:VAL:HG23	2.12	0.49
1:F:404:LEU:HD23	1:F:404:LEU:C	2.38	0.49
1:B:411:GLY:O	1:B:412:VAL:C	2.56	0.49
1:E:334:GLU:HG3	1:E:358:LEU:HD11	1.96	0.48
1:J:448:ASN:OD1	1:J:451:PHE:N	2.35	0.48
1:D:355:THR:HG21	1:D:358:LEU:CD1	2.44	0.48
1:A:420:ILE:O	1:A:424:MET:HG3	2.13	0.48
1:I:342:THR:O	1:I:346:LEU:HG	2.14	0.48
1:B:373:LEU:HD22	1:B:386:TYR:HB3	1.95	0.48
1:D:452:MET:HE2	2:D:501:CJA:N21	2.29	0.48
1:L:342:THR:O	1:L:346:LEU:HD13	2.14	0.48
1:C:408:CYS:SG	1:C:412:VAL:HA	2.54	0.47
1:I:323:THR:HG21	1:I:442:ARG:HB2	1.95	0.47
1:K:331:LEU:HD21	1:K:412:VAL:HB	1.97	0.47
1:L:430:THR:HG22	1:L:431:MET:N	2.29	0.47
1:C:432:THR:CG2	1:E:456:LEU:HD11	2.44	0.47
1:E:423:LEU:O	1:E:427:THR:HB	2.14	0.47
1:G:434:ALA:O	1:G:438:VAL:HG23	2.14	0.47
1:C:427:THR:HG22	1:C:429:MET:HG3	1.95	0.47
1:F:382:ASN:OD1	1:F:382:ASN:C	2.58	0.47
1:H:379:ASN:OD1	1:H:379:ASN:O	2.31	0.47
1:K:331:LEU:CD1	1:K:419:VAL:HG21	2.44	0.47
1:L:369:ASN:O	1:L:370:TYR:CD1	2.67	0.47
1:B:448:ASN:O	1:B:452:MET:HG3	2.14	0.47
1:C:456:LEU:CD1	1:E:432:THR:HG22	2.45	0.47
1:J:385:GLN:HG3	1:J:386:TYR:CD1	2.50	0.47
1:J:391:PHE:CE1	1:J:422:TYR:HA	2.50	0.47
1:C:343:MET:HE1	1:C:351:VAL:HG22	1.96	0.47
1:K:404:LEU:HD23	1:K:405:LEU:C	2.40	0.47
1:K:325:ILE:O	1:K:326:LEU:HD23	2.14	0.47
1:C:340:LEU:C	1:C:340:LEU:HD23	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:MET:O	1:C:428:ARG:NH1	2.48	0.47
1:C:453:GLY:O	1:C:457:GLU:HG3	2.15	0.47
1:F:457:GLU:OE2	1:F:457:GLU:HA	2.15	0.47
1:K:352:ILE:HB	1:K:406:ILE:HG13	1.97	0.47
1:J:357:HIS:CD2	1:K:363:TYR:HD2	2.33	0.46
1:K:355:THR:CG2	1:K:358:LEU:HD12	2.44	0.46
1:C:340:LEU:HD23	1:C:340:LEU:O	2.15	0.46
1:F:422:TYR:CE1	1:F:426:HIS:ND1	2.83	0.46
1:H:431:MET:HE2	1:H:456:LEU:HA	1.98	0.46
1:L:408:CYS:SG	1:L:412:VAL:HA	2.55	0.46
1:C:423:LEU:O	1:C:427:THR:HB	2.15	0.46
1:J:449:LEU:HD22	1:J:452:MET:HE3	1.97	0.46
1:K:329:LEU:HD12	1:K:330:PHE:N	2.30	0.46
1:K:411:GLY:O	1:K:412:VAL:HG22	2.16	0.46
1:L:384:ARG:NE	1:L:458:PHE:HD1	2.13	0.46
1:J:429:MET:HE1	1:J:437:PHE:CD1	2.50	0.46
1:K:326:LEU:HB3	1:K:327:PRO:HD2	1.98	0.46
1:G:330:PHE:CE1	1:G:346:LEU:HD13	2.51	0.46
1:I:365:LYS:O	1:I:367:LEU:HD23	2.16	0.46
1:I:424:MET:SD	1:I:455:LEU:HD22	2.55	0.46
1:J:342:THR:O	1:J:346:LEU:CD1	2.55	0.46
1:K:419:VAL:O	1:K:423:LEU:CD2	2.64	0.46
1:L:368:PHE:HB2	1:L:370:TYR:CE1	2.51	0.46
1:D:325:ILE:HD12	1:D:438:VAL:HG22	1.98	0.46
1:F:394:ILE:HG21	1:F:422:TYR:CE1	2.51	0.46
1:I:353:ASN:C	1:I:353:ASN:OD1	2.59	0.46
1:J:328:PHE:C	1:J:328:PHE:CD2	2.94	0.46
1:J:434:ALA:O	1:J:437:PHE:HB3	2.16	0.46
1:K:427:THR:HB	1:K:429:MET:HG2	1.97	0.46
1:K:437:PHE:CE1	1:K:441:LYS:HE3	2.51	0.46
1:C:450:ASN:O	1:C:454:GLN:HG3	2.15	0.46
1:E:355:THR:HG21	1:E:358:LEU:HD12	1.98	0.46
1:L:326:LEU:HB3	1:L:327:PRO:CD	2.45	0.46
1:B:456:LEU:HD12	1:B:456:LEU:C	2.42	0.45
1:B:326:LEU:HB3	1:B:327:PRO:CD	2.46	0.45
1:F:330:PHE:CE1	1:F:346:LEU:HD23	2.52	0.45
1:J:334:GLU:O	1:J:338:GLN:HG3	2.16	0.45
1:F:338:GLN:HG2	1:F:361:TYR:CE2	2.50	0.45
1:I:328:PHE:N	1:I:328:PHE:CD1	2.84	0.45
1:I:431:MET:CE	1:I:456:LEU:HD12	2.46	0.45
1:D:382:ASN:OD1	1:D:385:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:342:THR:C	1:J:346:LEU:CD1	2.89	0.45
1:L:331:LEU:HD23	1:L:331:LEU:C	2.42	0.45
1:K:322:LEU:HD23	1:K:322:LEU:N	2.31	0.45
1:D:349:GLY:C	1:D:350:TYR:CD1	2.95	0.45
1:L:376:THR:HG23	1:L:381:GLN:HB2	1.99	0.45
1:F:354:VAL:CG1	1:F:414:ARG:HB3	2.47	0.45
1:J:382:ASN:ND2	1:J:385:GLN:HB3	2.31	0.45
1:K:384:ARG:HA	1:K:387:PHE:CE1	2.51	0.45
1:B:394:ILE:HA	1:B:404:LEU:HD12	1.97	0.45
1:F:405:LEU:HD23	1:F:406:ILE:N	2.31	0.45
1:K:331:LEU:HD12	1:K:419:VAL:CG2	2.46	0.45
1:L:328:PHE:CD2	1:L:328:PHE:N	2.85	0.45
1:C:357:HIS:HB3	1:F:363:TYR:CD1	2.52	0.44
1:C:391:PHE:N	1:C:391:PHE:CD2	2.85	0.44
1:D:382:ASN:OD1	1:D:382:ASN:C	2.60	0.44
1:I:400:CYS:O	1:I:402:LYS:N	2.50	0.44
1:F:326:LEU:HB3	1:F:327:PRO:CD	2.47	0.44
1:K:350:TYR:N	1:K:350:TYR:CD1	2.84	0.44
1:L:342:THR:O	1:L:346:LEU:CD1	2.65	0.44
1:L:384:ARG:NH2	1:L:458:PHE:CD1	2.85	0.44
1:E:340:LEU:HD23	1:E:340:LEU:C	2.42	0.44
1:L:431:MET:HE1	1:L:456:LEU:HA	1.99	0.44
1:E:390:ALA:O	1:E:394:ILE:HG13	2.16	0.44
1:H:326:LEU:HB3	1:H:327:PRO:CD	2.48	0.44
1:I:390:ALA:O	1:I:394:ILE:HG12	2.18	0.44
1:I:411:GLY:O	1:I:412:VAL:C	2.61	0.44
1:J:412:VAL:HG23	1:J:412:VAL:O	2.18	0.44
1:B:347:ASN:O	1:B:403:GLY:N	2.50	0.44
1:H:412:VAL:HG21	1:H:442:ARG:HD3	2.00	0.44
1:K:387:PHE:HB3	1:K:391:PHE:CE2	2.52	0.44
1:L:444:ILE:HD12	1:L:444:ILE:H	1.82	0.44
1:I:419:VAL:HG12	1:I:423:LEU:CD2	2.46	0.44
1:J:346:LEU:HD12	1:J:346:LEU:N	2.26	0.44
1:K:404:LEU:HD23	1:K:405:LEU:N	2.32	0.44
1:E:365:LYS:CB	1:E:367:LEU:CD2	2.96	0.44
1:F:411:GLY:HA3	1:F:446:SER:HB3	1.99	0.44
1:K:349:GLY:O	1:K:368:PHE:HB3	2.18	0.44
1:K:444:ILE:C	1:K:445:ILE:HG13	2.43	0.44
1:L:384:ARG:NE	1:L:458:PHE:CD1	2.86	0.44
1:F:384:ARG:HD2	1:F:387:PHE:HD2	1.81	0.44
1:K:412:VAL:HG11	1:K:442:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:GLY:C	1:A:350:TYR:CD1	2.96	0.43
1:F:343:MET:O	1:F:348:ILE:HB	2.18	0.43
1:E:404:LEU:HD23	1:E:405:LEU:C	2.43	0.43
1:F:354:VAL:HG11	1:F:414:ARG:HB3	2.00	0.43
1:H:324:PRO:HB3	1:H:330:PHE:CE2	2.53	0.43
1:I:372:ARG:NH1	1:I:372:ARG:HG3	2.32	0.43
1:J:411:GLY:HA3	1:J:446:SER:HB2	1.99	0.43
1:K:374:PRO:HD2	1:K:386:TYR:CE1	2.53	0.43
1:E:382:ASN:C	1:E:382:ASN:OD1	2.60	0.43
1:G:427:THR:O	1:G:427:THR:CG2	2.65	0.43
1:K:384:ARG:HA	1:K:387:PHE:CD1	2.53	0.43
1:C:382:ASN:OD1	1:C:382:ASN:C	2.61	0.43
1:K:328:PHE:HE1	1:K:398:HIS:CE1	2.36	0.43
1:B:412:VAL:HG21	1:B:442:ARG:HD3	1.99	0.43
1:C:343:MET:HE2	1:C:343:MET:HB3	1.90	0.43
1:C:383:LEU:HD12	1:C:451:PHE:CE1	2.54	0.43
1:E:365:LYS:HB2	1:E:367:LEU:CD2	2.48	0.43
1:F:338:GLN:HG2	1:F:361:TYR:CD2	2.54	0.43
1:F:408:CYS:SG	1:F:409:GLN:N	2.92	0.43
1:K:412:VAL:O	1:K:412:VAL:HG23	2.18	0.43
1:L:339:ASP:OD2	1:L:342:THR:CB	2.67	0.43
1:L:381:GLN:OE1	1:L:381:GLN:HA	2.17	0.43
1:I:322:LEU:HD12	1:I:346:LEU:CD1	2.48	0.43
1:L:429:MET:HE1	1:L:434:ALA:HA	2.01	0.43
1:C:326:LEU:HB2	1:C:329:LEU:HB3	1.99	0.43
1:F:352:ILE:HG22	1:F:354:VAL:HG23	2.01	0.43
1:H:431:MET:HE2	1:H:456:LEU:CA	2.49	0.43
1:K:350:TYR:CD2	1:K:393:PHE:CE1	3.07	0.43
1:B:383:LEU:HD23	1:B:386:TYR:HD2	1.84	0.43
1:B:449:LEU:HD23	1:B:452:MET:SD	2.58	0.43
1:I:372:ARG:HG3	1:I:372:ARG:HH11	1.84	0.43
1:J:348:ILE:HG12	1:J:403:GLY:C	2.44	0.43
1:F:382:ASN:OD1	1:F:384:ARG:N	2.52	0.43
1:B:391:PHE:N	1:B:391:PHE:CD2	2.87	0.43
1:B:444:ILE:H	1:B:444:ILE:HD12	1.84	0.43
1:B:458:PHE:O	1:B:462:LEU:HG	2.19	0.43
1:C:349:GLY:C	1:C:350:TYR:CD1	2.97	0.43
1:D:330:PHE:CD2	1:D:330:PHE:N	2.87	0.43
1:D:359:PRO:HG2	1:D:361:TYR:CE1	2.54	0.43
1:F:322:LEU:HD12	1:F:322:LEU:N	2.34	0.43
1:H:376:THR:HA	1:H:414:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:350:TYR:CD1	1:J:397:ALA:HB2	2.49	0.43
1:J:394:ILE:CD1	1:J:404:LEU:HD13	2.48	0.43
1:I:420:ILE:HG23	1:I:434:ALA:HB3	2.01	0.42
1:B:382:ASN:OD1	1:B:382:ASN:C	2.62	0.42
1:C:383:LEU:HD12	1:C:451:PHE:CD1	2.54	0.42
1:F:412:VAL:HG21	1:F:442:ARG:HD3	2.02	0.42
1:G:322:LEU:HD23	1:G:322:LEU:HA	1.86	0.42
1:G:361:TYR:O	1:G:370:TYR:OH	2.30	0.42
1:I:431:MET:HE2	1:I:456:LEU:CA	2.49	0.42
1:A:425:LYS:HG2	1:A:426:HIS:ND1	2.34	0.42
1:F:354:VAL:O	1:F:354:VAL:CG1	2.66	0.42
1:F:447:PRO:HA	2:F:501:CJA:C14	2.49	0.42
1:A:353:ASN:OD1	1:A:353:ASN:C	2.62	0.42
1:C:339:ASP:O	1:C:343:MET:HG3	2.19	0.42
1:I:323:THR:O	1:I:330:PHE:HA	2.19	0.42
1:I:419:VAL:HG12	1:I:423:LEU:HD23	2.01	0.42
1:K:411:GLY:C	1:K:413:SER:N	2.74	0.42
1:A:373:LEU:HD13	1:A:386:TYR:HB3	2.02	0.42
1:F:349:GLY:C	1:F:350:TYR:CD1	2.98	0.42
1:A:338:GLN:HG2	1:A:361:TYR:CD2	2.54	0.42
1:G:456:LEU:C	1:G:456:LEU:HD23	2.45	0.42
1:K:328:PHE:C	1:K:328:PHE:CD2	2.98	0.42
1:K:372:ARG:C	1:K:373:LEU:HD23	2.45	0.42
1:A:356:THR:HG22	1:A:374:PRO:HB2	2.01	0.42
1:C:430:THR:OG1	1:C:433:ASP:CG	2.59	0.42
1:D:437:PHE:HE2	1:D:441:LYS:HD2	1.85	0.42
1:F:405:LEU:C	1:F:405:LEU:CD2	2.92	0.42
1:G:395:GLU:OE2	1:G:422:TYR:OH	2.32	0.42
1:J:331:LEU:HD23	1:J:332:GLY:N	2.33	0.42
1:J:342:THR:O	1:J:345:ARG:N	2.51	0.42
1:L:384:ARG:NH2	1:L:458:PHE:HD1	2.17	0.42
1:C:352:ILE:HD12	1:C:404:LEU:HD21	2.01	0.42
1:D:325:ILE:HG22	1:D:326:LEU:HD13	2.02	0.42
1:E:411:GLY:C	1:E:413:SER:N	2.75	0.42
1:B:444:ILE:HD12	1:B:444:ILE:N	2.35	0.42
1:D:340:LEU:HD11	1:D:367:LEU:CD1	2.50	0.42
1:D:437:PHE:C	1:D:437:PHE:CD2	2.95	0.42
1:F:363:TYR:C	1:F:363:TYR:CD2	2.97	0.42
1:K:429:MET:CE	1:K:437:PHE:CD2	3.01	0.42
1:L:449:LEU:CD1	1:L:452:MET:HE3	2.49	0.42
1:C:420:ILE:O	1:C:424:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:423:LEU:O	1:I:427:THR:CB	2.68	0.42
1:A:365:LYS:HB3	1:A:367:LEU:CD1	2.49	0.41
1:A:368:PHE:HB2	1:A:370:TYR:CE2	2.55	0.41
1:J:384:ARG:HA	1:J:387:PHE:CE2	2.55	0.41
1:K:384:ARG:HG2	1:K:384:ARG:NH1	2.29	0.41
1:K:405:LEU:CD2	1:K:407:HIS:HB3	2.50	0.41
1:F:431:MET:HE1	1:F:456:LEU:HD13	2.00	0.41
1:J:330:PHE:N	1:J:330:PHE:CD2	2.88	0.41
1:J:342:THR:HG22	1:J:346:LEU:CD1	2.39	0.41
1:J:342:THR:C	1:J:346:LEU:HD12	2.43	0.41
1:L:354:VAL:HA	1:L:373:LEU:HB2	2.03	0.41
1:E:408:CYS:SG	1:E:412:VAL:HA	2.61	0.41
1:E:452:MET:HE2	1:E:452:MET:HB3	1.95	0.41
1:G:437:PHE:CE2	1:G:441:LYS:HE3	2.56	0.41
1:C:342:THR:O	1:C:346:LEU:HG	2.20	0.41
1:D:431:MET:CE	2:D:501:CJA:S04	3.09	0.41
1:G:449:LEU:H	1:G:449:LEU:HD22	1.85	0.41
1:H:387:PHE:CD1	1:H:418:ILE:HD13	2.55	0.41
1:I:373:LEU:HD22	1:I:386:TYR:HB3	2.02	0.41
1:L:330:PHE:CD1	1:L:330:PHE:N	2.89	0.41
1:E:428:ARG:NH1	1:G:399:GLN:HA	2.36	0.41
1:G:320:ALA:HB1	1:G:336:ASP:HA	2.01	0.41
1:J:350:TYR:HB3	1:J:404:LEU:HG	2.01	0.41
1:F:417:THR:HG21	1:F:451:PHE:HB3	2.02	0.41
1:F:446:SER:HA	1:F:447:PRO:HD3	1.93	0.41
1:I:326:LEU:HB3	1:I:327:PRO:CD	2.51	0.41
1:J:437:PHE:C	1:J:437:PHE:CD2	2.99	0.41
1:D:361:TYR:O	1:D:370:TYR:OH	2.31	0.41
1:K:455:LEU:HD12	1:K:455:LEU:H	1.86	0.41
1:A:408:CYS:SG	1:A:409:GLN:N	2.94	0.41
1:B:323:THR:HG22	1:B:325:ILE:HD13	2.03	0.41
1:C:347:ASN:O	1:C:403:GLY:N	2.46	0.41
1:D:427:THR:CG2	1:D:428:ARG:N	2.83	0.41
1:G:413:SER:O	1:G:417:THR:OG1	2.35	0.41
1:H:322:LEU:HD12	1:H:322:LEU:C	2.44	0.41
1:I:330:PHE:CD1	1:I:330:PHE:N	2.88	0.41
1:L:352:ILE:HG13	1:L:404:LEU:HD11	2.03	0.41
1:L:431:MET:CE	1:L:456:LEU:HA	2.51	0.41
1:B:343:MET:HA	1:B:348:ILE:HD12	2.02	0.41
1:E:404:LEU:HD23	1:E:404:LEU:C	2.46	0.41
1:H:411:GLY:O	1:H:412:VAL:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:357:HIS:CG	1:K:363:TYR:HD2	2.38	0.41
1:J:385:GLN:CG	1:J:386:TYR:CD1	3.04	0.41
1:K:382:ASN:OD1	1:K:382:ASN:C	2.64	0.41
1:G:340:LEU:HD12	1:G:344:GLN:OE1	2.21	0.40
1:J:387:PHE:CE1	1:J:421:ALA:CB	3.04	0.40
1:K:330:PHE:N	1:K:330:PHE:CD2	2.88	0.40
1:L:449:LEU:CD1	1:L:452:MET:CE	2.99	0.40
1:A:379:ASN:OD1	1:A:379:ASN:O	2.39	0.40
1:C:360:LEU:HG	1:C:370:TYR:CD1	2.57	0.40
1:E:456:LEU:HD12	1:E:456:LEU:HA	1.95	0.40
1:H:420:ILE:O	1:H:424:MET:HG3	2.21	0.40
1:I:371:LYS:NZ	1:I:389:GLU:OE2	2.55	0.40
1:J:373:LEU:HD22	1:J:386:TYR:CB	2.51	0.40
1:K:435:TRP:O	1:K:439:LYS:N	2.40	0.40
1:E:340:LEU:HD21	1:E:344:GLN:CD	2.47	0.40
1:J:383:LEU:O	1:J:387:PHE:CD2	2.74	0.40
1:F:342:THR:O	1:F:346:LEU:CD1	2.68	0.40
1:I:437:PHE:CD2	1:I:437:PHE:C	2.99	0.40
1:J:417:THR:HG21	1:J:451:PHE:HB3	2.03	0.40
1:L:437:PHE:CE1	1:L:441:LYS:HE2	2.56	0.40
1:D:384:ARG:HA	1:D:387:PHE:CD2	2.57	0.40
1:H:379:ASN:OD1	1:H:379:ASN:C	2.65	0.40
1:H:444:ILE:O	1:H:445:ILE:HG13	2.21	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	146/148 (99%)	134 (92%)	12 (8%)	0	100	100
1	B	145/148 (98%)	135 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
1	D	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
1	E	145/148 (98%)	137 (94%)	7 (5%)	1 (1%)	19	49
1	F	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
1	G	145/148 (98%)	134 (92%)	10 (7%)	1 (1%)	19	49
1	H	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
1	I	145/148 (98%)	129 (89%)	15 (10%)	1 (1%)	19	49
1	J	144/148 (97%)	131 (91%)	13 (9%)	0	100	100
1	K	144/148 (97%)	131 (91%)	12 (8%)	1 (1%)	19	49
1	L	141/148 (95%)	131 (93%)	10 (7%)	0	100	100
All	All	1734/1776 (98%)	1601 (92%)	129 (7%)	4 (0%)	44	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	401	GLY
1	E	412	VAL
1	G	354	VAL
1	K	354	VAL

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	126/130 (97%)	119 (94%)	7 (6%)	17	47
1	B	126/130 (97%)	124 (98%)	2 (2%)	58	84
1	C	125/130 (96%)	122 (98%)	3 (2%)	44	76
1	D	120/130 (92%)	114 (95%)	6 (5%)	20	52
1	E	122/130 (94%)	113 (93%)	9 (7%)	11	34
1	F	120/130 (92%)	116 (97%)	4 (3%)	33	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	123/130 (95%)	117 (95%)	6 (5%)	21 53
1	H	124/130 (95%)	120 (97%)	4 (3%)	34 69
1	I	115/130 (88%)	107 (93%)	8 (7%)	12 36
1	J	110/130 (85%)	97 (88%)	13 (12%)	4 13
1	K	111/130 (85%)	103 (93%)	8 (7%)	12 35
1	L	110/130 (85%)	99 (90%)	11 (10%)	6 20
All	All	1432/1560 (92%)	1351 (94%)	81 (6%)	17 47

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	LEU
1	A	333	ASN
1	A	378	SER
1	A	400	CYS
1	A	412	VAL
1	A	425	LYS
1	A	439	LYS
1	B	413	SER
1	B	414	ARG
1	C	325	ILE
1	C	340	LEU
1	C	342	THR
1	D	323	THR
1	D	378	SER
1	D	396	GLU
1	D	446	SER
1	D	449	LEU
1	D	456	LEU
1	E	322	LEU
1	E	354	VAL
1	E	356	THR
1	E	376	THR
1	E	415	SER
1	E	418	ILE
1	E	432	THR
1	E	441	LYS
1	E	442	ARG
1	F	376	THR
1	F	378	SER

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Mol	Chain	Res	Type
1	F	405	LEU
1	F	444	ILE
1	G	340	LEU
1	G	356	THR
1	G	376	THR
1	G	415	SER
1	G	430	THR
1	G	466	VAL
1	H	342	THR
1	H	413	SER
1	H	444	ILE
1	H	466	VAL
1	I	325	ILE
1	I	340	LEU
1	I	347	ASN
1	I	413	SER
1	I	427	THR
1	I	431	MET
1	I	444	ILE
1	I	445	ILE
1	J	341	ASP
1	J	342	THR
1	J	346	LEU
1	J	356	THR
1	J	368	PHE
1	J	382	ASN
1	J	405	LEU
1	J	407	HIS
1	J	408	CYS
1	J	412	VAL
1	J	413	SER
1	J	415	SER
1	J	423	LEU
1	K	330	PHE
1	K	342	THR
1	K	348	ILE
1	K	376	THR
1	K	405	LEU
1	K	412	VAL
1	K	430	THR
1	K	452	MET
1	L	330	PHE

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Mol	Chain	Res	Type
1	L	346	LEU
1	L	347	ASN
1	L	354	VAL
1	L	400	CYS
1	L	409	GLN
1	L	415	SER
1	L	427	THR
1	L	432	THR
1	L	445	ILE
1	L	462	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	ASN
1	B	353	ASN
1	B	369	ASN
1	B	379	ASN
1	B	426	HIS
1	B	463	ASN
1	B	464	ASN
1	C	347	ASN
1	C	369	ASN
1	C	385	GLN
1	D	426	HIS
1	D	450	ASN
1	E	344	GLN
1	E	426	HIS
1	F	338	GLN
1	F	463	ASN
1	G	426	HIS
1	G	450	ASN
1	G	454	GLN
1	H	347	ASN
1	H	464	ASN
1	I	338	GLN
1	I	362	HIS
1	I	398	HIS
1	I	463	ASN
1	J	347	ASN
1	J	381	GLN
1	J	385	GLN

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Mol	Chain	Res	Type
1	K	344	GLN
1	K	347	ASN
1	K	398	HIS
1	K	426	HIS
1	L	333	ASN
1	L	357	HIS
1	L	407	HIS

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

12 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	7.75	20 (86%)	24,37,37	2.06	7 (29%)
2	CJA	G	501	-	23,25,25	7.53	19 (82%)	24,37,37	2.41	7 (29%)
2	CJA	J	501	-	23,25,25	7.54	20 (86%)	24,37,37	2.57	7 (29%)
2	CJA	C	501	-	23,25,25	7.71	19 (82%)	24,37,37	2.22	8 (33%)
2	CJA	L	501	-	23,25,25	7.52	20 (86%)	24,37,37	2.39	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CJA	B	501	-	23,25,25	7.53	20 (86%)	24,37,37	2.45	7 (29%)
2	CJA	F	501	-	23,25,25	7.99	20 (86%)	24,37,37	2.33	7 (29%)
2	CJA	A	501	-	23,25,25	7.59	18 (78%)	24,37,37	2.53	7 (29%)
2	CJA	I	501	-	23,25,25	7.29	20 (86%)	24,37,37	2.15	7 (29%)
2	CJA	E	501	-	23,25,25	7.43	20 (86%)	24,37,37	2.70	7 (29%)
2	CJA	K	501	-	23,25,25	7.54	20 (86%)	24,37,37	2.58	7 (29%)
2	CJA	H	501	-	23,25,25	7.50	20 (86%)	24,37,37	2.25	7 (29%)

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	-	-	4/13/22/22	0/3/3/3
2	CJA	G	501	-	-	0/13/22/22	0/3/3/3
2	CJA	J	501	-	-	5/13/22/22	0/3/3/3
2	CJA	C	501	-	-	2/13/22/22	0/3/3/3
2	CJA	L	501	-	-	2/13/22/22	0/3/3/3
2	CJA	B	501	-	-	4/13/22/22	0/3/3/3
2	CJA	F	501	-	-	2/13/22/22	0/3/3/3
2	CJA	A	501	-	-	0/13/22/22	0/3/3/3
2	CJA	I	501	-	-	0/13/22/22	0/3/3/3
2	CJA	E	501	-	-	3/13/22/22	0/3/3/3
2	CJA	K	501	-	-	0/13/22/22	0/3/3/3
2	CJA	H	501	-	-	0/13/22/22	0/3/3/3

All (236) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	CJA	C05-C06	29.63	1.55	1.37
2	C	501	CJA	C05-C06	28.81	1.54	1.37
2	A	501	CJA	C05-C06	28.11	1.54	1.37
2	G	501	CJA	C05-C06	28.10	1.54	1.37
2	D	501	CJA	C05-C06	28.07	1.54	1.37
2	K	501	CJA	C05-C06	27.97	1.54	1.37
2	L	501	CJA	C05-C06	27.94	1.54	1.37
2	J	501	CJA	C05-C06	27.86	1.54	1.37
2	H	501	CJA	C05-C06	27.84	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	CJA	C05-C06	27.68	1.54	1.37
2	E	501	CJA	C05-C06	26.98	1.53	1.37
2	I	501	CJA	C05-C06	26.53	1.53	1.37
2	D	501	CJA	C23-C06	12.15	1.64	1.40
2	F	501	CJA	C23-C06	12.04	1.64	1.40
2	B	501	CJA	C23-C06	12.00	1.64	1.40
2	H	501	CJA	C23-C06	11.98	1.64	1.40
2	E	501	CJA	C23-C06	11.96	1.64	1.40
2	J	501	CJA	C23-C06	11.81	1.63	1.40
2	C	501	CJA	C23-C06	11.79	1.63	1.40
2	K	501	CJA	C23-C06	11.78	1.63	1.40
2	A	501	CJA	C23-C06	11.77	1.63	1.40
2	L	501	CJA	C23-C06	11.71	1.63	1.40
2	I	501	CJA	C23-C06	11.67	1.63	1.40
2	G	501	CJA	C23-C06	11.54	1.63	1.40
2	F	501	CJA	C08-C09	9.74	1.67	1.51
2	D	501	CJA	C08-C09	9.15	1.66	1.51
2	J	501	CJA	C08-C09	8.99	1.66	1.51
2	H	501	CJA	C08-C09	8.95	1.66	1.51
2	C	501	CJA	C08-C09	8.94	1.66	1.51
2	A	501	CJA	C08-C09	8.88	1.66	1.51
2	E	501	CJA	C08-C09	8.86	1.66	1.51
2	L	501	CJA	C08-C09	8.78	1.65	1.51
2	G	501	CJA	C08-C09	8.72	1.65	1.51
2	I	501	CJA	C08-C09	8.70	1.65	1.51
2	K	501	CJA	C08-C09	8.62	1.65	1.51
2	B	501	CJA	C08-C09	8.61	1.65	1.51
2	F	501	CJA	C12-S13	7.92	1.91	1.75
2	J	501	CJA	C12-S13	7.17	1.90	1.75
2	D	501	CJA	C12-S13	7.15	1.90	1.75
2	D	501	CJA	C12-N11	7.10	1.46	1.33
2	F	501	CJA	C14-C15	7.10	1.61	1.51
2	E	501	CJA	C12-S13	7.09	1.89	1.75
2	K	501	CJA	C12-S13	6.99	1.89	1.75
2	G	501	CJA	C12-S13	6.98	1.89	1.75
2	B	501	CJA	C12-S13	6.97	1.89	1.75
2	C	501	CJA	C12-S13	6.97	1.89	1.75
2	A	501	CJA	C12-S13	6.95	1.89	1.75
2	A	501	CJA	C03-S04	-6.93	1.60	1.72
2	D	501	CJA	C14-C15	6.89	1.61	1.51
2	H	501	CJA	C12-S13	6.86	1.89	1.75
2	L	501	CJA	C12-S13	6.82	1.89	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	CJA	C12-N11	6.62	1.45	1.33
2	I	501	CJA	C12-S13	6.56	1.88	1.75
2	B	501	CJA	C12-N11	6.46	1.45	1.33
2	H	501	CJA	C03-S04	-6.44	1.61	1.72
2	B	501	CJA	C14-C15	6.43	1.60	1.51
2	L	501	CJA	C12-N11	6.40	1.45	1.33
2	K	501	CJA	C12-N11	6.40	1.45	1.33
2	G	501	CJA	C12-N11	6.39	1.45	1.33
2	G	501	CJA	C03-S04	-6.38	1.61	1.72
2	C	501	CJA	C03-S04	-6.36	1.61	1.72
2	E	501	CJA	C12-N11	6.34	1.45	1.33
2	I	501	CJA	C12-N11	6.34	1.45	1.33
2	J	501	CJA	C12-N11	6.32	1.44	1.33
2	D	501	CJA	C03-S04	-6.31	1.61	1.72
2	A	501	CJA	C12-N11	6.26	1.44	1.33
2	E	501	CJA	C14-C15	6.24	1.60	1.51
2	C	501	CJA	C12-N11	6.22	1.44	1.33
2	A	501	CJA	C05-S04	-6.18	1.60	1.70
2	E	501	CJA	C03-S04	-6.15	1.61	1.72
2	H	501	CJA	C12-N11	6.12	1.44	1.33
2	B	501	CJA	C03-S04	-6.09	1.61	1.72
2	I	501	CJA	C14-C15	6.04	1.59	1.51
2	J	501	CJA	C03-S04	-6.02	1.61	1.72
2	K	501	CJA	C03-S04	-6.01	1.61	1.72
2	C	501	CJA	C14-C15	5.92	1.59	1.51
2	I	501	CJA	C03-S04	-5.92	1.61	1.72
2	L	501	CJA	C03-S04	-5.88	1.62	1.72
2	A	501	CJA	C14-C15	5.83	1.59	1.51
2	J	501	CJA	C14-C15	5.81	1.59	1.51
2	F	501	CJA	C03-S04	-5.76	1.62	1.72
2	F	501	CJA	C12-N21	5.71	1.42	1.34
2	G	501	CJA	C14-C15	5.70	1.59	1.51
2	L	501	CJA	C14-C15	5.59	1.59	1.51
2	C	501	CJA	C05-S04	-5.59	1.61	1.70
2	I	501	CJA	C05-S04	-5.59	1.61	1.70
2	E	501	CJA	C05-S04	-5.57	1.61	1.70
2	K	501	CJA	C12-N21	5.57	1.42	1.34
2	E	501	CJA	C12-N21	5.47	1.42	1.34
2	K	501	CJA	C14-C15	5.43	1.59	1.51
2	I	501	CJA	C12-N21	5.43	1.42	1.34
2	D	501	CJA	C12-N21	5.42	1.42	1.34
2	B	501	CJA	C12-N21	5.38	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	501	CJA	C12-N21	5.38	1.42	1.34
2	K	501	CJA	C05-S04	-5.37	1.62	1.70
2	C	501	CJA	C12-N21	5.29	1.42	1.34
2	H	501	CJA	C12-N21	5.26	1.42	1.34
2	D	501	CJA	C14-S13	5.26	1.92	1.80
2	L	501	CJA	C05-S04	-5.24	1.62	1.70
2	J	501	CJA	C12-N21	5.24	1.42	1.34
2	B	501	CJA	C05-S04	-5.23	1.62	1.70
2	H	501	CJA	C14-C15	5.20	1.58	1.51
2	H	501	CJA	C05-S04	-5.19	1.62	1.70
2	G	501	CJA	C05-S04	-5.19	1.62	1.70
2	F	501	CJA	C14-S13	5.09	1.92	1.80
2	G	501	CJA	C12-N21	5.03	1.41	1.34
2	J	501	CJA	C05-S04	-5.00	1.62	1.70
2	A	501	CJA	C12-N21	4.85	1.41	1.34
2	J	501	CJA	C14-S13	4.46	1.91	1.80
2	A	501	CJA	C14-S13	4.42	1.90	1.80
2	K	501	CJA	C14-S13	4.38	1.90	1.80
2	C	501	CJA	C14-S13	4.36	1.90	1.80
2	G	501	CJA	C14-S13	4.34	1.90	1.80
2	E	501	CJA	C14-S13	4.31	1.90	1.80
2	B	501	CJA	C14-S13	4.29	1.90	1.80
2	L	501	CJA	C14-S13	4.19	1.90	1.80
2	H	501	CJA	C14-S13	4.18	1.90	1.80
2	I	501	CJA	C14-S13	4.15	1.90	1.80
2	D	501	CJA	C05-S04	-4.01	1.64	1.70
2	L	501	CJA	C17-C15	3.79	1.60	1.52
2	D	501	CJA	C10-N11	3.74	1.42	1.34
2	B	501	CJA	C17-C15	3.61	1.60	1.52
2	F	501	CJA	C10-N11	3.57	1.41	1.34
2	E	501	CJA	C17-C15	3.50	1.59	1.52
2	D	501	CJA	C17-C15	3.49	1.59	1.52
2	J	501	CJA	C17-C15	3.48	1.59	1.52
2	F	501	CJA	C23-C22	3.37	1.53	1.48
2	G	501	CJA	C17-C15	3.34	1.59	1.52
2	C	501	CJA	C17-C15	3.33	1.59	1.52
2	F	501	CJA	C05-S04	-3.29	1.65	1.70
2	D	501	CJA	C23-C22	3.28	1.53	1.48
2	J	501	CJA	C10-N11	3.25	1.41	1.34
2	I	501	CJA	C17-C15	3.23	1.59	1.52
2	A	501	CJA	C10-N11	3.22	1.41	1.34
2	C	501	CJA	C10-N11	3.22	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	501	CJA	C10-N11	3.16	1.40	1.34
2	D	501	CJA	C10-C09	3.16	1.44	1.37
2	K	501	CJA	C10-N11	3.13	1.40	1.34
2	B	501	CJA	C10-N11	3.13	1.40	1.34
2	K	501	CJA	C17-C15	3.12	1.59	1.52
2	F	501	CJA	C10-C09	3.12	1.43	1.37
2	D	501	CJA	C22-C09	3.11	1.47	1.41
2	F	501	CJA	C22-C09	3.08	1.47	1.41
2	G	501	CJA	C10-N11	3.07	1.40	1.34
2	A	501	CJA	C17-C15	3.04	1.58	1.52
2	C	501	CJA	C23-C22	3.01	1.52	1.48
2	I	501	CJA	C10-N11	3.00	1.40	1.34
2	E	501	CJA	C10-N11	2.99	1.40	1.34
2	H	501	CJA	C23-C22	2.94	1.52	1.48
2	H	501	CJA	C10-N11	2.94	1.40	1.34
2	D	501	CJA	C01-S02	2.92	1.91	1.79
2	F	501	CJA	C17-C15	2.91	1.58	1.52
2	K	501	CJA	C23-C22	2.90	1.52	1.48
2	H	501	CJA	C17-C15	2.89	1.58	1.52
2	B	501	CJA	C23-C22	2.80	1.52	1.48
2	B	501	CJA	C01-S02	2.79	1.90	1.79
2	F	501	CJA	C01-S02	2.78	1.90	1.79
2	K	501	CJA	C01-S02	2.78	1.90	1.79
2	D	501	CJA	C18-C17	2.77	1.61	1.53
2	H	501	CJA	C01-S02	2.76	1.90	1.79
2	L	501	CJA	C23-C22	2.72	1.52	1.48
2	B	501	CJA	C22-C09	2.68	1.46	1.41
2	J	501	CJA	C23-C22	2.68	1.52	1.48
2	L	501	CJA	C01-S02	2.68	1.90	1.79
2	I	501	CJA	C01-S02	2.68	1.90	1.79
2	I	501	CJA	C22-C09	2.67	1.46	1.41
2	D	501	CJA	C19-C17	2.66	1.60	1.53
2	C	501	CJA	C22-C09	2.65	1.46	1.41
2	E	501	CJA	C23-C22	2.65	1.52	1.48
2	C	501	CJA	C10-C09	2.65	1.43	1.37
2	K	501	CJA	C22-C09	2.64	1.46	1.41
2	J	501	CJA	C22-C09	2.64	1.46	1.41
2	I	501	CJA	C23-C22	2.64	1.52	1.48
2	J	501	CJA	C01-S02	2.63	1.89	1.79
2	A	501	CJA	C01-S02	2.63	1.89	1.79
2	H	501	CJA	C22-C09	2.62	1.46	1.41
2	L	501	CJA	C20-C17	2.61	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	CJA	C01-S02	2.58	1.89	1.79
2	F	501	CJA	C19-C17	2.55	1.60	1.53
2	L	501	CJA	C22-C09	2.53	1.46	1.41
2	G	501	CJA	C01-S02	2.52	1.89	1.79
2	I	501	CJA	C10-C09	2.51	1.42	1.37
2	F	501	CJA	C18-C17	2.51	1.60	1.53
2	H	501	CJA	C18-C17	2.51	1.60	1.53
2	C	501	CJA	C01-S02	2.51	1.89	1.79
2	G	501	CJA	C22-C09	2.51	1.46	1.41
2	L	501	CJA	C10-C09	2.50	1.42	1.37
2	K	501	CJA	C19-C17	2.49	1.60	1.53
2	K	501	CJA	C22-N21	2.49	1.38	1.34
2	E	501	CJA	C22-C09	2.49	1.46	1.41
2	J	501	CJA	C19-C17	2.48	1.60	1.53
2	G	501	CJA	C18-C17	2.48	1.60	1.53
2	J	501	CJA	C18-C17	2.48	1.60	1.53
2	G	501	CJA	C23-C22	2.47	1.52	1.48
2	F	501	CJA	C20-C17	2.47	1.60	1.53
2	E	501	CJA	C18-C17	2.47	1.60	1.53
2	I	501	CJA	C20-C17	2.47	1.60	1.53
2	J	501	CJA	C10-C09	2.46	1.42	1.37
2	K	501	CJA	C20-C17	2.46	1.60	1.53
2	I	501	CJA	C19-C17	2.45	1.60	1.53
2	L	501	CJA	C18-C17	2.44	1.60	1.53
2	A	501	CJA	C19-C17	2.43	1.60	1.53
2	E	501	CJA	C22-N21	2.43	1.38	1.34
2	K	501	CJA	C10-C09	2.42	1.42	1.37
2	B	501	CJA	C19-C17	2.42	1.60	1.53
2	J	501	CJA	C20-C17	2.41	1.60	1.53
2	A	501	CJA	C23-C22	2.40	1.52	1.48
2	A	501	CJA	C10-C09	2.39	1.42	1.37
2	E	501	CJA	C20-C17	2.38	1.59	1.53
2	C	501	CJA	C20-C17	2.37	1.59	1.53
2	I	501	CJA	C18-C17	2.37	1.59	1.53
2	G	501	CJA	C19-C17	2.37	1.59	1.53
2	A	501	CJA	C18-C17	2.35	1.59	1.53
2	B	501	CJA	C20-C17	2.35	1.59	1.53
2	H	501	CJA	C19-C17	2.33	1.59	1.53
2	J	501	CJA	C22-N21	2.31	1.38	1.34
2	E	501	CJA	C19-C17	2.31	1.59	1.53
2	H	501	CJA	C20-C17	2.30	1.59	1.53
2	D	501	CJA	C20-C17	2.30	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	CJA	C19-C17	2.29	1.59	1.53
2	A	501	CJA	C22-C09	2.29	1.45	1.41
2	H	501	CJA	C10-C09	2.29	1.42	1.37
2	K	501	CJA	C18-C17	2.28	1.59	1.53
2	G	501	CJA	C10-C09	2.27	1.42	1.37
2	F	501	CJA	C22-N21	2.26	1.38	1.34
2	C	501	CJA	C18-C17	2.26	1.59	1.53
2	B	501	CJA	C18-C17	2.24	1.59	1.53
2	G	501	CJA	C20-C17	2.23	1.59	1.53
2	B	501	CJA	C10-C09	2.22	1.42	1.37
2	E	501	CJA	C10-C09	2.20	1.42	1.37
2	I	501	CJA	C22-N21	2.17	1.38	1.34
2	L	501	CJA	C19-C17	2.16	1.59	1.53
2	D	501	CJA	O16-C15	2.15	1.24	1.21
2	B	501	CJA	C22-N21	2.14	1.38	1.34
2	L	501	CJA	C22-N21	2.13	1.38	1.34
2	H	501	CJA	C22-N21	2.04	1.37	1.34

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	CJA	C14-S13-C12	7.58	111.39	101.65
2	K	501	CJA	C14-S13-C12	6.24	109.67	101.65
2	B	501	CJA	C14-S13-C12	6.19	109.60	101.65
2	A	501	CJA	C14-S13-C12	6.08	109.46	101.65
2	F	501	CJA	N11-C12-N21	-6.06	120.06	127.57
2	J	501	CJA	C14-S13-C12	5.95	109.29	101.65
2	J	501	CJA	N11-C12-N21	-5.83	120.34	127.57
2	L	501	CJA	C14-S13-C12	5.69	108.96	101.65
2	A	501	CJA	N11-C12-N21	-5.68	120.54	127.57
2	J	501	CJA	C10-N11-C12	5.52	119.91	115.39
2	E	501	CJA	C10-N11-C12	5.47	119.87	115.39
2	E	501	CJA	N11-C12-N21	-5.42	120.85	127.57
2	G	501	CJA	C14-S13-C12	5.28	108.43	101.65
2	K	501	CJA	N11-C12-N21	-5.23	121.09	127.57
2	A	501	CJA	C10-N11-C12	5.18	119.63	115.39
2	B	501	CJA	C10-N11-C12	5.16	119.61	115.39
2	G	501	CJA	C10-N11-C12	5.14	119.60	115.39
2	G	501	CJA	N11-C12-N21	-5.13	121.21	127.57
2	B	501	CJA	N11-C12-N21	-5.09	121.27	127.57
2	F	501	CJA	C10-N11-C12	5.07	119.54	115.39
2	C	501	CJA	N11-C12-N21	-5.05	121.31	127.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	CJA	C06-C05-S04	-5.01	106.92	112.26
2	H	501	CJA	N11-C12-N21	-4.92	121.48	127.57
2	K	501	CJA	C10-N11-C12	4.90	119.40	115.39
2	D	501	CJA	N11-C12-N21	-4.85	121.56	127.57
2	C	501	CJA	C14-S13-C12	4.84	107.88	101.65
2	L	501	CJA	N11-C12-N21	-4.81	121.61	127.57
2	K	501	CJA	C06-C05-S04	-4.73	107.22	112.26
2	B	501	CJA	C06-C05-S04	-4.68	107.28	112.26
2	E	501	CJA	C06-C05-S04	-4.59	107.37	112.26
2	G	501	CJA	C06-C05-S04	-4.34	107.64	112.26
2	I	501	CJA	C06-C05-S04	-4.32	107.66	112.26
2	J	501	CJA	C06-C05-S04	-4.31	107.67	112.26
2	L	501	CJA	C10-N11-C12	4.31	118.92	115.39
2	H	501	CJA	C06-C05-S04	-4.30	107.68	112.26
2	I	501	CJA	N11-C12-N21	-4.25	122.30	127.57
2	L	501	CJA	C06-C05-S04	-4.23	107.75	112.26
2	C	501	CJA	C10-N11-C12	4.17	118.80	115.39
2	I	501	CJA	C14-S13-C12	4.04	106.84	101.65
2	I	501	CJA	C10-N11-C12	4.02	118.68	115.39
2	H	501	CJA	C14-S13-C12	3.99	106.77	101.65
2	H	501	CJA	C10-N11-C12	3.97	118.64	115.39
2	A	501	CJA	C06-C05-S04	-3.84	108.17	112.26
2	F	501	CJA	C14-S13-C12	3.66	106.36	101.65
2	F	501	CJA	C07-C08-C09	3.64	119.61	110.71
2	A	501	CJA	C07-C08-C09	3.62	119.55	110.71
2	K	501	CJA	C07-C08-C09	3.60	119.51	110.71
2	F	501	CJA	C08-C07-C06	3.59	119.50	110.71
2	D	501	CJA	C10-N11-C12	3.59	118.33	115.39
2	L	501	CJA	C07-C08-C09	3.54	119.36	110.71
2	K	501	CJA	C08-C07-C06	3.52	119.31	110.71
2	I	501	CJA	C07-C08-C09	3.48	119.21	110.71
2	J	501	CJA	C07-C08-C09	3.44	119.11	110.71
2	L	501	CJA	C08-C07-C06	3.40	119.02	110.71
2	C	501	CJA	C06-C05-S04	-3.37	108.67	112.26
2	E	501	CJA	C07-C08-C09	3.36	118.93	110.71
2	H	501	CJA	C07-C08-C09	3.33	118.86	110.71
2	F	501	CJA	C06-C05-S04	-3.30	108.75	112.26
2	A	501	CJA	C08-C07-C06	3.26	118.68	110.71
2	H	501	CJA	C08-C07-C06	3.21	118.56	110.71
2	I	501	CJA	C08-C07-C06	3.13	118.36	110.71
2	G	501	CJA	C07-C08-C09	3.09	118.27	110.71
2	J	501	CJA	C08-C07-C06	3.07	118.20	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	CJA	C08-C07-C06	2.99	118.03	110.71
2	C	501	CJA	C07-C08-C09	2.95	117.92	110.71
2	G	501	CJA	C08-C07-C06	2.88	117.74	110.71
2	B	501	CJA	C09-C10-N11	-2.75	119.35	123.83
2	G	501	CJA	C09-C10-N11	-2.73	119.39	123.83
2	H	501	CJA	O16-C15-C14	-2.70	118.29	120.96
2	E	501	CJA	C08-C07-C06	2.59	117.04	110.71
2	B	501	CJA	C07-C08-C09	2.59	117.03	110.71
2	I	501	CJA	C09-C10-N11	-2.58	119.64	123.83
2	E	501	CJA	C09-C10-N11	-2.56	119.66	123.83
2	L	501	CJA	C09-C10-N11	-2.47	119.81	123.83
2	D	501	CJA	S13-C12-N11	2.46	125.05	115.69
2	K	501	CJA	C09-C10-N11	-2.43	119.87	123.83
2	A	501	CJA	C09-C10-N11	-2.39	119.94	123.83
2	D	501	CJA	C09-C10-N11	-2.36	119.99	123.83
2	J	501	CJA	C09-C10-N11	-2.34	120.03	123.83
2	C	501	CJA	C09-C10-N11	-2.29	120.11	123.83
2	D	501	CJA	C14-S13-C12	-2.18	98.85	101.65
2	C	501	CJA	C09-C22-N21	-2.14	120.38	122.70
2	F	501	CJA	C09-C10-N11	-2.11	120.39	123.83
2	D	501	CJA	C08-C07-C06	2.03	115.66	110.71
2	B	501	CJA	O16-C15-C14	-2.02	118.97	120.96

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	CJA	C23-C03-S02-C01
2	C	501	CJA	S04-C03-S02-C01
2	D	501	CJA	S13-C14-C15-C17
2	D	501	CJA	S13-C14-C15-O16
2	F	501	CJA	N11-C12-S13-C14
2	F	501	CJA	N21-C12-S13-C14
2	L	501	CJA	N11-C12-S13-C14
2	L	501	CJA	N21-C12-S13-C14
2	D	501	CJA	N11-C12-S13-C14
2	D	501	CJA	N21-C12-S13-C14
2	B	501	CJA	C14-C15-C17-C20
2	B	501	CJA	C14-C15-C17-C18
2	E	501	CJA	C14-C15-C17-C18
2	E	501	CJA	C14-C15-C17-C19
2	J	501	CJA	C14-C15-C17-C20

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Mol	Chain	Res	Type	Atoms
2	J	501	CJA	C14-C15-C17-C19
2	J	501	CJA	O16-C15-C17-C19
2	J	501	CJA	O16-C15-C17-C20
2	B	501	CJA	O16-C15-C17-C20
2	B	501	CJA	C14-C15-C17-C19
2	E	501	CJA	C14-C15-C17-C20
2	J	501	CJA	C14-C15-C17-C18

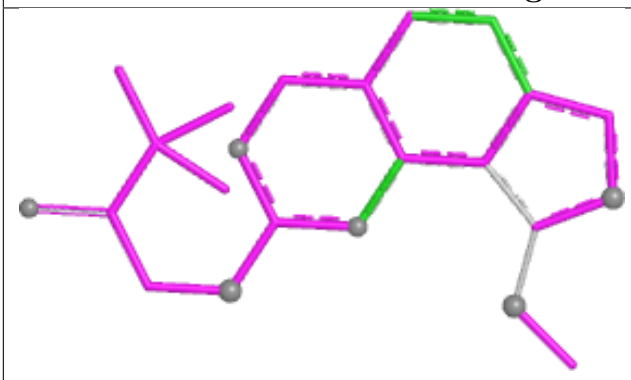
There are no ring outliers.

2 monomers are involved in 4 short contacts:

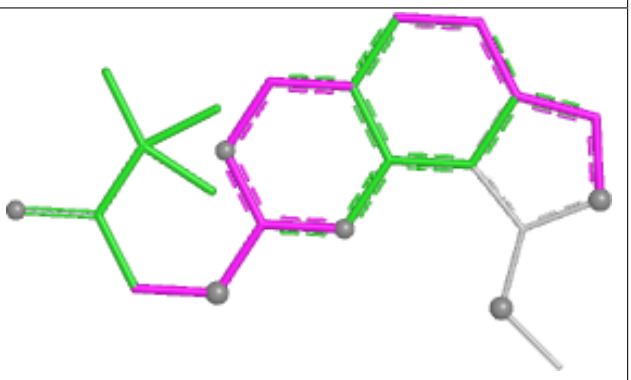
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	CJA	3	0
2	F	501	CJA	1	0

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 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.

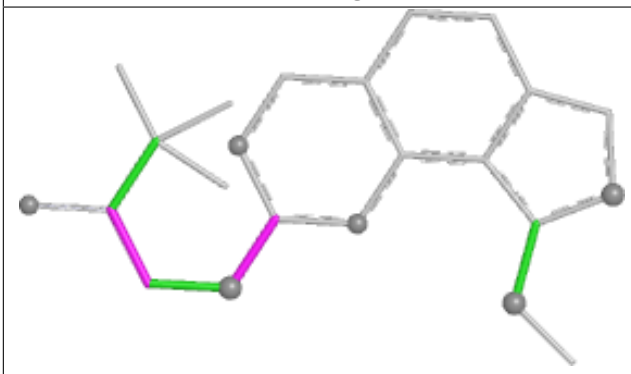
Ligand CJA D 501



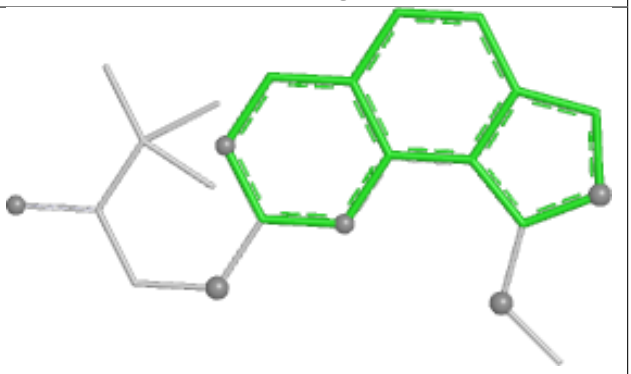
Bond lengths



Bond angles

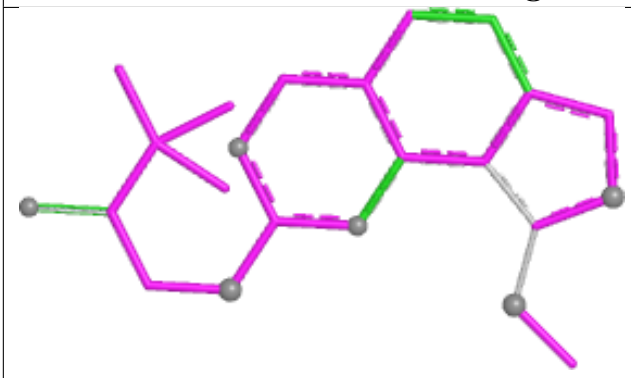


Torsions

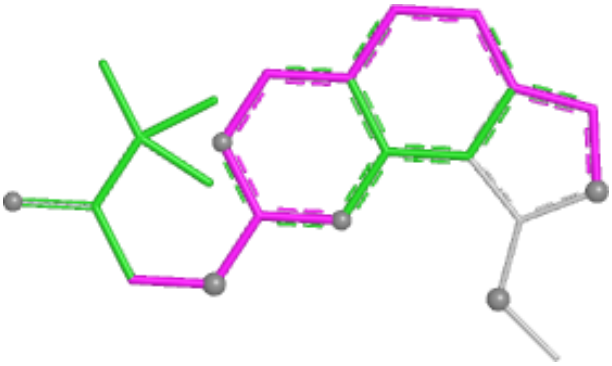


Rings

Ligand CJA G 501



Bond lengths



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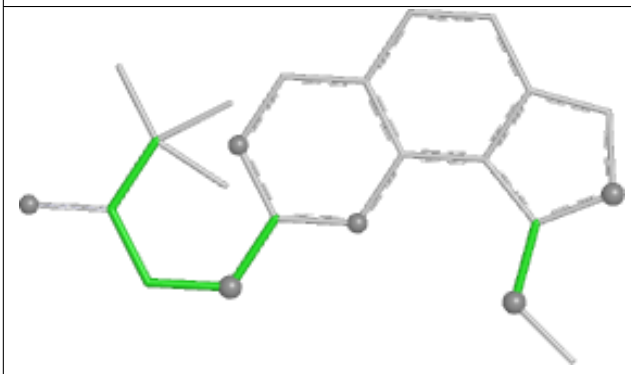

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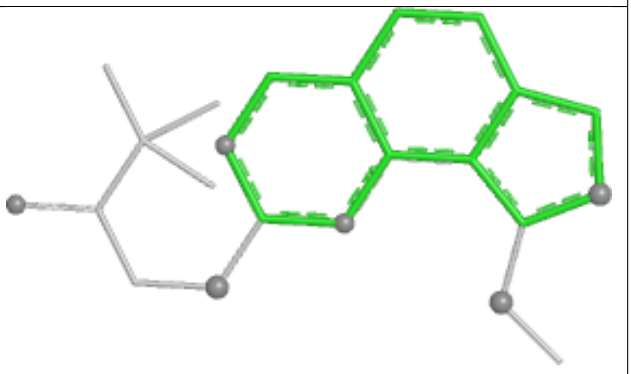
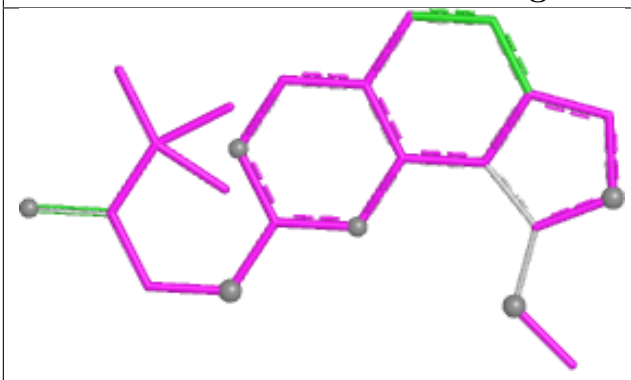


Rings

Ligand CJA J 501



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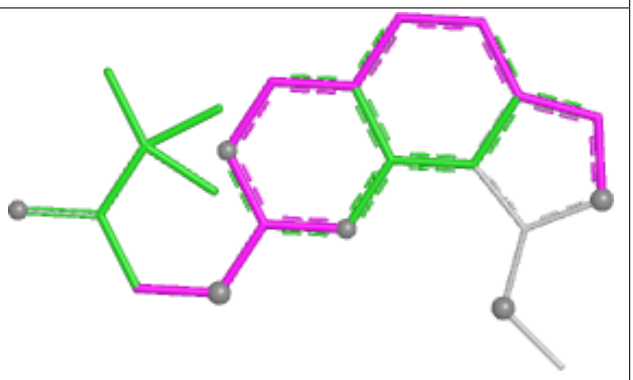
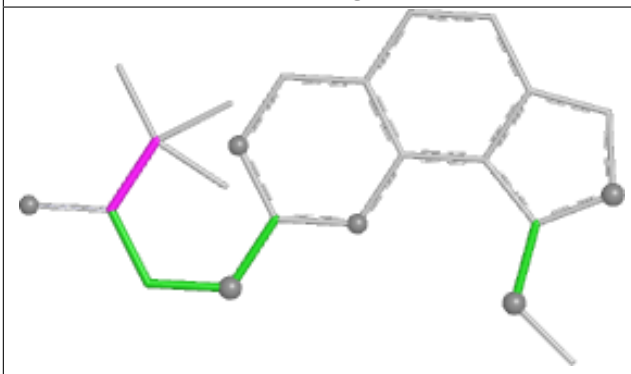


Bond angles



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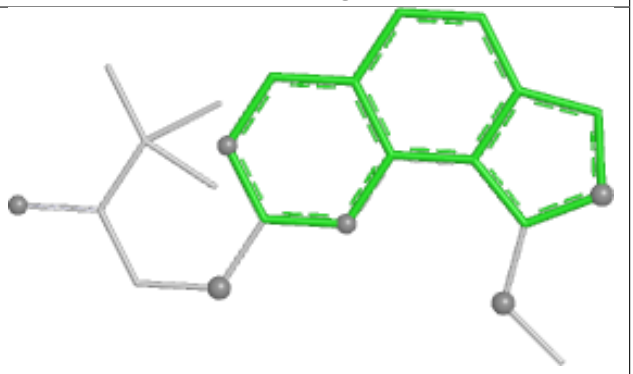
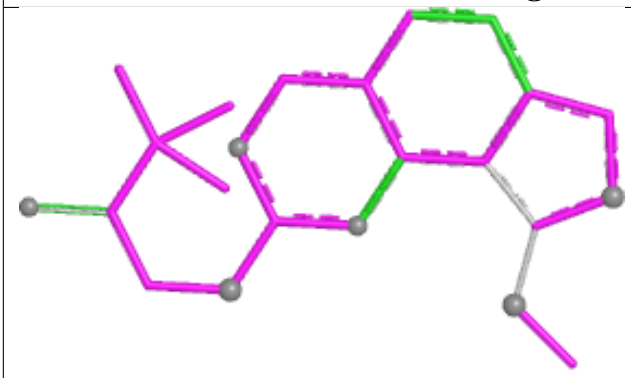


Rings

Ligand CJA C 501



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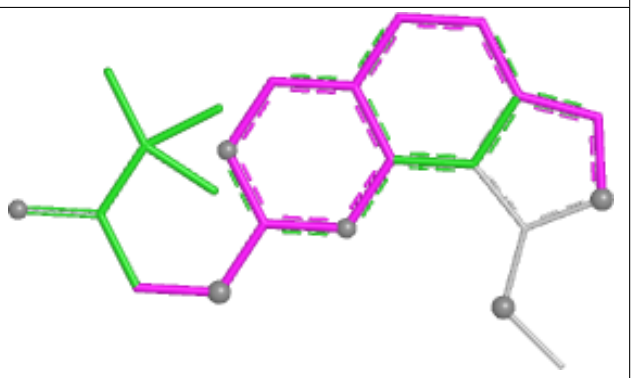
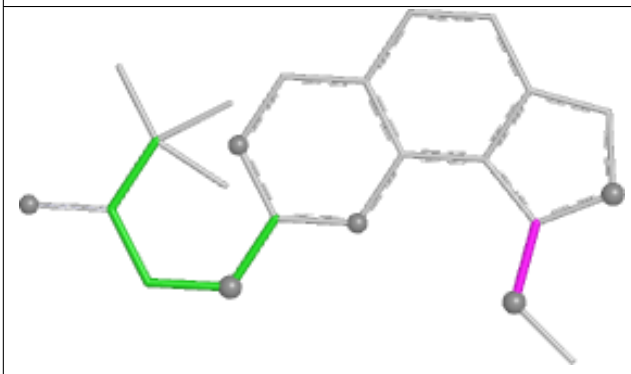


Bond angles



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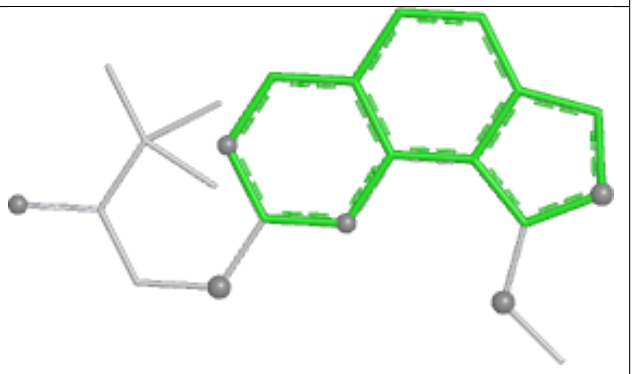
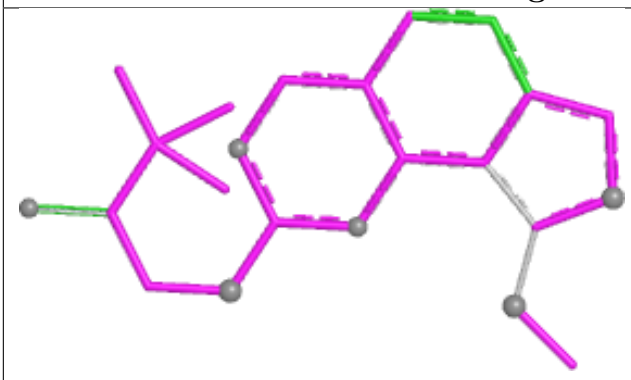


Rings

Ligand CJA L 501



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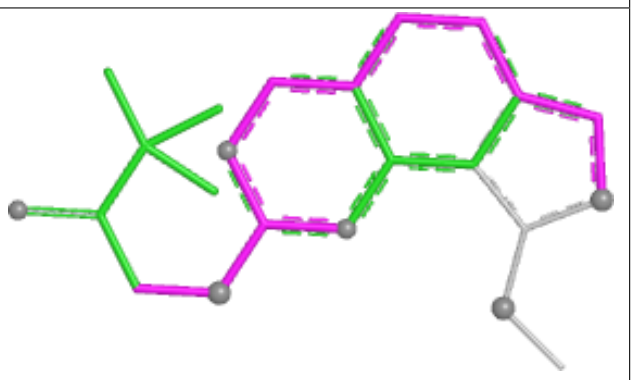
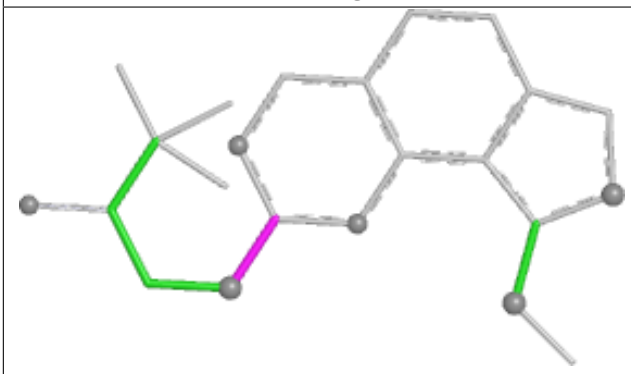


Bond angles



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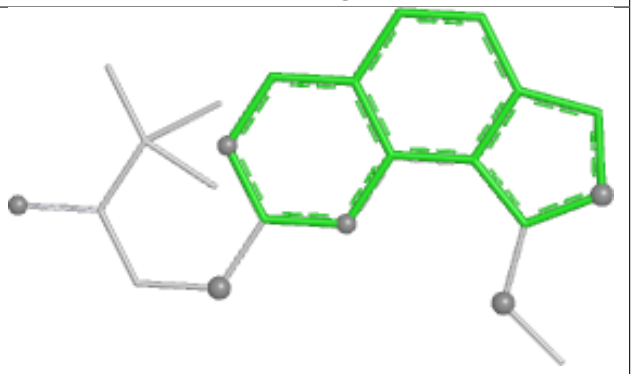
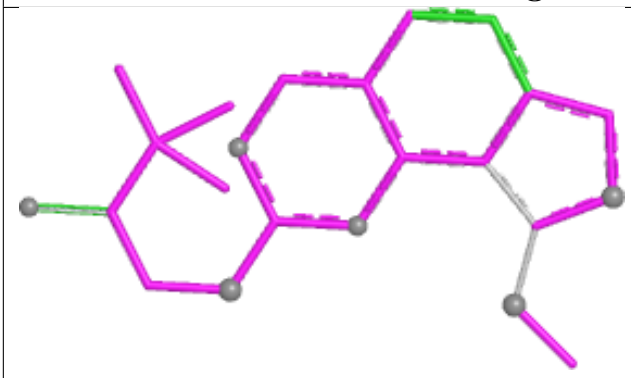
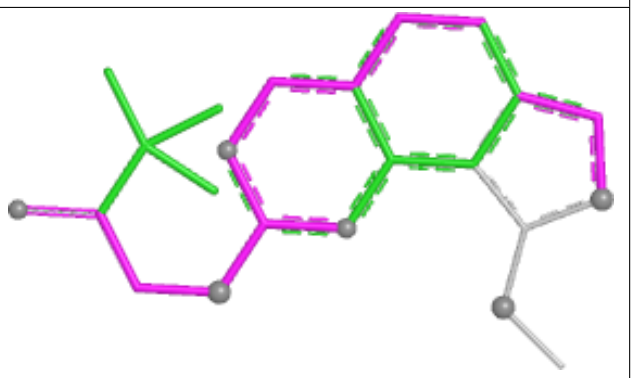


Rings

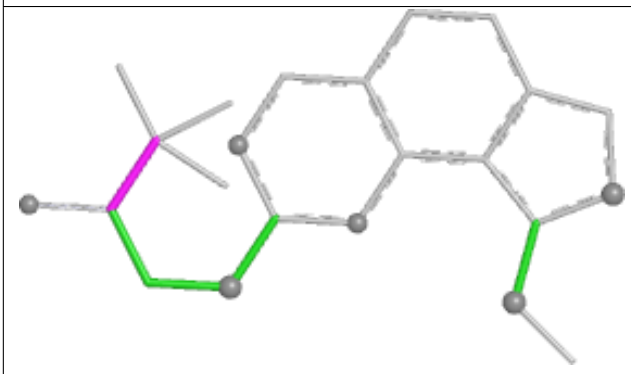
Ligand CJA B 501



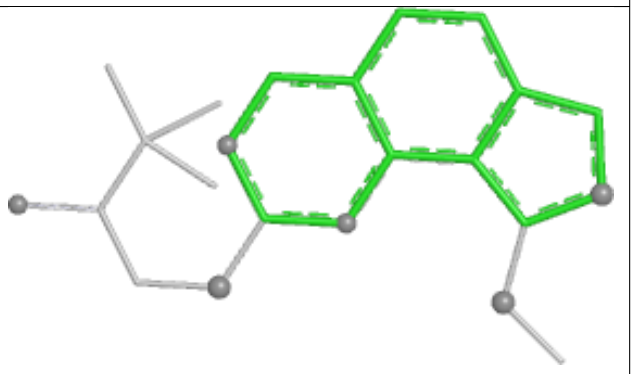
Bond lengths



Bond angles

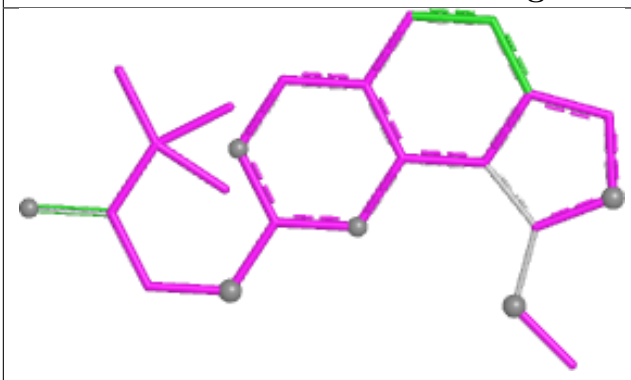


Torsions

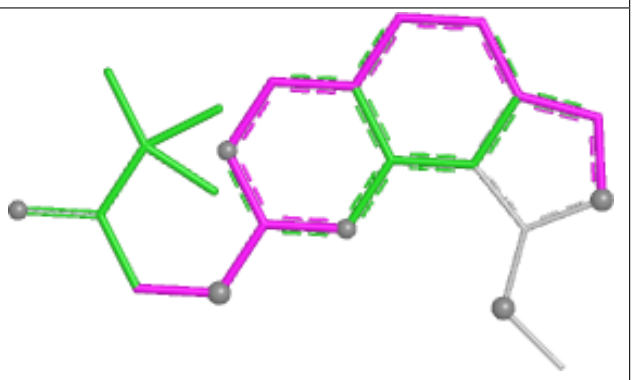


Rings

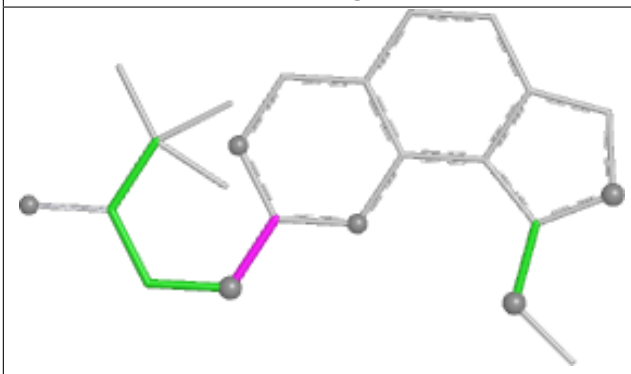
Ligand CJA F 501



Bond lengths



Bond angles



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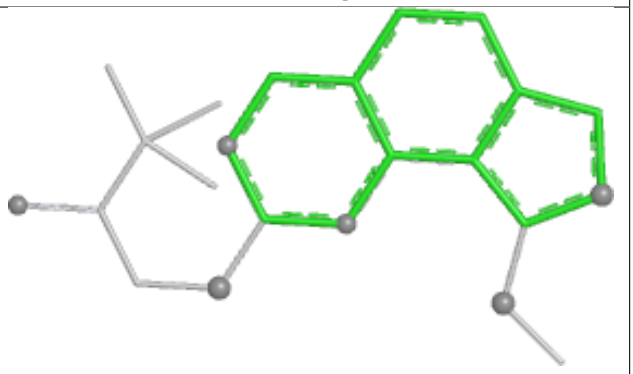
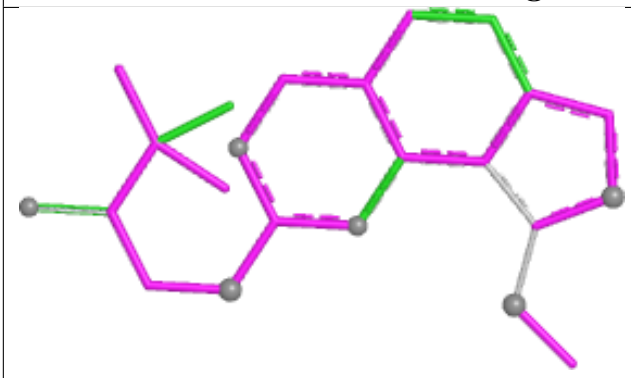
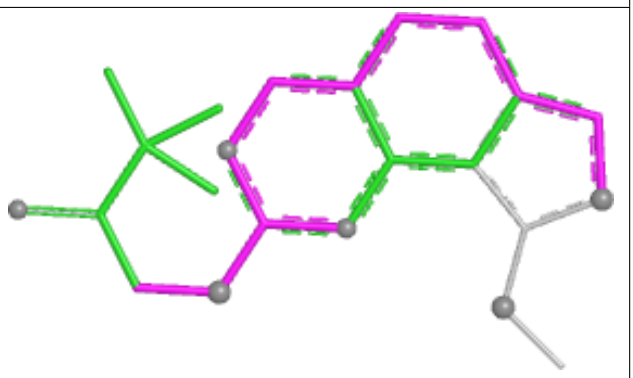


Rings

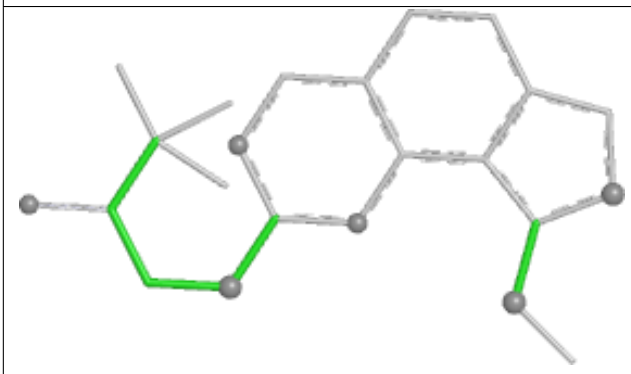
Ligand CJA A 501



Bond lengths



Bond angles



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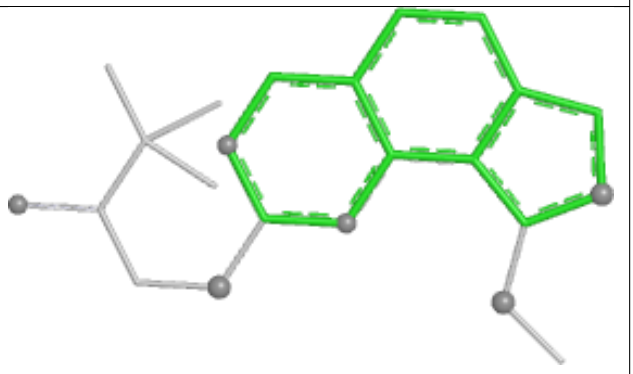
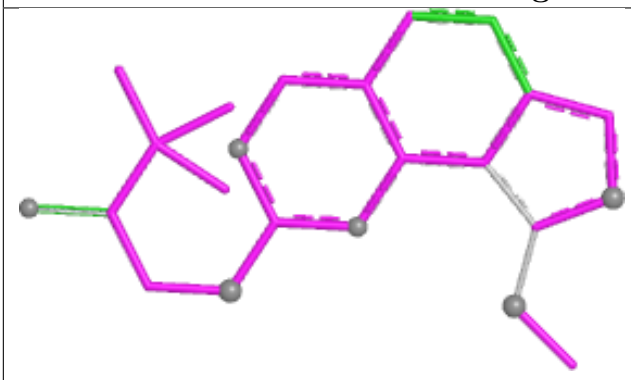


Rings

Ligand CJA I 501



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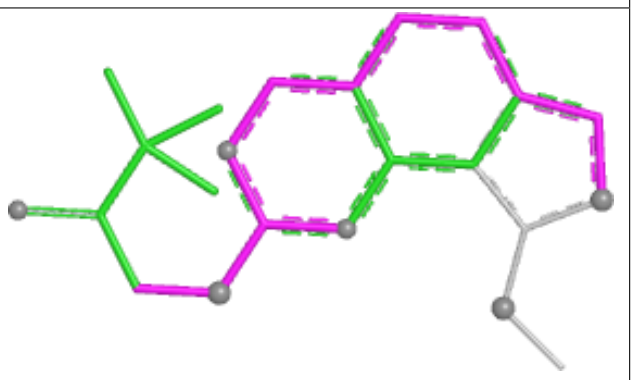
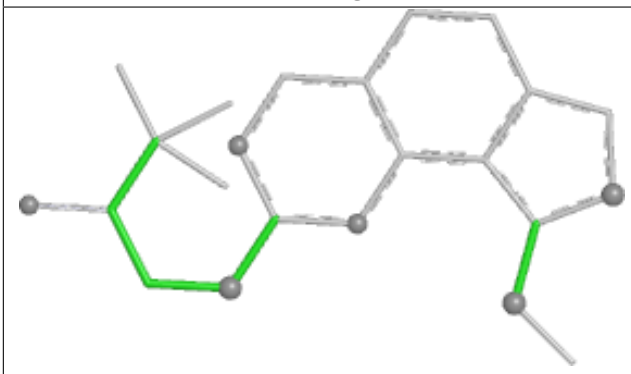
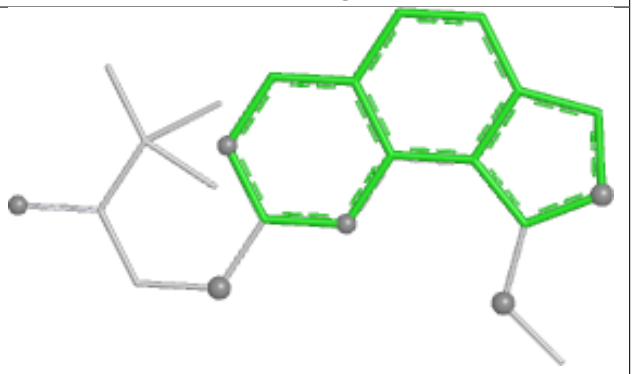


Bond angles

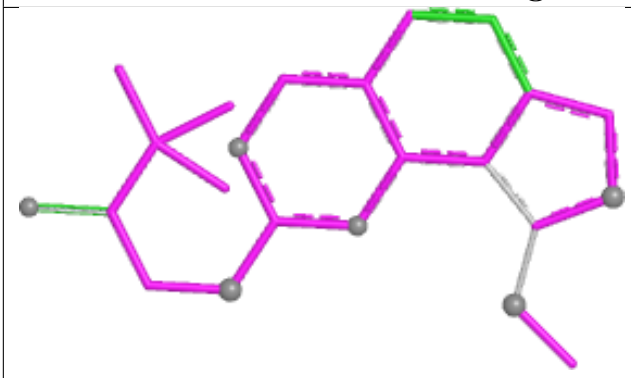


Torsions

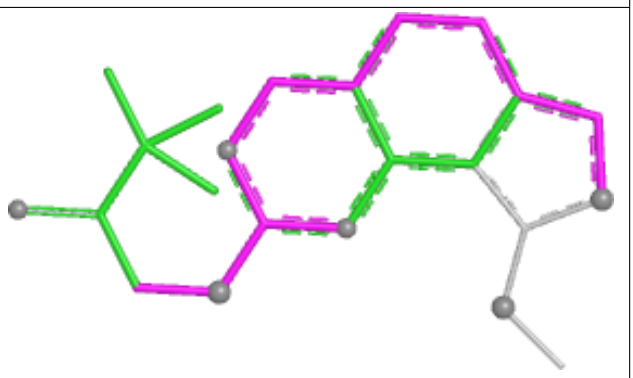


Rings

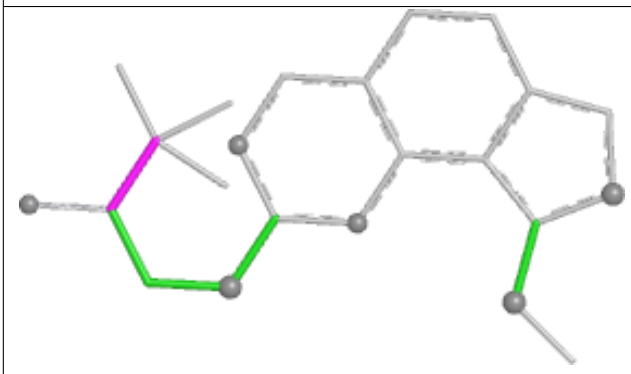
Ligand CJA E 501



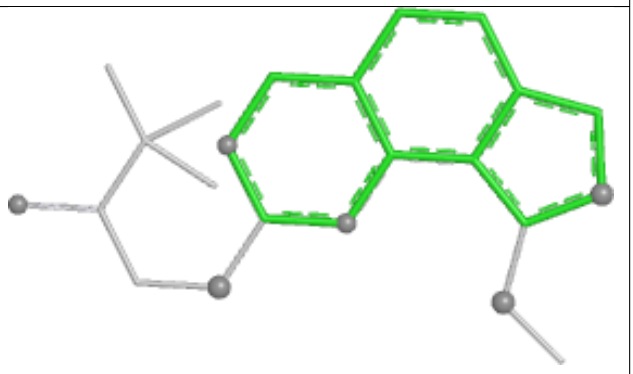
Bond lengths



Bond angles

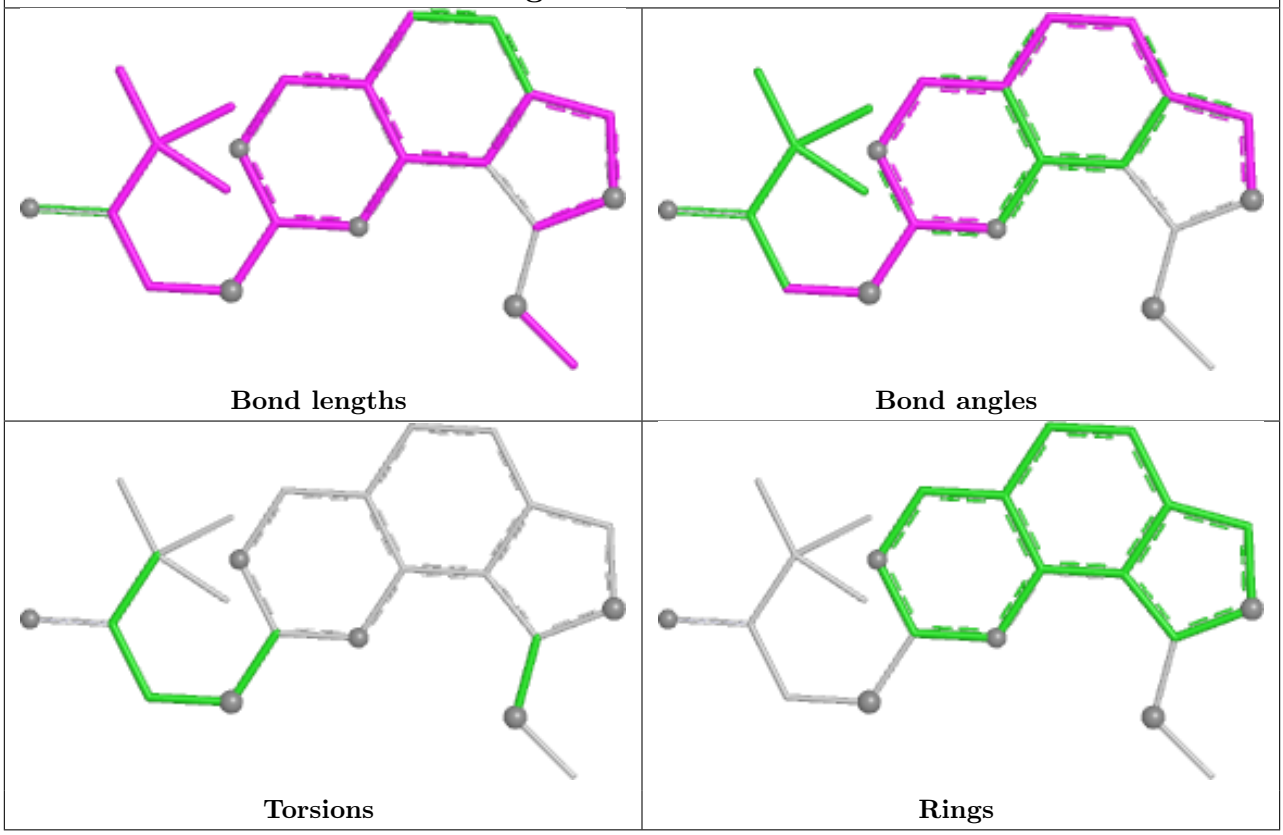


Torsions

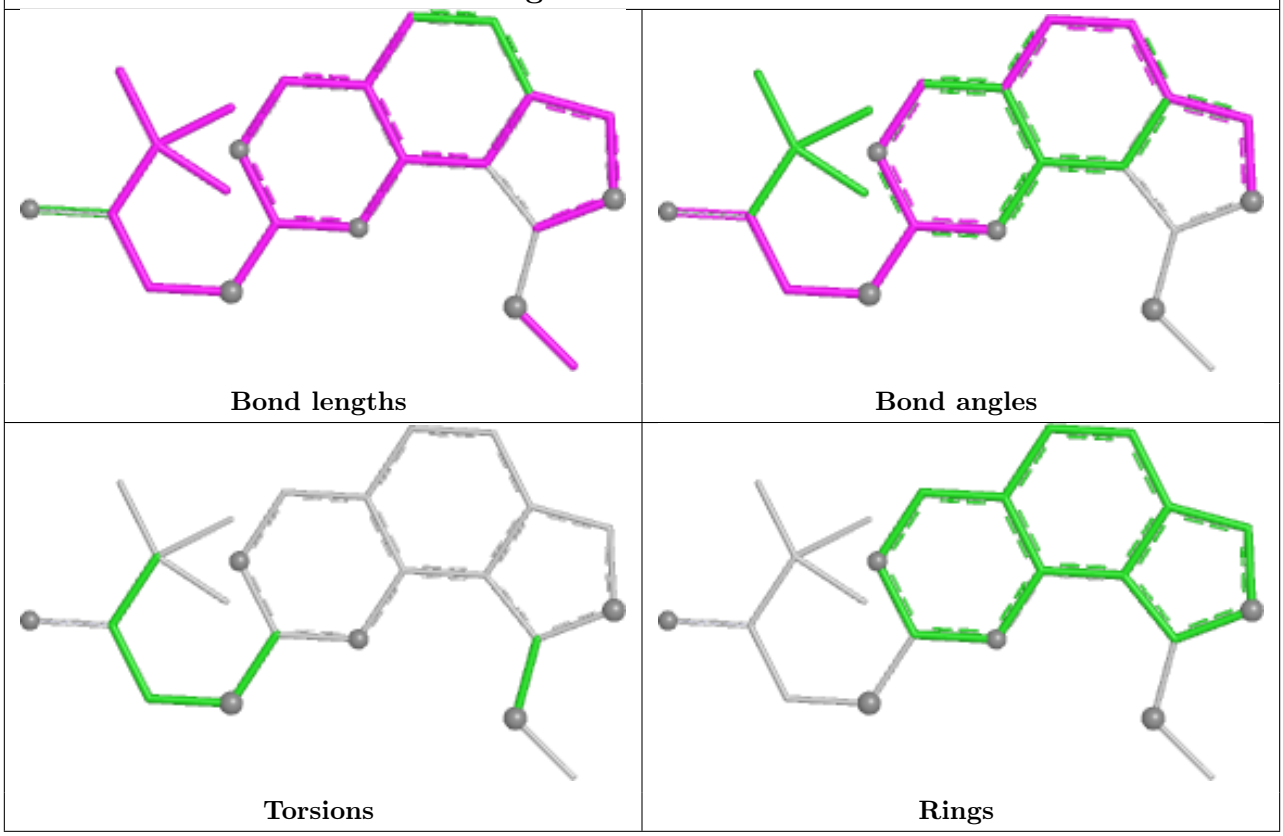


Rings

Ligand CJA K 501



Ligand CJA H 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, 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	148/148 (100%)	-0.13	4 (2%) 56 50	51, 68, 91, 114	0
1	B	147/148 (99%)	-0.08	1 (0%) 84 80	51, 69, 99, 120	0
1	C	147/148 (99%)	-0.03	2 (1%) 73 68	55, 74, 107, 125	0
1	D	147/148 (99%)	-0.08	1 (0%) 84 80	51, 74, 105, 125	0
1	E	147/148 (99%)	0.04	6 (4%) 42 35	55, 73, 100, 127	0
1	F	146/148 (98%)	-0.02	0 100 100	54, 78, 103, 126	0
1	G	147/148 (99%)	0.10	3 (2%) 64 58	53, 79, 104, 135	0
1	H	147/148 (99%)	0.02	3 (2%) 64 58	55, 73, 101, 120	0
1	I	147/148 (99%)	0.72	12 (8%) 19 16	74, 105, 130, 140	0
1	J	146/148 (98%)	0.74	13 (8%) 17 14	71, 104, 129, 138	0
1	K	146/148 (98%)	0.71	6 (4%) 42 35	79, 108, 128, 146	0
1	L	143/148 (96%)	0.78	17 (11%) 10 9	88, 115, 140, 148	0
All	All	1758/1776 (98%)	0.23	68 (3%) 44 37	51, 83, 127, 148	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	466	VAL	6.1
1	B	466	VAL	4.3
1	K	394	ILE	4.3
1	K	466	VAL	4.2
1	I	335	GLN	3.9
1	J	399	GLN	3.6
1	J	466	VAL	3.4
1	C	466	VAL	3.4
1	I	412	VAL	3.1
1	L	343	MET	3.1
1	J	322	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	466	VAL	3.1
1	K	362	HIS	3.1
1	L	428	ARG	3.1
1	H	466	VAL	3.1
1	I	395	GLU	3.1
1	L	389	GLU	3.0
1	J	339	ASP	2.9
1	J	420	ILE	2.8
1	I	320	ALA	2.8
1	A	466	VAL	2.7
1	J	389	GLU	2.7
1	E	441	LYS	2.7
1	L	459	GLU	2.7
1	A	375	ALA	2.7
1	L	334	GLU	2.7
1	A	319	MET	2.6
1	L	328	PHE	2.6
1	L	420	ILE	2.6
1	L	368	PHE	2.5
1	L	340	LEU	2.5
1	J	337	ALA	2.5
1	I	441	LYS	2.5
1	J	398	HIS	2.5
1	L	398	HIS	2.4
1	G	466	VAL	2.4
1	J	406	ILE	2.4
1	L	354	VAL	2.4
1	L	350	TYR	2.3
1	L	367	LEU	2.3
1	L	402	LYS	2.3
1	J	395	GLU	2.3
1	K	402	LYS	2.3
1	C	320	ALA	2.3
1	G	399	GLN	2.2
1	I	406	ILE	2.2
1	L	399	GLN	2.2
1	E	321	GLU	2.2
1	E	442	ARG	2.2
1	I	427	THR	2.2
1	D	466	VAL	2.2
1	E	320	ALA	2.2
1	I	343	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	339	ASP	2.2
1	L	430	THR	2.1
1	I	362	HIS	2.1
1	E	327	PRO	2.1
1	J	325	ILE	2.1
1	G	428	ARG	2.1
1	J	441	LYS	2.1
1	I	460	GLU	2.1
1	H	465	GLY	2.1
1	L	322	LEU	2.1
1	J	444	ILE	2.1
1	A	449	LEU	2.0
1	H	408	CYS	2.0
1	K	399	GLN	2.0
1	I	321	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	CJA	B	501	23/23	0.90	0.19	41,71,96,116	0
2	CJA	G	501	23/23	0.91	0.18	66,83,107,127	0
2	CJA	L	501	23/23	0.91	0.19	77,101,120,131	0
2	CJA	K	501	23/23	0.92	0.19	72,95,130,156	0
2	CJA	I	501	23/23	0.92	0.18	66,96,117,137	0
2	CJA	D	501	23/23	0.93	0.17	66,93,117,128	0
2	CJA	E	501	23/23	0.94	0.16	35,73,92,98	0
2	CJA	C	501	23/23	0.94	0.14	48,69,91,98	0

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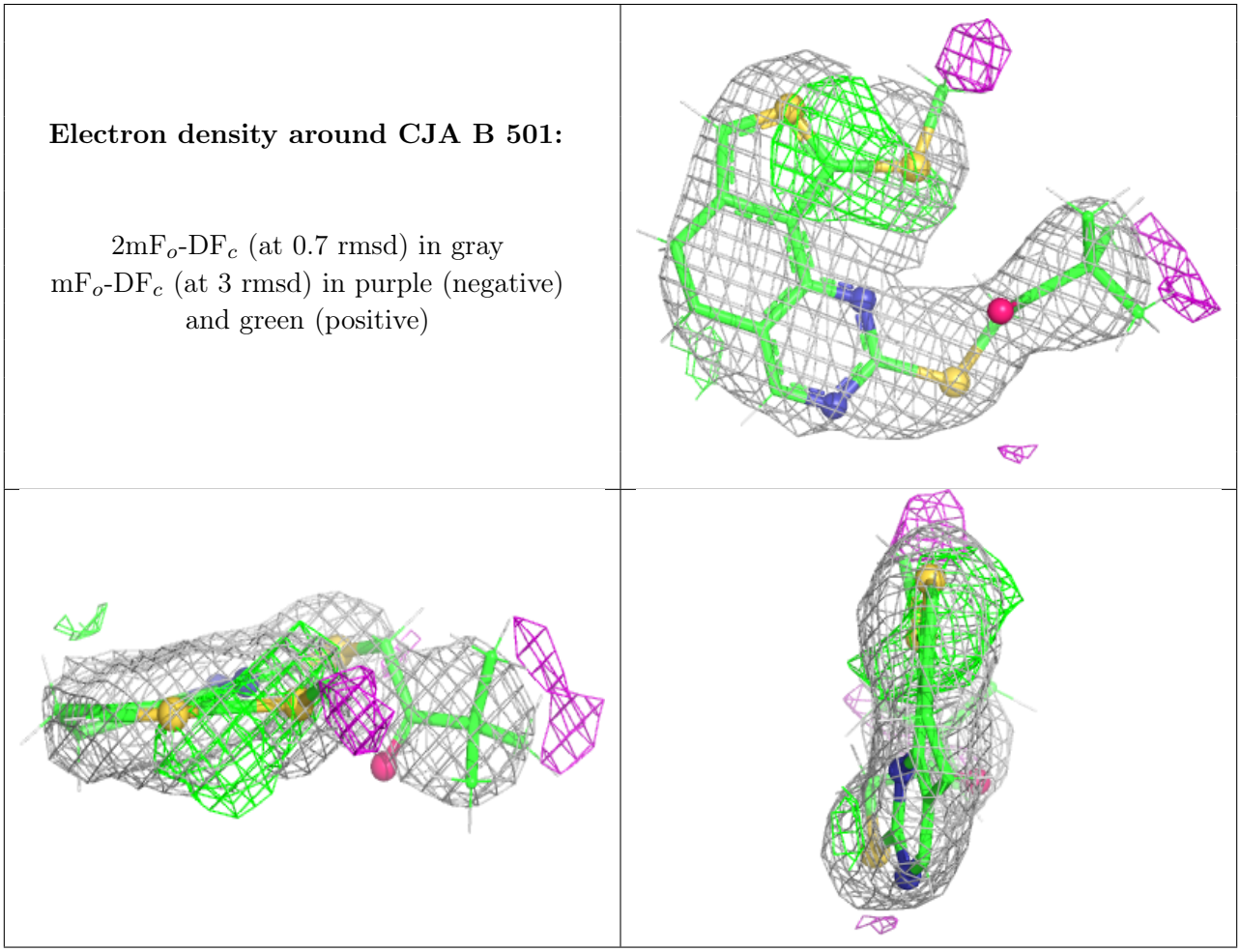
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CJA	H	501	23/23	0.94	0.16	58,79,101,117	0
2	CJA	F	501	23/23	0.95	0.16	67,87,100,120	0
2	CJA	J	501	23/23	0.95	0.14	72,91,111,125	0
2	CJA	A	501	23/23	0.96	0.14	45,64,88,93	0

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

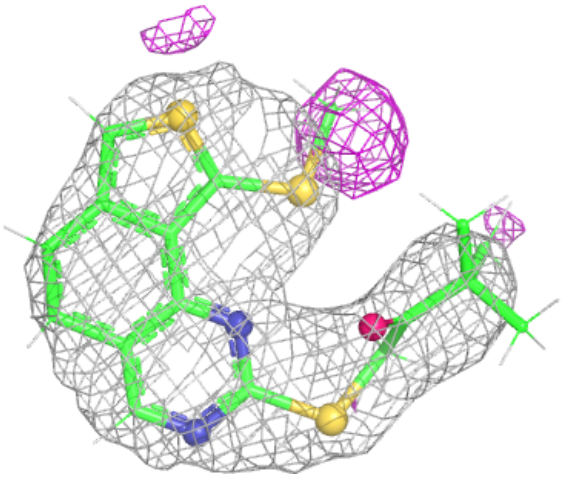
Electron density around CJA B 501:

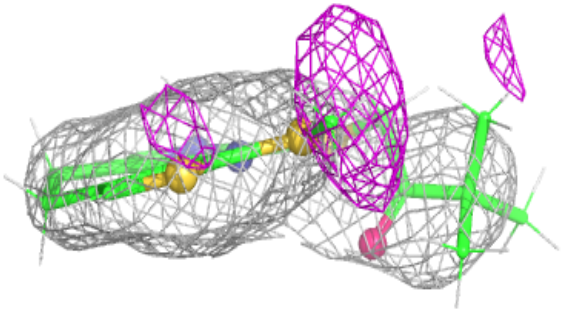
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

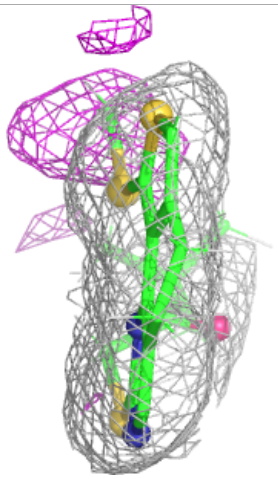


Electron density around CJA G 501:

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

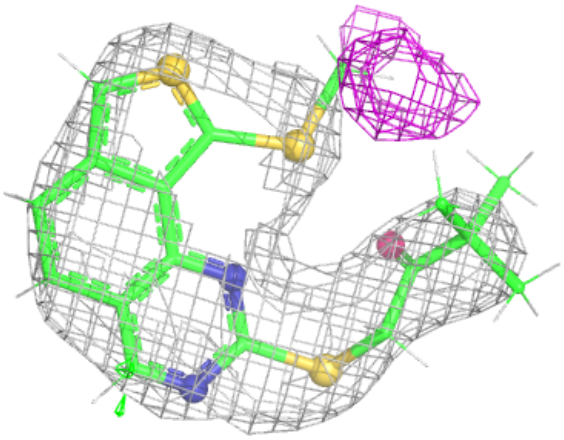


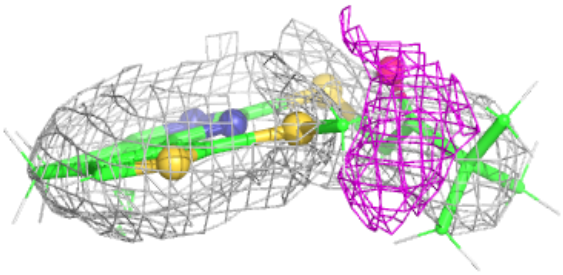


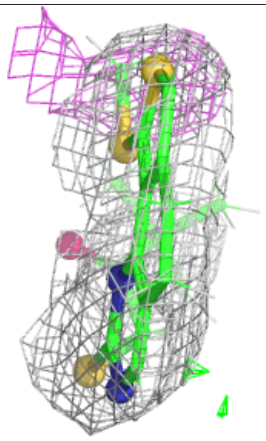


Electron density around CJA L 501:

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

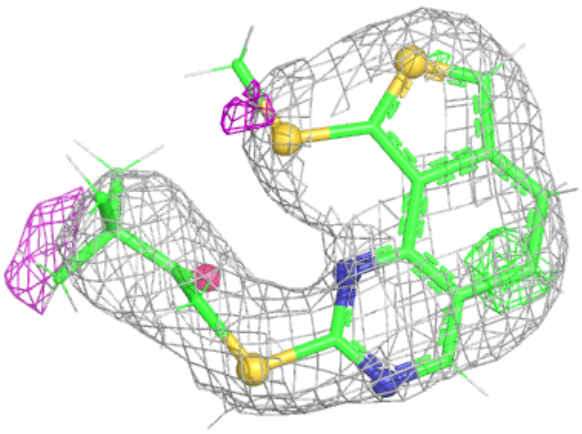


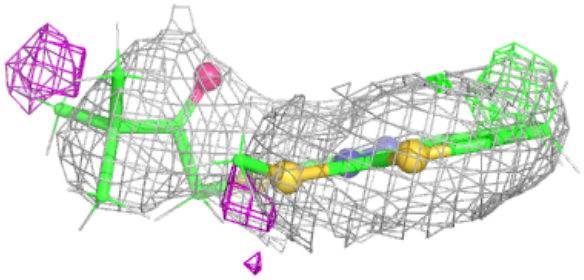


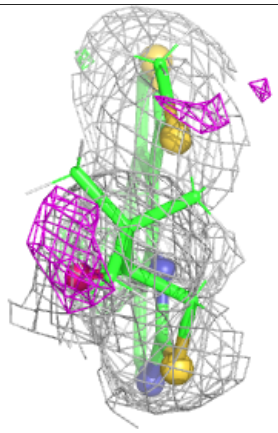


Electron density around CJA K 501:

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

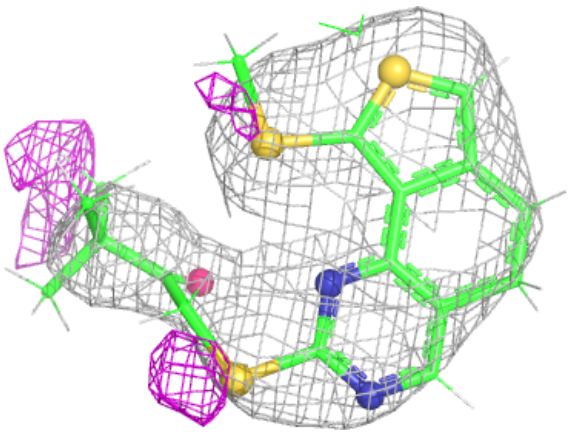


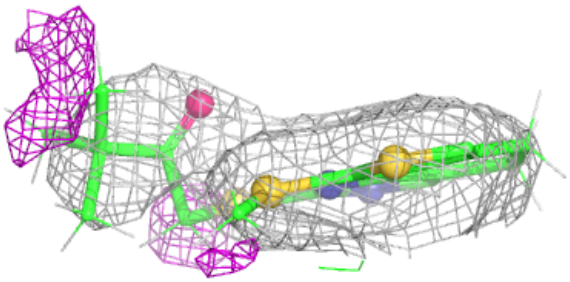


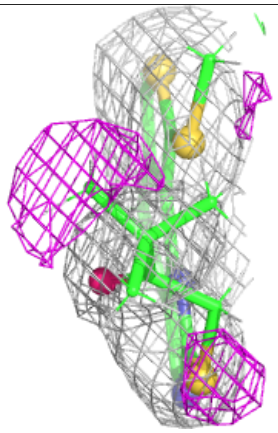


Electron density around CJA I 501:

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

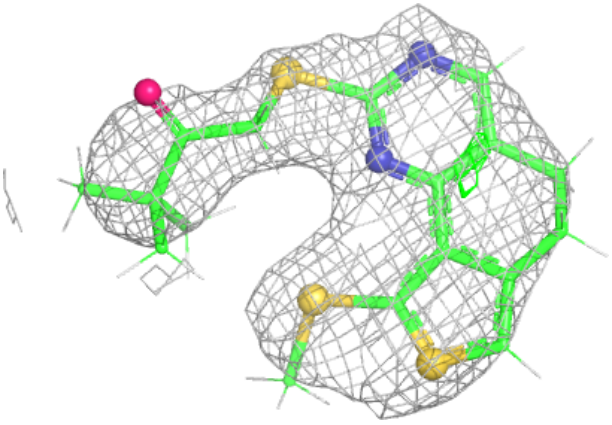


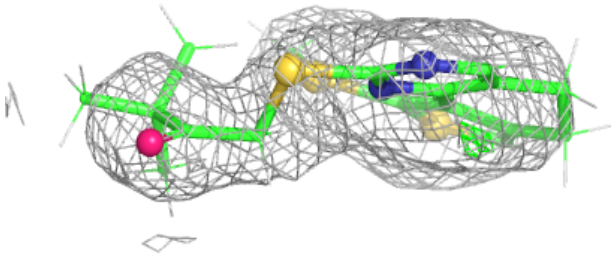


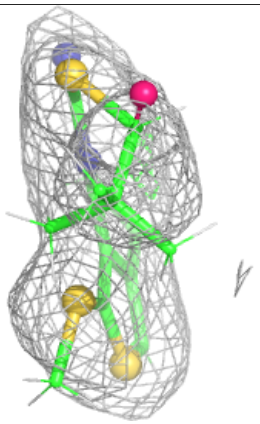


Electron density around CJA D 501:

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

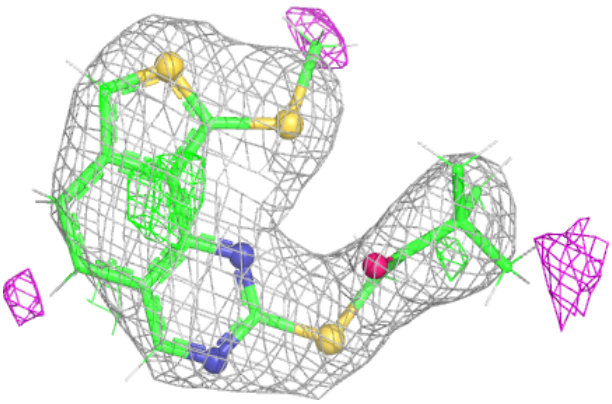


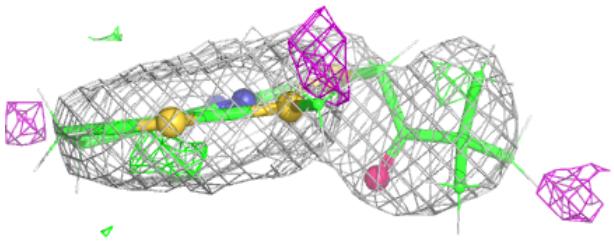


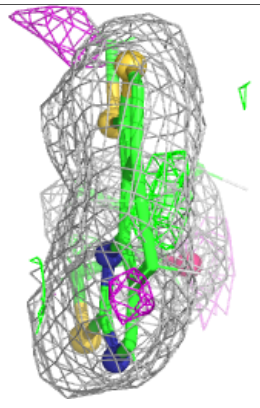


Electron density around CJA E 501:

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

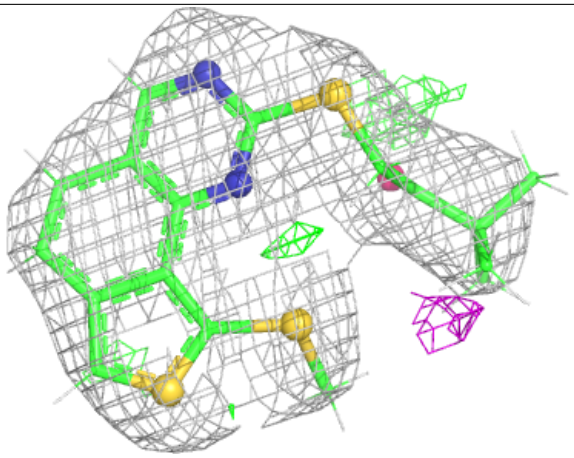


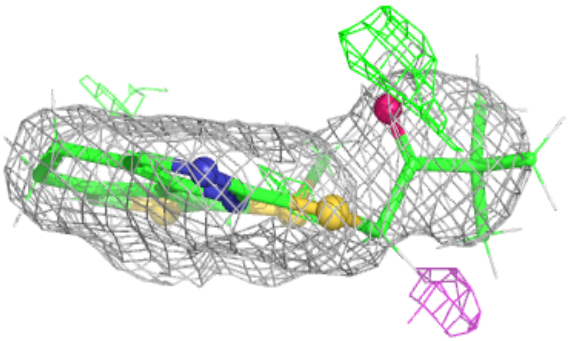


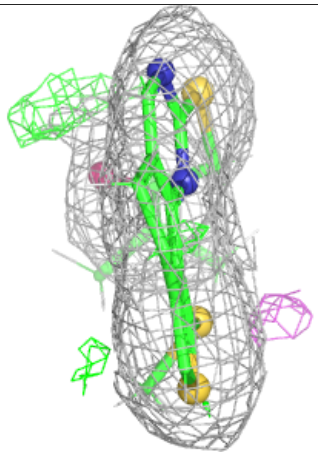


Electron density around CJA C 501:

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

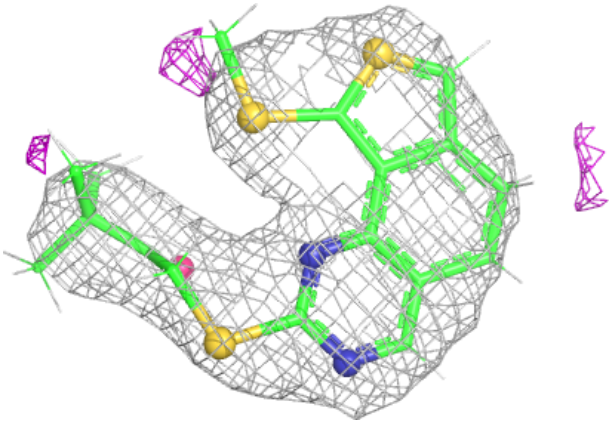


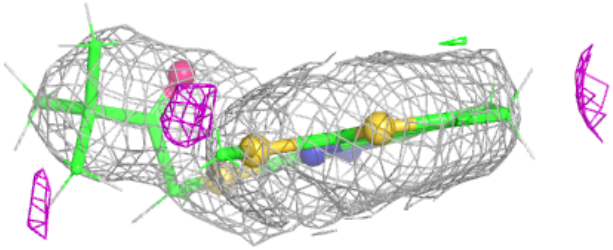


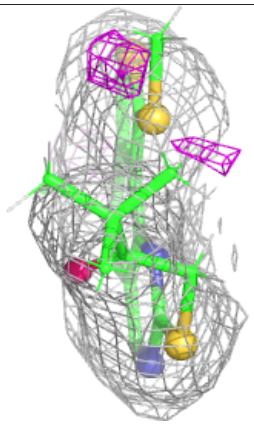


Electron density around CJA H 501:

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

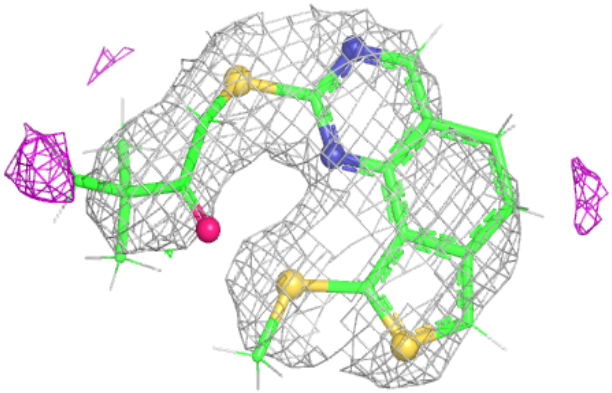


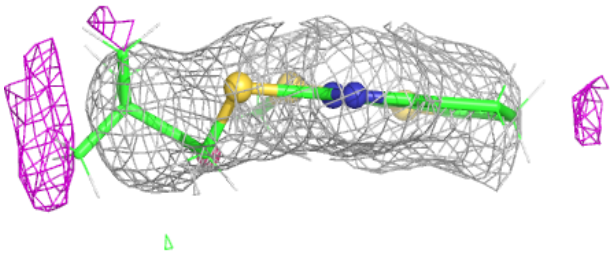


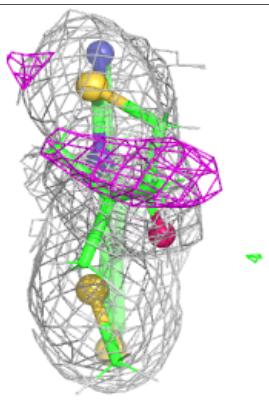


Electron density around CJA F 501:

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

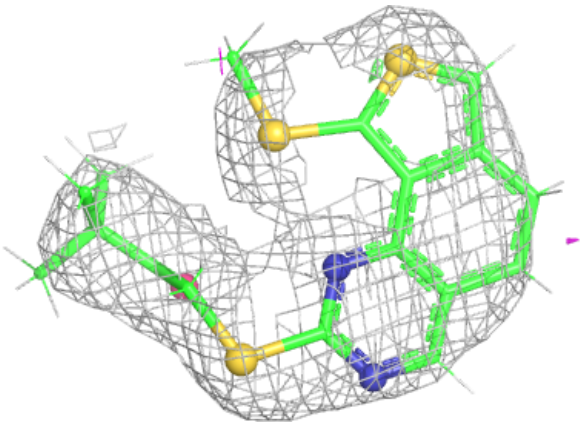


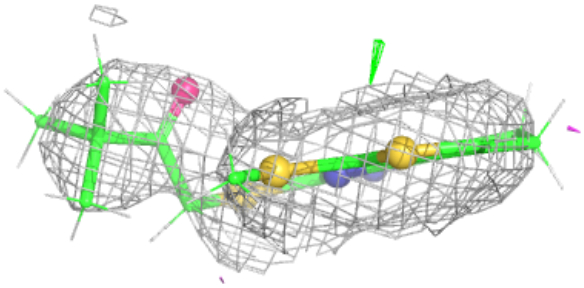


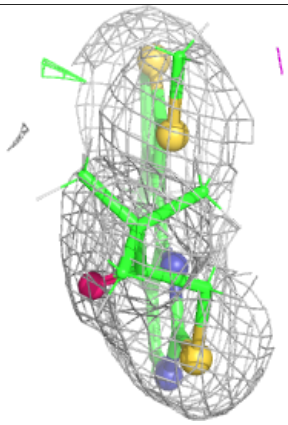


Electron density around CJA J 501:

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

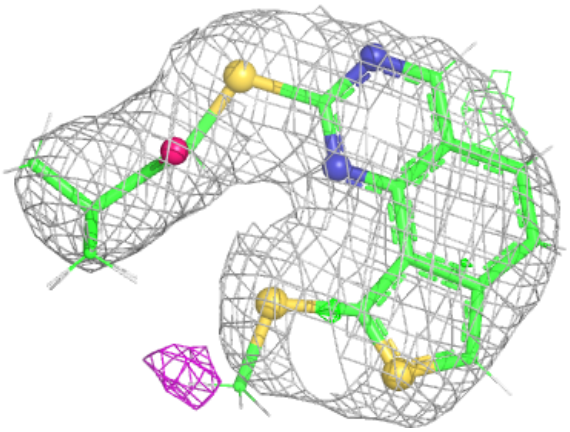


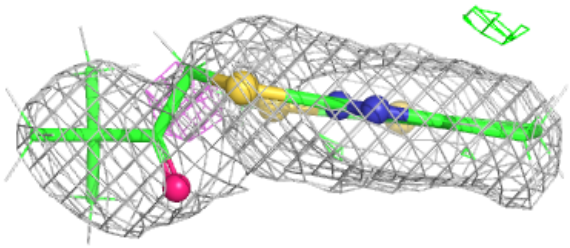


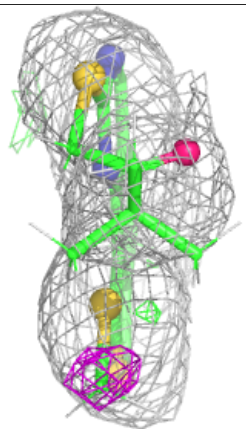


Electron density around CJA A 501:

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







6.5 Other polymers

There are no such residues in this entry.