



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2020 – 07:13 PM EST

PDB ID : 2A3W
Title : Decameric structure of human serum amyloid P-component bound to Bis-1,2-
-{[(Z)-2-carboxy-2-methyl-1,3-dioxane]-5-yloxy carbamoyl}-ethane
Authors : Ho, J.G.; Kitov, P.I.; Paszkiewicz, E.; Sadowska, J.; Bundle, D.R.; Ng, K.K.
Deposited on : 2005-06-27
Resolution : 2.20 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

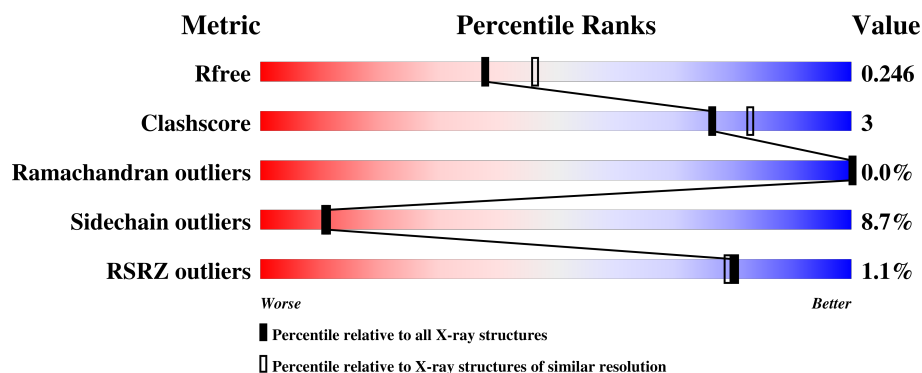
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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. 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	204	<div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	B	204	<div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	C	204	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	D	204	<div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	E	204	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	204	 82% 15% .
1	G	204	 83% 15% .
1	H	204	 85% 14% .
1	I	204	 79% 18% .
1	J	204	 85% 13% .
1	K	204	 83% 15% .
1	L	204	 85% 13% .
1	M	204	 83% 14% .
1	N	204	 83% 16% .
1	O	204	 79% 18% .
1	P	204	 83% 15% .
1	Q	204	 84% 13% .
1	R	204	 88% 11% .
1	S	204	 83% 15% .
1	T	204	 85% 13% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35698 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 Serum amyloid P-component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	B	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	C	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	D	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	E	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	F	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	G	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	H	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	I	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	J	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	K	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	L	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	M	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	N	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	O	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	P	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	R	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	S	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0
1	T	204	Total 1649	C 1071	N 272	O 303	S 3	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

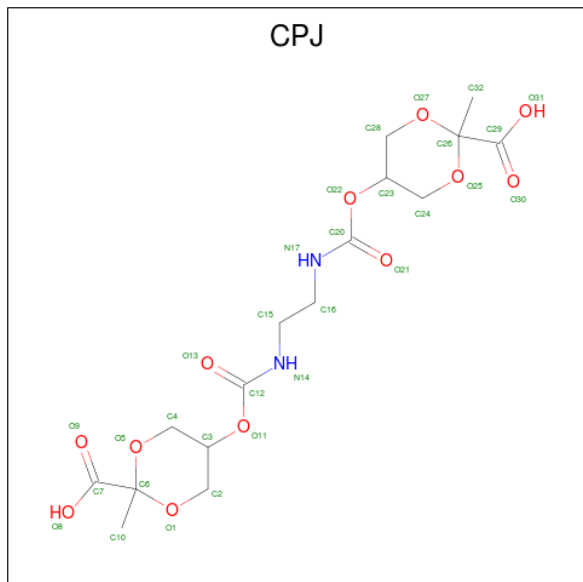
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	2	Total 2	Ca 2	0	0
2	G	2	Total 2	Ca 2	0	0
2	J	2	Total 2	Ca 2	0	0
2	Q	2	Total 2	Ca 2	0	0
2	D	2	Total 2	Ca 2	0	0
2	K	2	Total 2	Ca 2	0	0
2	E	2	Total 2	Ca 2	0	0
2	H	2	Total 2	Ca 2	0	0
2	B	2	Total 2	Ca 2	0	0
2	I	2	Total 2	Ca 2	0	0
2	C	2	Total 2	Ca 2	0	0
2	A	2	Total 2	Ca 2	0	0
2	T	2	Total 2	Ca 2	0	0
2	N	2	Total 2	Ca 2	0	0
2	O	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	2	Total	Ca	0	0
			2	2		
2	L	2	Total	Ca	0	0
			2	2		
2	S	2	Total	Ca	0	0
			2	2		
2	F	2	Total	Ca	0	0
			2	2		
2	M	2	Total	Ca	0	0
			2	2		

- Molecule 3 is BIS-1,2-{[(Z)-2-CARBOXY-2-METHYL-1,3-DIOXANE]-5-YLOXYCARBA MOYL}-ETHANE (three-letter code: CPJ) (formula: C₁₆H₂₄N₂O₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	16	2	12		
3	B	1	Total	C	N	O	0	0
			30	16	2	12		
3	C	1	Total	C	N	O	0	0
			30	16	2	12		
3	D	1	Total	C	N	O	0	0
			30	16	2	12		
3	E	1	Total	C	N	O	0	0
			30	16	2	12		
3	L	1	Total	C	N	O	0	0
			30	16	2	12		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	1	Total	C	N	O	0	0
			30	16	2	12		
3	N	1	Total	C	N	O	0	0
			30	16	2	12		
3	P	1	Total	C	N	O	0	0
			30	16	2	12		
3	Q	1	Total	C	N	O	0	0
			30	16	2	12		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	153	Total	O	0	0
			153	153		
4	C	154	Total	O	0	0
			154	154		
4	D	138	Total	O	0	0
			138	138		
4	E	139	Total	O	0	0
			139	139		
4	F	138	Total	O	0	0
			138	138		
4	G	122	Total	O	0	0
			122	122		
4	H	126	Total	O	0	0
			126	126		
4	I	144	Total	O	0	0
			144	144		
4	J	142	Total	O	0	0
			142	142		
4	K	65	Total	O	0	0
			65	65		
4	L	129	Total	O	0	0
			129	129		
4	M	98	Total	O	0	0
			98	98		
4	N	72	Total	O	0	0
			72	72		
4	O	95	Total	O	0	0
			95	95		

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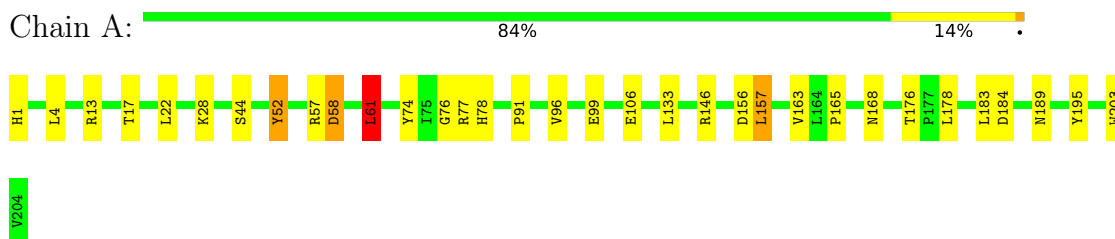
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	104	Total 104	O 104	0	0
4	Q	90	Total 90	O 90	0	0
4	R	84	Total 84	O 84	0	0
4	S	109	Total 109	O 109	0	0
4	T	89	Total 89	O 89	0	0

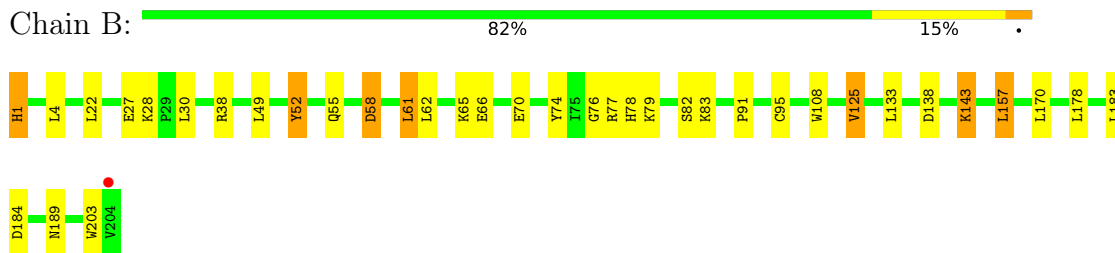
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

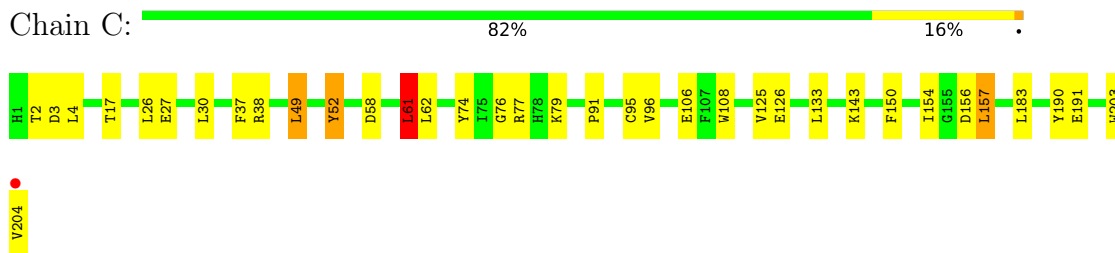
- Molecule 1: Serum amyloid P-component



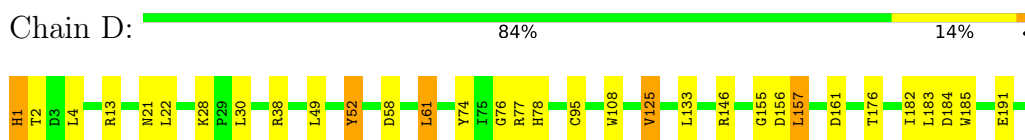
- Molecule 1: Serum amyloid P-component




- Molecule 1: Serum amyloid P-component



- Molecule 1: Serum amyloid P-component




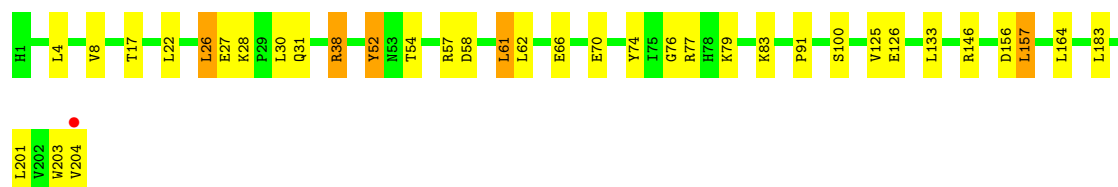
- Molecule 1: Serum amyloid P-component

Chain E:  84% 15%




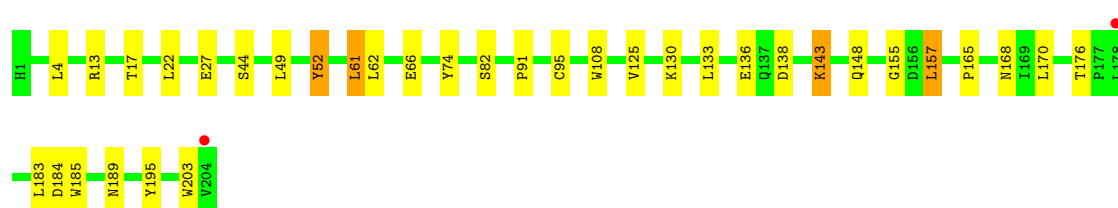
- Molecule 1: Serum amyloid P-component

Chain F:  82% 15%




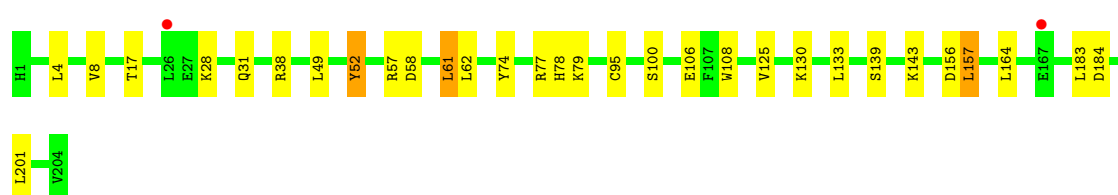
- Molecule 1: Serum amyloid P-component

Chain G:  83% 15%




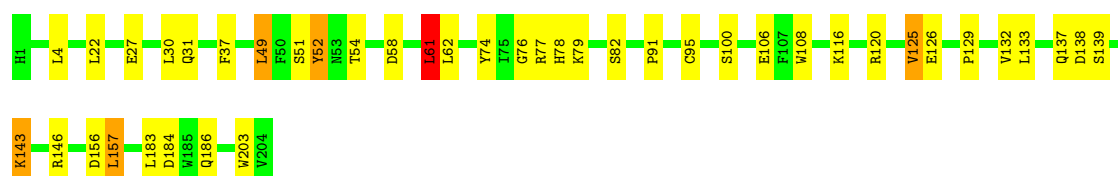
- Molecule 1: Serum amyloid P-component

Chain H:  85% 14%




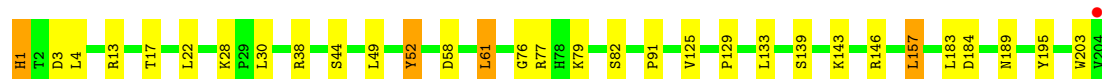
- Molecule 1: Serum amyloid P-component

Chain I:  79% 18%

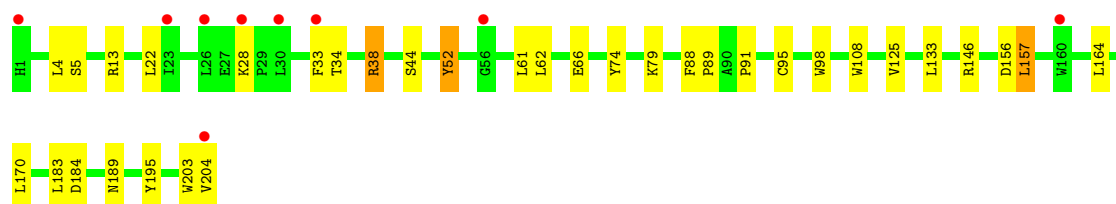
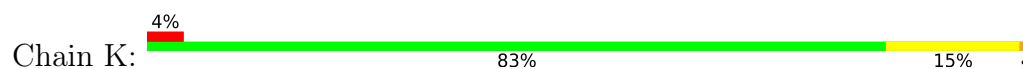


- Molecule 1: Serum amyloid P-component

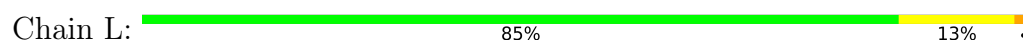
Chain J:  85% 13%



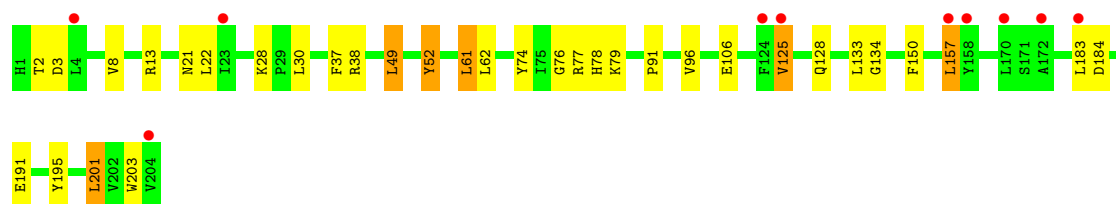
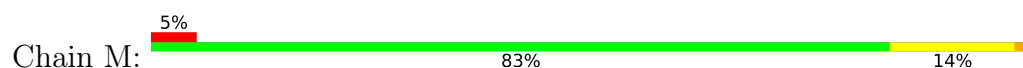
- Molecule 1: Serum amyloid P-component



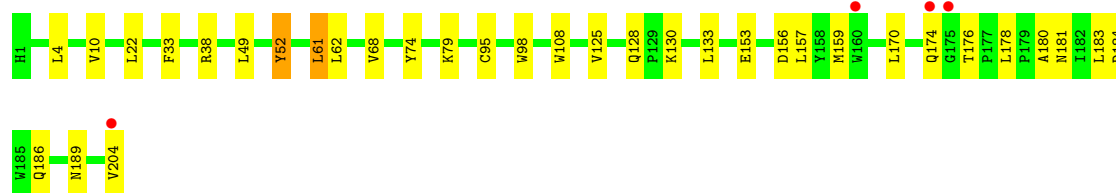
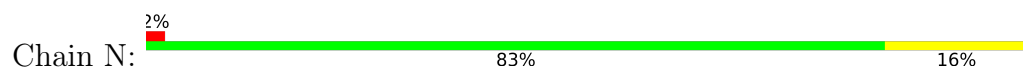
- Molecule 1: Serum amyloid P-component



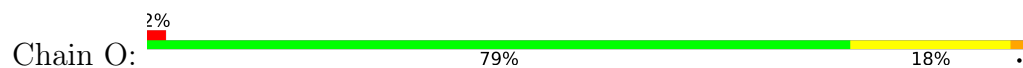
- Molecule 1: Serum amyloid P-component

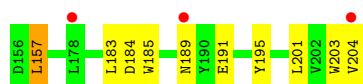


- Molecule 1: Serum amyloid P-component



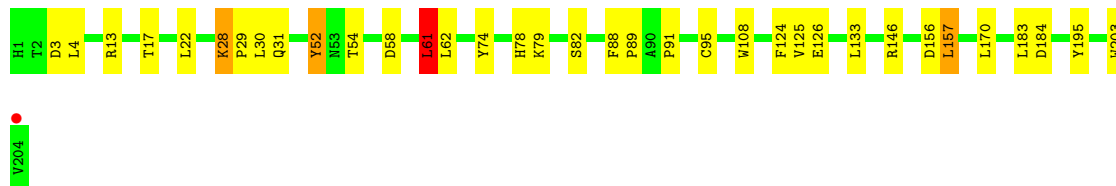
- Molecule 1: Serum amyloid P-component





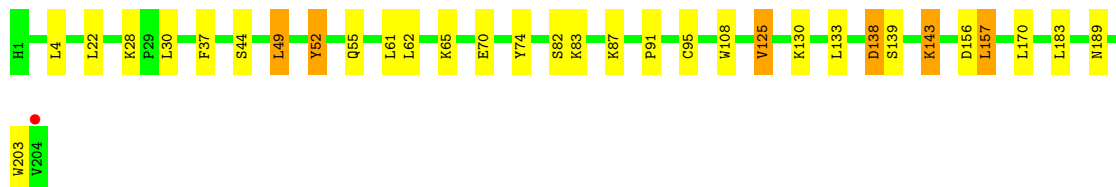
- Molecule 1: Serum amyloid P-component

Chain P: 83% 15% .



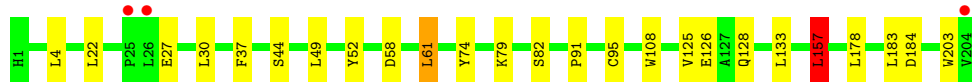
- Molecule 1: Serum amyloid P-component

Chain Q: 84% 13% .



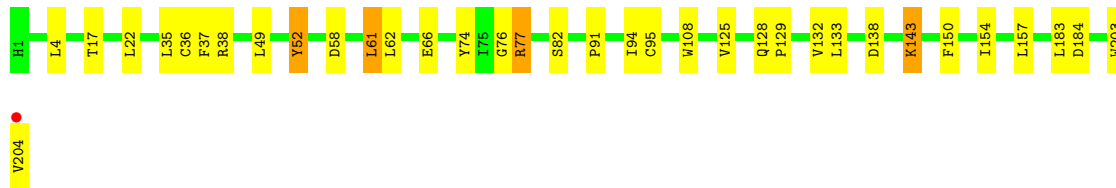
- Molecule 1: Serum amyloid P-component

Chain R: 88% 11% .



- Molecule 1: Serum amyloid P-component

Chain S: 83% 15% .



- Molecule 1: Serum amyloid P-component

Chain T: 85% 13% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.71Å 105.33Å 146.01Å 86.53° 78.15° 76.78°	Depositor
Resolution (Å)	100.00 – 2.20 59.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (100.00-2.20) 97.1 (59.73-2.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.188 , 0.229 0.214 , 0.246	Depositor DCC
R_{free} test set	13598 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35698	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CPJ, 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	0.39	0/1696	0.72	5/2306 (0.2%)
1	B	0.37	0/1696	0.70	3/2306 (0.1%)
1	C	0.37	0/1696	0.70	5/2306 (0.2%)
1	D	0.36	0/1696	0.70	4/2306 (0.2%)
1	E	0.36	0/1696	0.69	3/2306 (0.1%)
1	F	0.36	0/1696	0.69	3/2306 (0.1%)
1	G	0.36	0/1696	0.68	2/2306 (0.1%)
1	H	0.38	0/1696	0.70	3/2306 (0.1%)
1	I	0.36	0/1696	0.69	5/2306 (0.2%)
1	J	0.36	0/1696	0.71	4/2306 (0.2%)
1	K	0.33	0/1696	0.65	3/2306 (0.1%)
1	L	0.36	0/1696	0.70	4/2306 (0.2%)
1	M	0.34	0/1696	0.66	3/2306 (0.1%)
1	N	0.33	0/1696	0.65	2/2306 (0.1%)
1	O	0.35	0/1696	0.68	3/2306 (0.1%)
1	P	0.35	0/1696	0.68	6/2306 (0.3%)
1	Q	0.35	0/1696	0.68	3/2306 (0.1%)
1	R	0.35	0/1696	0.67	3/2306 (0.1%)
1	S	0.36	0/1696	0.67	2/2306 (0.1%)
1	T	0.34	0/1696	0.67	4/2306 (0.2%)
All	All	0.36	0/33920	0.69	70/46120 (0.2%)

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	157	LEU	CA-CB-CG	6.77	130.87	115.30
1	L	157	LEU	CA-CB-CG	6.52	130.29	115.30
1	J	157	LEU	CA-CB-CG	6.46	130.17	115.30
1	H	157	LEU	CA-CB-CG	6.41	130.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	157	LEU	CA-CB-CG	6.30	129.79	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1649	0	1624	11	0
1	B	1649	0	1624	11	0
1	C	1649	0	1624	11	0
1	D	1649	0	1624	13	0
1	E	1649	0	1624	9	0
1	F	1649	0	1624	12	0
1	G	1649	0	1624	10	0
1	H	1649	0	1624	9	0
1	I	1649	0	1624	19	0
1	J	1649	0	1624	9	0
1	K	1649	0	1624	9	0
1	L	1649	0	1624	10	0
1	M	1649	0	1624	12	0
1	N	1649	0	1624	7	0
1	O	1649	0	1624	17	0
1	P	1649	0	1624	11	0
1	Q	1649	0	1624	9	0
1	R	1649	0	1624	6	0
1	S	1649	0	1624	12	0
1	T	1649	0	1624	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
3	A	30	0	22	0	0
3	B	30	0	22	0	0
3	C	30	0	22	0	0
3	D	30	0	22	1	0
3	E	30	0	22	0	0
3	L	30	0	22	0	0
3	M	30	0	22	0	0
3	N	30	0	22	0	0
3	P	30	0	22	0	0
3	Q	30	0	22	0	0
4	A	187	0	0	1	0
4	B	153	0	0	1	0
4	C	154	0	0	0	0
4	D	138	0	0	1	0
4	E	139	0	0	0	0
4	F	138	0	0	1	0
4	G	122	0	0	3	0
4	H	126	0	0	1	0
4	I	144	0	0	0	0
4	J	142	0	0	0	0
4	K	65	0	0	0	0
4	L	129	0	0	1	0
4	M	98	0	0	0	0
4	N	72	0	0	0	0
4	O	95	0	0	0	0
4	P	104	0	0	0	0
4	Q	90	0	0	0	0
4	R	84	0	0	0	0
4	S	109	0	0	0	0
4	T	89	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35698	0	32700	220	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 3.

The worst 5 of 220 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:HIS:HA	1:D:2:THR:OG1	1.70	0.91
3:D:344:CPJ:H322	4:G:3324:HOH:O	1.79	0.82
1:M:30:LEU:HB2	1:M:125:VAL:HG22	1.71	0.72
1:A:176:THR:HG23	4:A:1005:HOH:O	1.92	0.69
1:B:30:LEU:HB2	1:B:125:VAL:HG22	1.76	0.68

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
1	B	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
1	C	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
1	D	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
1	E	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
1	F	202/204 (99%)	197 (98%)	4 (2%)	1 (0%)	31	33
1	G	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
1	H	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
1	I	202/204 (99%)	199 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
1	K	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
1	L	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
1	M	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
1	N	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
1	O	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
1	P	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
1	Q	202/204 (99%)	195 (96%)	7 (4%)	0	100	100
1	R	202/204 (99%)	199 (98%)	3 (2%)	0	100	100
1	S	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
1	T	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
All	All	4040/4080 (99%)	3937 (98%)	102 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	26	LEU

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	181/181 (100%)	167 (92%)	14 (8%)	14	14
1	B	181/181 (100%)	159 (88%)	22 (12%)	5	4
1	C	181/181 (100%)	165 (91%)	16 (9%)	11	11
1	D	181/181 (100%)	167 (92%)	14 (8%)	14	14
1	E	181/181 (100%)	166 (92%)	15 (8%)	12	12
1	F	181/181 (100%)	167 (92%)	14 (8%)	14	14
1	G	181/181 (100%)	162 (90%)	19 (10%)	7	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	181/181 (100%)	166 (92%)	15 (8%)	12	12
1	I	181/181 (100%)	165 (91%)	16 (9%)	11	11
1	J	181/181 (100%)	165 (91%)	16 (9%)	11	11
1	K	181/181 (100%)	165 (91%)	16 (9%)	11	11
1	L	181/181 (100%)	164 (91%)	17 (9%)	9	9
1	M	181/181 (100%)	167 (92%)	14 (8%)	14	14
1	N	181/181 (100%)	161 (89%)	20 (11%)	7	6
1	O	181/181 (100%)	165 (91%)	16 (9%)	11	11
1	P	181/181 (100%)	168 (93%)	13 (7%)	16	17
1	Q	181/181 (100%)	163 (90%)	18 (10%)	8	8
1	R	181/181 (100%)	168 (93%)	13 (7%)	16	17
1	S	181/181 (100%)	167 (92%)	14 (8%)	14	14
1	T	181/181 (100%)	168 (93%)	13 (7%)	16	17
All	All	3620/3620 (100%)	3305 (91%)	315 (9%)	11	11

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	157	LEU
1	K	189	ASN
1	S	49	LEU
1	J	4	LEU
1	J	157	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	186	GLN
1	K	189	ASN
1	Q	189	ASN
1	J	1	HIS
1	J	189	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 40 are monoatomic - leaving 10 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$
3	CPJ	A	341	2	25,31,31	2.02	4 (16%)	28,44,44	2.15	12 (42%)
3	CPJ	B	342	2	25,31,31	2.00	3 (12%)	28,44,44	2.17	11 (39%)
3	CPJ	C	343	2	25,31,31	1.93	2 (8%)	28,44,44	1.81	8 (28%)
3	CPJ	D	344	2	25,31,31	1.86	2 (8%)	28,44,44	1.75	9 (32%)
3	CPJ	E	345	2	25,31,31	1.92	2 (8%)	28,44,44	1.78	9 (32%)
3	CPJ	L	347	2	25,31,31	1.97	2 (8%)	28,44,44	2.15	12 (42%)
3	CPJ	M	348	2	25,31,31	1.87	3 (12%)	28,44,44	1.82	8 (28%)
3	CPJ	N	349	2	25,31,31	1.90	3 (12%)	28,44,44	1.87	8 (28%)
3	CPJ	P	346	2	25,31,31	1.95	2 (8%)	28,44,44	1.98	12 (42%)
3	CPJ	Q	350	2	25,31,31	1.91	2 (8%)	28,44,44	1.80	9 (32%)

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
3	CPJ	A	341	2	-	0/15/51/51	0/2/2/2
3	CPJ	B	342	2	-	0/15/51/51	0/2/2/2
3	CPJ	C	343	2	-	0/15/51/51	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPJ	D	344	2	-	0/15/51/51	0/2/2/2
3	CPJ	E	345	2	-	0/15/51/51	0/2/2/2
3	CPJ	L	347	2	-	0/15/51/51	0/2/2/2
3	CPJ	M	348	2	-	0/15/51/51	0/2/2/2
3	CPJ	N	349	2	-	0/15/51/51	0/2/2/2
3	CPJ	P	346	2	-	0/15/51/51	0/2/2/2
3	CPJ	Q	350	2	-	0/15/51/51	0/2/2/2

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	341	CPJ	O22-C20	6.34	1.46	1.35
3	B	342	CPJ	O11-C12	6.32	1.46	1.35
3	L	347	CPJ	O11-C12	6.25	1.46	1.35
3	L	347	CPJ	O22-C20	6.18	1.45	1.35
3	B	342	CPJ	O22-C20	6.17	1.45	1.35

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	348	CPJ	O1-C6-C10	4.13	111.52	106.25
3	Q	350	CPJ	O1-C6-C10	4.08	111.45	106.25
3	N	349	CPJ	O1-C6-C10	4.00	111.35	106.25
3	A	341	CPJ	O1-C6-C10	3.96	111.30	106.25
3	P	346	CPJ	O1-C6-C10	3.95	111.29	106.25

There are no chirality outliers.

There are no torsion outliers.

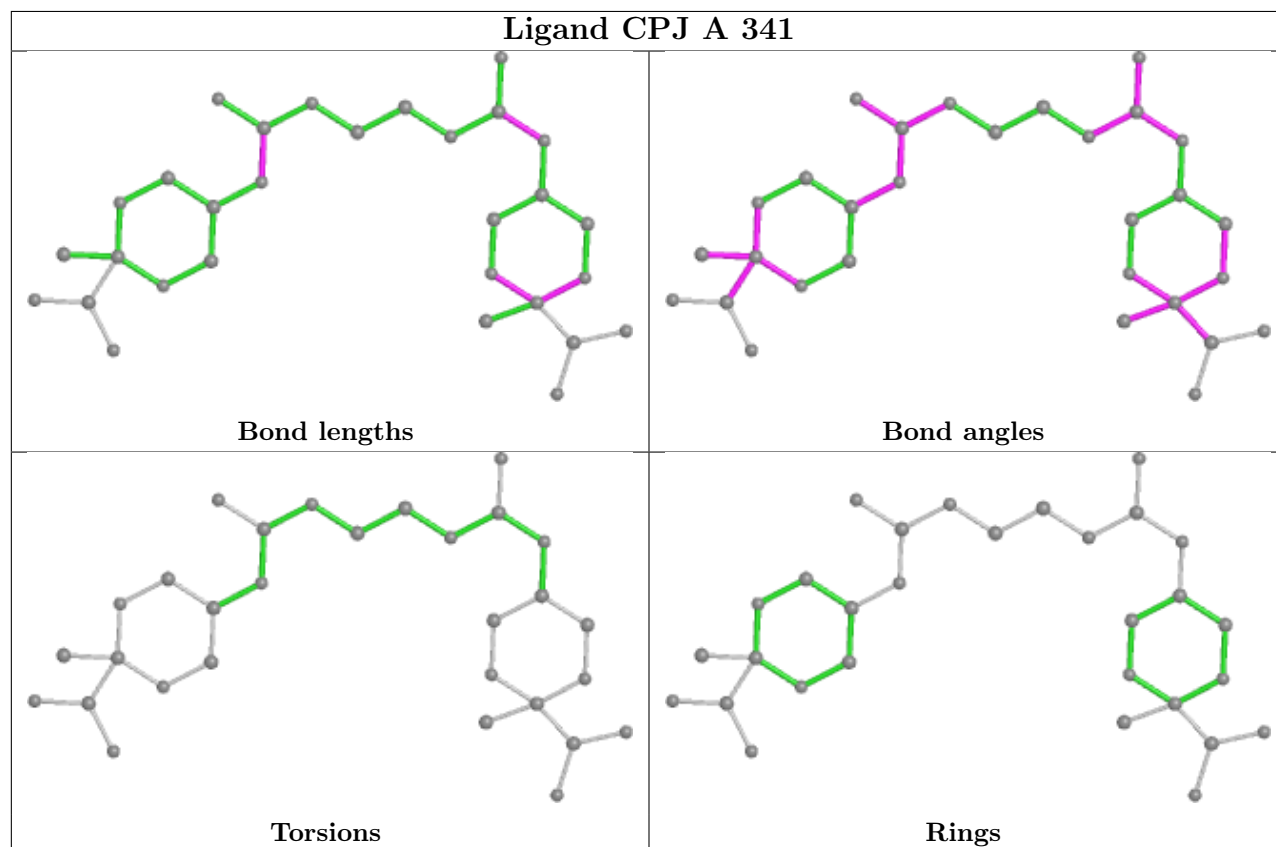
There are no ring outliers.

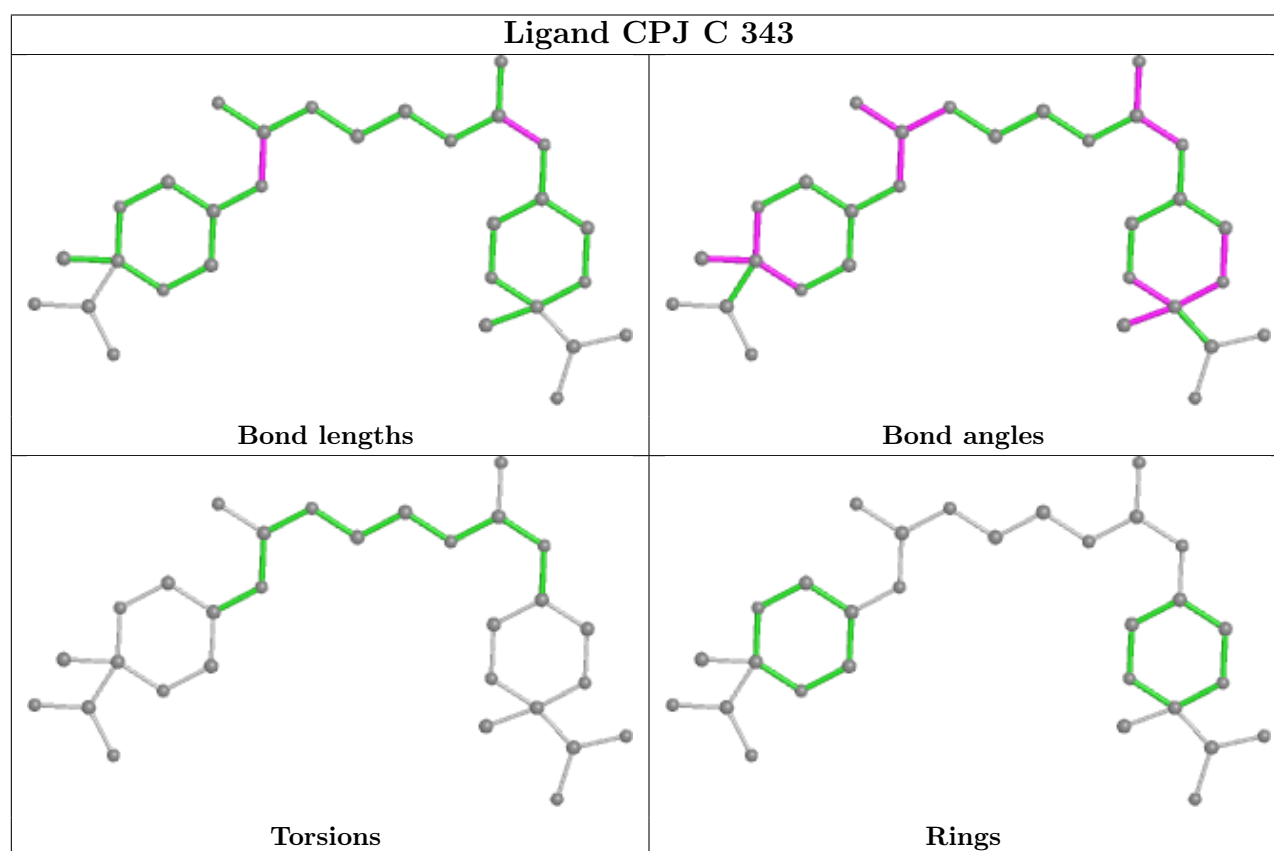
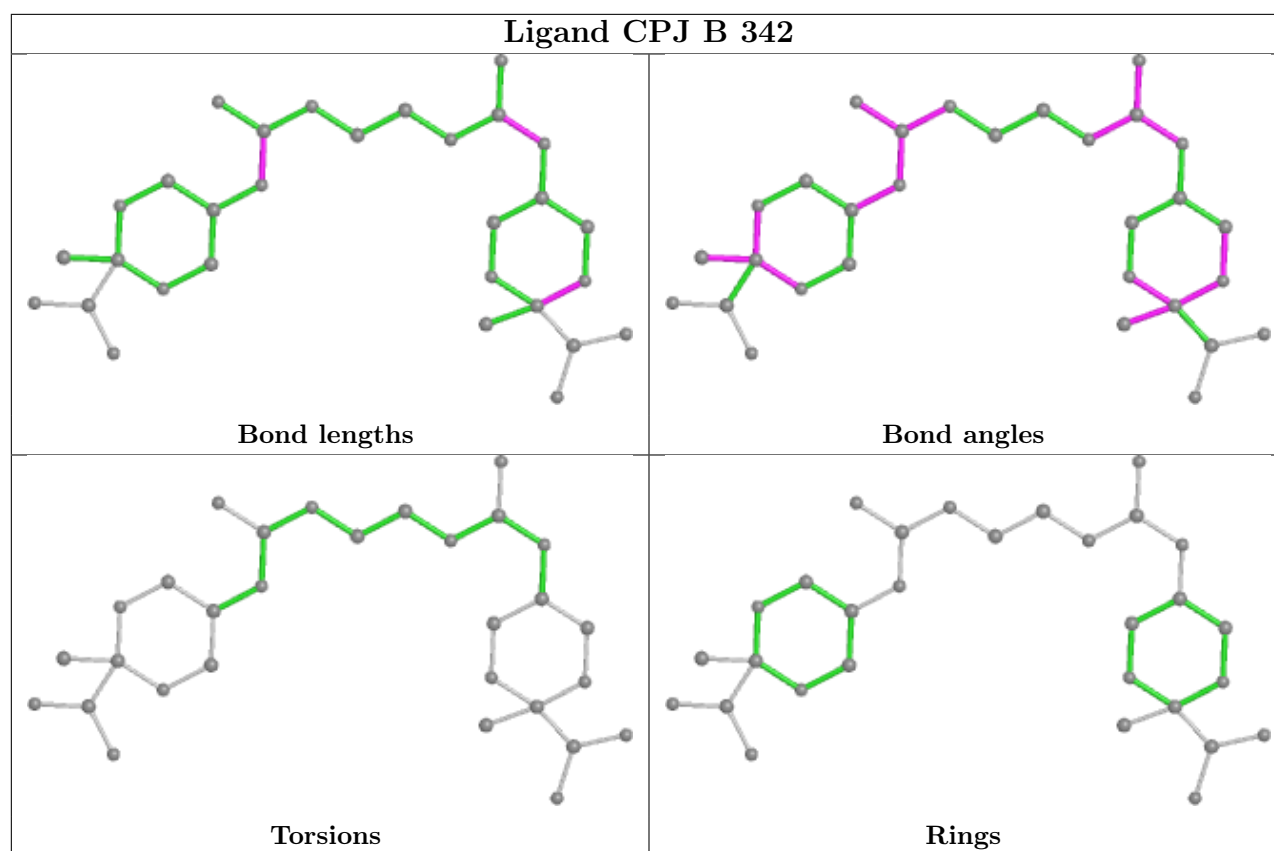
1 monomer is involved in 1 short contact:

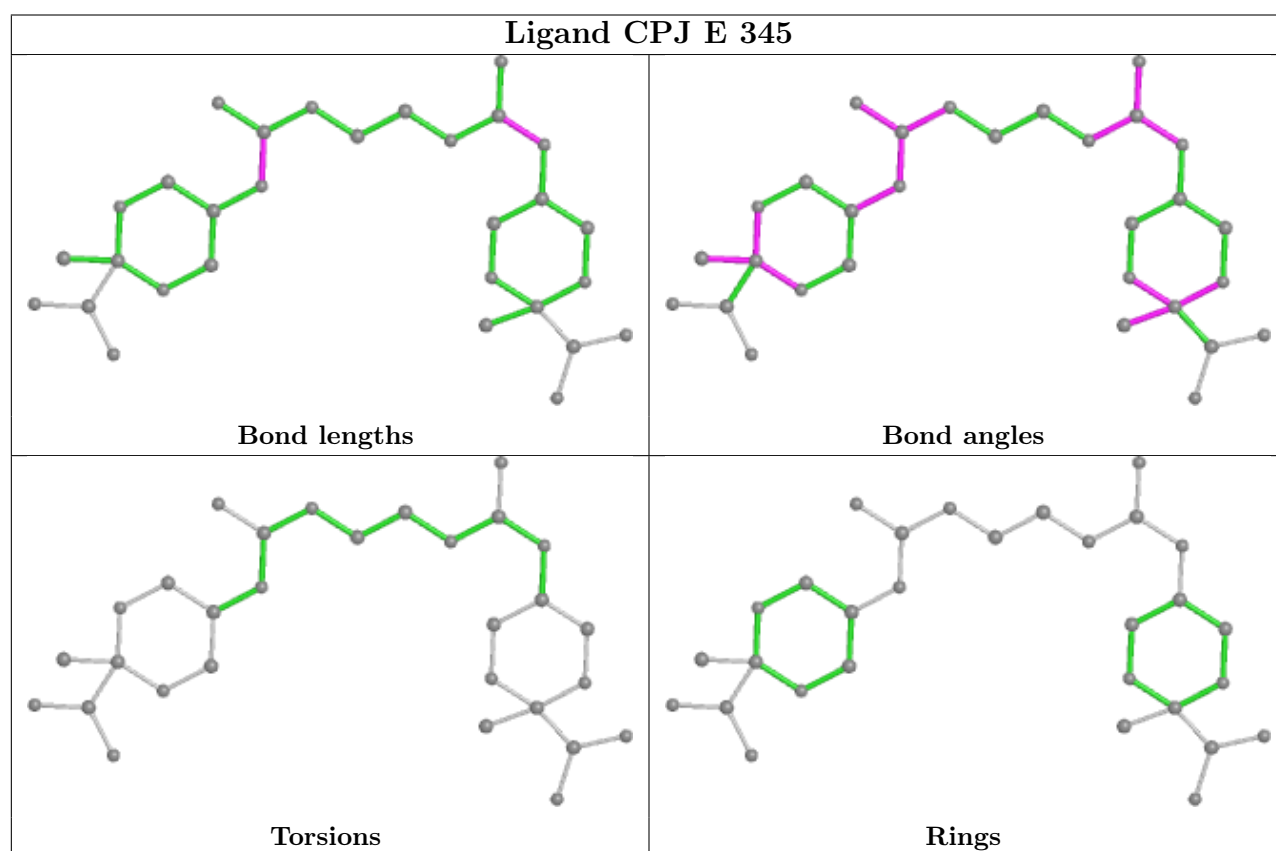
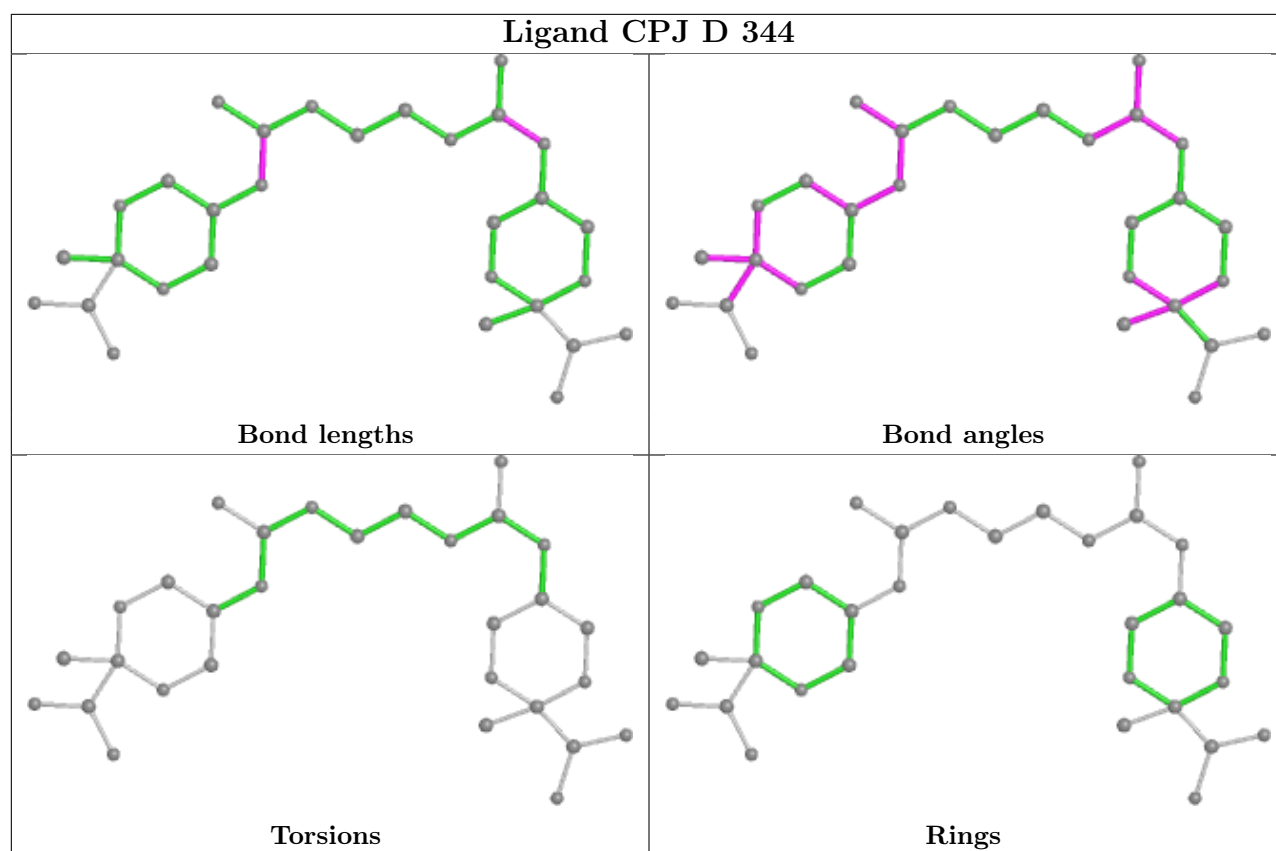
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	344	CPJ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

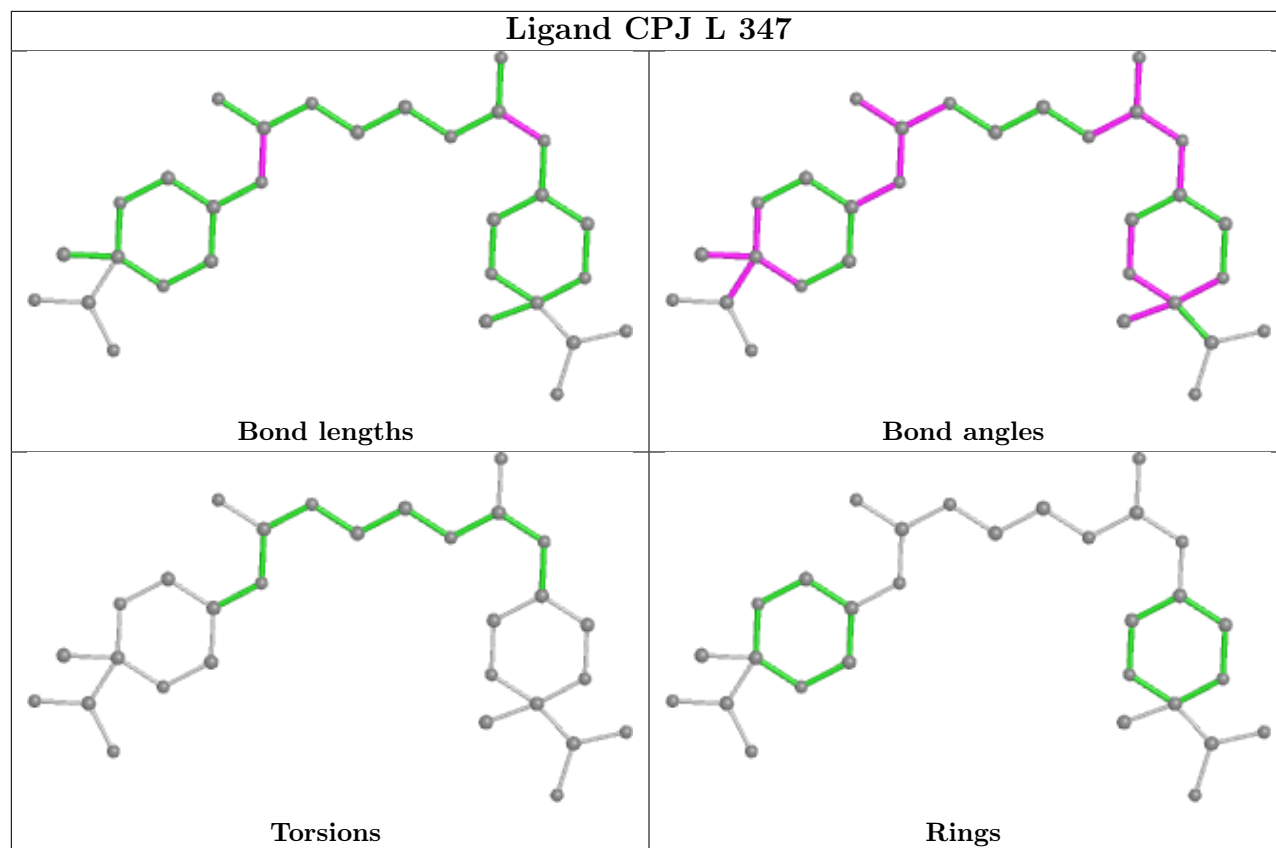
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



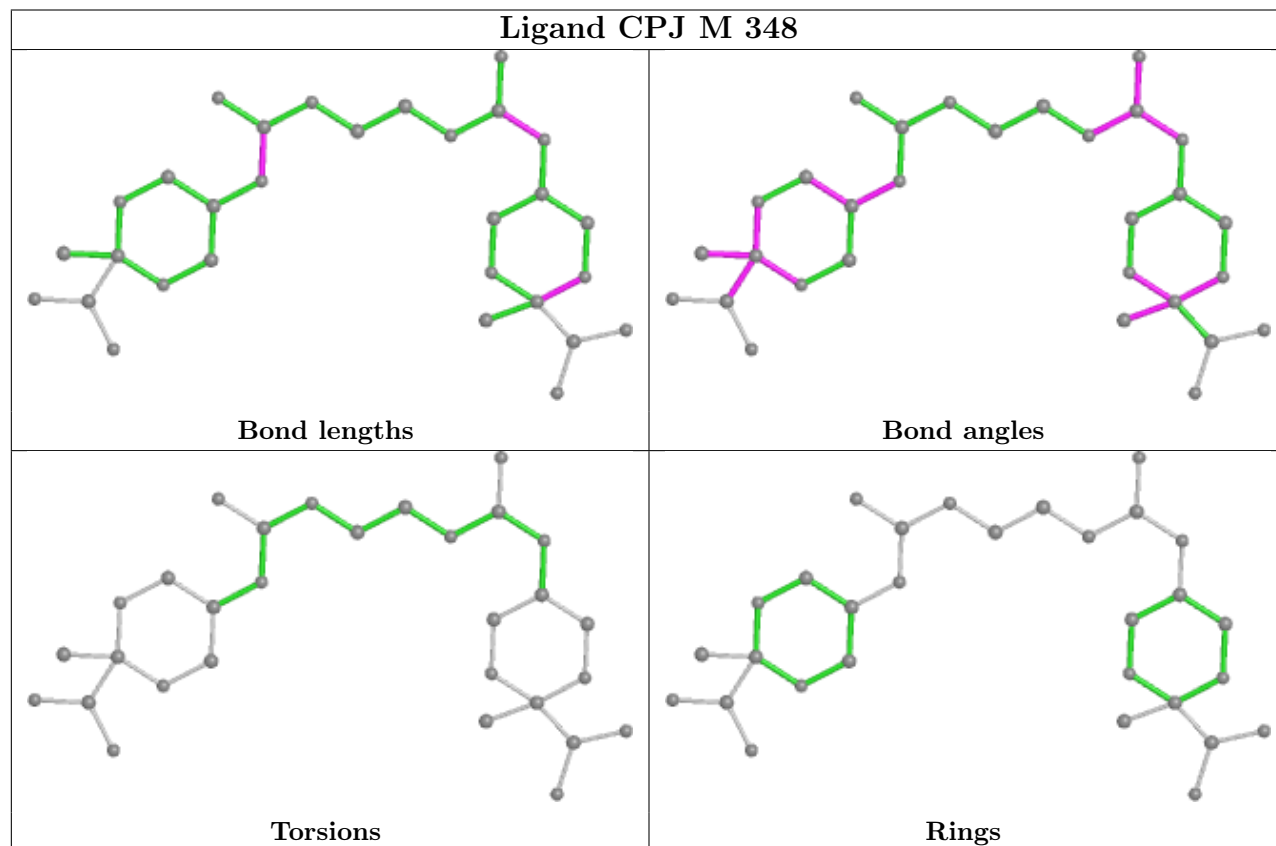


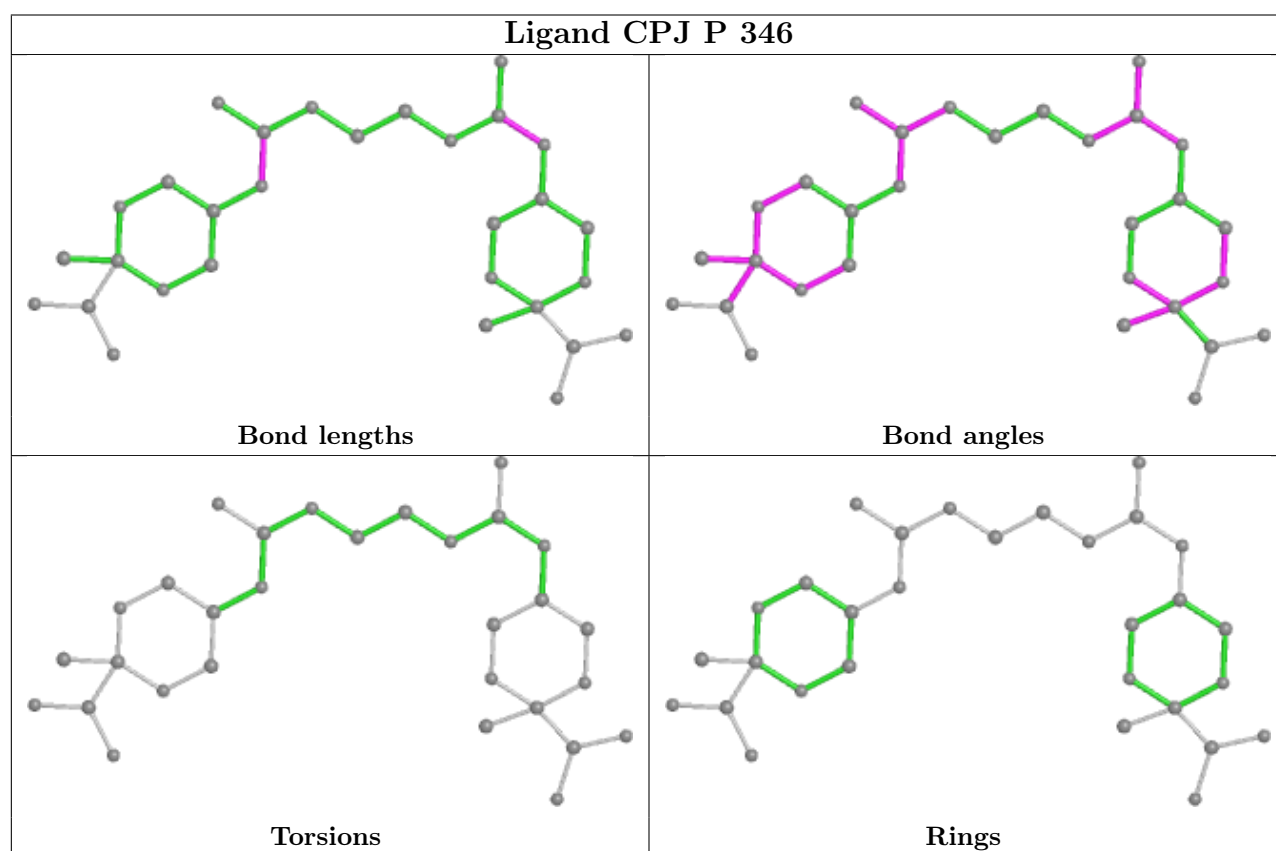
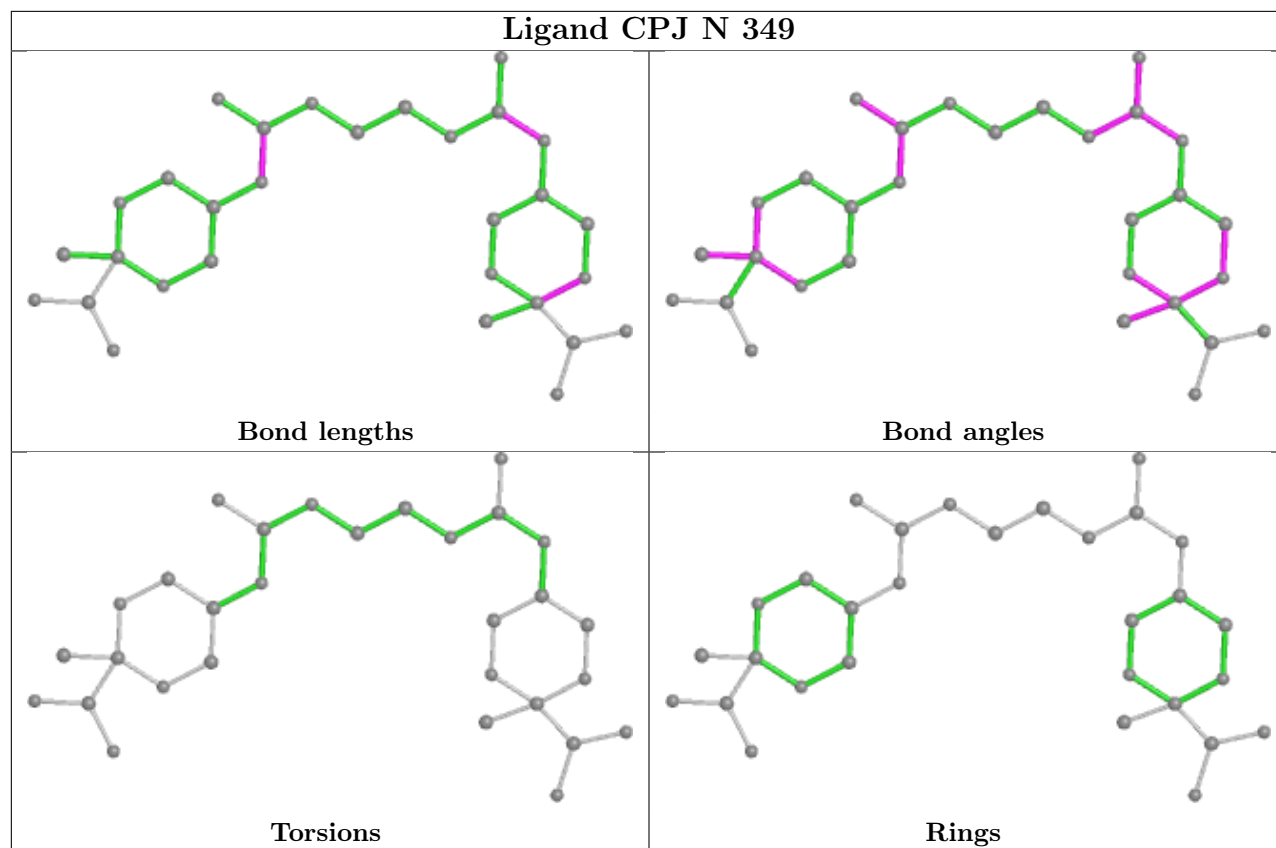


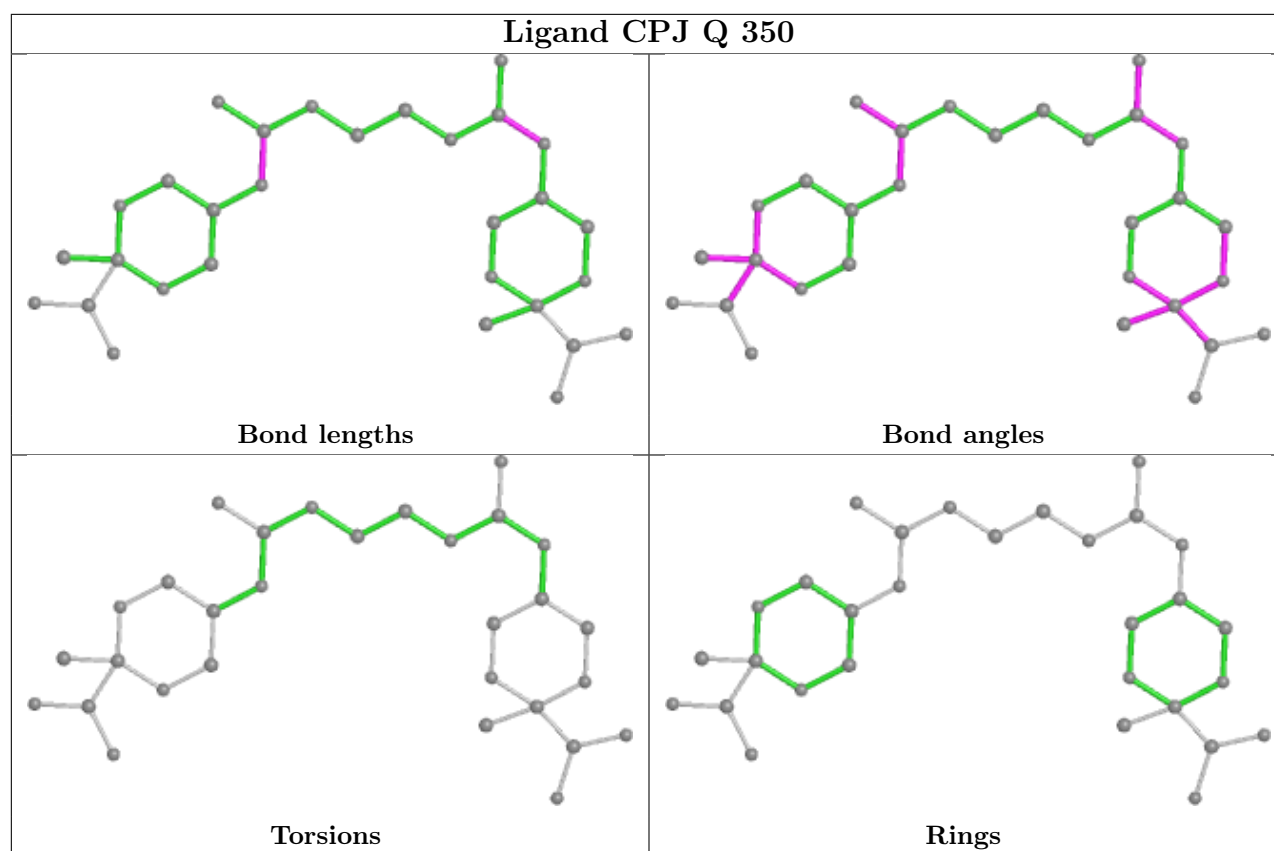
Ligand CPJ L 347



Ligand CPJ M 348







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	204/204 (100%)	-0.11	0 100 100	8, 13, 22, 36	0
1	B	204/204 (100%)	-0.10	1 (0%) 90 90	8, 13, 23, 31	0
1	C	204/204 (100%)	-0.14	1 (0%) 90 90	7, 14, 23, 33	0
1	D	204/204 (100%)	-0.15	0 100 100	8, 13, 21, 34	0
1	E	204/204 (100%)	-0.14	0 100 100	8, 13, 24, 30	0
1	F	204/204 (100%)	0.04	1 (0%) 90 90	9, 14, 25, 37	0
1	G	204/204 (100%)	0.11	2 (0%) 82 81	8, 13, 22, 32	0
1	H	204/204 (100%)	0.15	2 (0%) 82 81	8, 13, 23, 36	0
1	I	204/204 (100%)	0.07	0 100 100	8, 13, 23, 33	0
1	J	204/204 (100%)	0.03	1 (0%) 90 90	6, 14, 23, 32	0
1	K	204/204 (100%)	0.49	9 (4%) 34 32	9, 15, 24, 35	0
1	L	204/204 (100%)	0.38	0 100 100	9, 15, 25, 37	0
1	M	204/204 (100%)	0.48	10 (4%) 29 28	10, 16, 24, 35	0
1	N	204/204 (100%)	0.41	4 (1%) 65 63	6, 15, 25, 28	0
1	O	204/204 (100%)	0.24	4 (1%) 65 63	9, 15, 24, 37	0
1	P	204/204 (100%)	-0.03	1 (0%) 90 90	7, 13, 22, 33	0
1	Q	204/204 (100%)	-0.04	1 (0%) 90 90	9, 15, 25, 37	0
1	R	204/204 (100%)	0.07	3 (1%) 73 72	10, 15, 24, 35	0
1	S	204/204 (100%)	0.03	1 (0%) 90 90	7, 13, 24, 32	0
1	T	204/204 (100%)	0.10	3 (1%) 73 72	8, 13, 23, 39	0
All	All	4080/4080 (100%)	0.09	44 (1%) 80 79	6, 14, 24, 39	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	204	VAL	8.1
1	F	204	VAL	5.4
1	N	204	VAL	4.9
1	R	204	VAL	4.7
1	C	204	VAL	4.6

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	M	326	1/1	0.84	0.09	38,38,38,38	0
2	CA	O	329	1/1	0.86	0.10	30,30,30,30	0
2	CA	R	336	1/1	0.87	0.14	37,37,37,37	0
2	CA	N	327	1/1	0.88	0.09	42,42,42,42	0
3	CPJ	M	348	30/30	0.88	0.21	27,64,76,77	0
2	CA	K	321	1/1	0.88	0.08	45,45,45,45	0
3	CPJ	L	347	30/30	0.90	0.19	29,53,68,68	0
3	CPJ	N	349	30/30	0.91	0.22	51,67,83,84	0
2	CA	Q	334	1/1	0.92	0.12	35,35,35,35	0
3	CPJ	P	346	30/30	0.92	0.14	28,62,70,71	0
2	CA	L	324	1/1	0.92	0.13	31,31,31,31	0
2	CA	J	319	1/1	0.92	0.11	27,27,27,27	0
2	CA	T	340	1/1	0.93	0.10	39,39,39,39	0
3	CPJ	D	344	30/30	0.93	0.14	27,36,58,59	0
2	CA	F	312	1/1	0.93	0.12	24,24,24,24	0
3	CPJ	B	342	30/30	0.93	0.16	20,41,58,61	0
2	CA	T	339	1/1	0.94	0.11	39,39,39,39	0
2	CA	G	313	1/1	0.94	0.09	28,28,28,28	0
2	CA	M	325	1/1	0.94	0.10	44,44,44,44	0

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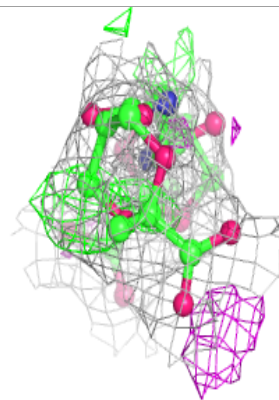
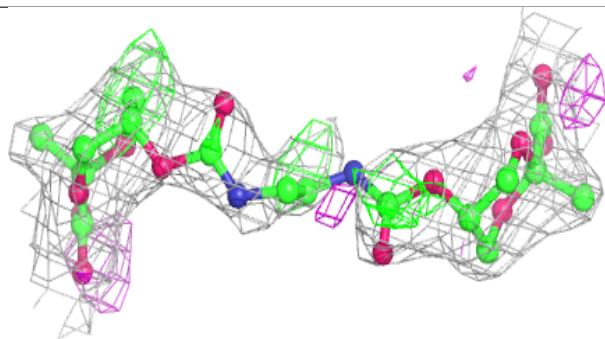
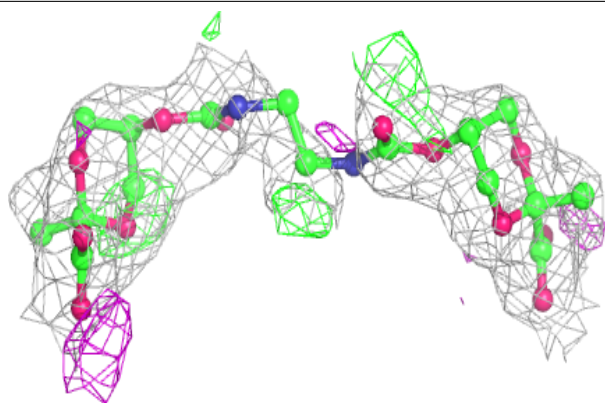
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CPJ	C	343	30/30	0.94	0.14	26,34,55,56	0
3	CPJ	Q	350	30/30	0.94	0.16	31,51,71,72	0
2	CA	S	338	1/1	0.94	0.10	27,27,27,27	0
3	CPJ	A	341	30/30	0.94	0.13	19,35,52,54	0
2	CA	C	306	1/1	0.95	0.13	26,26,26,26	0
2	CA	D	308	1/1	0.95	0.11	26,26,26,26	0
2	CA	B	304	1/1	0.95	0.12	23,23,23,23	0
2	CA	H	315	1/1	0.95	0.08	25,25,25,25	0
2	CA	N	328	1/1	0.95	0.08	42,42,42,42	0
2	CA	E	309	1/1	0.96	0.10	24,24,24,24	0
2	CA	P	332	1/1	0.96	0.09	28,28,28,28	0
3	CPJ	E	345	30/30	0.96	0.15	20,34,56,57	0
2	CA	G	314	1/1	0.96	0.12	27,27,27,27	0
2	CA	J	320	1/1	0.97	0.10	27,27,27,27	0
2	CA	Q	333	1/1	0.97	0.11	36,36,36,36	0
2	CA	L	323	1/1	0.97	0.10	30,30,30,30	0
2	CA	D	307	1/1	0.97	0.10	26,26,26,26	0
2	CA	R	335	1/1	0.97	0.10	36,36,36,36	0
2	CA	H	316	1/1	0.97	0.09	28,28,28,28	0
2	CA	F	311	1/1	0.97	0.13	24,24,24,24	0
2	CA	A	301	1/1	0.97	0.09	19,19,19,19	0
2	CA	K	322	1/1	0.97	0.09	46,46,46,46	0
2	CA	B	303	1/1	0.97	0.11	23,23,23,23	0
2	CA	E	310	1/1	0.98	0.10	23,23,23,23	0
2	CA	O	330	1/1	0.98	0.13	28,28,28,28	0
2	CA	I	318	1/1	0.98	0.10	28,28,28,28	0
2	CA	C	305	1/1	0.98	0.09	28,28,28,28	0
2	CA	I	317	1/1	0.98	0.10	26,26,26,26	0
2	CA	P	331	1/1	0.98	0.10	29,29,29,29	0
2	CA	S	337	1/1	0.98	0.09	26,26,26,26	0
2	CA	A	302	1/1	0.99	0.11	20,20,20,20	0

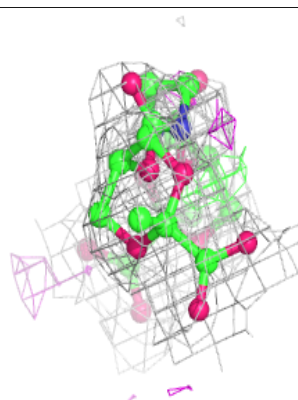
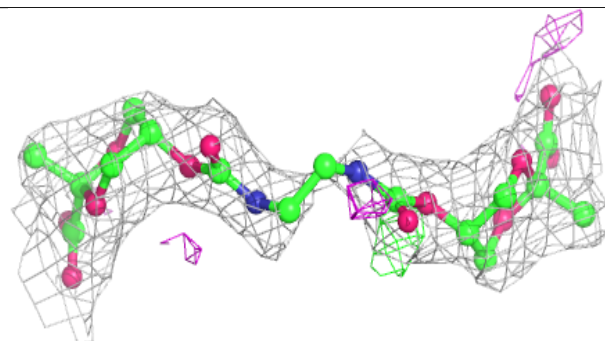
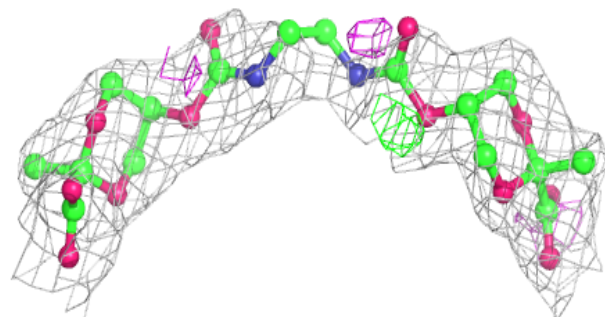
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CPJ M 348:

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

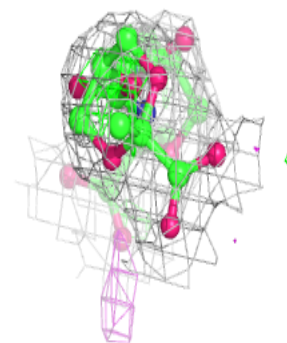
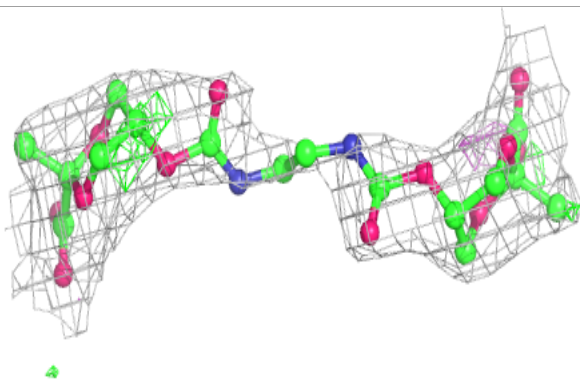
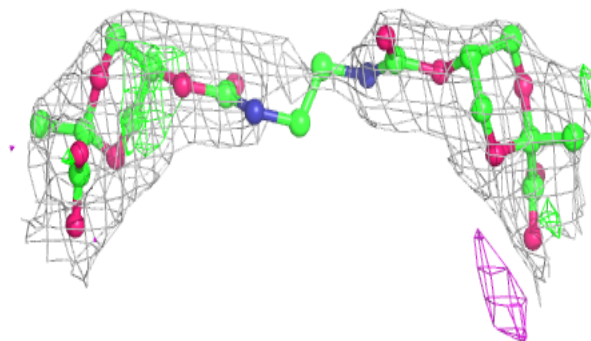
**Electron density around CPJ L 347:**

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

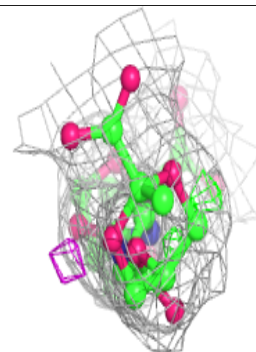
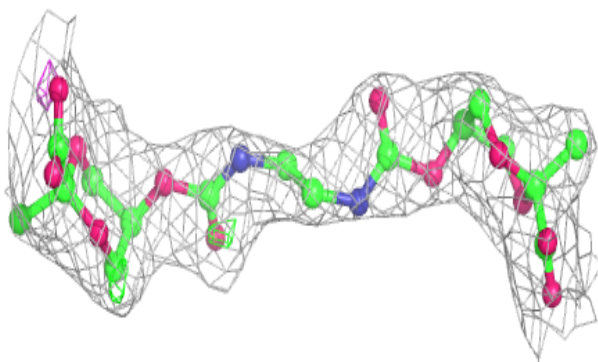
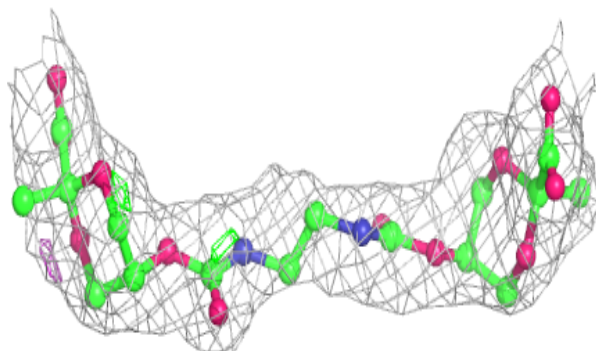


Electron density around CPJ N 349:

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

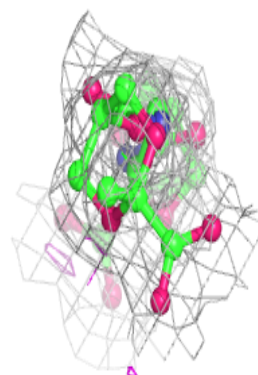
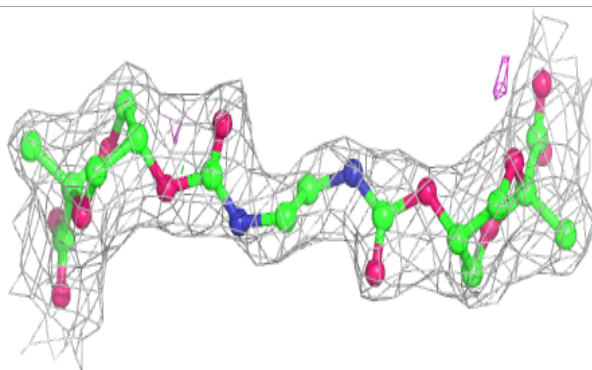
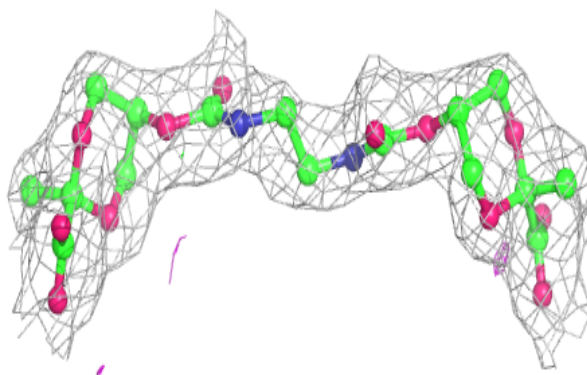
**Electron density around CPJ P 346:**

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

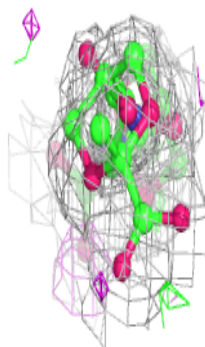
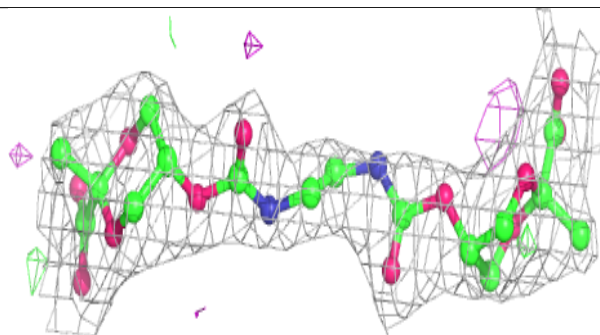
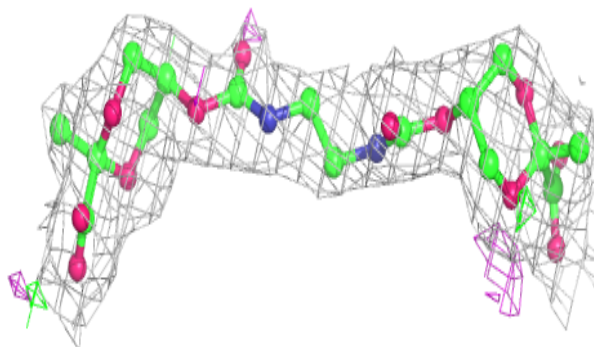


Electron density around CPJ D 344:

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

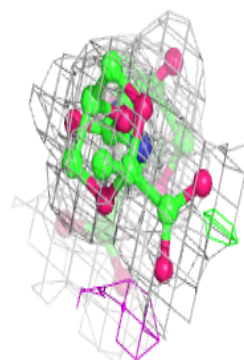
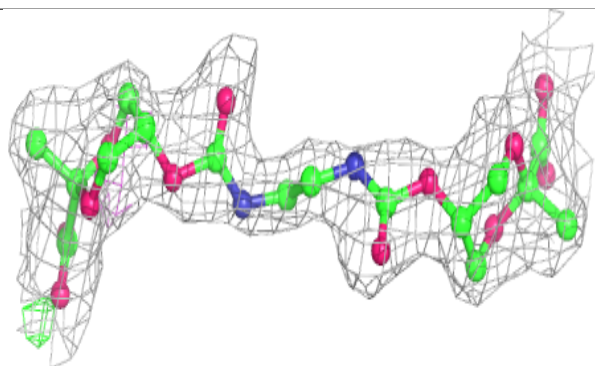
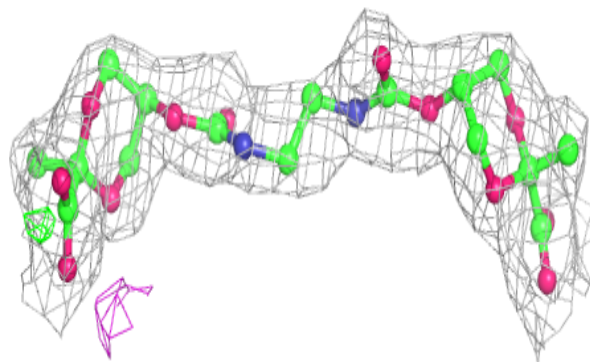
**Electron density around CPJ B 342:**

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

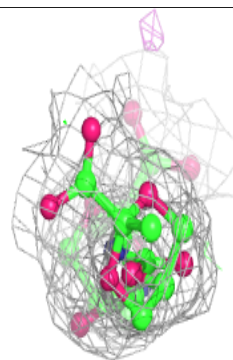
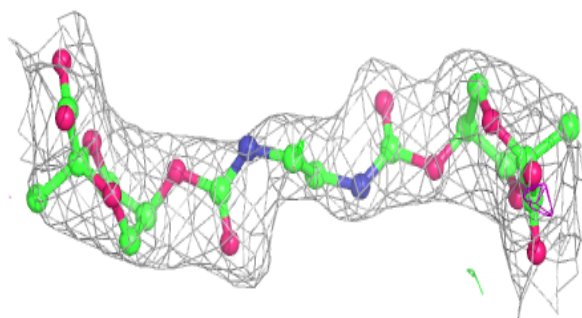
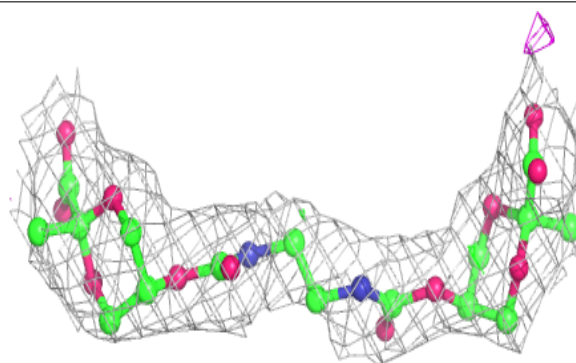


Electron density around CPJ C 343:

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

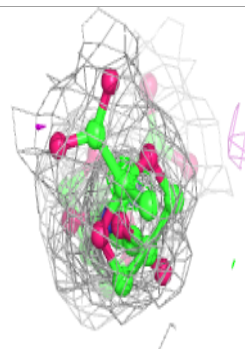
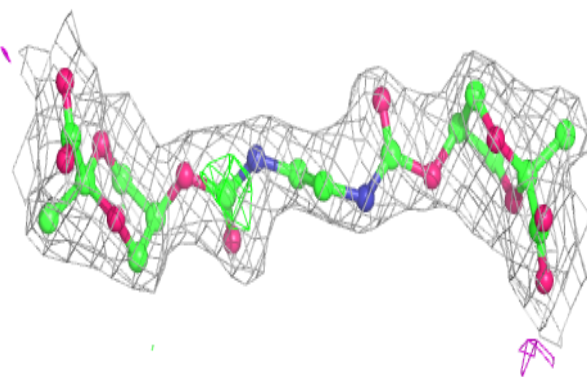
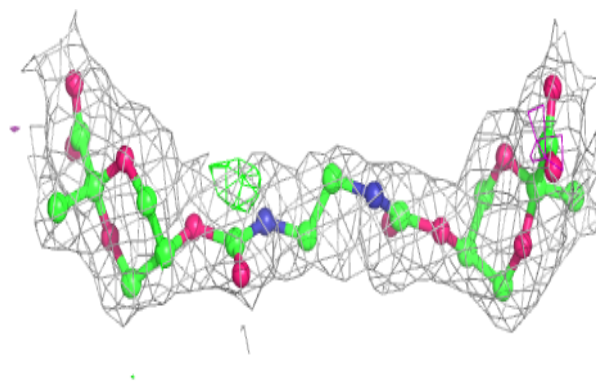
**Electron density around CPJ Q 350:**

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

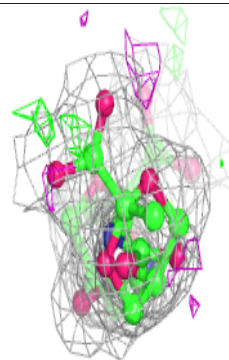
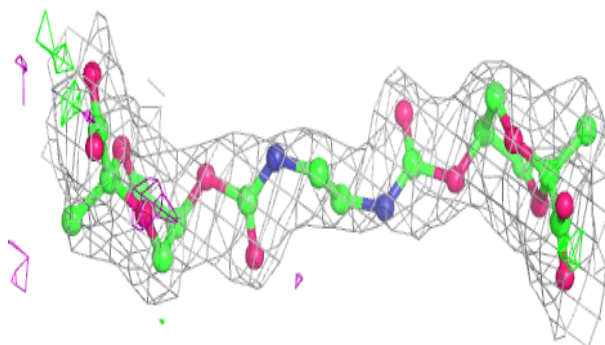
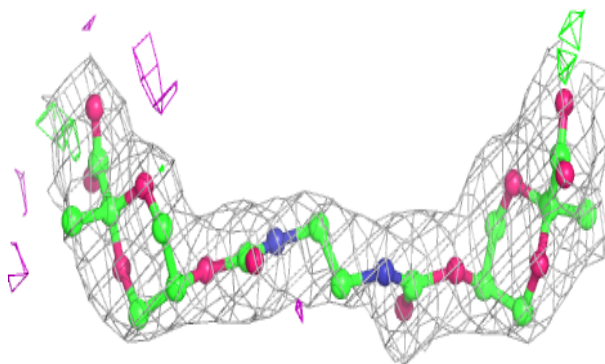


Electron density around CPJ A 341:

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

**Electron density around CPJ E 345:**

$2mF_o-DF_c$ (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.