



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:40 PM BST

PDB ID : 6ISP
Title : structure of Candida antarctica Lipase B mutant
Authors : Cen, Y.X.; Zhou, J.H.; Wu, Q.
Deposited on : 2018-11-18
Resolution : 1.88 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

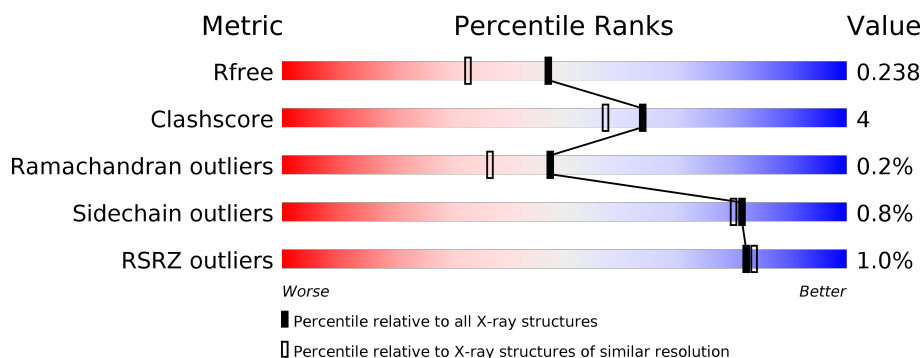
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 on 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	321	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	321	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	321	<div> <div></div> <div> <div></div> <div>90%</div> <div>10%</div> <div>.</div> </div> </div>
1	D	321	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10930 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	317	Total	C	N	O	S	0	1	0
			2336	1479	392	455	10			
1	A	317	Total	C	N	O	S	0	0	0
			2326	1474	388	453	11			
1	C	319	Total	C	N	O	S	0	0	0
			2341	1483	390	457	11			
1	B	317	Total	C	N	O	S	0	1	0
			2333	1478	389	455	11			

There are 40 discrepancies between the modelled and reference sequences:

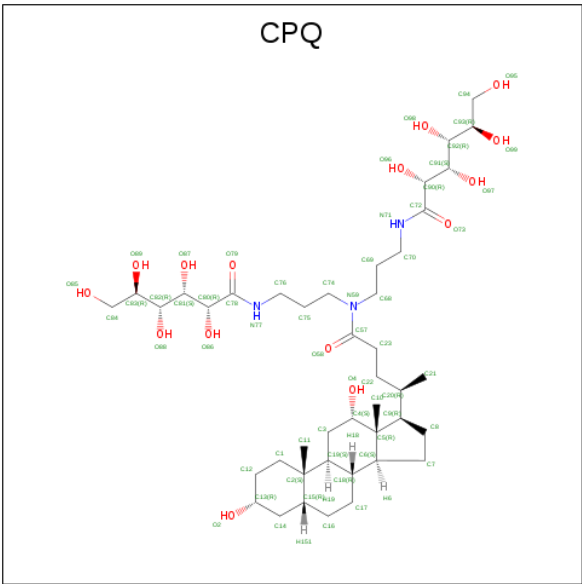
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP P41365
D	-2	ALA	-	expression tag	UNP P41365
D	-1	MET	-	expression tag	UNP P41365
D	0	ALA	-	expression tag	UNP P41365
D	57	ALA	THR	engineered mutation	UNP P41365
D	89	THR	ALA	engineered mutation	UNP P41365
D	104	VAL	TRP	engineered mutation	UNP P41365
D	149	GLY	VAL	engineered mutation	UNP P41365
D	281	TYR	ALA	engineered mutation	UNP P41365
D	282	TYR	ALA	engineered mutation	UNP P41365
A	-3	GLY	-	expression tag	UNP P41365
A	-2	ALA	-	expression tag	UNP P41365
A	-1	MET	-	expression tag	UNP P41365
A	0	ALA	-	expression tag	UNP P41365
A	57	ALA	THR	engineered mutation	UNP P41365
A	89	THR	ALA	engineered mutation	UNP P41365
A	104	VAL	TRP	engineered mutation	UNP P41365
A	149	GLY	VAL	engineered mutation	UNP P41365
A	281	TYR	ALA	engineered mutation	UNP P41365
A	282	TYR	ALA	engineered mutation	UNP P41365
C	-3	GLY	-	expression tag	UNP P41365

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ALA	-	expression tag	UNP P41365
C	-1	MET	-	expression tag	UNP P41365
C	0	ALA	-	expression tag	UNP P41365
C	57	ALA	THR	engineered mutation	UNP P41365
C	89	THR	ALA	engineered mutation	UNP P41365
C	104	VAL	TRP	engineered mutation	UNP P41365
C	149	GLY	VAL	engineered mutation	UNP P41365
C	281	TYR	ALA	engineered mutation	UNP P41365
C	282	TYR	ALA	engineered mutation	UNP P41365
B	-3	GLY	-	expression tag	UNP P41365
B	-2	ALA	-	expression tag	UNP P41365
B	-1	MET	-	expression tag	UNP P41365
B	0	ALA	-	expression tag	UNP P41365
B	57	ALA	THR	engineered mutation	UNP P41365
B	89	THR	ALA	engineered mutation	UNP P41365
B	104	VAL	TRP	engineered mutation	UNP P41365
B	149	GLY	VAL	engineered mutation	UNP P41365
B	281	TYR	ALA	engineered mutation	UNP P41365
B	282	TYR	ALA	engineered mutation	UNP P41365

- Molecule 2 is N,N-BIS(3-D-GLUCONAMIDOPROPYL)DEOXYCHOLAMIDE (three-letter code: CPQ) (formula: C₄₂H₇₅N₃O₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			45	34	2	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 22 20 2	0	0
2	A	1	Total C N O 60 42 3 15	0	0
2	A	1	Total C N O 28 24 1 3	0	0
2	A	1	Total C N O 35 29 2 4	0	0
2	A	1	Total C O 27 24 3	0	0
2	C	1	Total C O 22 20 2	0	0
2	C	1	Total C N O 30 26 1 3	0	0
2	C	1	Total C O 28 24 4	0	0
2	B	1	Total C N O 45 34 2 9	0	0
2	B	1	Total C O 22 20 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0

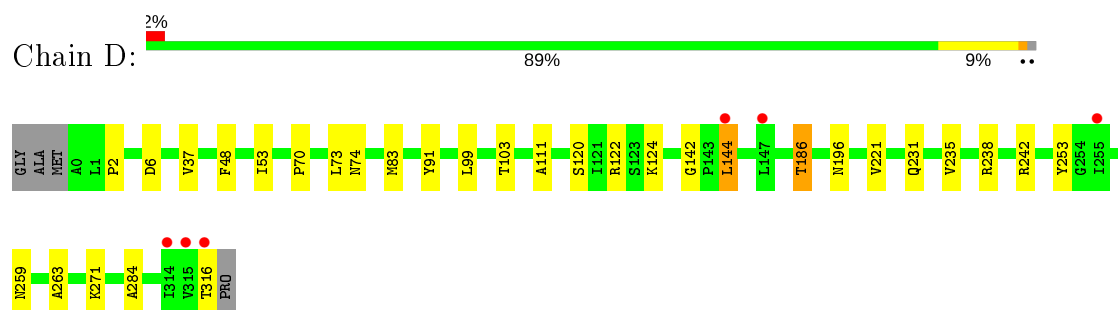
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	286	Total O 286 286	0	0
4	A	312	Total O 312 312	0	0
4	C	319	Total O 319 319	0	0
4	B	311	Total O 311 311	0	0

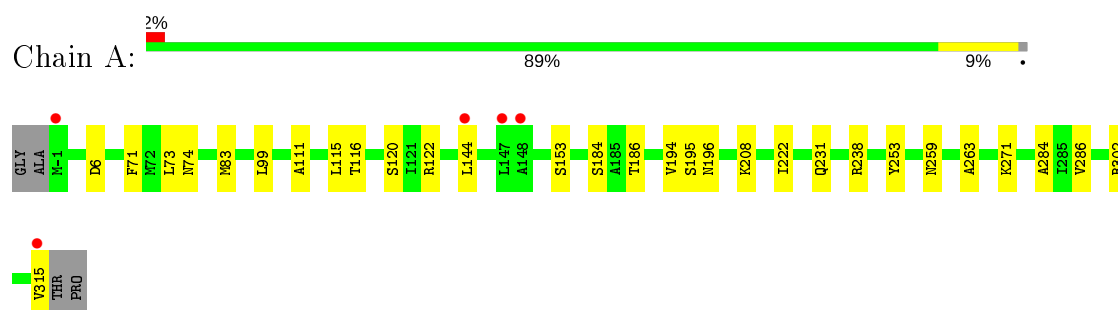
3 Residue-property plots [i](#)

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.

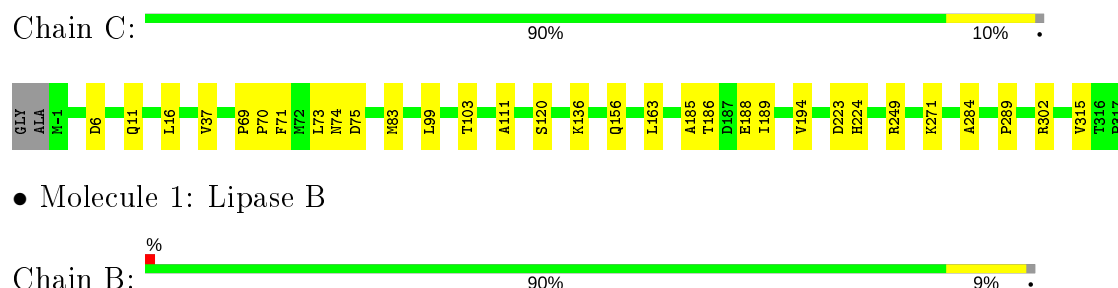
- Molecule 1: Lipase B



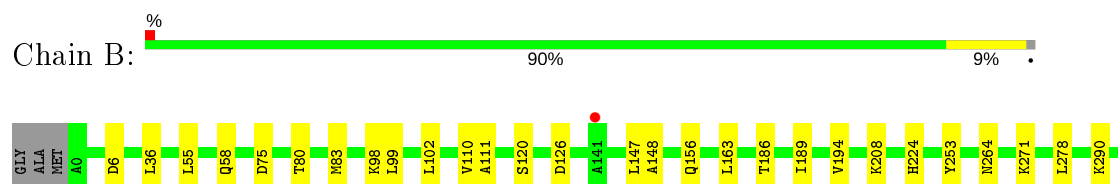
- Molecule 1: Lipase B



- Molecule 1: Lipase B



- Molecule 1: Lipase B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.98Å 155.97Å 92.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.27 – 1.88 46.27 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.27-1.88) 98.7 (46.27-1.88)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.88Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.213 , 0.238 0.214 , 0.238	Depositor DCC
R_{free} test set	5444 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10930	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3305e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: CPQ, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/2384	0.47	0/3271
1	B	0.25	0/2391	0.46	0/3281
1	C	0.25	0/2400	0.47	0/3293
1	D	0.26	0/2394	0.51	1/3286 (0.0%)
All	All	0.25	0/9569	0.48	1/13131 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	144	LEU	CB-CG-CD1	-11.08	92.16	111.00

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	2326	0	2301	18	0
1	B	2333	0	2307	16	0
1	C	2341	0	2315	20	0
1	D	2336	0	2312	18	0
2	A	150	0	199	14	0
2	B	67	0	88	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	80	0	109	4	0
2	D	67	0	88	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	312	0	0	0	0
4	B	311	0	0	2	0
4	C	319	0	0	5	0
4	D	286	0	0	2	0
All	All	10930	0	9719	82	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402:CPQ:H161	2:A:404:CPQ:H111	1.76	0.68
1:D:238:ARG:HD3	1:D:242:ARG:CZ	2.27	0.64
1:D:144:LEU:HD11	2:A:404:CPQ:C57	2.27	0.64
1:C:186:THR:HB	2:C:402:CPQ:H13	1.81	0.62
1:A:194:VAL:HB	2:A:402:CPQ:H71	1.82	0.62
2:B:402:CPQ:N77	2:B:402:CPQ:O88	2.35	0.59
1:A:302:ARG:HG3	1:A:315:VAL:HG13	1.85	0.58
1:C:271:LYS:NZ	4:C:516:HOH:O	2.35	0.58
1:B:208:LYS:NZ	1:B:253:TYR:OH	2.37	0.58
1:A:208:LYS:NZ	1:A:253:TYR:OH	2.38	0.57
1:D:70:PRO:HD2	1:D:74:ASN:HB2	1.86	0.57
1:A:238:ARG:HG2	1:A:238:ARG:HH11	1.69	0.57
1:A:231:GLN:HB3	1:A:259:ASN:HB3	1.87	0.56
1:D:73:LEU:HD11	1:D:284:ALA:HB1	1.87	0.56
1:C:6:ASP:OD1	1:C:120:SER:OG	2.22	0.56
1:D:231:GLN:HB3	1:D:259:ASN:HB3	1.89	0.54
1:C:194:VAL:HB	2:C:402:CPQ:H71	1.90	0.54
1:A:195:SER:O	2:A:402:CPQ:H741	2.08	0.54
2:D:401:CPQ:H161	2:A:403:CPQ:H111	1.92	0.52
1:D:196:ASN:ND2	4:D:516:HOH:O	2.42	0.52
1:A:115:LEU:O	1:A:122:ARG:NE	2.34	0.51
1:C:189:ILE:HD12	1:C:224:HIS:CD2	2.45	0.51
1:D:144:LEU:HD11	2:A:404:CPQ:O58	2.10	0.51
1:B:6:ASP:OD2	1:B:120:SER:OG	2.22	0.51
1:A:116:THR:O	1:A:122:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:VAL:HB	2:B:402:CPQ:H71	1.93	0.50
1:D:83:MET:SD	1:D:111:ALA:HA	2.52	0.50
1:D:142:GLY:O	1:D:144:LEU:N	2.45	0.50
1:C:185:ALA:HB1	1:C:194:VAL:HG12	1.94	0.49
1:A:73:LEU:HD11	1:A:284:ALA:HB1	1.93	0.49
1:B:156:GLN:HB3	1:B:163:LEU:HG	1.94	0.48
2:A:403:CPQ:H212	2:A:403:CPQ:H103	1.95	0.48
1:C:11:GLN:HB2	1:C:16:LEU:HD21	1.95	0.48
1:A:196:ASN:HD22	2:A:402:CPQ:H701	1.79	0.47
1:C:71:PHE:CE2	2:C:403:CPQ:H171	2.49	0.47
2:A:402:CPQ:H752	2:A:402:CPQ:H702	1.95	0.47
1:A:83:MET:SD	1:A:111:ALA:HA	2.55	0.47
1:C:156:GLN:HB3	1:C:163:LEU:HG	1.97	0.46
1:D:37:VAL:HB	1:D:103:THR:HG22	1.96	0.46
1:D:6:ASP:OD2	1:D:120:SER:OG	2.26	0.46
2:A:402:CPQ:O87	2:A:402:CPQ:N77	2.49	0.46
1:C:83:MET:SD	1:C:111:ALA:HA	2.56	0.45
1:A:284:ALA:HA	2:A:405:CPQ:H162	1.98	0.45
1:D:186:THR:HG21	1:D:221:VAL:HG13	1.98	0.45
1:C:188:GLU:OE2	1:C:223:ASP:HB2	2.17	0.45
1:A:71:PHE:CE2	2:A:405:CPQ:H171	2.50	0.45
1:D:48:PHE:HB2	1:D:53:ILE:HG13	1.99	0.45
1:A:6:ASP:OD2	1:A:120:SER:OG	2.25	0.44
1:D:235:VAL:HG12	1:D:253:TYR:HB3	1.99	0.44
1:B:83[A]:MET:SD	1:B:111:ALA:HA	2.57	0.44
1:B:189:ILE:HD12	1:B:224:HIS:CD2	2.53	0.43
1:D:2:PRO:O	1:D:122:ARG:NH2	2.46	0.43
1:C:249:ARG:NH2	4:C:535:HOH:O	2.51	0.43
1:C:73:LEU:HD11	1:C:284:ALA:HB1	2.00	0.43
1:C:69:PRO:HA	1:C:70:PRO:HA	1.75	0.43
1:B:75:ASP:OD1	1:B:156:GLN:NE2	2.33	0.43
1:C:37:VAL:HB	1:C:103:THR:HG22	2.01	0.43
1:C:223:ASP:OD1	4:C:501:HOH:O	2.21	0.43
1:A:184:SER:HB2	1:A:222:ILE:HG23	2.01	0.42
1:B:278:LEU:HD23	4:B:699:HOH:O	2.19	0.42
2:C:403:CPQ:H19	2:C:403:CPQ:H141	1.82	0.42
1:B:98:LYS:HB3	1:B:126:ASP:HB2	2.00	0.42
1:A:144:LEU:HD21	1:A:286:VAL:HG13	2.02	0.42
2:A:405:CPQ:H212	2:A:405:CPQ:H103	2.00	0.42
1:A:74:ASN:O	1:A:153:SER:HB3	2.20	0.42
1:B:290:LYS:HE3	4:B:710:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ALA:O	1:B:290:LYS:HD3	2.20	0.41
1:A:263:ALA:O	1:A:271:LYS:HE2	2.20	0.41
1:B:264:ASN:HA	1:B:271:LYS:NZ	2.35	0.41
1:C:136:LYS:O	4:C:502:HOH:O	2.21	0.41
1:C:73:LEU:CD1	1:C:289:PRO:HD2	2.50	0.41
1:D:263:ALA:O	1:D:271:LYS:NZ	2.51	0.41
1:B:55:LEU:O	1:B:58:GLN:HG2	2.21	0.41
1:D:316:THR:HA	4:D:638:HOH:O	2.21	0.41
2:D:401:CPQ:H701	2:D:401:CPQ:H911	2.01	0.41
1:B:264:ASN:HA	1:B:271:LYS:HZ1	1.86	0.41
1:B:36:LEU:HA	1:B:102:LEU:O	2.21	0.41
1:D:91:TYR:CD2	1:D:124:LYS:HE2	2.56	0.40
2:A:403:CPQ:H18	2:A:403:CPQ:H102	1.80	0.40
1:C:74:ASN:OD1	1:C:75:ASP:N	2.49	0.40
1:B:80:THR:HA	1:B:110:VAL:HG13	2.03	0.40
1:C:302:ARG:HD3	4:C:591:HOH:O	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	315/321 (98%)	304 (96%)	11 (4%)	0	100	100
1	B	316/321 (98%)	306 (97%)	9 (3%)	1 (0%)	41	30
1	C	317/321 (99%)	304 (96%)	12 (4%)	1 (0%)	41	30
1	D	316/321 (98%)	304 (96%)	12 (4%)	0	100	100
All	All	1264/1284 (98%)	1218 (96%)	44 (4%)	2 (0%)	47	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	315	VAL
1	B	315	VAL

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	255/257 (99%)	253 (99%)	2 (1%)	81	80
1	B	256/257 (100%)	253 (99%)	3 (1%)	71	67
1	C	257/257 (100%)	256 (100%)	1 (0%)	91	90
1	D	256/257 (100%)	254 (99%)	2 (1%)	81	80
All	All	1024/1028 (100%)	1016 (99%)	8 (1%)	81	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	99	LEU
1	D	186	THR
1	A	99	LEU
1	A	186	THR
1	C	99	LEU
1	B	99	LEU
1	B	147	LEU
1	B	186	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	196	ASN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CPQ	A	405	-	30,30,63	0.83	1 (3%)	47,47,92	1.43	7 (14%)
2	CPQ	B	403	-	25,25,63	0.89	1 (4%)	38,41,92	1.22	3 (7%)
2	CPQ	A	403	-	31,31,63	0.78	1 (3%)	49,49,92	1.54	9 (18%)
2	CPQ	C	402	-	33,33,63	0.77	1 (3%)	51,52,92	1.43	8 (15%)
2	CPQ	D	402	-	25,25,63	0.82	1 (4%)	38,41,92	1.79	5 (13%)
2	CPQ	A	402	-	63,63,63	0.63	1 (1%)	91,92,92	0.92	4 (4%)
2	CPQ	B	402	-	48,48,63	0.72	1 (2%)	70,72,92	1.28	8 (11%)
2	CPQ	D	401	-	48,48,63	0.71	1 (2%)	70,72,92	1.18	5 (7%)
2	CPQ	C	403	-	30,30,63	0.82	1 (3%)	47,47,92	1.31	3 (6%)
2	CPQ	A	404	-	38,38,63	0.73	1 (2%)	54,57,92	1.37	8 (14%)
2	CPQ	C	401	-	25,25,63	0.90	2 (8%)	38,41,92	1.16	2 (5%)

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	CPQ	A	405	-	-	6/7/70/125	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CPQ	B	403	-	-	-	0/4/4/4
2	CPQ	A	403	-	-	7/9/71/125	0/4/4/4
2	CPQ	C	402	-	-	10/13/75/125	0/4/4/4
2	CPQ	D	402	-	-	-	0/4/4/4
2	CPQ	A	402	-	-	35/63/125/125	0/4/4/4
2	CPQ	B	402	-	-	23/38/100/125	0/4/4/4
2	CPQ	D	401	-	-	22/38/100/125	0/4/4/4
2	CPQ	C	403	-	-	3/7/70/125	0/4/4/4
2	CPQ	A	404	-	-	12/19/81/125	0/4/4/4
2	CPQ	C	401	-	-	-	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	402	CPQ	C5-C6	-2.48	1.51	1.55
2	B	403	CPQ	C5-C6	-2.27	1.51	1.55
2	C	401	CPQ	C5-C6	-2.21	1.51	1.55
2	B	402	CPQ	C5-C6	-2.21	1.51	1.55
2	A	403	CPQ	C5-C6	-2.18	1.51	1.55
2	A	402	CPQ	C5-C6	-2.17	1.51	1.55
2	A	404	CPQ	C5-C6	-2.16	1.51	1.55
2	A	405	CPQ	C5-C6	-2.12	1.51	1.55
2	C	403	CPQ	C5-C6	-2.08	1.52	1.55
2	D	401	CPQ	C5-C6	-2.03	1.52	1.55
2	C	402	CPQ	C5-C6	-2.03	1.52	1.55
2	C	401	CPQ	C5-C9	-2.01	1.52	1.55

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	402	CPQ	C5-C6-C18	-6.21	107.86	114.71
2	C	403	CPQ	C19-C3-C4	-4.74	108.05	114.30
2	A	403	CPQ	C21-C20-C22	-3.93	104.21	110.36
2	D	402	CPQ	C9-C5-C6	3.77	103.92	100.10
2	B	402	CPQ	C22-C20-C9	-3.74	102.57	110.28
2	C	402	CPQ	C5-C9-C20	3.73	123.95	119.50
2	B	403	CPQ	C5-C6-C18	-3.72	110.60	114.71
2	A	403	CPQ	C10-C5-C4	3.70	112.83	109.07
2	A	403	CPQ	C5-C6-C18	-3.69	110.64	114.71
2	D	401	CPQ	C70-N71-C72	3.54	128.89	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	402	CPQ	C14-C15-C2	-3.51	108.93	112.66
2	A	405	CPQ	C19-C3-C4	-3.43	109.77	114.30
2	C	402	CPQ	C21-C20-C9	3.40	118.13	112.92
2	A	402	CPQ	C5-C9-C20	-3.40	115.43	119.50
2	C	401	CPQ	C5-C6-C18	-3.37	111.00	114.71
2	A	403	CPQ	C21-C20-C9	3.36	118.06	112.92
2	A	405	CPQ	C21-C20-C9	3.35	118.05	112.92
2	A	404	CPQ	C9-C5-C6	3.33	103.45	100.09
2	A	405	CPQ	C21-C20-C22	-3.14	105.44	110.36
2	B	402	CPQ	C5-C6-C18	-3.07	111.32	114.71
2	D	402	CPQ	C1-C2-C15	3.06	112.29	107.77
2	A	405	CPQ	C10-C5-C4	2.98	112.10	109.07
2	C	402	CPQ	C1-C12-C13	2.96	114.27	110.47
2	A	404	CPQ	C5-C9-C20	-2.93	115.99	119.50
2	A	404	CPQ	C5-C6-C18	-2.93	111.48	114.71
2	B	403	CPQ	C9-C5-C6	2.92	103.06	100.10
2	A	403	CPQ	C9-C5-C6	2.91	103.03	100.09
2	C	401	CPQ	C9-C5-C6	2.90	103.04	100.10
2	D	402	CPQ	C16-C15-C2	2.78	117.30	112.31
2	A	404	CPQ	C2-C19-C18	-2.71	109.57	112.42
2	C	402	CPQ	C5-C6-C18	-2.61	111.83	114.71
2	C	402	CPQ	C3-C19-C2	-2.57	111.07	113.73
2	A	404	CPQ	C3-C4-C5	-2.55	108.62	111.24
2	A	405	CPQ	C5-C6-C18	-2.55	111.90	114.71
2	A	403	CPQ	C3-C19-C2	-2.53	111.12	113.73
2	B	402	CPQ	C10-C5-C4	2.52	111.63	109.07
2	C	403	CPQ	C9-C5-C6	2.51	102.62	100.09
2	B	402	CPQ	C21-C20-C9	2.51	116.76	112.92
2	D	402	CPQ	C11-C2-C19	-2.50	107.73	111.18
2	D	401	CPQ	C69-C68-N59	-2.48	103.89	112.55
2	A	405	CPQ	C10-C5-C6	-2.47	107.34	111.21
2	A	403	CPQ	C10-C5-C6	-2.47	107.35	111.21
2	C	403	CPQ	C3-C4-C5	-2.47	108.71	111.24
2	A	404	CPQ	O73-C72-N71	-2.45	122.41	124.89
2	B	402	CPQ	C21-C20-C22	-2.40	106.61	110.36
2	D	401	CPQ	C23-C57-N59	-2.37	113.93	118.14
2	A	402	CPQ	C5-C6-C18	-2.36	112.10	114.71
2	B	402	CPQ	C19-C3-C4	-2.36	111.18	114.30
2	B	402	CPQ	C3-C19-C2	-2.33	111.33	113.73
2	B	402	CPQ	C23-C57-N59	2.26	122.16	118.14
2	A	403	CPQ	C19-C3-C4	-2.24	111.34	114.30
2	C	402	CPQ	C1-C2-C19	-2.22	107.86	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	CPQ	C23-C22-C20	-2.18	110.54	114.52
2	B	403	CPQ	C3-C19-C2	-2.15	111.50	113.73
2	A	404	CPQ	C3-C19-C2	-2.12	111.55	113.73
2	D	401	CPQ	C5-C9-C20	-2.09	117.00	119.50
2	C	402	CPQ	C10-C5-C6	-2.06	107.98	111.21
2	A	403	CPQ	C6-C5-C4	-2.05	105.49	107.40
2	D	401	CPQ	C7-C6-C18	-2.04	115.71	119.08
2	A	404	CPQ	C1-C2-C15	2.03	110.76	107.77
2	A	402	CPQ	C82-C81-C80	-2.02	110.02	113.60
2	A	405	CPQ	C3-C19-C2	-2.02	111.65	113.73

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	402	CPQ	C20-C22-C23-C57
2	C	402	CPQ	C23-C57-N59-C74
2	C	402	CPQ	C23-C57-N59-C68
2	C	402	CPQ	O58-C57-N59-C74
2	C	402	CPQ	O58-C57-N59-C68
2	A	402	CPQ	C78-C80-C81-O87
2	A	402	CPQ	C78-C80-C81-C82
2	A	402	CPQ	O86-C80-C81-O87
2	A	402	CPQ	O86-C80-C81-C82
2	A	402	CPQ	C90-C72-N71-C70
2	A	402	CPQ	O73-C72-N71-C70
2	A	402	CPQ	C72-C90-C91-O97
2	A	402	CPQ	C90-C91-C92-O98
2	A	402	CPQ	C90-C91-C92-C93
2	A	402	CPQ	O97-C91-C92-C93
2	A	402	CPQ	O99-C93-C94-O95
2	B	402	CPQ	O58-C57-N59-C74
2	B	402	CPQ	O58-C57-N59-C68
2	B	402	CPQ	C80-C78-N77-C76
2	B	402	CPQ	N77-C78-C80-C81
2	B	402	CPQ	O79-C78-C80-C81
2	B	402	CPQ	C80-C81-C82-C83
2	D	401	CPQ	C23-C57-N59-C74
2	D	401	CPQ	C23-C57-N59-C68
2	D	401	CPQ	O58-C57-N59-C74
2	D	401	CPQ	O58-C57-N59-C68
2	D	401	CPQ	C90-C72-N71-C70

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Mol	Chain	Res	Type	Atoms
2	D	401	CPQ	O73-C72-N71-C70
2	D	401	CPQ	N71-C72-C90-O96
2	D	401	CPQ	N71-C72-C90-C91
2	D	401	CPQ	O73-C72-C90-O96
2	D	401	CPQ	O73-C72-C90-C91
2	D	401	CPQ	C90-C91-C92-O98
2	D	401	CPQ	C90-C91-C92-C93
2	D	401	CPQ	O97-C91-C92-C93
2	A	404	CPQ	O58-C57-N59-C74
2	A	404	CPQ	C69-C68-N59-C57
2	A	404	CPQ	C69-C68-N59-C74
2	A	404	CPQ	O73-C72-N71-C70
2	B	402	CPQ	O79-C78-N77-C76
2	A	404	CPQ	C21-C20-C22-C23
2	D	401	CPQ	C68-C69-C70-N71
2	A	402	CPQ	C92-C93-C94-O95
2	C	402	CPQ	C9-C20-C22-C23
2	B	402	CPQ	C9-C20-C22-C23
2	A	404	CPQ	C9-C20-C22-C23
2	D	401	CPQ	O97-C91-C92-O98
2	A	403	CPQ	C21-C20-C22-C23
2	B	402	CPQ	C21-C20-C22-C23
2	C	402	CPQ	C22-C20-C9-C8
2	A	405	CPQ	C9-C20-C22-C23
2	C	403	CPQ	C9-C20-C22-C23
2	B	402	CPQ	C74-C75-C76-N77
2	C	403	CPQ	C21-C20-C22-C23
2	D	401	CPQ	N59-C68-C69-C70
2	A	403	CPQ	C9-C20-C22-C23
2	A	404	CPQ	N59-C68-C69-C70
2	A	405	CPQ	C21-C20-C22-C23
2	A	403	CPQ	C20-C22-C23-C57
2	C	402	CPQ	C21-C20-C22-C23
2	A	403	CPQ	C22-C20-C9-C8
2	B	402	CPQ	C23-C57-N59-C68
2	C	402	CPQ	C21-C20-C9-C8
2	C	402	CPQ	C22-C20-C9-C5
2	D	401	CPQ	O96-C90-C91-O97
2	A	405	CPQ	C22-C20-C9-C8
2	A	402	CPQ	O87-C81-C82-C83
2	A	402	CPQ	C80-C81-C82-C83
2	A	405	CPQ	C21-C20-C9-C5

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Mol	Chain	Res	Type	Atoms
2	B	402	CPQ	C82-C83-C84-O85
2	A	404	CPQ	C68-C69-C70-N71
2	D	401	CPQ	C69-C70-N71-C72
2	A	403	CPQ	C21-C20-C9-C5
2	B	402	CPQ	O87-C81-C82-C83
2	B	402	CPQ	O87-C81-C82-O88
2	A	402	CPQ	O98-C92-C93-O99
2	A	402	CPQ	C91-C92-C93-O99
2	A	404	CPQ	O58-C57-N59-C68
2	A	402	CPQ	O87-C81-C82-O88
2	A	402	CPQ	O97-C91-C92-O98
2	A	402	CPQ	N59-C68-C69-C70
2	B	402	CPQ	O89-C83-C84-O85
2	A	402	CPQ	C23-C57-N59-C74
2	A	402	CPQ	N71-C72-C90-O96
2	B	402	CPQ	N77-C78-C80-O86
2	A	404	CPQ	C23-C57-N59-C74
2	A	402	CPQ	C72-C90-C91-C92
2	A	402	CPQ	C91-C92-C93-C94
2	B	402	CPQ	C80-C81-C82-O88
2	C	403	CPQ	C20-C22-C23-C57
2	A	402	CPQ	C80-C81-C82-O88
2	A	405	CPQ	C22-C20-C9-C5
2	A	403	CPQ	C22-C20-C9-C5
2	A	402	CPQ	O73-C72-C90-O96
2	B	402	CPQ	O79-C78-C80-O86
2	B	402	CPQ	C22-C23-C57-O58
2	B	402	CPQ	O88-C82-C83-C84
2	D	401	CPQ	C69-C68-N59-C57
2	A	402	CPQ	O96-C90-C91-C92
2	D	401	CPQ	O96-C90-C91-C92
2	A	405	CPQ	C21-C20-C9-C8
2	A	403	CPQ	C21-C20-C9-C8
2	A	402	CPQ	C74-C75-C76-N77
2	A	402	CPQ	O96-C90-C91-O97
2	A	404	CPQ	C20-C22-C23-C57
2	D	401	CPQ	C72-C90-C91-O97
2	B	402	CPQ	C23-C57-N59-C74
2	A	404	CPQ	C23-C57-N59-C68
2	D	401	CPQ	C69-C68-N59-C74
2	B	402	CPQ	O88-C82-C83-O89
2	A	402	CPQ	C21-C20-C9-C5

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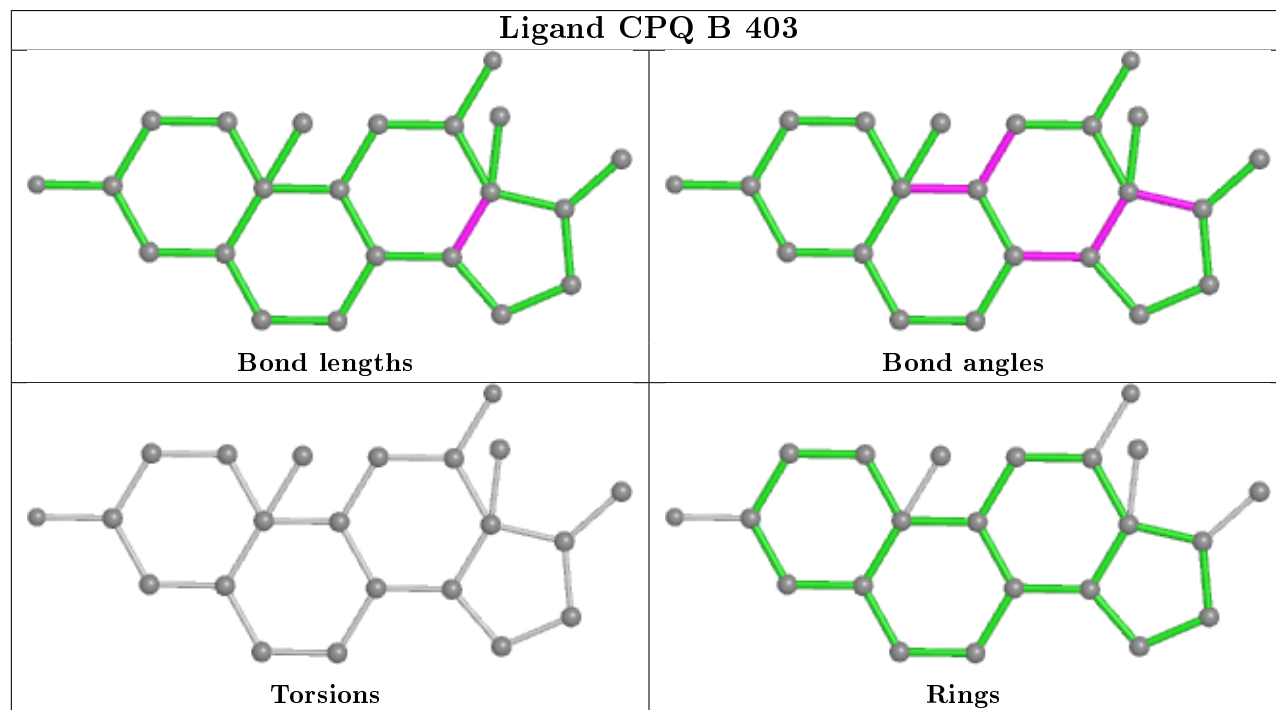
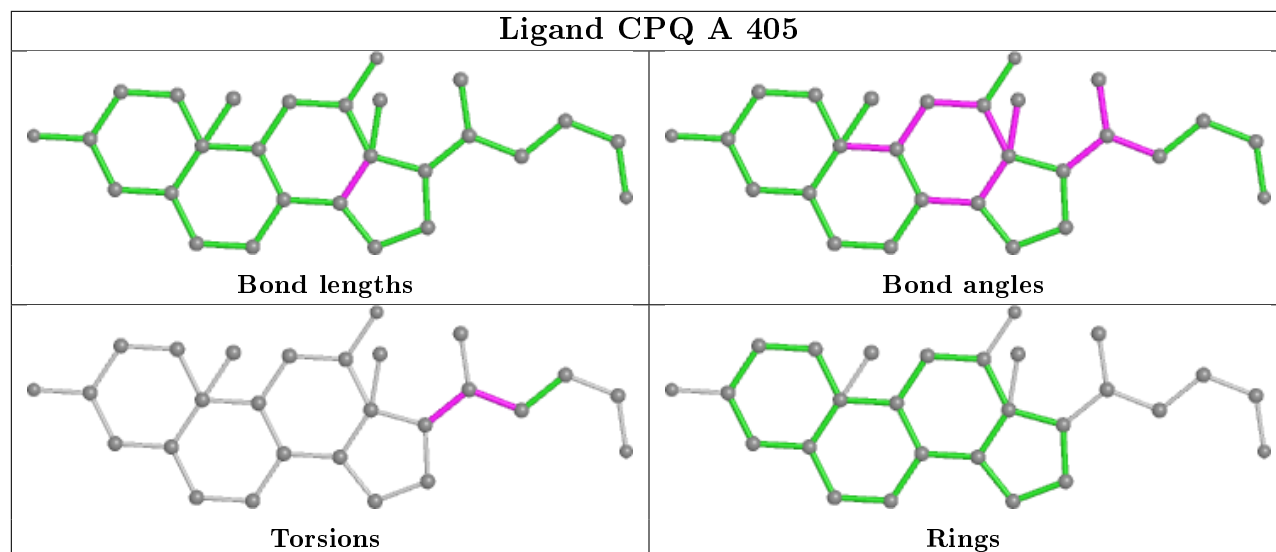
Mol	Chain	Res	Type	Atoms
2	A	402	CPQ	O98-C92-C93-C94
2	A	402	CPQ	O79-C78-C80-O86
2	B	402	CPQ	C22-C23-C57-N59
2	A	402	CPQ	O58-C57-N59-C74
2	A	402	CPQ	O79-C78-C80-C81
2	A	402	CPQ	N77-C78-C80-O86
2	A	402	CPQ	C22-C20-C9-C5

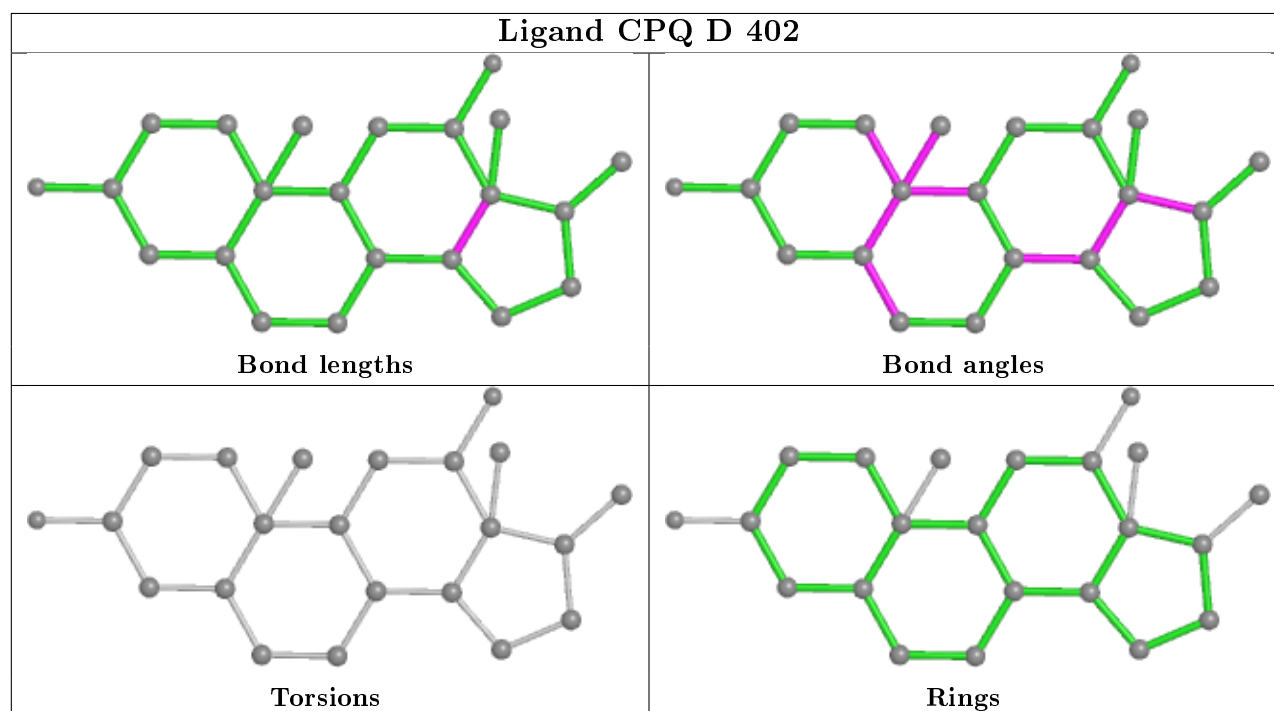
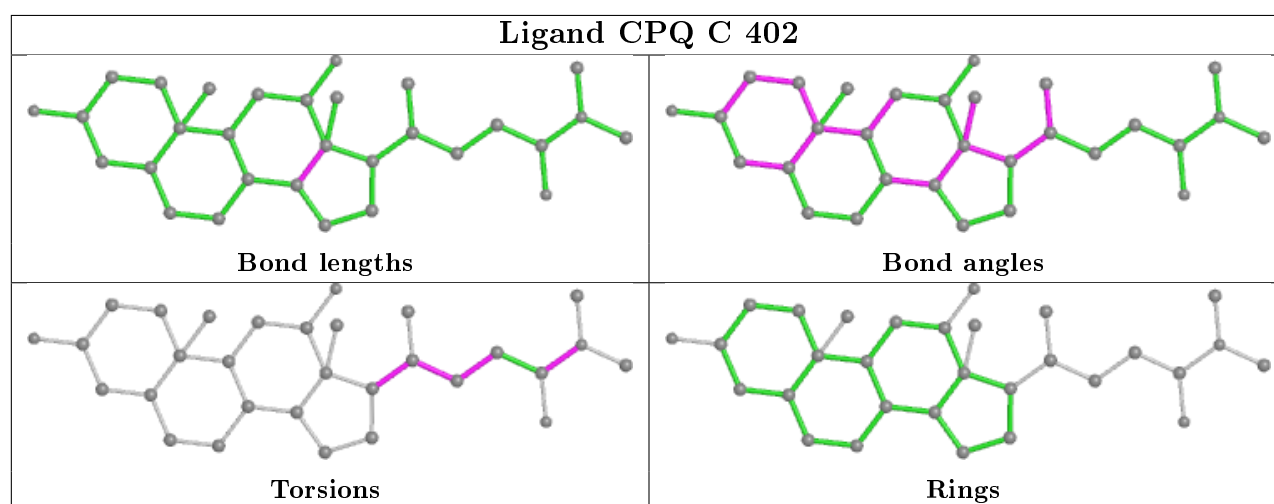
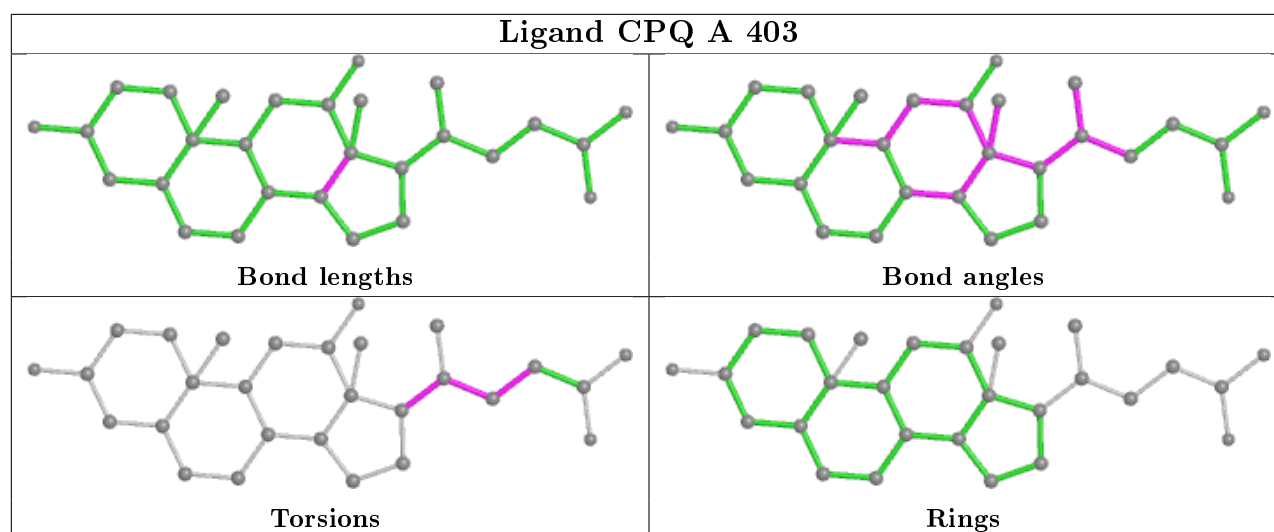
There are no ring outliers.

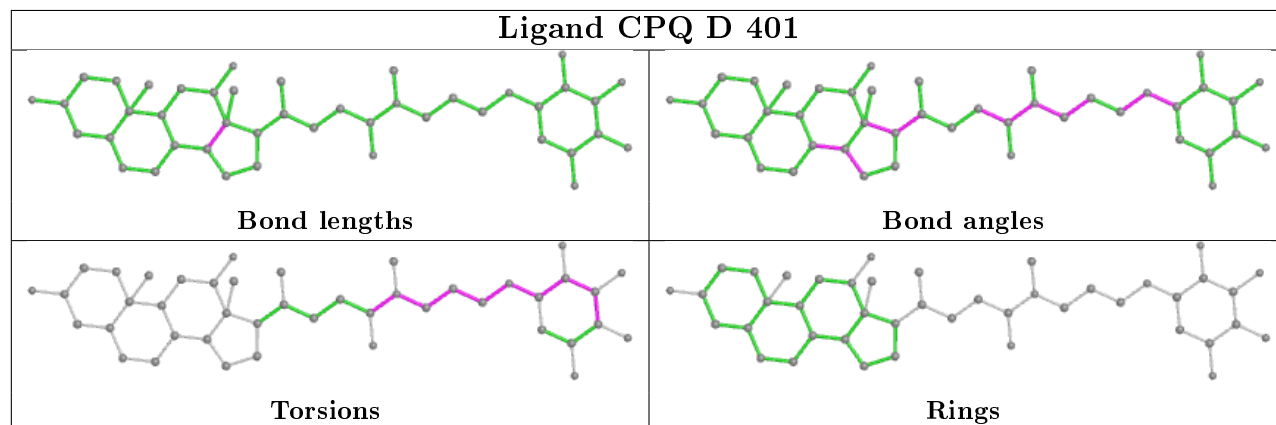
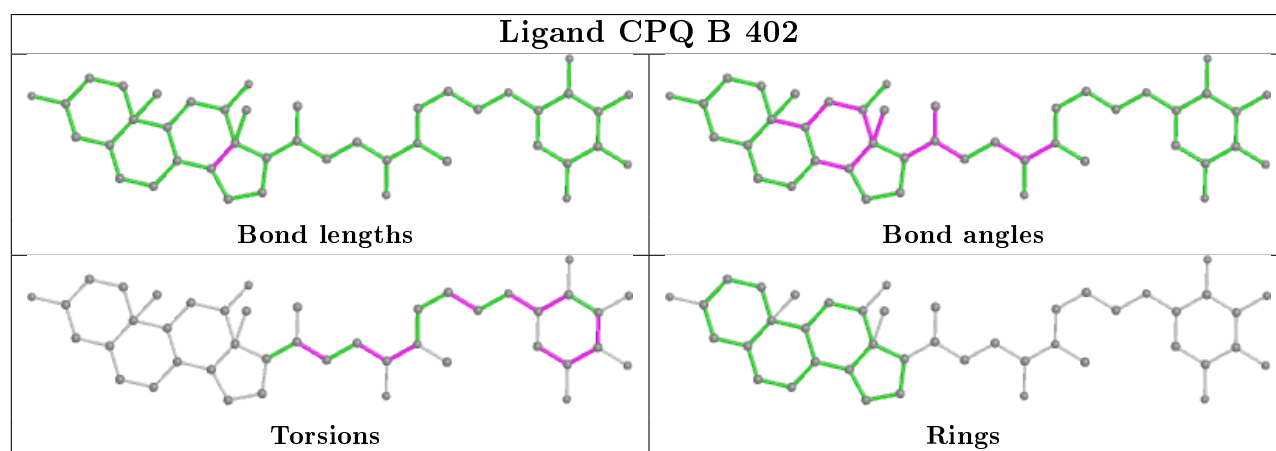
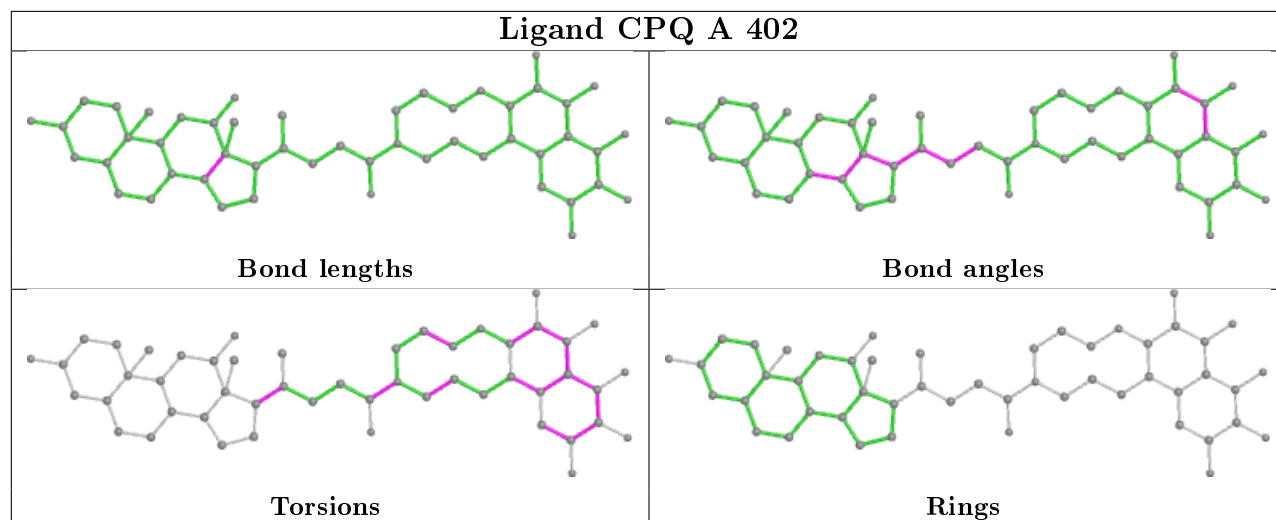
8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	CPQ	3	0
2	A	403	CPQ	3	0
2	C	402	CPQ	2	0
2	A	402	CPQ	6	0
2	B	402	CPQ	2	0
2	D	401	CPQ	2	0
2	C	403	CPQ	2	0
2	A	404	CPQ	3	0

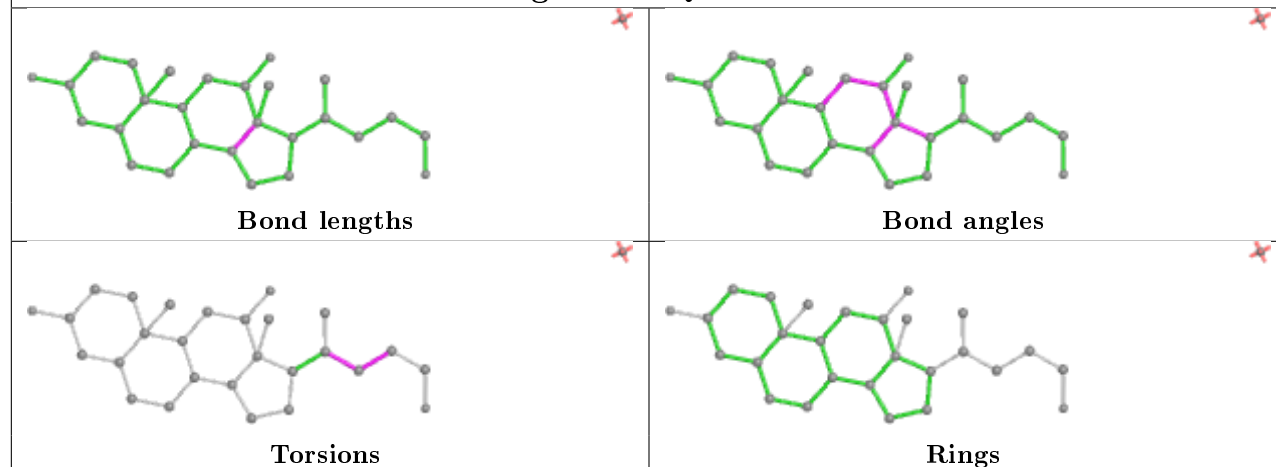
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



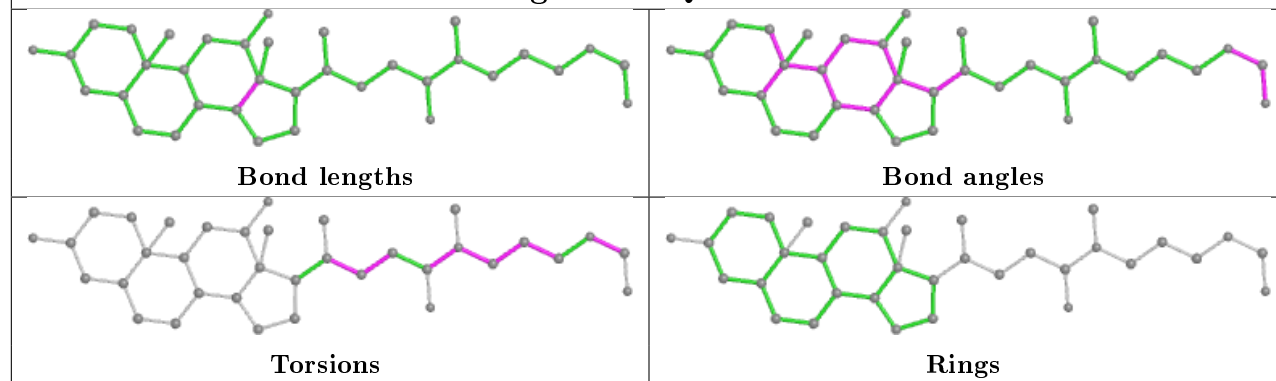




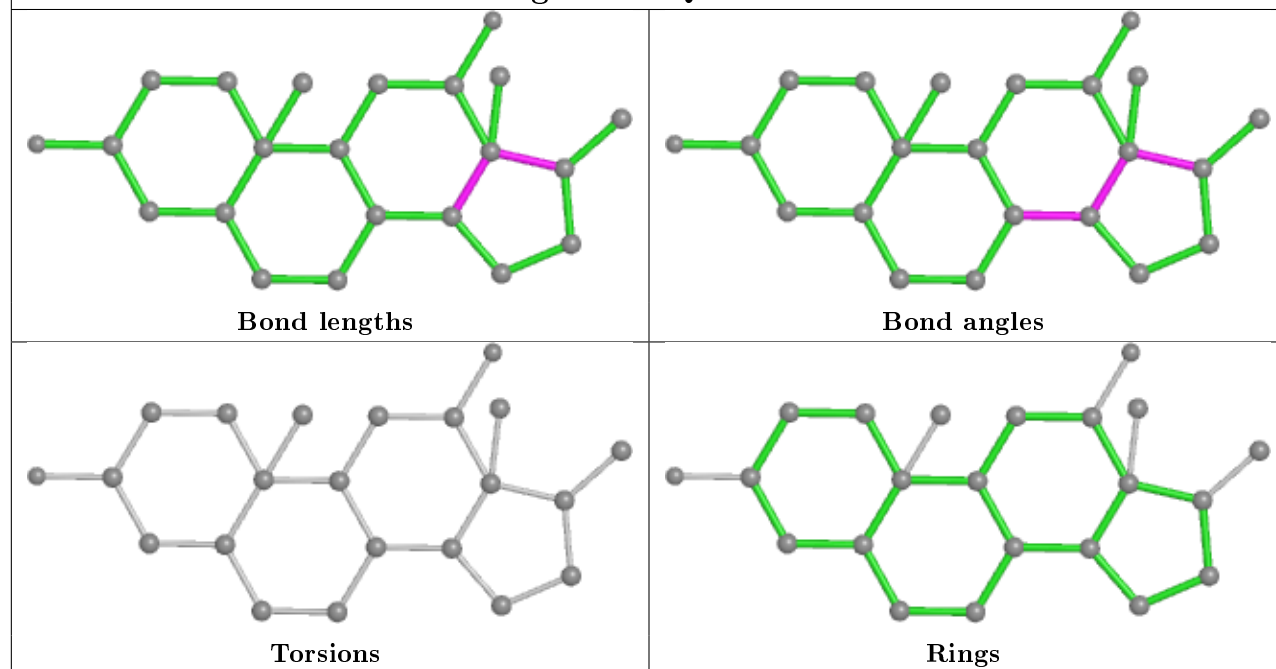
Ligand CPQ C 403



Ligand CPQ A 404



Ligand CPQ C 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	317/321 (98%)	0.06	5 (1%) 72 74	18, 24, 35, 79	0
1	B	317/321 (98%)	-0.03	2 (0%) 89 90	16, 22, 31, 64	0
1	C	319/321 (99%)	-0.01	0 100 100	16, 22, 33, 72	0
1	D	317/321 (98%)	0.11	6 (1%) 66 68	18, 25, 38, 71	0
All	All	1270/1284 (98%)	0.04	13 (1%) 82 83	16, 23, 35, 79	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	316	THR	5.0
1	A	144	LEU	4.8
1	D	144	LEU	3.7
1	D	314	ILE	2.6
1	A	315	VAL	2.6
1	D	147	LEU	2.4
1	B	316	THR	2.3
1	A	-1	MET	2.3
1	A	148	ALA	2.1
1	D	255	ILE	2.1
1	D	315	VAL	2.1
1	B	141	ALA	2.1
1	A	147	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

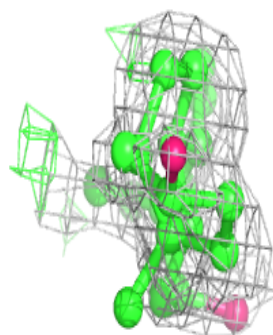
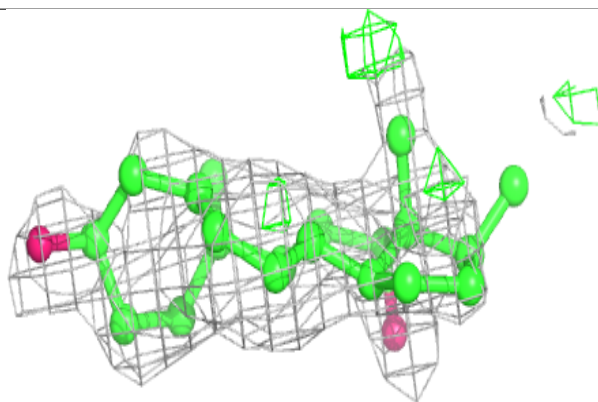
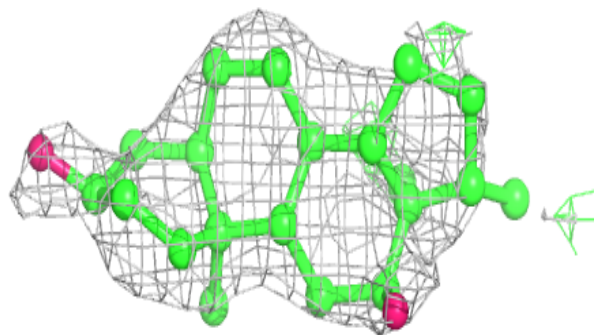
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CPQ	D	402	22/60	0.69	0.27	57,60,61,62	0
2	CPQ	C	403	28/60	0.74	0.24	32,36,47,52	0
2	CPQ	B	402	45/60	0.79	0.23	25,41,52,55	0
2	CPQ	C	402	30/60	0.80	0.20	31,37,45,48	0
2	CPQ	A	405	27/60	0.80	0.21	34,38,45,48	0
2	CPQ	A	402	60/60	0.81	0.17	34,38,51,54	0
2	CPQ	B	403	22/60	0.83	0.21	34,41,42,42	0
2	CPQ	A	404	35/60	0.85	0.17	25,28,54,61	0
2	CPQ	C	401	22/60	0.85	0.14	31,35,44,44	0
2	CPQ	D	401	45/60	0.88	0.16	25,35,48,50	0
2	CPQ	A	403	28/60	0.88	0.14	28,31,49,51	0
3	CA	A	401	1/1	0.99	0.04	25,25,25,25	0
3	CA	B	401	1/1	0.99	0.10	22,22,22,22	0

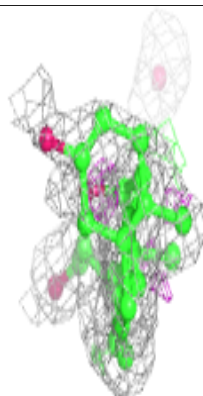
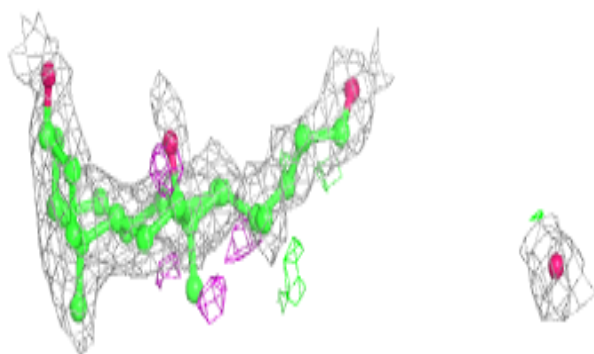
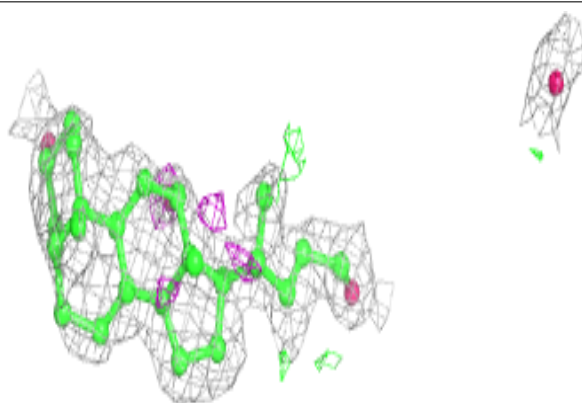
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CPQ D 402:

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

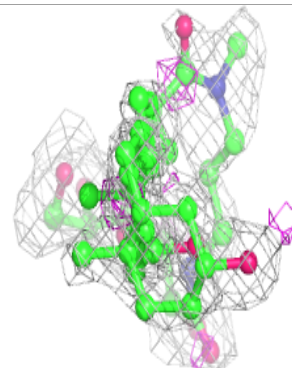
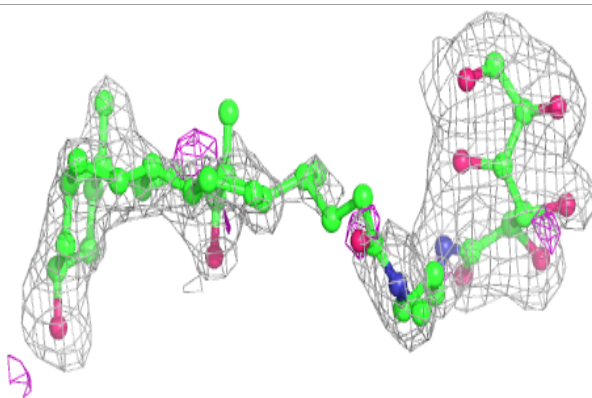
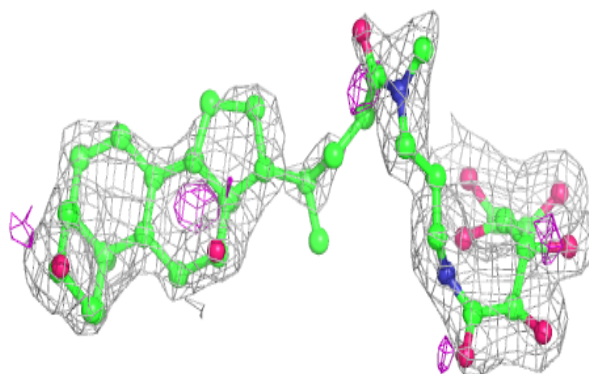
**Electron density around CPQ C 403:**

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

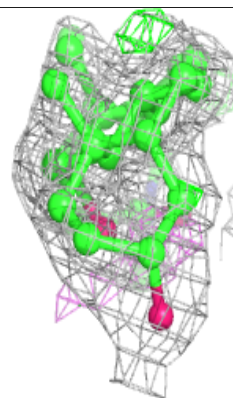
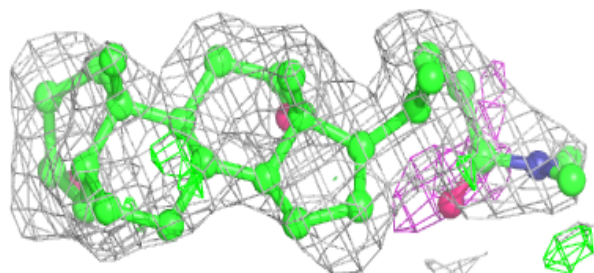
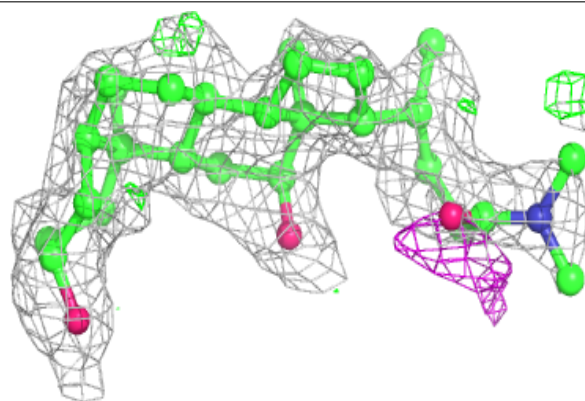


Electron density around CPQ B 402:

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

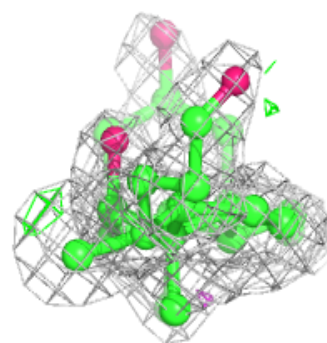
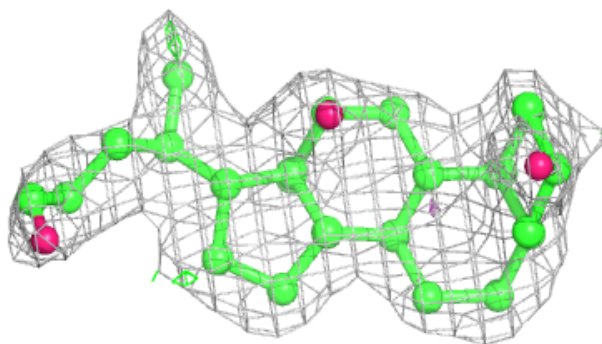
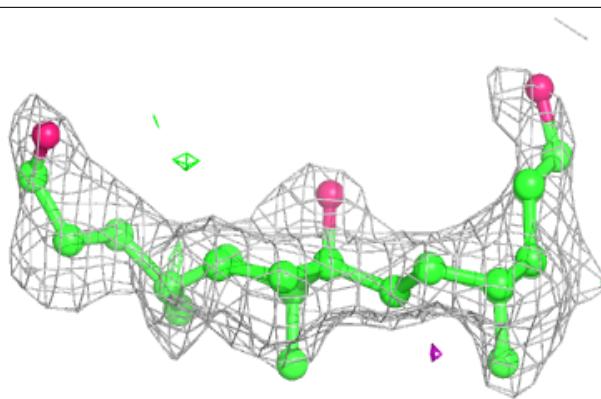
**Electron density around CPQ C 402:**

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



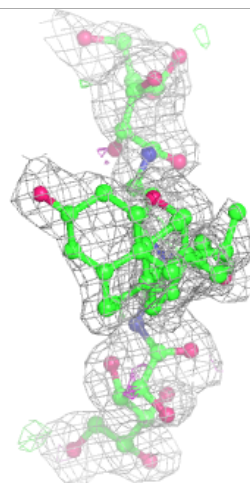
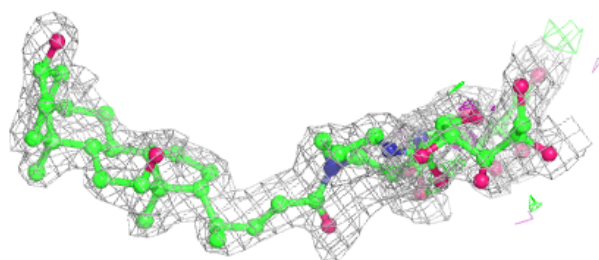
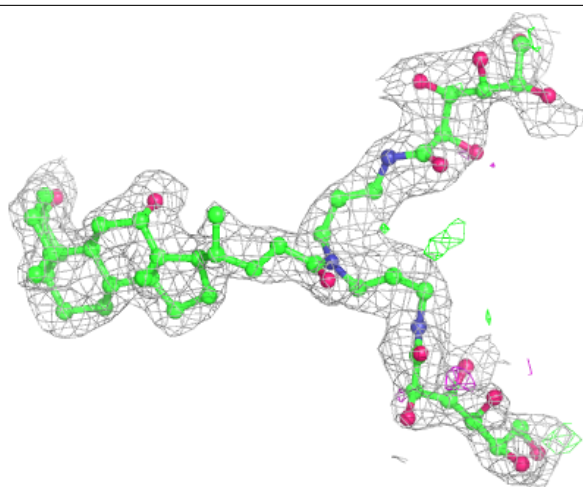
Electron density around CPQ A 405:

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



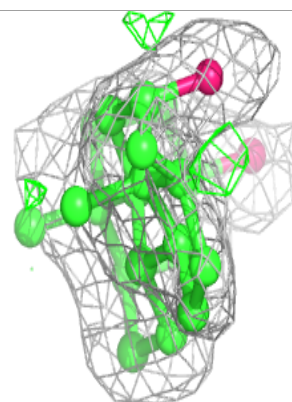
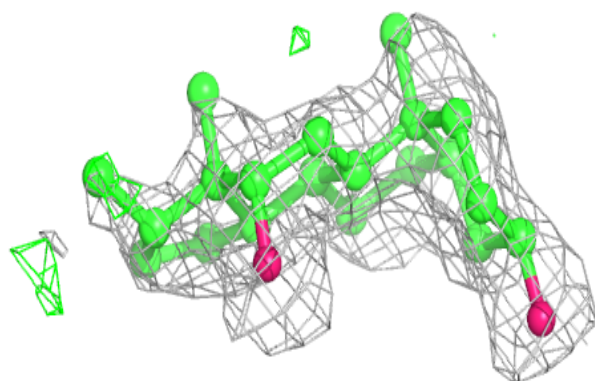
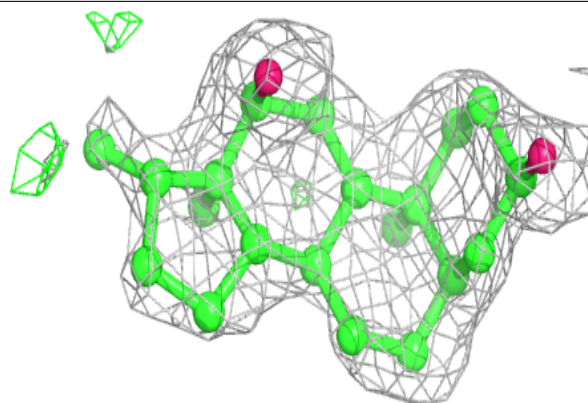
Electron density around CPQ A 402:

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

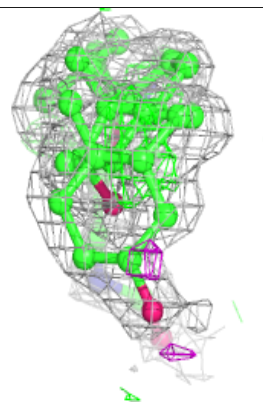
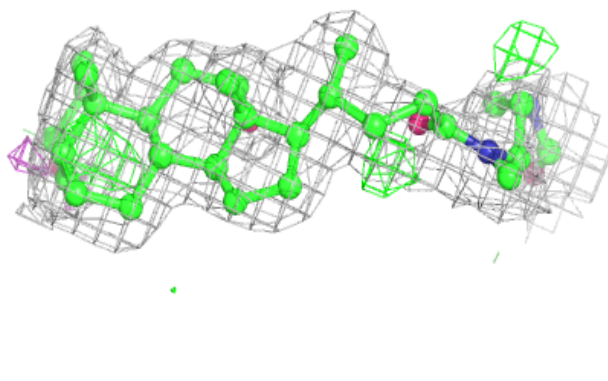
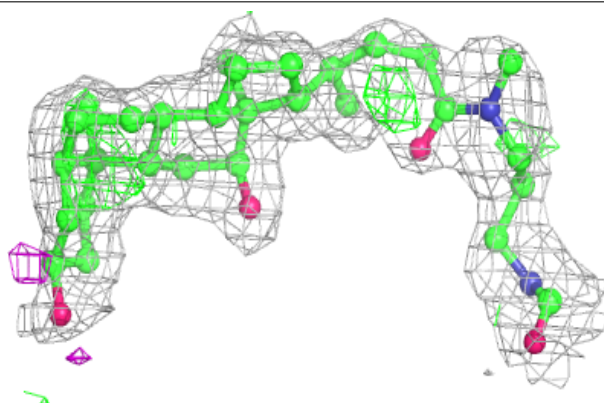


Electron density around CPQ B 403:

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

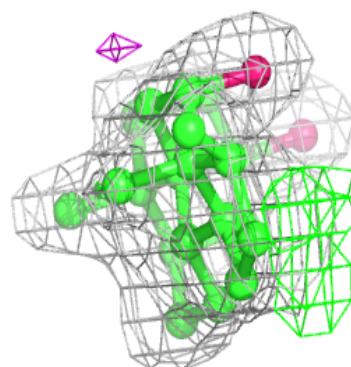
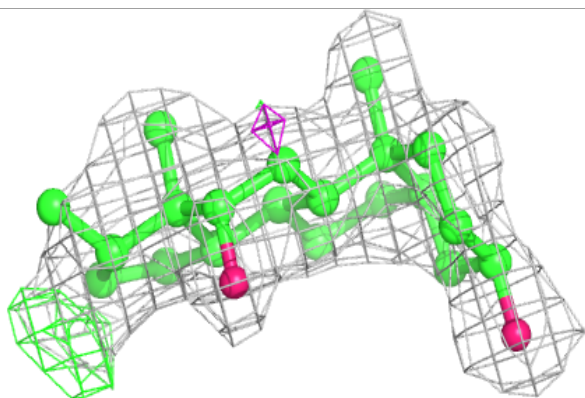
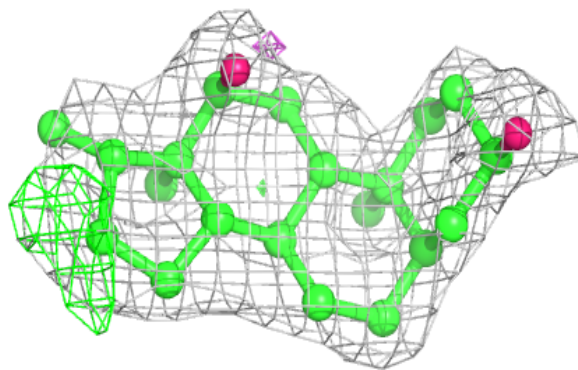
**Electron density around CPQ A 404:**

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

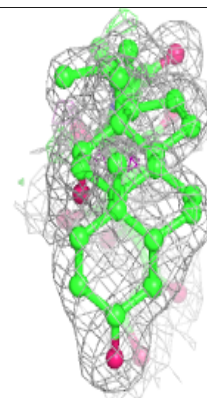
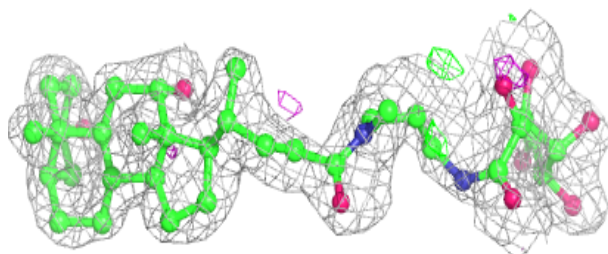
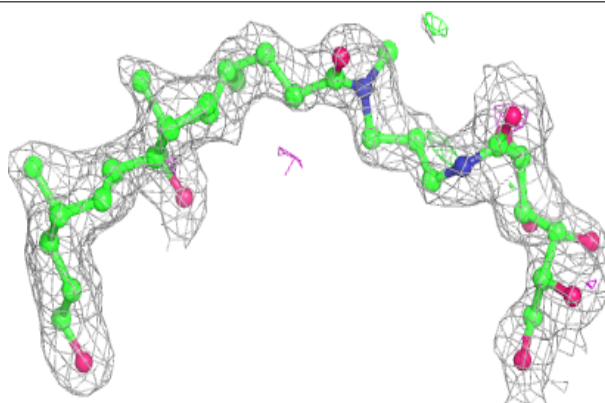


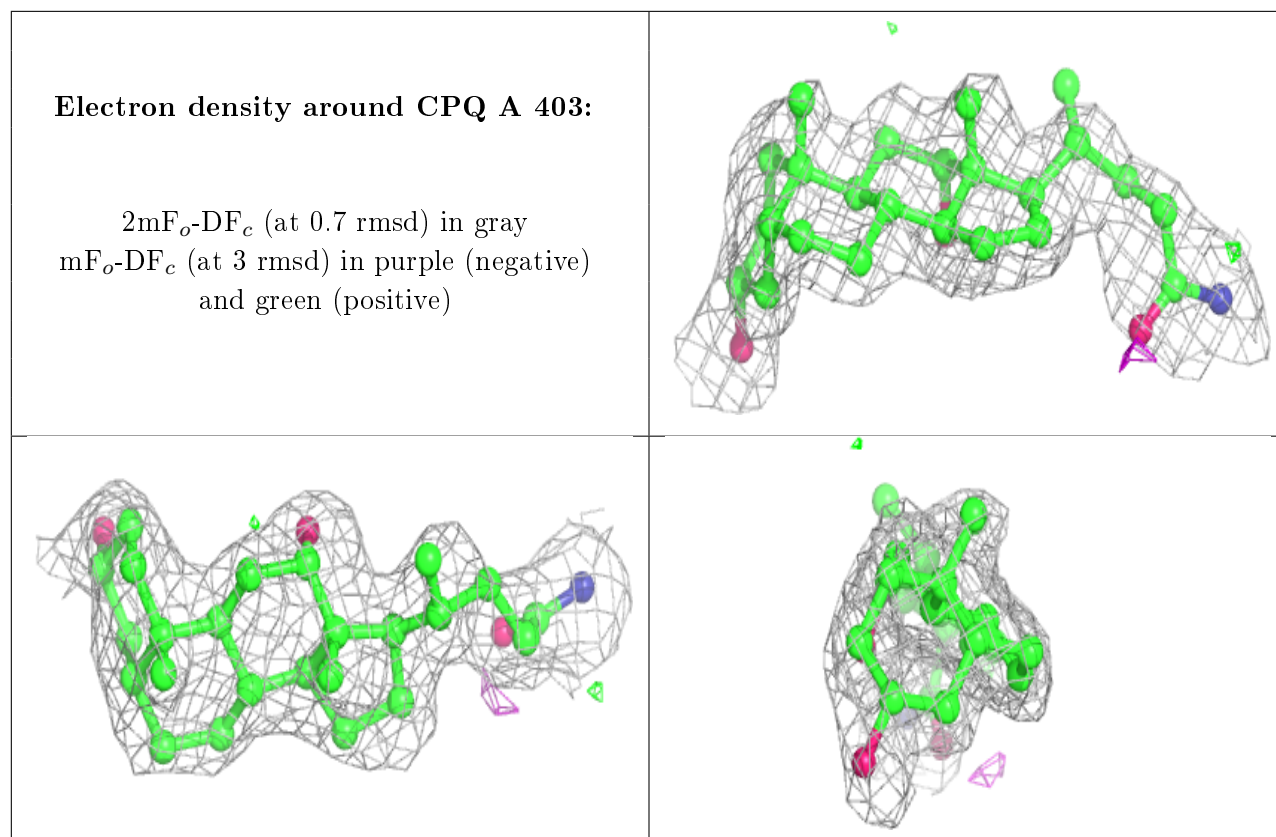
Electron density around CPQ C 401:

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

**Electron density around CPQ D 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.