Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 03:26 PM EDT

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-yloxycarbamoyl}-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 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 (i) 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 (i)) were used in the production of this report:

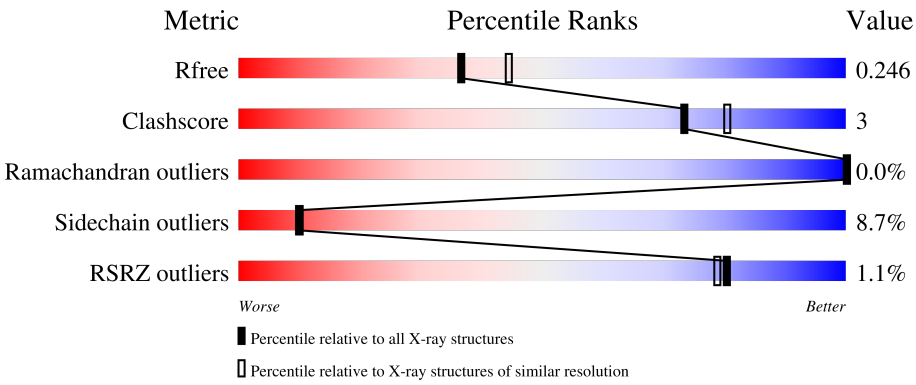
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	204	84% 14% •
1	B	204	82% 15% •
1	C	204	82% 16% •
1	D	204	84% 14% •
1	E	204	84% 15%

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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	4% 83% 15%
1	L	204	85% 13%
1	M	204	5% 83% 14%
1	N	204	2% 83% 16%
1	O	204	2% 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 (i)

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
			Total	C	N	O	S			
1	A	204	1649	1071	272	303	3	0	0	0
1	B	204	1649	1071	272	303	3	0	0	0
1	C	204	1649	1071	272	303	3	0	0	0
1	D	204	1649	1071	272	303	3	0	0	0
1	E	204	1649	1071	272	303	3	0	0	0
1	F	204	1649	1071	272	303	3	0	0	0
1	G	204	1649	1071	272	303	3	0	0	0
1	H	204	1649	1071	272	303	3	0	0	0
1	I	204	1649	1071	272	303	3	0	0	0
1	J	204	1649	1071	272	303	3	0	0	0
1	K	204	1649	1071	272	303	3	0	0	0
1	L	204	1649	1071	272	303	3	0	0	0
1	M	204	1649	1071	272	303	3	0	0	0
1	N	204	1649	1071	272	303	3	0	0	0
1	O	204	1649	1071	272	303	3	0	0	0
1	P	204	1649	1071	272	303	3	0	0	0

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	2	2	2	0	0
			Total	Ca		
2	B	2	2	2	0	0
			Total	Ca		
2	C	2	2	2	0	0
			Total	Ca		
2	D	2	2	2	0	0
			Total	Ca		
2	E	2	2	2	0	0
			Total	Ca		
2	F	2	2	2	0	0
			Total	Ca		
2	G	2	2	2	0	0
			Total	Ca		
2	H	2	2	2	0	0
			Total	Ca		
2	I	2	2	2	0	0
			Total	Ca		
2	J	2	2	2	0	0
			Total	Ca		
2	K	2	2	2	0	0
			Total	Ca		
2	L	2	2	2	0	0
			Total	Ca		
2	M	2	2	2	0	0
			Total	Ca		
2	N	2	2	2	0	0
			Total	Ca		
2	O	2	2	2	0	0

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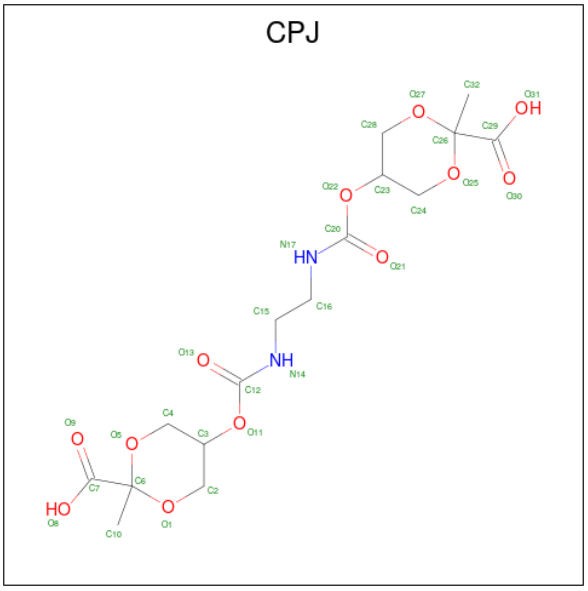
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	P	2	2	2	0	0
2	Q	2	2	2	0	0
2	R	2	2	2	0	0
2	S	2	2	2	0	0
2	T	2	2	2	0	0

- Molecule 3 is BIS-1,2-{[(Z)-2-CARBOXY-2-METHYL-1,3-DIOXANE]-5-YLOXYCARBAMOYL}-ETHANE (three-letter code: CPJ) (formula: $C_{16}H_{24}N_2O_{12}$).



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

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

- Molecule 4 is water.

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

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

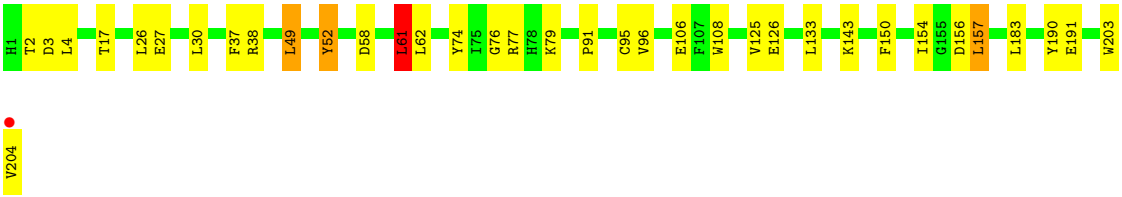
Chain A:

• Molecule 1: Serum amyloid P-component

Chain B:

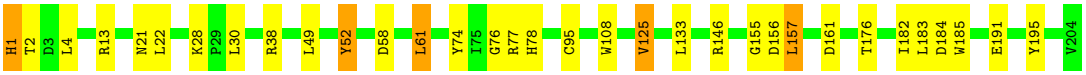
• Molecule 1: Serum amyloid P-component

Chain C:



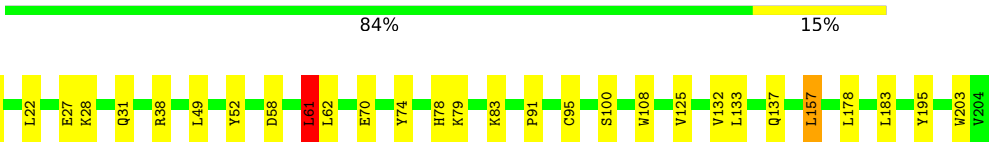
• Molecule 1: Serum amyloid P-component

Chain D:



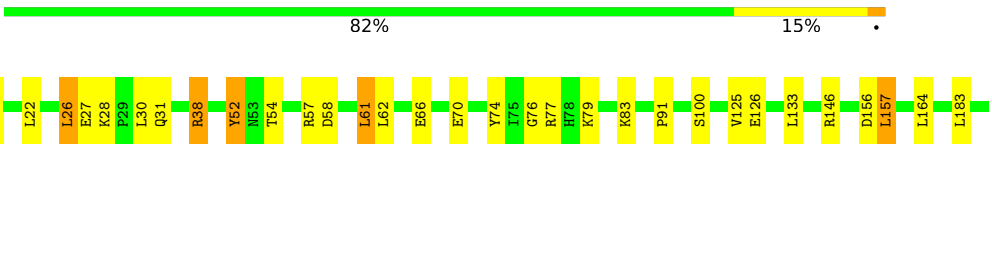
• Molecule 1: Serum amyloid P-component

Chain E:



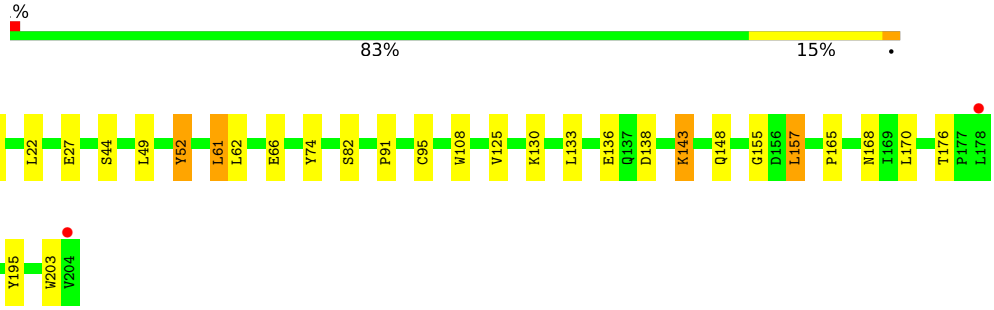
• Molecule 1: Serum amyloid P-component

Chain F:



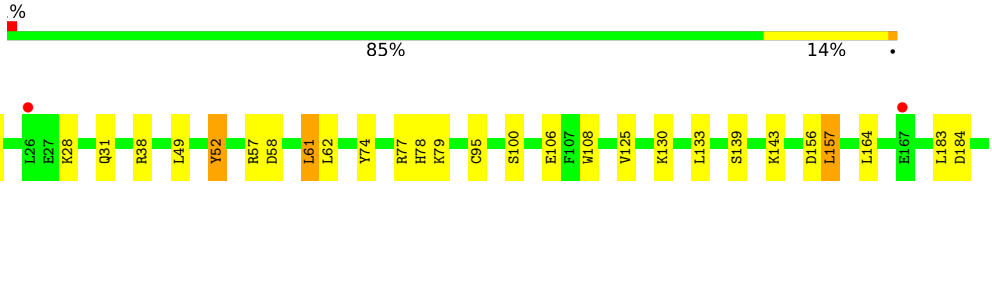
• Molecule 1: Serum amyloid P-component

Chain G:



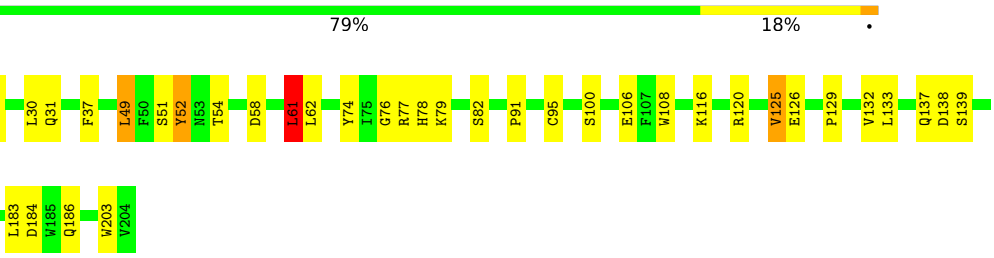
• Molecule 1: Serum amyloid P-component

Chain H:



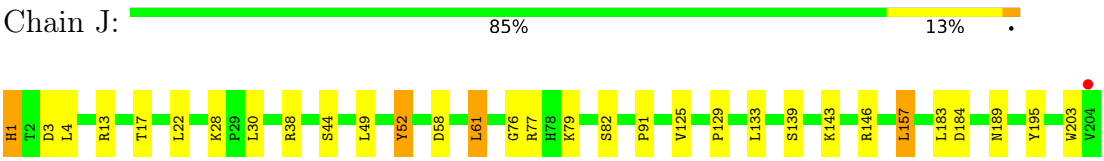
• Molecule 1: Serum amyloid P-component

Chain I:



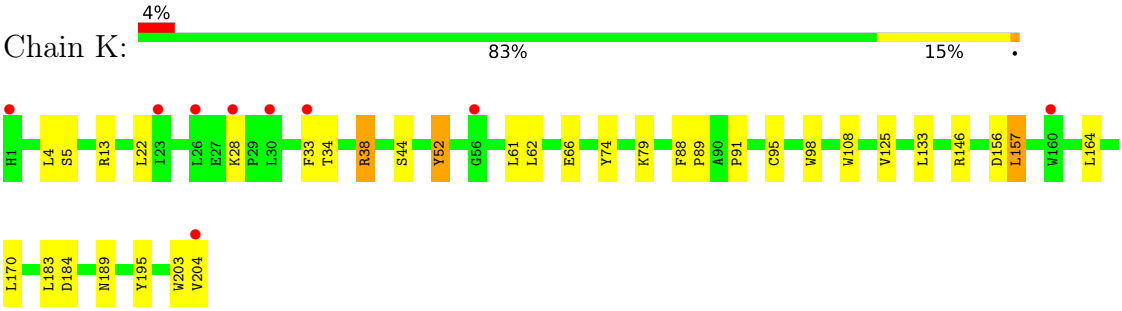
• Molecule 1: Serum amyloid P-component

Chain J:



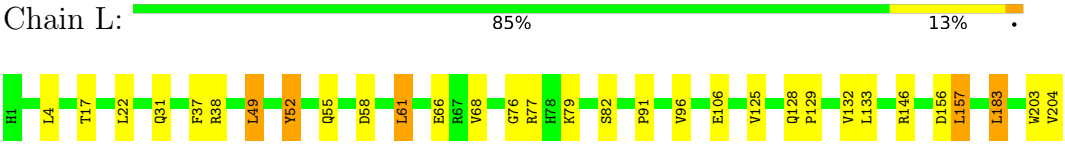
• Molecule 1: Serum amyloid P-component

Chain K:



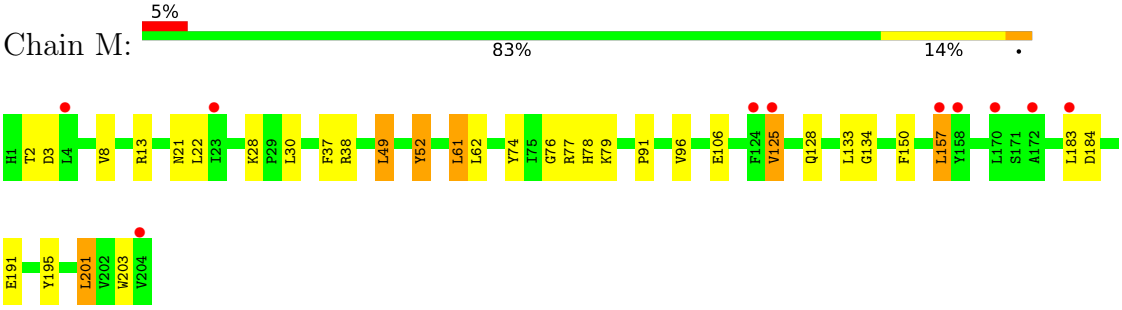
• Molecule 1: Serum amyloid P-component

Chain L:



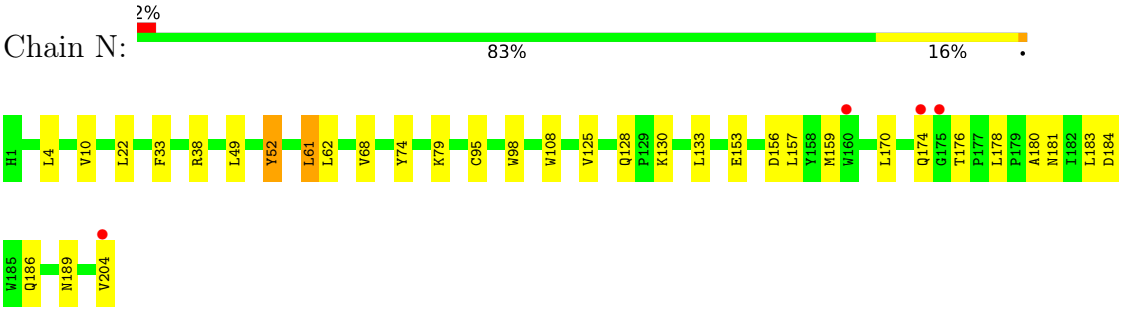
• Molecule 1: Serum amyloid P-component

Chain M:



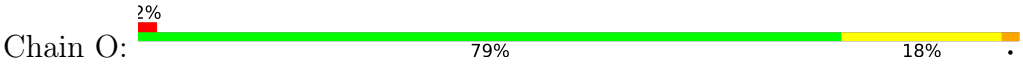
• Molecule 1: Serum amyloid P-component

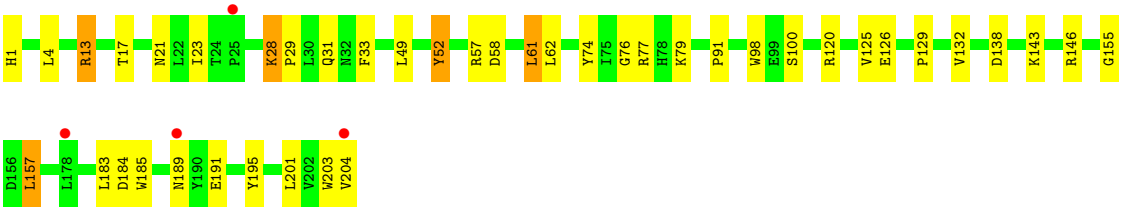
Chain N:



• Molecule 1: Serum amyloid P-component

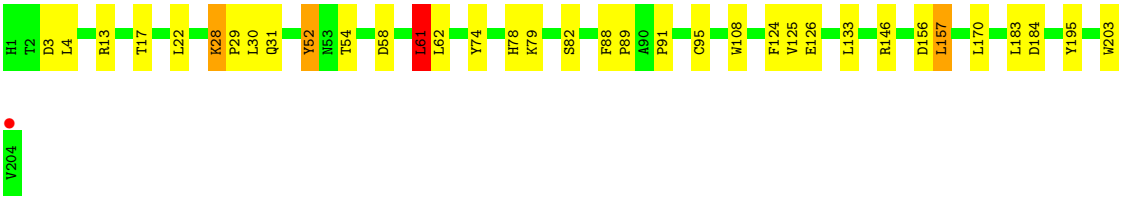
Chain O:





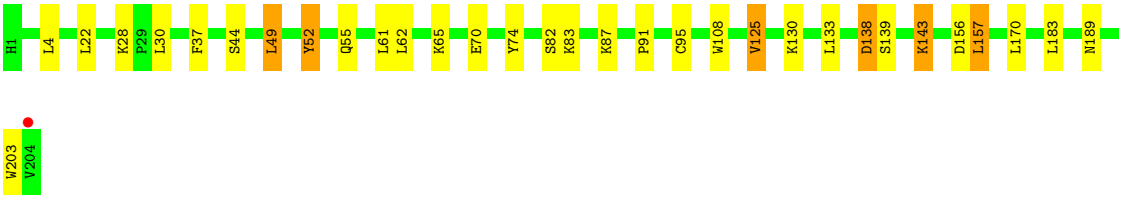
• Molecule 1: Serum amyloid P-component

Chain P: 83% 15%



• Molecule 1: Serum amyloid P-component

Chain Q: 84% 13%

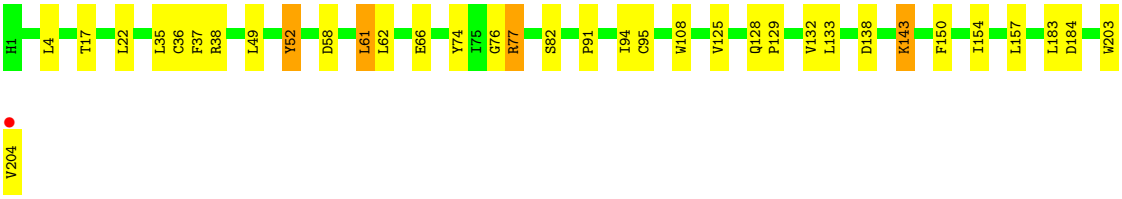


• Molecule 1: Serum amyloid P-component

Chain R: % 88% 11%

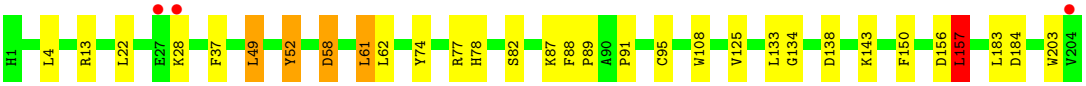
• Molecule 1: Serum amyloid P-component

Chain S: 83% 15%



• Molecule 1: Serum amyloid P-component

Chain T: % 85% 13%


H1
L4
R13
L22
E27
K28
F37
L49
Y52
D58
L61
L62
Y74
R77
H78
S82
K87
F88
P89
A90
P91
C95
W108
V125
L133
G134
D138
K143
F150
D156
L157
L183
D184
W203
V204

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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 (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.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
1	P	157	LEU	CA-CB-CG	6.30	129.79	115.30
1	B	157	LEU	CA-CB-CG	6.25	129.68	115.30
1	C	157	LEU	CA-CB-CG	6.18	129.52	115.30
1	J	184	ASP	CB-CG-OD2	6.17	123.85	118.30
1	G	157	LEU	CA-CB-CG	6.13	129.41	115.30
1	Q	157	LEU	CA-CB-CG	6.01	129.12	115.30
1	D	58	ASP	CB-CG-OD2	5.98	123.69	118.30
1	A	156	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	157	LEU	CA-CB-CG	5.95	128.98	115.30
1	I	157	LEU	CA-CB-CG	5.95	128.97	115.30
1	B	58	ASP	CB-CG-OD2	5.94	123.64	118.30
1	D	157	LEU	CA-CB-CG	5.88	128.83	115.30
1	F	157	LEU	CA-CB-CG	5.87	128.80	115.30
1	T	184	ASP	CB-CG-OD2	5.85	123.56	118.30
1	H	184	ASP	CB-CG-OD2	5.84	123.55	118.30
1	Q	138	ASP	CB-CG-OD2	5.72	123.45	118.30
1	L	156	ASP	CB-CG-OD2	5.66	123.40	118.30
1	O	58	ASP	CB-CG-OD2	5.66	123.39	118.30
1	I	58	ASP	CB-CG-OD2	5.63	123.36	118.30
1	N	184	ASP	CB-CG-OD2	5.62	123.36	118.30
1	M	157	LEU	CA-CB-CG	5.60	128.19	115.30
1	C	58	ASP	CB-CG-OD2	5.56	123.31	118.30
1	H	156	ASP	CB-CG-OD2	5.53	123.28	118.30
1	I	184	ASP	CB-CG-OD2	5.50	123.25	118.30
1	T	157	LEU	CA-CB-CG	5.50	127.96	115.30
1	O	184	ASP	CB-CG-OD2	5.49	123.24	118.30
1	S	184	ASP	CB-CG-OD2	5.49	123.24	118.30
1	J	58	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	184	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	3	ASP	CB-CG-OD2	5.47	123.22	118.30
1	R	58	ASP	CB-CG-OD2	5.43	123.19	118.30
1	R	157	LEU	CA-CB-CG	5.43	127.78	115.30
1	K	157	LEU	CA-CB-CG	5.42	127.78	115.30
1	N	156	ASP	CB-CG-OD2	5.40	123.16	118.30
1	M	184	ASP	CB-CG-OD2	5.39	123.16	118.30
1	P	184	ASP	CB-CG-OD2	5.38	123.14	118.30
1	T	58	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	58	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	156	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	184	ASP	CB-CG-OD2	5.33	123.09	118.30
1	L	183	LEU	CA-CB-CG	5.32	127.53	115.30
1	O	157	LEU	CA-CB-CG	5.27	127.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	184	ASP	CB-CG-OD2	5.26	123.04	118.30
1	S	58	ASP	CB-CG-OD2	5.26	123.04	118.30
1	G	184	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	61	LEU	CA-CB-CG	5.21	127.27	115.30
1	P	58	ASP	CB-CG-OD2	5.20	122.98	118.30
1	K	156	ASP	CB-CG-OD2	5.19	122.97	118.30
1	P	3	ASP	CB-CG-OD2	5.18	122.96	118.30
1	F	156	ASP	CB-CG-OD2	5.18	122.96	118.30
1	F	58	ASP	CB-CG-OD2	5.17	122.95	118.30
1	R	184	ASP	CB-CG-OD2	5.17	122.95	118.30
1	L	58	ASP	CB-CG-OD2	5.15	122.94	118.30
1	I	61	LEU	CA-CB-CG	5.14	127.13	115.30
1	T	156	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	58	ASP	CB-CG-OD2	5.11	122.90	118.30
1	P	61	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	156	ASP	CB-CG-OD2	5.09	122.88	118.30
1	E	61	LEU	CA-CB-CG	5.08	126.99	115.30
1	B	184	ASP	CB-CG-OD2	5.07	122.86	118.30
1	J	3	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	61	LEU	CA-CB-CG	5.05	126.92	115.30
1	M	3	ASP	CB-CG-OD2	5.04	122.84	118.30
1	P	156	ASP	CB-CG-OD2	5.04	122.84	118.30
1	Q	156	ASP	CB-CG-OD2	5.04	122.83	118.30
1	I	156	ASP	CB-CG-OD2	5.01	122.81	118.30

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
1:S:38:ARG:HD3	1:S:204:VAL:HG21	1.76	0.67
1:I:30:LEU:HB2	1:I:125:VAL:HG22	1.76	0.66
1:S:35:LEU:HD11	1:S:157:LEU:HD21	1.78	0.65
1:P:30:LEU:HB2	1:P:125:VAL:HG22	1.78	0.65
1:N:52:TYR:HB3	1:N:61:LEU:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LEU:HB2	1:D:125:VAL:HG22	1.79	0.63
1:R:52:TYR:HB3	1:R:61:LEU:O	1.99	0.63
1:T:52:TYR:HB3	1:T:61:LEU:O	1.98	0.63
1:Q:30:LEU:HB2	1:Q:125:VAL:HG13	1.82	0.62
1:E:70:GLU:HG2	1:E:83:LYS:HG2	1.82	0.61
1:D:52:TYR:HB3	1:D:61:LEU:O	2.00	0.61
1:L:52:TYR:HB3	1:L:61:LEU:O	2.01	0.61
1:O:31:GLN:HG2	1:O:100:SER:HB3	1.83	0.61
1:F:17:THR:HB	4:F:928:HOH:O	2.01	0.60
1:B:138:ASP:HB2	1:B:143:LYS:HB3	1.85	0.59
1:K:52:TYR:HB3	1:K:61:LEU:O	2.03	0.59
1:O:52:TYR:HB3	1:O:61:LEU:O	2.04	0.58
1:Q:52:TYR:HB3	1:Q:61:LEU:O	2.04	0.58
1:E:52:TYR:HB3	1:E:61:LEU:O	2.02	0.57
1:L:37:PHE:CE2	1:L:49:LEU:HG	2.39	0.56
1:A:52:TYR:HB3	1:A:61:LEU:O	2.04	0.56
1:I:132:VAL:HG11	1:I:137:GLN:HG3	1.87	0.56
1:H:52:TYR:HB3	1:H:61:LEU:O	2.06	0.56
1:M:52:TYR:HB3	1:M:61:LEU:O	2.05	0.56
1:P:52:TYR:HB3	1:P:61:LEU:O	2.05	0.56
1:K:38:ARG:HD3	1:K:204:VAL:HG21	1.86	0.56
1:K:95:CYS:HB2	1:K:108:TRP:HB2	1.88	0.55
1:J:52:TYR:HB3	1:J:61:LEU:O	2.06	0.55
1:M:21:ASN:HB2	1:M:191:GLU:HB2	1.88	0.55
1:N:38:ARG:HD3	1:N:204:VAL:HG21	1.88	0.55
1:O:1:HIS:CE1	1:O:189:ASN:HD21	2.25	0.55
1:R:30:LEU:HB2	1:R:125:VAL:HG22	1.88	0.55
1:S:37:PHE:HB3	1:S:157:LEU:HD23	1.89	0.54
1:H:31:GLN:HG2	1:H:100:SER:HB3	1.88	0.54
1:O:62:LEU:HB3	1:O:74:TYR:HB2	1.89	0.54
1:N:95:CYS:HB2	1:N:108:TRP:HB2	1.89	0.54
1:I:52:TYR:HB3	1:I:61:LEU:O	2.07	0.54
1:E:62:LEU:HB3	1:E:74:TYR:HB2	1.89	0.53
1:E:132:VAL:HG13	1:E:137:GLN:NE2	2.24	0.53
1:L:37:PHE:HE2	1:L:49:LEU:HG	1.73	0.53
1:G:136:GLU:HG3	4:G:3324:HOH:O	2.08	0.53
1:T:138:ASP:HB2	1:T:143:LYS:HB3	1.90	0.52
1:D:1:HIS:HA	1:D:2:THR:CB	2.40	0.52
1:O:13:ARG:HG2	1:O:195:TYR:HD2	1.75	0.52
1:I:51:SER:HB3	1:I:132:VAL:HG13	1.92	0.52
1:J:1:HIS:N	1:J:1:HIS:CD2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:31:GLN:HG2	1:F:100:SER:HB3	1.90	0.51
1:P:95:CYS:HB2	1:P:108:TRP:HB2	1.92	0.51
1:C:52:TYR:HB3	1:C:61:LEU:O	2.11	0.51
1:F:52:TYR:HB3	1:F:61:LEU:O	2.10	0.51
1:K:62:LEU:HB3	1:K:74:TYR:HB2	1.93	0.51
1:G:148:GLN:NE2	4:G:3324:HOH:O	2.44	0.51
1:I:106:GLU:HG2	1:I:116:LYS:HG2	1.93	0.51
1:S:52:TYR:HB3	1:S:61:LEU:O	2.11	0.50
1:G:95:CYS:HB2	1:G:108:TRP:HB2	1.93	0.49
1:J:13:ARG:HG2	1:J:195:TYR:HD2	1.77	0.49
1:F:26:LEU:O	1:F:27:GLU:HB2	2.12	0.49
1:I:138:ASP:HB2	1:I:143:LYS:HB3	1.93	0.49
1:P:54:THR:HG21	1:P:126:GLU:HB2	1.95	0.49
1:C:62:LEU:HB3	1:C:74:TYR:HB2	1.95	0.49
1:R:37:PHE:HB3	1:R:157:LEU:HD22	1.95	0.49
1:J:91:PRO:HB3	1:J:203:TRP:CE3	2.48	0.49
1:M:76:GLY:O	1:M:77:ARG:HB2	2.13	0.49
1:F:30:LEU:HB2	1:F:125:VAL:HG22	1.94	0.49
1:M:62:LEU:HB3	1:M:74:TYR:HB2	1.95	0.49
1:N:62:LEU:HB3	1:N:74:TYR:HB2	1.94	0.49
1:T:62:LEU:HB3	1:T:74:TYR:HB2	1.95	0.48
1:E:91:PRO:HB3	1:E:203:TRP:CE3	2.48	0.48
1:E:95:CYS:HB2	1:E:108:TRP:HB2	1.94	0.48
1:O:155:GLY:HA2	1:O:185:TRP:CZ2	2.48	0.48
1:I:37:PHE:CE2	1:I:49:LEU:HG	2.47	0.48
1:F:38:ARG:HD3	1:F:204:VAL:HG21	1.95	0.48
1:C:37:PHE:CE1	1:C:49:LEU:HG	2.48	0.48
1:A:58:ASP:O	1:A:77:ARG:HG3	2.14	0.48
1:J:30:LEU:HB2	1:J:125:VAL:HG22	1.96	0.48
1:I:54:THR:HG21	1:I:126:GLU:HB3	1.94	0.48
1:T:37:PHE:HB3	1:T:157:LEU:HD22	1.95	0.48
1:G:13:ARG:HG2	1:G:195:TYR:HD2	1.78	0.48
1:H:106:GLU:HG2	4:H:3681:HOH:O	2.13	0.48
1:T:37:PHE:CE2	1:T:49:LEU:HG	2.49	0.47
1:I:31:GLN:HG2	1:I:100:SER:HB3	1.96	0.47
1:Q:62:LEU:HB3	1:Q:74:TYR:HB2	1.95	0.47
1:T:37:PHE:HE2	1:T:49:LEU:HG	1.80	0.47
1:Q:95:CYS:HB2	1:Q:108:TRP:HB2	1.97	0.47
1:S:62:LEU:HB3	1:S:74:TYR:HB2	1.96	0.47
1:S:76:GLY:O	1:S:77:ARG:HB2	2.15	0.47
1:I:132:VAL:HG12	1:I:137:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:28:LYS:HE3	1:O:29:PRO:HD2	1.97	0.47
1:M:13:ARG:HG2	1:M:195:TYR:HD2	1.79	0.47
1:A:91:PRO:HB3	1:A:203:TRP:CE3	2.50	0.46
1:D:76:GLY:O	1:D:77:ARG:HB2	2.16	0.46
1:O:77:ARG:HG3	1:O:77:ARG:HH11	1.80	0.46
1:B:74:TYR:HA	1:B:78:HIS:O	2.15	0.46
1:H:139:SER:HB3	1:H:143:LYS:HG3	1.97	0.46
1:B:58:ASP:O	1:B:77:ARG:HG3	2.16	0.46
1:C:37:PHE:HE1	1:C:49:LEU:HG	1.81	0.46
1:D:74:TYR:HA	1:D:78:HIS:O	2.14	0.46
1:F:62:LEU:HB3	1:F:74:TYR:HB2	1.97	0.46
1:S:91:PRO:HB3	1:S:203:TRP:CE3	2.50	0.46
1:I:76:GLY:O	1:I:77:ARG:HB2	2.16	0.46
1:H:95:CYS:HB2	1:H:108:TRP:HB2	1.98	0.46
1:N:10:VAL:HG22	1:N:153:GLU:HG2	1.98	0.46
1:P:74:TYR:HA	1:P:78:HIS:O	2.16	0.45
1:M:8:VAL:HG13	1:M:201:LEU:HB2	1.97	0.45
1:O:138:ASP:HB2	1:O:143:LYS:HB3	1.99	0.45
1:F:76:GLY:O	1:F:77:ARG:HB2	2.16	0.45
1:L:38:ARG:HD3	1:L:204:VAL:HG21	1.99	0.45
1:Q:91:PRO:HB3	1:Q:203:TRP:CE3	2.51	0.45
1:G:52:TYR:HB3	1:G:61:LEU:O	2.16	0.45
1:Q:139:SER:HB3	1:Q:143:LYS:HD3	1.97	0.45
1:D:1:HIS:HB2	4:D:1262:HOH:O	2.16	0.45
1:O:21:ASN:HB2	1:O:191:GLU:HB2	1.97	0.45
1:O:201:LEU:HD11	1:O:204:VAL:HG23	1.98	0.45
1:R:91:PRO:HB3	1:R:203:TRP:CE3	2.51	0.45
1:A:1:HIS:N	1:A:1:HIS:CD2	2.84	0.45
1:C:76:GLY:O	1:C:77:ARG:HB2	2.17	0.45
1:H:8:VAL:HG13	1:H:201:LEU:HB2	1.99	0.45
1:O:23:ILE:HB	1:O:189:ASN:HB2	1.98	0.45
1:S:150:PHE:CE2	1:S:154:ILE:HG13	2.52	0.45
1:J:52:TYR:CZ	1:J:129:PRO:HB3	2.52	0.45
1:A:76:GLY:O	1:A:77:ARG:HB2	2.17	0.45
1:C:150:PHE:CE2	1:C:154:ILE:HG13	2.53	0.44
1:E:31:GLN:HG2	1:E:100:SER:HB3	1.98	0.44
1:H:62:LEU:HB3	1:H:74:TYR:HB2	1.98	0.44
1:T:134:GLY:HA2	1:T:150:PHE:HB3	1.99	0.44
1:B:95:CYS:HB2	1:B:108:TRP:HB2	2.00	0.44
1:G:91:PRO:HB3	1:G:203:TRP:CE3	2.53	0.44
1:Q:37:PHE:CE2	1:Q:49:LEU:HG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:GLY:HA2	1:D:185:TRP:CZ2	2.53	0.44
1:A:165:PRO:HD2	1:A:168:ASN:ND2	2.33	0.43
1:D:21:ASN:HB2	1:D:191:GLU:HB2	1.99	0.43
1:D:95:CYS:HB2	1:D:108:TRP:HB2	2.00	0.43
1:I:132:VAL:HG12	1:I:137:GLN:HE21	1.83	0.43
1:K:34:THR:HG21	1:K:164:LEU:HB2	2.00	0.43
1:S:128:GLN:N	1:S:129:PRO:HD3	2.34	0.43
1:G:138:ASP:HB2	1:G:143:LYS:HB3	2.01	0.43
1:S:36:CYS:HA	1:S:94:ILE:O	2.18	0.43
1:S:138:ASP:HB2	1:S:143:LYS:HB3	1.99	0.43
1:B:76:GLY:O	1:B:77:ARG:HB2	2.19	0.43
1:F:70:GLU:HG2	1:F:83:LYS:HG2	2.01	0.43
1:G:62:LEU:HB3	1:G:74:TYR:HB2	2.00	0.43
1:I:62:LEU:HB3	1:I:74:TYR:HB2	2.00	0.43
1:M:96:VAL:HA	1:M:106:GLU:O	2.18	0.43
1:Q:70:GLU:HG3	1:Q:83:LYS:HG2	1.99	0.43
1:T:91:PRO:HB3	1:T:203:TRP:CE3	2.53	0.43
1:T:74:TYR:HA	1:T:78:HIS:O	2.19	0.43
1:B:70:GLU:HG2	1:B:83:LYS:HG2	2.00	0.43
1:G:155:GLY:HA2	1:G:185:TRP:CZ2	2.54	0.43
1:J:1:HIS:CE1	1:J:189:ASN:HD21	2.36	0.43
1:B:52:TYR:HB3	1:B:61:LEU:O	2.19	0.43
1:I:37:PHE:HE2	1:I:49:LEU:HG	1.82	0.43
1:R:95:CYS:HB2	1:R:108:TRP:HB2	2.00	0.43
1:E:13:ARG:HG2	1:E:195:TYR:HD2	1.84	0.43
1:M:91:PRO:HB3	1:M:203:TRP:CE3	2.54	0.43
1:S:95:CYS:HB2	1:S:108:TRP:HB2	2.00	0.43
1:B:91:PRO:HB3	1:B:203:TRP:CE3	2.53	0.43
1:H:58:ASP:O	1:H:77:ARG:HG3	2.18	0.43
1:I:52:TYR:CZ	1:I:129:PRO:HB3	2.53	0.43
1:L:38:ARG:HD3	1:L:204:VAL:CG2	2.48	0.43
1:J:76:GLY:O	1:J:77:ARG:HB2	2.19	0.42
1:N:33:PHE:CE2	1:N:98:TRP:HB3	2.54	0.42
1:O:76:GLY:O	1:O:77:ARG:HB2	2.19	0.42
1:T:95:CYS:HB2	1:T:108:TRP:HB2	2.01	0.42
1:H:74:TYR:HA	1:H:78:HIS:O	2.19	0.42
1:K:33:PHE:CE2	1:K:98:TRP:HB3	2.54	0.42
1:L:128:GLN:N	1:L:129:PRO:HD3	2.33	0.42
1:D:13:ARG:HG2	1:D:195:TYR:HD2	1.85	0.42
1:E:74:TYR:HA	1:E:78:HIS:O	2.20	0.42
1:L:91:PRO:HB3	1:L:203:TRP:CE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:PRO:HD2	1:G:168:ASN:HD22	1.85	0.42
1:P:31:GLN:HG3	1:P:124:PHE:HD1	1.85	0.42
1:T:88:PHE:HA	1:T:89:PRO:HA	1.86	0.42
1:I:95:CYS:HB2	1:I:108:TRP:HB2	2.01	0.42
1:N:159:MET:O	1:N:180:ALA:HB1	2.20	0.42
1:P:13:ARG:HG2	1:P:195:TYR:HD2	1.85	0.42
1:A:13:ARG:HG2	1:A:195:TYR:HD2	1.83	0.42
1:B:1:HIS:HD2	4:B:1828:HOH:O	2.03	0.42
1:C:91:PRO:HB3	1:C:203:TRP:CE3	2.55	0.42
1:C:95:CYS:HB2	1:C:108:TRP:HB2	2.02	0.42
1:A:96:VAL:HA	1:A:106:GLU:O	2.20	0.42
1:M:134:GLY:HA2	1:M:150:PHE:HB3	2.02	0.41
1:Q:138:ASP:HB2	1:Q:143:LYS:HB3	2.02	0.41
1:A:99:GLU:HB2	1:A:163:VAL:HG21	2.02	0.41
1:I:91:PRO:HB3	1:I:203:TRP:CE3	2.55	0.41
1:K:91:PRO:HB3	1:K:203:TRP:CE3	2.55	0.41
1:M:37:PHE:CE1	1:M:49:LEU:HG	2.55	0.41
1:C:2:THR:HB	1:C:190:TYR:HE2	1.85	0.41
1:F:91:PRO:HB3	1:F:203:TRP:CE3	2.55	0.41
1:C:30:LEU:HB2	1:C:125:VAL:HG22	2.02	0.41
1:D:161:ASP:HB3	1:D:182:ILE:HD11	2.02	0.41
1:L:96:VAL:HA	1:L:106:GLU:O	2.21	0.41
1:M:74:TYR:HA	1:M:78:HIS:O	2.21	0.41
1:O:91:PRO:HB3	1:O:203:TRP:CE3	2.56	0.41
1:P:62:LEU:HB3	1:P:74:TYR:HB2	2.02	0.41
1:B:62:LEU:HB3	1:B:74:TYR:HB2	2.03	0.41
1:K:13:ARG:HG2	1:K:195:TYR:HD2	1.86	0.41
1:K:88:PHE:HA	1:K:89:PRO:HA	1.83	0.41
1:P:28:LYS:HA	1:P:29:PRO:HD2	1.91	0.41
1:C:96:VAL:HA	1:C:106:GLU:O	2.21	0.41
1:F:8:VAL:HG13	1:F:201:LEU:HB2	2.03	0.41
1:O:52:TYR:CZ	1:O:129:PRO:HB3	2.56	0.41
1:R:74:TYR:CZ	1:R:79:LYS:HG3	2.56	0.41
1:L:76:GLY:O	1:L:77:ARG:HB2	2.21	0.41
1:I:74:TYR:HA	1:I:78:HIS:O	2.21	0.40
1:I:139:SER:HB3	1:I:143:LYS:HD3	2.03	0.40
1:F:54:THR:HG21	1:F:126:GLU:HB2	2.02	0.40
1:J:139:SER:HB3	1:J:143:LYS:HG3	2.03	0.40
1:O:28:LYS:HA	1:O:29:PRO:HD3	1.97	0.40
1:A:74:TYR:HA	1:A:78:HIS:O	2.21	0.40
1:T:58:ASP:O	1:T:77:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:VAL:HG23	4:L:3702:HOH:O	2.21	0.40
1:O:33:PHE:CE2	1:O:98:TRP:HB3	2.57	0.40
1:P:88:PHE:HA	1:P:89:PRO:HA	1.87	0.40
1:D:1:HIS:O	1:D:1:HIS:CG	2.75	0.40
1:P:91:PRO:HB3	1:P:203:TRP:CE3	2.55	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	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%)	29	31
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (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	181/181 (100%)	167 (92%)	14 (8%)	13	13
1	B	181/181 (100%)	159 (88%)	22 (12%)	5	4
1	C	181/181 (100%)	165 (91%)	16 (9%)	10	10
1	D	181/181 (100%)	167 (92%)	14 (8%)	13	13
1	E	181/181 (100%)	166 (92%)	15 (8%)	11	11
1	F	181/181 (100%)	167 (92%)	14 (8%)	13	13
1	G	181/181 (100%)	162 (90%)	19 (10%)	7	6
1	H	181/181 (100%)	166 (92%)	15 (8%)	11	11
1	I	181/181 (100%)	165 (91%)	16 (9%)	10	10
1	J	181/181 (100%)	165 (91%)	16 (9%)	10	10
1	K	181/181 (100%)	165 (91%)	16 (9%)	10	10
1	L	181/181 (100%)	164 (91%)	17 (9%)	8	8
1	M	181/181 (100%)	167 (92%)	14 (8%)	13	13
1	N	181/181 (100%)	161 (89%)	20 (11%)	6	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	181/181 (100%)	165 (91%)	16 (9%)	10	10
1	P	181/181 (100%)	168 (93%)	13 (7%)	14	15
1	Q	181/181 (100%)	163 (90%)	18 (10%)	8	7
1	R	181/181 (100%)	168 (93%)	13 (7%)	14	15
1	S	181/181 (100%)	167 (92%)	14 (8%)	13	13
1	T	181/181 (100%)	168 (93%)	13 (7%)	14	15
All	All	3620/3620 (100%)	3305 (91%)	315 (9%)	10	10

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	17	THR
1	A	22	LEU
1	A	28	LYS
1	A	44	SER
1	A	52	TYR
1	A	57	ARG
1	A	61	LEU
1	A	133	LEU
1	A	146	ARG
1	A	157	LEU
1	A	178	LEU
1	A	183	LEU
1	A	189	ASN
1	B	1	HIS
1	B	4	LEU
1	B	22	LEU
1	B	27	GLU
1	B	28	LYS
1	B	38	ARG
1	B	49	LEU
1	B	52	TYR
1	B	55	GLN
1	B	61	LEU
1	B	65	LYS
1	B	66	GLU
1	B	79	LYS
1	B	82	SER
1	B	125	VAL

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Mol	Chain	Res	Type
1	B	133	LEU
1	B	143	LYS
1	B	157	LEU
1	B	170	LEU
1	B	178	LEU
1	B	183	LEU
1	B	189	ASN
1	C	4	LEU
1	C	17	THR
1	C	26	LEU
1	C	27	GLU
1	C	38	ARG
1	C	49	LEU
1	C	52	TYR
1	C	61	LEU
1	C	79	LYS
1	C	126	GLU
1	C	133	LEU
1	C	143	LYS
1	C	157	LEU
1	C	183	LEU
1	C	191	GLU
1	C	204	VAL
1	D	1	HIS
1	D	4	LEU
1	D	22	LEU
1	D	28	LYS
1	D	38	ARG
1	D	49	LEU
1	D	52	TYR
1	D	61	LEU
1	D	125	VAL
1	D	133	LEU
1	D	146	ARG
1	D	157	LEU
1	D	176	THR
1	D	183	LEU
1	E	1	HIS
1	E	4	LEU
1	E	17	THR
1	E	22	LEU
1	E	27	GLU

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Mol	Chain	Res	Type
1	E	28	LYS
1	E	38	ARG
1	E	49	LEU
1	E	61	LEU
1	E	79	LYS
1	E	125	VAL
1	E	133	LEU
1	E	157	LEU
1	E	178	LEU
1	E	183	LEU
1	F	4	LEU
1	F	22	LEU
1	F	28	LYS
1	F	38	ARG
1	F	52	TYR
1	F	57	ARG
1	F	61	LEU
1	F	66	GLU
1	F	79	LYS
1	F	133	LEU
1	F	146	ARG
1	F	157	LEU
1	F	164	LEU
1	F	183	LEU
1	G	4	LEU
1	G	17	THR
1	G	22	LEU
1	G	27	GLU
1	G	44	SER
1	G	49	LEU
1	G	52	TYR
1	G	61	LEU
1	G	66	GLU
1	G	82	SER
1	G	125	VAL
1	G	130	LYS
1	G	133	LEU
1	G	143	LYS
1	G	157	LEU
1	G	170	LEU
1	G	176	THR
1	G	183	LEU

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Mol	Chain	Res	Type
1	G	189	ASN
1	H	4	LEU
1	H	17	THR
1	H	28	LYS
1	H	38	ARG
1	H	49	LEU
1	H	52	TYR
1	H	57	ARG
1	H	61	LEU
1	H	79	LYS
1	H	125	VAL
1	H	130	LYS
1	H	133	LEU
1	H	157	LEU
1	H	164	LEU
1	H	183	LEU
1	I	4	LEU
1	I	22	LEU
1	I	27	GLU
1	I	49	LEU
1	I	52	TYR
1	I	61	LEU
1	I	79	LYS
1	I	82	SER
1	I	120	ARG
1	I	125	VAL
1	I	133	LEU
1	I	143	LYS
1	I	146	ARG
1	I	157	LEU
1	I	183	LEU
1	I	186	GLN
1	J	1	HIS
1	J	4	LEU
1	J	17	THR
1	J	22	LEU
1	J	28	LYS
1	J	38	ARG
1	J	44	SER
1	J	49	LEU
1	J	52	TYR
1	J	61	LEU

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Mol	Chain	Res	Type
1	J	79	LYS
1	J	82	SER
1	J	133	LEU
1	J	146	ARG
1	J	157	LEU
1	J	183	LEU
1	K	4	LEU
1	K	5	SER
1	K	22	LEU
1	K	28	LYS
1	K	38	ARG
1	K	44	SER
1	K	52	TYR
1	K	66	GLU
1	K	79	LYS
1	K	125	VAL
1	K	133	LEU
1	K	146	ARG
1	K	157	LEU
1	K	170	LEU
1	K	183	LEU
1	K	189	ASN
1	L	4	LEU
1	L	17	THR
1	L	22	LEU
1	L	31	GLN
1	L	49	LEU
1	L	52	TYR
1	L	55	GLN
1	L	61	LEU
1	L	66	GLU
1	L	79	LYS
1	L	82	SER
1	L	125	VAL
1	L	132	VAL
1	L	133	LEU
1	L	146	ARG
1	L	157	LEU
1	L	183	LEU
1	M	2	THR
1	M	22	LEU
1	M	28	LYS

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Mol	Chain	Res	Type
1	M	38	ARG
1	M	49	LEU
1	M	52	TYR
1	M	61	LEU
1	M	79	LYS
1	M	125	VAL
1	M	128	GLN
1	M	133	LEU
1	M	157	LEU
1	M	183	LEU
1	M	201	LEU
1	N	4	LEU
1	N	22	LEU
1	N	49	LEU
1	N	52	TYR
1	N	61	LEU
1	N	68	VAL
1	N	79	LYS
1	N	125	VAL
1	N	128	GLN
1	N	130	LYS
1	N	133	LEU
1	N	157	LEU
1	N	170	LEU
1	N	174	GLN
1	N	176	THR
1	N	178	LEU
1	N	181	ASN
1	N	183	LEU
1	N	186	GLN
1	N	189	ASN
1	O	4	LEU
1	O	13	ARG
1	O	17	THR
1	O	28	LYS
1	O	49	LEU
1	O	52	TYR
1	O	57	ARG
1	O	61	LEU
1	O	79	LYS
1	O	120	ARG
1	O	125	VAL

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Mol	Chain	Res	Type
1	O	126	GLU
1	O	132	VAL
1	O	146	ARG
1	O	157	LEU
1	O	183	LEU
1	P	4	LEU
1	P	17	THR
1	P	22	LEU
1	P	28	LYS
1	P	52	TYR
1	P	61	LEU
1	P	79	LYS
1	P	82	SER
1	P	133	LEU
1	P	146	ARG
1	P	157	LEU
1	P	170	LEU
1	P	183	LEU
1	Q	4	LEU
1	Q	22	LEU
1	Q	28	LYS
1	Q	44	SER
1	Q	49	LEU
1	Q	52	TYR
1	Q	55	GLN
1	Q	65	LYS
1	Q	82	SER
1	Q	87	LYS
1	Q	125	VAL
1	Q	130	LYS
1	Q	133	LEU
1	Q	143	LYS
1	Q	157	LEU
1	Q	170	LEU
1	Q	183	LEU
1	Q	189	ASN
1	R	4	LEU
1	R	22	LEU
1	R	27	GLU
1	R	44	SER
1	R	49	LEU
1	R	61	LEU

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Mol	Chain	Res	Type
1	R	82	SER
1	R	126	GLU
1	R	128	GLN
1	R	133	LEU
1	R	157	LEU
1	R	178	LEU
1	R	183	LEU
1	S	4	LEU
1	S	17	THR
1	S	22	LEU
1	S	49	LEU
1	S	52	TYR
1	S	61	LEU
1	S	66	GLU
1	S	77	ARG
1	S	82	SER
1	S	125	VAL
1	S	132	VAL
1	S	133	LEU
1	S	143	LYS
1	S	183	LEU
1	T	4	LEU
1	T	13	ARG
1	T	22	LEU
1	T	28	LYS
1	T	49	LEU
1	T	52	TYR
1	T	61	LEU
1	T	82	SER
1	T	87	LYS
1	T	125	VAL
1	T	133	LEU
1	T	157	LEU
1	T	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	189	ASN
1	B	31	GLN
1	B	55	GLN

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Mol	Chain	Res	Type
1	B	128	GLN
1	B	189	ASN
1	C	1	HIS
1	D	1	HIS
1	F	1	HIS
1	G	1	HIS
1	G	168	ASN
1	G	189	ASN
1	I	186	GLN
1	J	1	HIS
1	J	189	ASN
1	K	189	ASN
1	M	186	GLN
1	N	31	GLN
1	N	93	HIS
1	N	189	ASN
1	O	1	HIS
1	O	93	HIS
1	Q	1	HIS
1	Q	128	GLN
1	Q	168	ASN
1	Q	189	ASN
1	R	31	GLN
1	T	1	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	C	343	2	29,31,31	1.85	3 (10%)	30,44,44	1.77	8 (26%)
3	CPJ	L	347	2	29,31,31	1.88	2 (6%)	30,44,44	2.09	11 (36%)
3	CPJ	N	349	2	29,31,31	1.83	3 (10%)	30,44,44	1.82	8 (26%)
3	CPJ	D	344	2	29,31,31	1.79	2 (6%)	30,44,44	1.73	8 (26%)
3	CPJ	A	341	2	29,31,31	1.93	5 (17%)	30,44,44	2.09	10 (33%)
3	CPJ	E	345	2	29,31,31	1.84	2 (6%)	30,44,44	1.73	9 (30%)
3	CPJ	Q	350	2	29,31,31	1.83	2 (6%)	30,44,44	1.74	7 (23%)
3	CPJ	B	342	2	29,31,31	1.91	4 (13%)	30,44,44	2.12	10 (33%)
3	CPJ	M	348	2	29,31,31	1.80	4 (13%)	30,44,44	1.78	7 (23%)
3	CPJ	P	346	2	29,31,31	1.88	4 (13%)	30,44,44	1.92	11 (36%)

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	C	343	2	-	2/25/51/51	0/2/2/2
3	CPJ	L	347	2	-	2/25/51/51	0/2/2/2
3	CPJ	N	349	2	-	2/25/51/51	0/2/2/2
3	CPJ	D	344	2	-	4/25/51/51	0/2/2/2
3	CPJ	A	341	2	-	2/25/51/51	0/2/2/2
3	CPJ	E	345	2	-	3/25/51/51	0/2/2/2
3	CPJ	Q	350	2	-	2/25/51/51	0/2/2/2
3	CPJ	B	342	2	-	2/25/51/51	0/2/2/2
3	CPJ	M	348	2	-	4/25/51/51	0/2/2/2
3	CPJ	P	346	2	-	2/25/51/51	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	341	CPJ	O22-C20	6.36	1.46	1.35
3	B	342	CPJ	O11-C12	6.34	1.46	1.35
3	L	347	CPJ	O11-C12	6.27	1.46	1.35
3	L	347	CPJ	O22-C20	6.19	1.45	1.35
3	B	342	CPJ	O22-C20	6.19	1.45	1.35
3	P	346	CPJ	O22-C20	6.13	1.45	1.35
3	A	341	CPJ	O11-C12	6.04	1.45	1.35
3	E	345	CPJ	O22-C20	6.04	1.45	1.35
3	P	346	CPJ	O11-C12	6.01	1.45	1.35
3	C	343	CPJ	O11-C12	5.99	1.45	1.35
3	Q	350	CPJ	O22-C20	5.98	1.45	1.35
3	D	344	CPJ	O22-C20	5.90	1.45	1.35
3	C	343	CPJ	O22-C20	5.89	1.45	1.35
3	N	349	CPJ	O22-C20	5.87	1.45	1.35
3	E	345	CPJ	O11-C12	5.82	1.45	1.35
3	Q	350	CPJ	O11-C12	5.82	1.45	1.35
3	M	348	CPJ	O11-C12	5.69	1.45	1.35
3	N	349	CPJ	O11-C12	5.67	1.45	1.35
3	M	348	CPJ	O22-C20	5.53	1.44	1.35
3	D	344	CPJ	O11-C12	5.28	1.44	1.35
3	B	342	CPJ	O25-C26	2.38	1.44	1.42
3	A	341	CPJ	O27-C26	2.32	1.44	1.42
3	M	348	CPJ	O25-C26	2.23	1.44	1.42
3	A	341	CPJ	O25-C26	2.16	1.44	1.42
3	N	349	CPJ	O25-C26	2.16	1.44	1.42
3	P	346	CPJ	O27-C26	2.13	1.44	1.42
3	P	346	CPJ	O1-C6	2.09	1.44	1.42
3	A	341	CPJ	O5-C6	2.09	1.44	1.42
3	M	348	CPJ	O27-C26	2.06	1.44	1.42
3	C	343	CPJ	O27-C26	2.01	1.44	1.42
3	B	342	CPJ	O27-C26	2.01	1.44	1.42

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	348	CPJ	O1-C6-C10	4.40	111.52	106.27
3	Q	350	CPJ	O1-C6-C10	4.34	111.45	106.27
3	N	349	CPJ	O1-C6-C10	4.26	111.35	106.27
3	A	341	CPJ	O1-C6-C10	4.21	111.30	106.27
3	P	346	CPJ	O1-C6-C10	4.21	111.29	106.27
3	B	342	CPJ	O1-C6-C10	4.11	111.17	106.27
3	L	347	CPJ	O27-C26-C32	4.10	111.16	106.27
3	P	346	CPJ	O27-C26-C32	4.07	111.12	106.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	344	CPJ	O1-C6-C10	4.00	111.04	106.27
3	Q	350	CPJ	O27-C26-C32	3.93	110.96	106.27
3	L	347	CPJ	O5-C6-C10	3.90	110.92	106.27
3	M	348	CPJ	O27-C26-C32	3.89	110.92	106.27
3	L	347	CPJ	O1-C6-C10	3.87	110.88	106.27
3	N	349	CPJ	O27-C26-C32	3.83	110.83	106.27
3	C	343	CPJ	O1-C6-C10	3.78	110.77	106.27
3	E	345	CPJ	O1-C6-C10	3.70	110.68	106.27
3	D	344	CPJ	O25-C26-C32	3.61	110.57	106.27
3	A	341	CPJ	O5-C6-C10	3.60	110.56	106.27
3	B	342	CPJ	C24-O25-C26	3.59	117.07	113.94
3	B	342	CPJ	O11-C12-N14	3.56	117.35	111.11
3	B	342	CPJ	O27-C26-C32	3.51	110.45	106.27
3	A	341	CPJ	O11-C12-N14	3.47	117.20	111.11
3	A	341	CPJ	C3-O11-C12	-3.46	111.53	116.48
3	E	345	CPJ	O27-C26-C32	3.44	110.37	106.27
3	A	341	CPJ	O27-C26-C32	3.35	110.27	106.27
3	C	343	CPJ	O27-C26-C32	3.30	110.20	106.27
3	A	341	CPJ	O25-C26-C32	3.29	110.19	106.27
3	B	342	CPJ	O25-C26-C32	3.23	110.12	106.27
3	L	347	CPJ	O11-C12-N14	3.21	116.75	111.11
3	A	341	CPJ	O11-C12-O13	-3.14	119.80	124.53
3	B	342	CPJ	O22-C20-O21	-3.11	119.84	124.53
3	L	347	CPJ	O25-C26-C32	3.11	109.97	106.27
3	Q	350	CPJ	O5-C6-C10	3.07	109.93	106.27
3	L	347	CPJ	O22-C20-N17	3.03	116.43	111.11
3	C	343	CPJ	O25-C26-C32	3.03	109.88	106.27
3	M	348	CPJ	O25-C26-C32	3.02	109.86	106.27
3	C	343	CPJ	O22-C20-O21	-3.01	120.00	124.53
3	B	342	CPJ	O11-C12-O13	-2.99	120.02	124.53
3	B	342	CPJ	C3-O11-C12	-2.99	112.19	116.48
3	A	341	CPJ	O22-C20-O21	-2.98	120.03	124.53
3	B	342	CPJ	O5-C6-C10	2.98	109.83	106.27
3	P	346	CPJ	O5-C6-C10	2.96	109.81	106.27
3	E	345	CPJ	O5-C6-C10	2.96	109.80	106.27
3	E	345	CPJ	O22-C20-O21	-2.96	120.07	124.53
3	D	344	CPJ	O5-C6-C10	2.95	109.79	106.27
3	E	345	CPJ	O25-C26-C32	2.92	109.75	106.27
3	L	347	CPJ	O11-C12-O13	-2.91	120.14	124.53
3	L	347	CPJ	C3-O11-C12	-2.90	112.33	116.48
3	L	347	CPJ	O22-C20-O21	-2.89	120.17	124.53
3	M	348	CPJ	O22-C20-O21	-2.89	120.17	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	346	CPJ	O22-C20-O21	-2.84	120.24	124.53
3	D	344	CPJ	O22-C20-O21	-2.83	120.26	124.53
3	P	346	CPJ	O25-C26-C32	2.83	109.65	106.27
3	C	343	CPJ	O5-C6-C10	2.81	109.62	106.27
3	N	349	CPJ	O25-C26-C32	2.79	109.59	106.27
3	M	348	CPJ	O11-C3-C4	-2.76	103.16	108.94
3	A	341	CPJ	O22-C20-N17	2.72	115.89	111.11
3	N	349	CPJ	C24-O25-C26	2.72	116.31	113.94
3	N	349	CPJ	O22-C20-O21	-2.71	120.45	124.53
3	E	345	CPJ	O11-C12-O13	-2.69	120.48	124.53
3	B	342	CPJ	O22-C20-N17	2.69	115.82	111.11
3	Q	350	CPJ	O25-C26-C32	2.67	109.45	106.27
3	L	347	CPJ	C28-O27-C26	2.62	116.22	113.94
3	E	345	CPJ	O22-C20-N17	2.61	115.70	111.11
3	D	344	CPJ	O11-C12-O13	-2.56	120.67	124.53
3	P	346	CPJ	O22-C20-N17	2.54	115.56	111.11
3	D	344	CPJ	O11-C3-C4	-2.54	103.62	108.94
3	P	346	CPJ	O11-C12-O13	-2.53	120.72	124.53
3	P	346	CPJ	C4-O5-C6	2.52	116.14	113.94
3	C	343	CPJ	O11-C12-N14	2.51	115.51	111.11
3	P	346	CPJ	O11-C12-N14	2.50	115.50	111.11
3	M	348	CPJ	O5-C6-C10	2.50	109.25	106.27
3	P	346	CPJ	C2-O1-C6	2.49	116.11	113.94
3	N	349	CPJ	O5-C6-C10	2.48	109.23	106.27
3	A	341	CPJ	C24-O25-C26	2.43	116.06	113.94
3	C	343	CPJ	C24-O25-C26	2.41	116.04	113.94
3	Q	350	CPJ	O22-C20-O21	-2.41	120.90	124.53
3	E	345	CPJ	O11-C12-N14	2.40	115.32	111.11
3	M	348	CPJ	O22-C20-N17	2.39	115.31	111.11
3	C	343	CPJ	O11-C12-O13	-2.36	120.98	124.53
3	D	344	CPJ	O22-C20-N17	2.31	115.16	111.11
3	Q	350	CPJ	O11-C12-O13	-2.27	121.11	124.53
3	D	344	CPJ	O27-C26-C32	2.26	108.97	106.27
3	N	349	CPJ	O11-C12-O13	-2.25	121.13	124.53
3	N	349	CPJ	O22-C20-N17	2.16	114.90	111.11
3	L	347	CPJ	C23-O22-C20	-2.12	113.45	116.48
3	E	345	CPJ	C3-O11-C12	-2.08	113.50	116.48
3	P	346	CPJ	C24-O25-C26	2.05	115.72	113.94
3	Q	350	CPJ	C24-O25-C26	2.01	115.70	113.94

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	343	CPJ	O1-C6-C7-O8
3	D	344	CPJ	O1-C6-C7-O8
3	D	344	CPJ	O5-C6-C7-O8
3	D	344	CPJ	C10-C6-C7-O9
3	E	345	CPJ	O1-C6-C7-O8
3	E	345	CPJ	O5-C6-C7-O8
3	M	348	CPJ	O1-C6-C7-O8
3	M	348	CPJ	O5-C6-C7-O8
3	M	348	CPJ	C10-C6-C7-O9
3	N	349	CPJ	O1-C6-C7-O8
3	P	346	CPJ	O1-C6-C7-O8
3	Q	350	CPJ	O1-C6-C7-O8
3	M	348	CPJ	O1-C6-C7-O9
3	A	341	CPJ	O5-C6-C7-O8
3	B	342	CPJ	O1-C6-C7-O8
3	B	342	CPJ	O5-C6-C7-O8
3	C	343	CPJ	O5-C6-C7-O8
3	L	347	CPJ	O5-C6-C7-O8
3	N	349	CPJ	O5-C6-C7-O8
3	P	346	CPJ	O5-C6-C7-O8
3	Q	350	CPJ	O5-C6-C7-O8
3	A	341	CPJ	O1-C6-C7-O9
3	D	344	CPJ	O1-C6-C7-O9
3	E	345	CPJ	O1-C6-C7-O9
3	L	347	CPJ	O1-C6-C7-O9

There are no ring outliers.

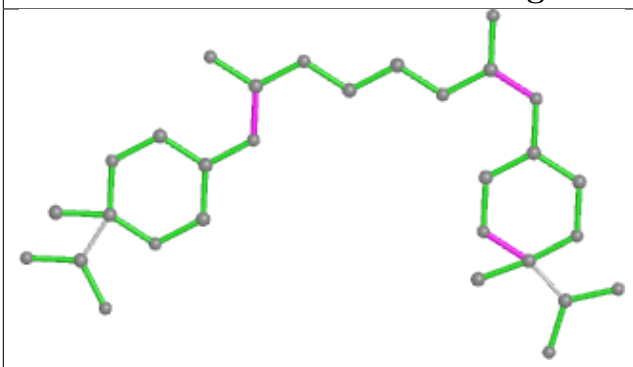
1 monomer is involved in 1 short contact:

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

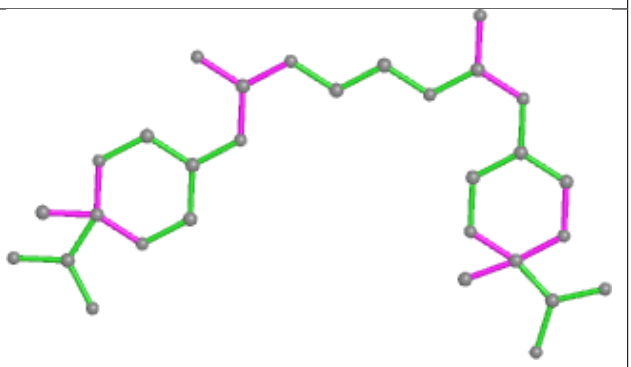
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

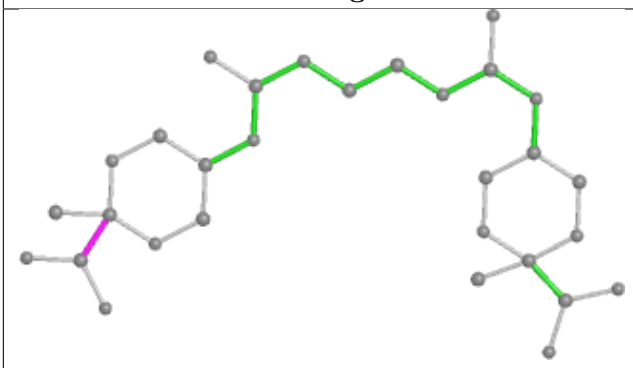
Ligand CPJ C 343



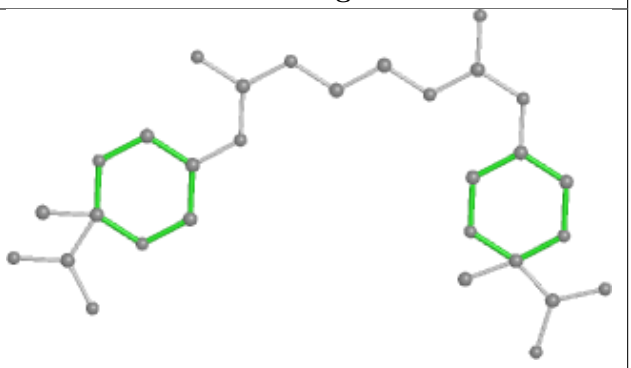
Bond lengths



Bond angles

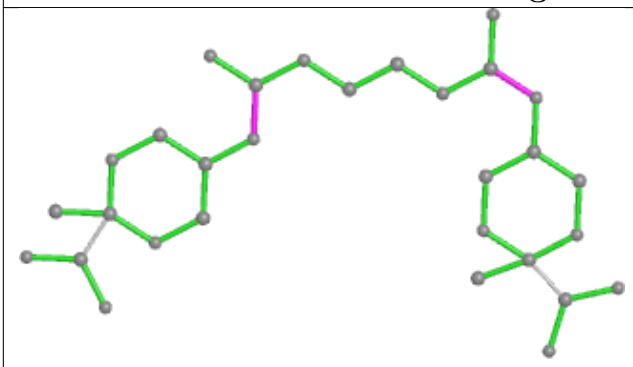


Torsions

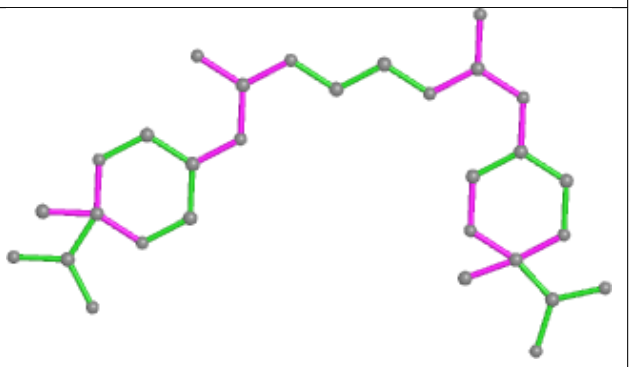


Rings

Ligand CPJ L 347



Bond lengths



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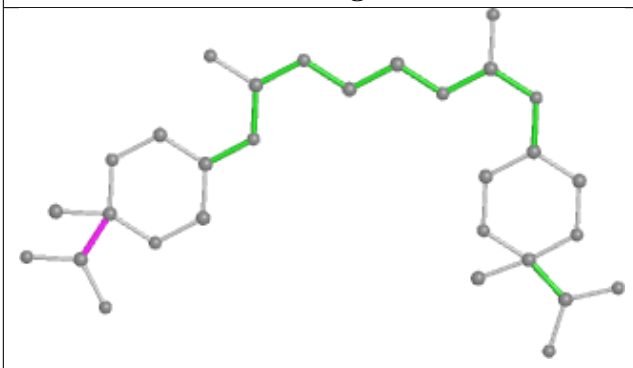

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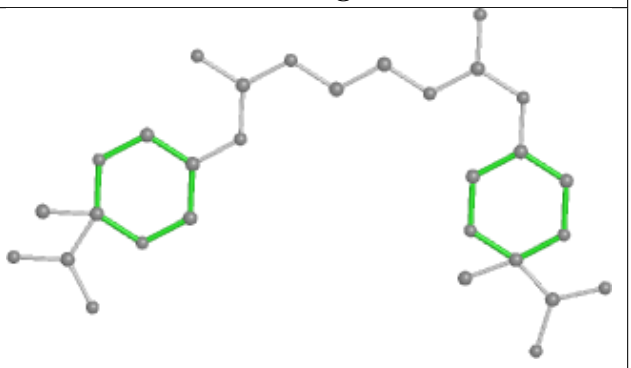
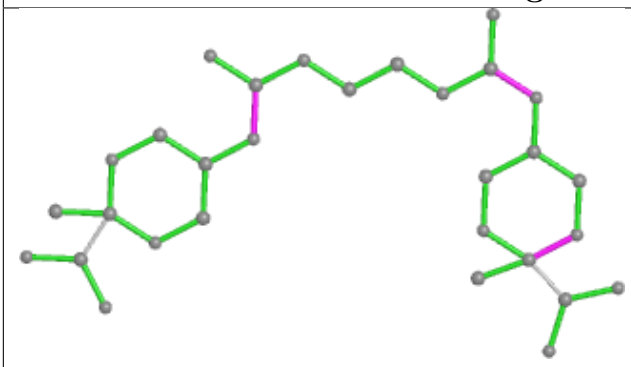
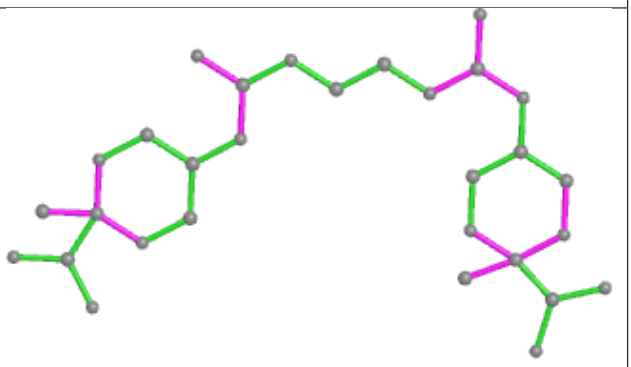


Rings

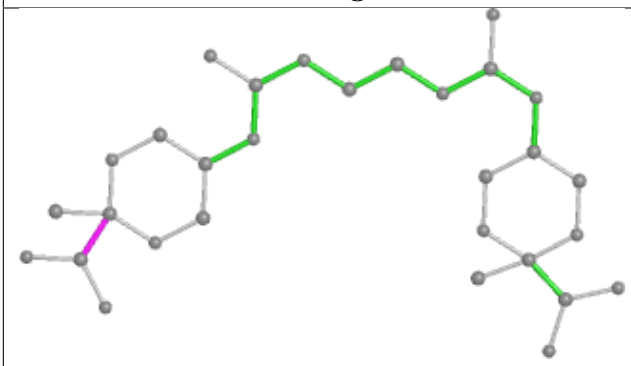
Ligand CPJ N 349



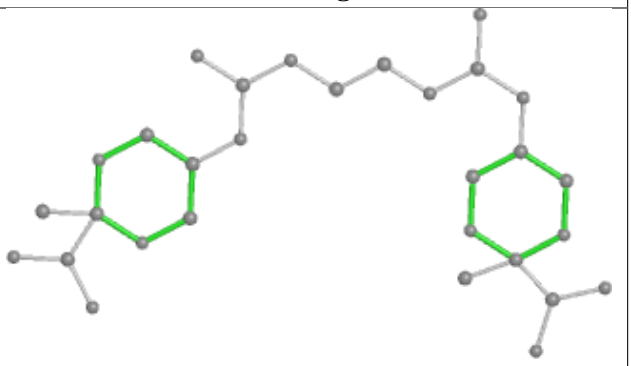
Bond lengths



Bond angles

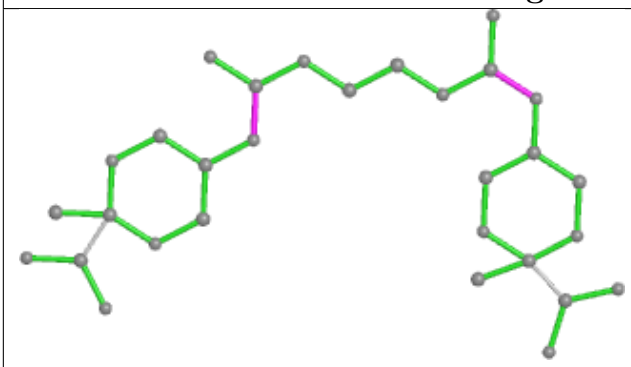


Torsions

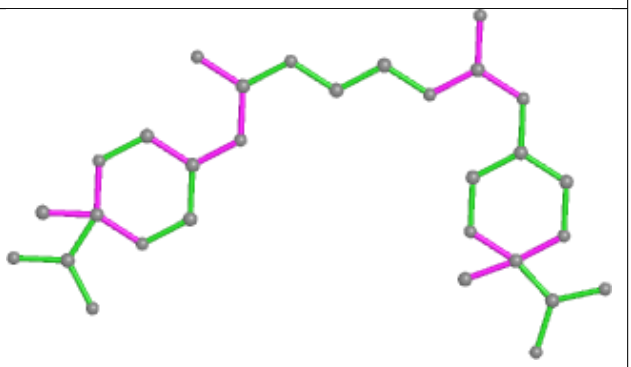


Rings

Ligand CPJ D 344



Bond lengths



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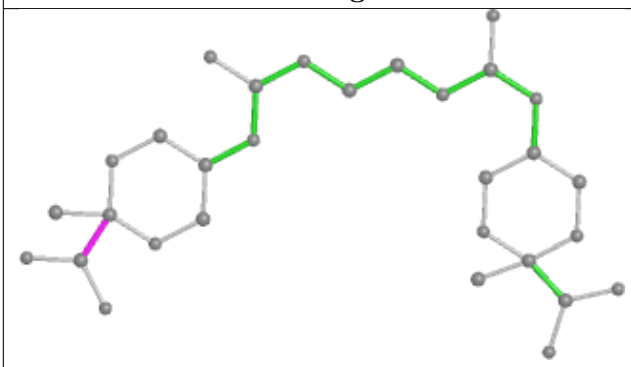

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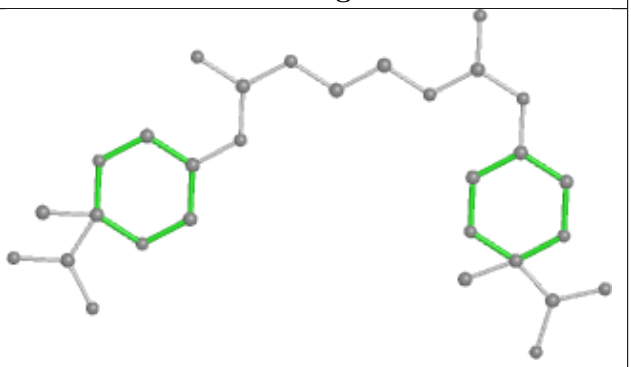
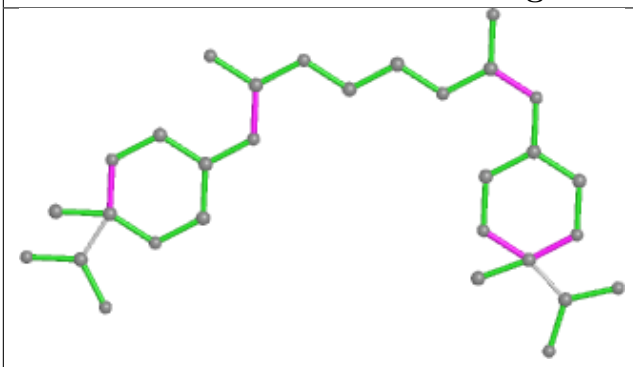
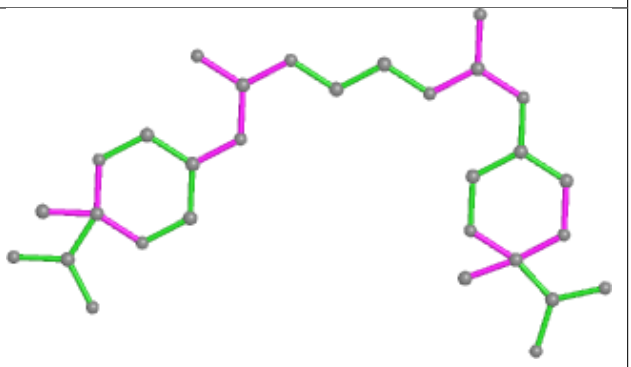


Rings

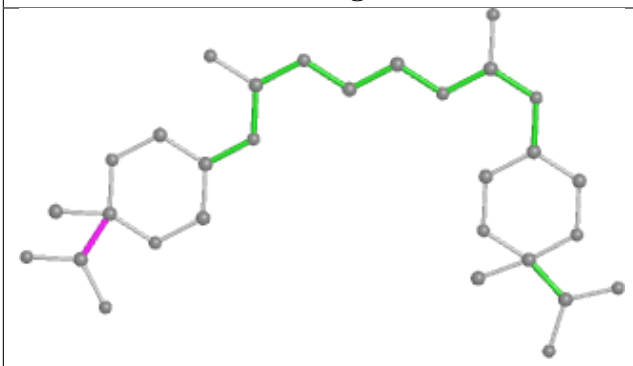
Ligand CPJ A 341



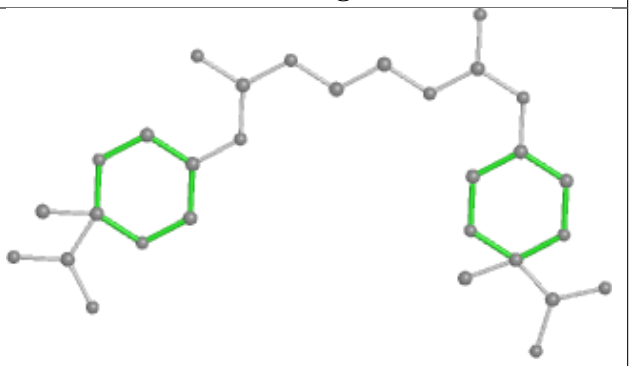
Bond lengths



Bond angles

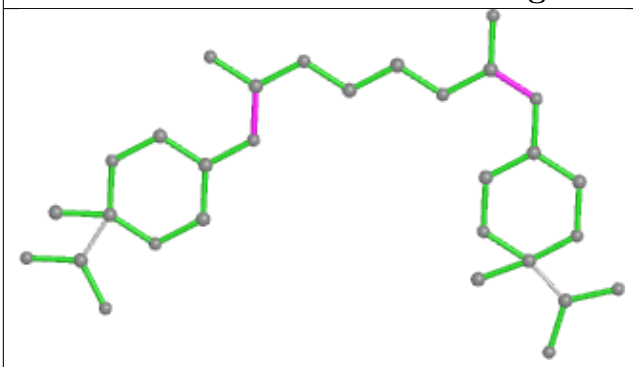


Torsions

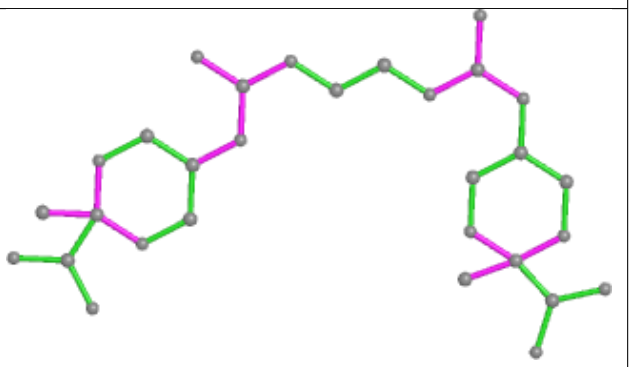


Rings

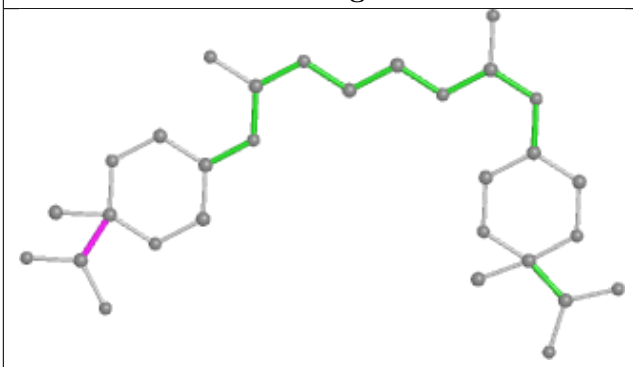
Ligand CPJ E 345



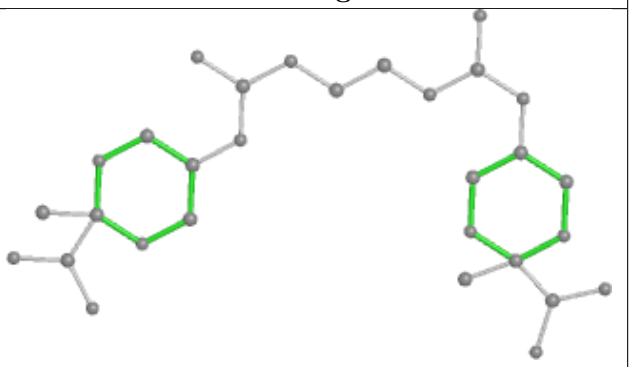
Bond lengths



Bond angles

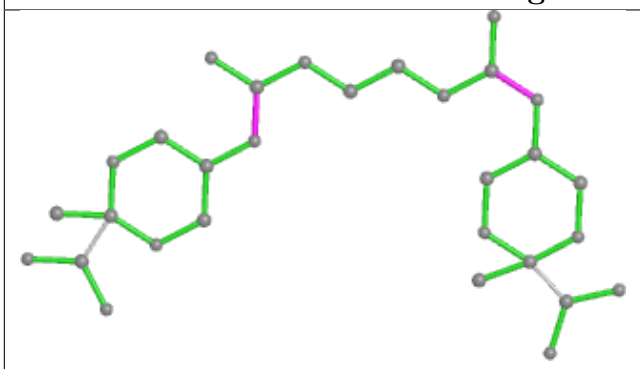


Torsions

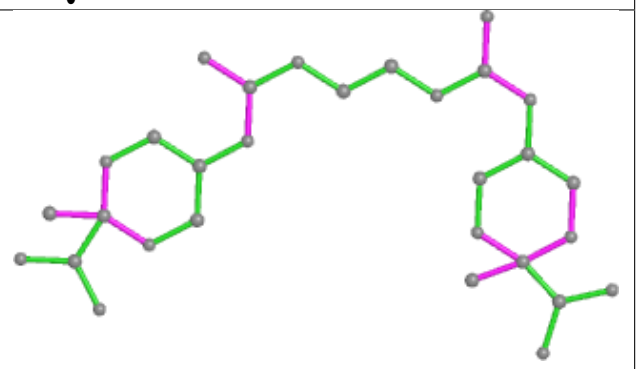


Rings

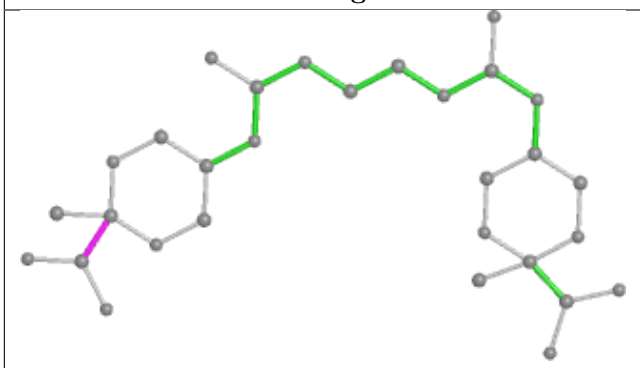
Ligand CPJ Q 350



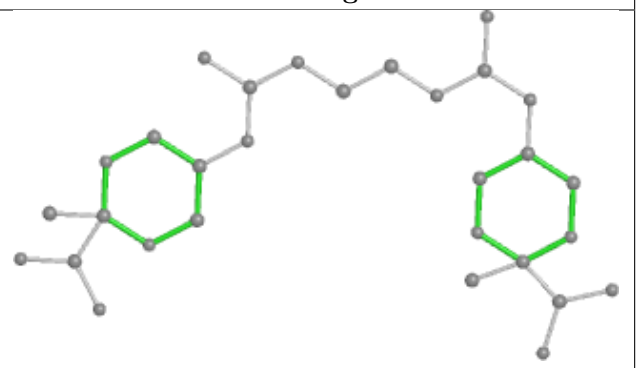
Bond lengths



Bond angles

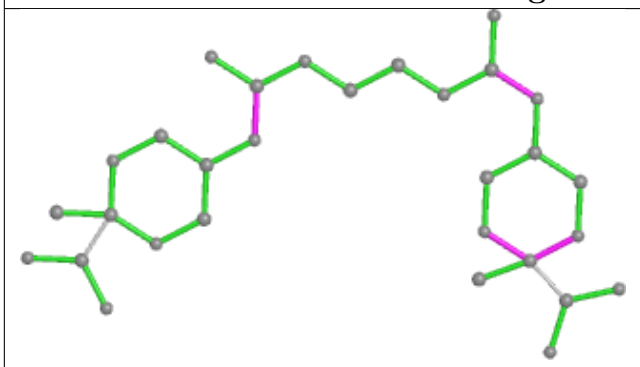


Torsions

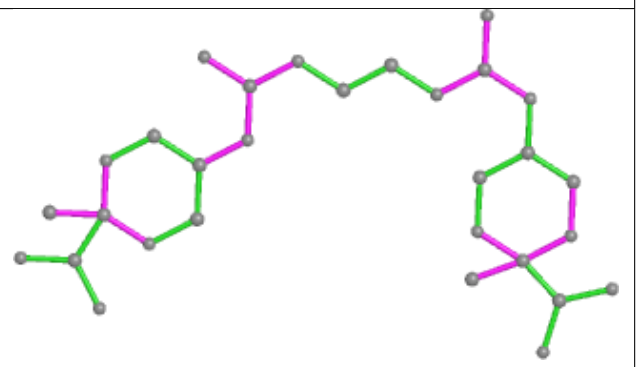


Rings

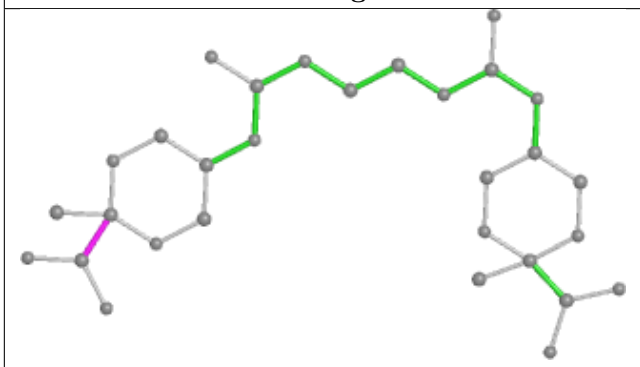
Ligand CPJ B 342



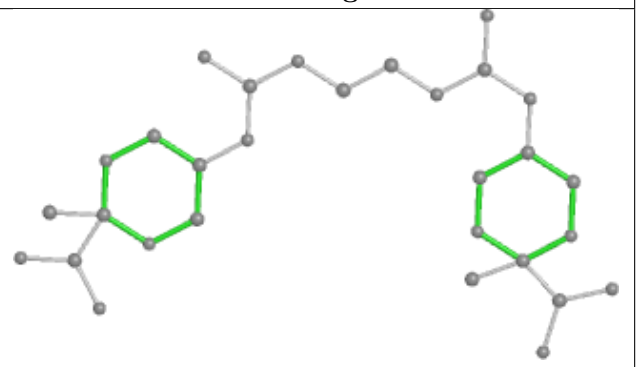
Bond lengths



Bond angles

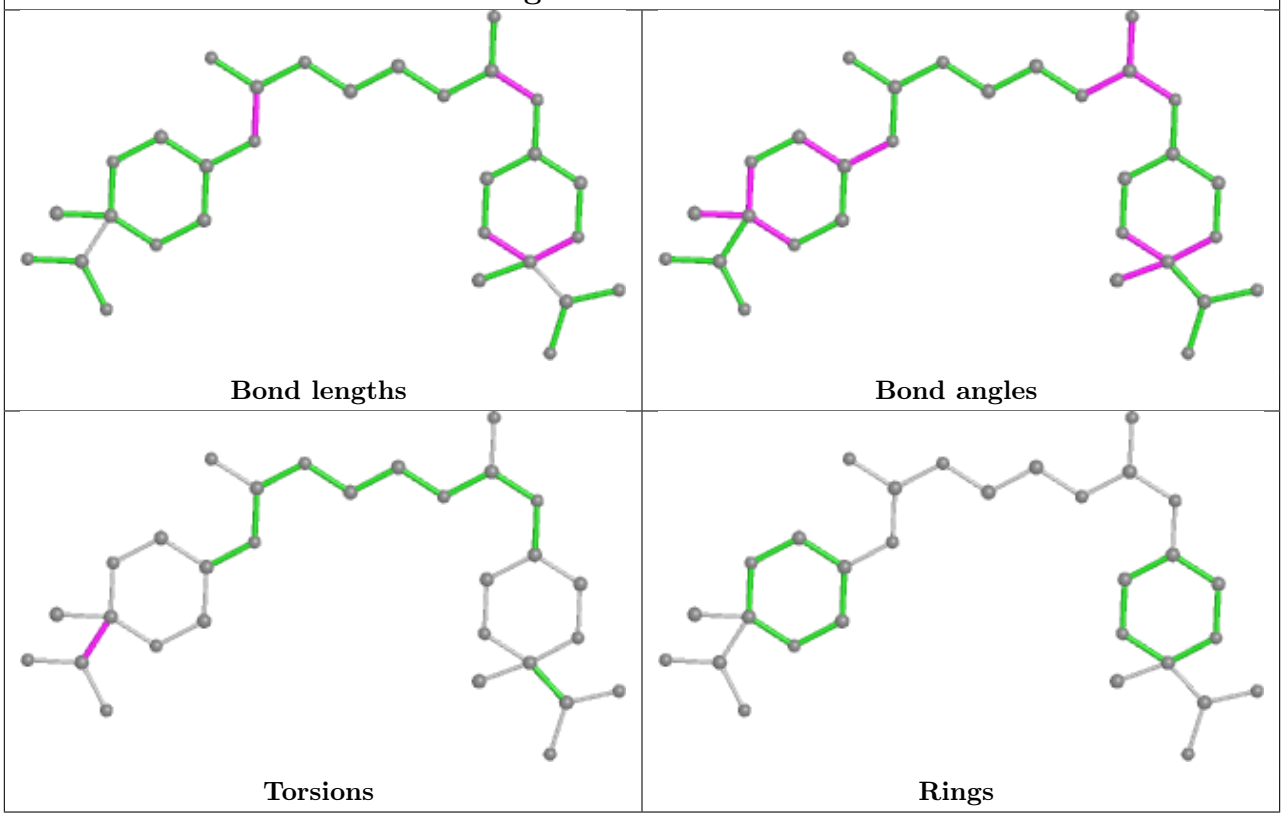


Torsions

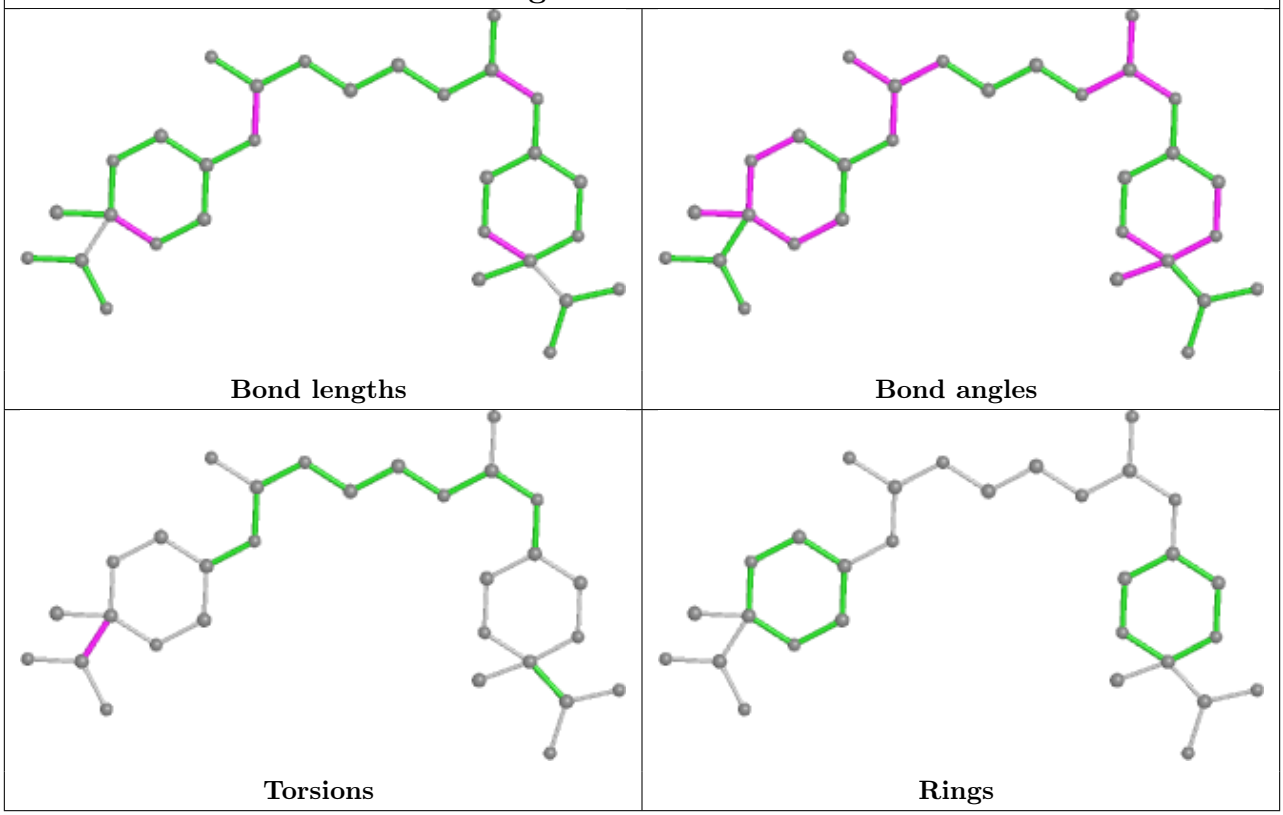


Rings

Ligand CPJ M 348



Ligand CPJ P 346



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	91	90	8, 13, 23, 31	0
1	C	204/204 (100%)	-0.14	1 (0%)	91	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%)	91	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%)	91	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, 24, 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%)	91	90	7, 13, 22, 33	0
1	Q	204/204 (100%)	-0.04	1 (0%)	91	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%)	91	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

All (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
1	M	204	VAL	4.2
1	K	26	LEU	3.6
1	S	204	VAL	3.5
1	M	172	ALA	3.4
1	K	204	VAL	3.3
1	B	204	VAL	2.9
1	M	183	LEU	2.9
1	O	178	LEU	2.8
1	O	204	VAL	2.7
1	N	175	GLY	2.6
1	K	56	GLY	2.6
1	M	23	ILE	2.5
1	M	125	VAL	2.5
1	G	204	VAL	2.4
1	P	204	VAL	2.4
1	H	26	LEU	2.4
1	M	124	PHE	2.3
1	M	170	LEU	2.3
1	K	28	LYS	2.3
1	R	25	PRO	2.2
1	K	23	ILE	2.2
1	K	33	PHE	2.2
1	K	30	LEU	2.2
1	J	204	VAL	2.1
1	K	160	TRP	2.1
1	N	160	TRP	2.1
1	N	174	GLN	2.1
1	Q	204	VAL	2.1
1	R	26	LEU	2.1
1	H	167	GLU	2.1
1	O	25	PRO	2.1
1	M	4	LEU	2.1
1	M	158	TYR	2.1
1	T	28	LYS	2.1
1	T	27	GLU	2.1
1	K	1	HIS	2.0
1	O	189	ASN	2.0
1	G	178	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	157	LEU	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, 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	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	K	321	1/1	0.88	0.08	45,45,45,45	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
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	J	319	1/1	0.92	0.11	27,27,27,27	0
2	CA	Q	334	1/1	0.92	0.12	35,35,35,35	0
2	CA	L	324	1/1	0.92	0.13	31,31,31,31	0
3	CPJ	P	346	30/30	0.92	0.14	28,62,70,71	0
2	CA	F	312	1/1	0.93	0.12	24,24,24,24	0
2	CA	T	340	1/1	0.93	0.10	39,39,39,39	0
3	CPJ	B	342	30/30	0.93	0.16	20,41,58,61	0
3	CPJ	D	344	30/30	0.93	0.14	27,36,58,59	0
3	CPJ	C	343	30/30	0.94	0.14	26,34,55,56	0
2	CA	S	338	1/1	0.94	0.10	27,27,27,27	0
2	CA	T	339	1/1	0.94	0.11	39,39,39,39	0
2	CA	M	325	1/1	0.94	0.10	44,44,44,44	0
3	CPJ	A	341	30/30	0.94	0.13	19,35,52,54	0
2	CA	G	313	1/1	0.94	0.09	28,28,28,28	0

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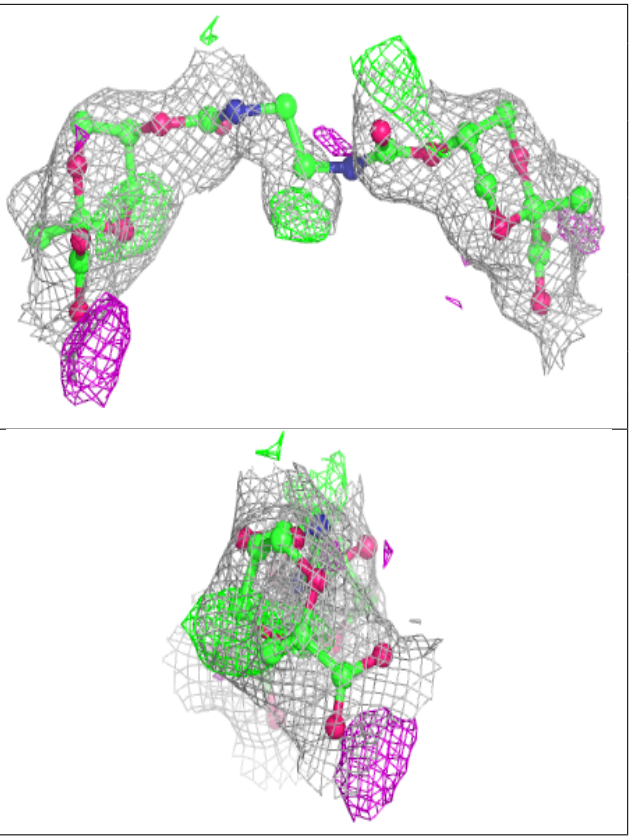
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CPJ	Q	350	30/30	0.94	0.16	31,51,71,72	0
2	CA	C	306	1/1	0.95	0.13	26,26,26,26	0
2	CA	H	315	1/1	0.95	0.08	25,25,25,25	0
2	CA	D	308	1/1	0.95	0.11	26,26,26,26	0
2	CA	B	304	1/1	0.95	0.12	23,23,23,23	0
2	CA	N	328	1/1	0.95	0.08	42,42,42,42	0
2	CA	E	309	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	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	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	R	335	1/1	0.97	0.10	36,36,36,36	0
2	CA	B	303	1/1	0.97	0.11	23,23,23,23	0
2	CA	F	311	1/1	0.97	0.13	24,24,24,24	0
2	CA	H	316	1/1	0.97	0.09	28,28,28,28	0
2	CA	D	307	1/1	0.97	0.10	26,26,26,26	0
2	CA	S	337	1/1	0.98	0.09	26,26,26,26	0
2	CA	P	331	1/1	0.98	0.10	29,29,29,29	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	E	310	1/1	0.98	0.10	23,23,23,23	0
2	CA	I	317	1/1	0.98	0.10	26,26,26,26	0
2	CA	O	330	1/1	0.98	0.13	28,28,28,28	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.

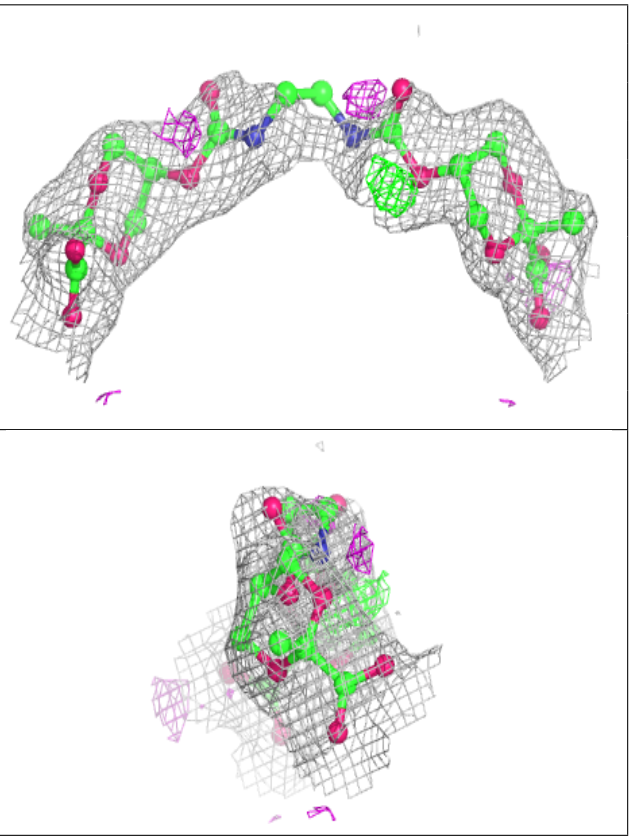
Electron density around CPJ M 348:

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



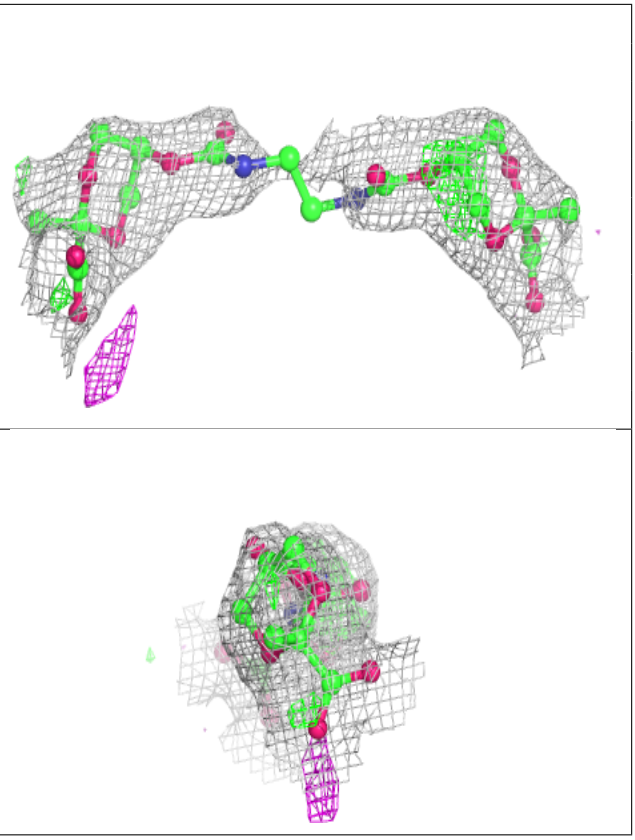
Electron density around CPJ L 347:

$2mF_o$-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:

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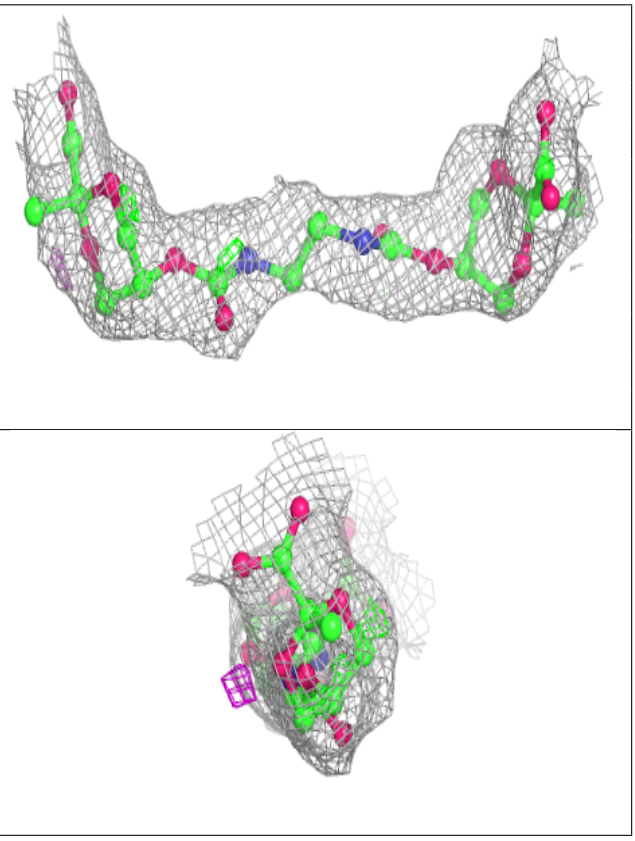
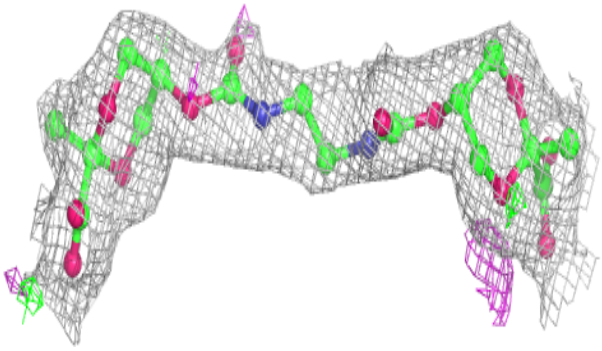
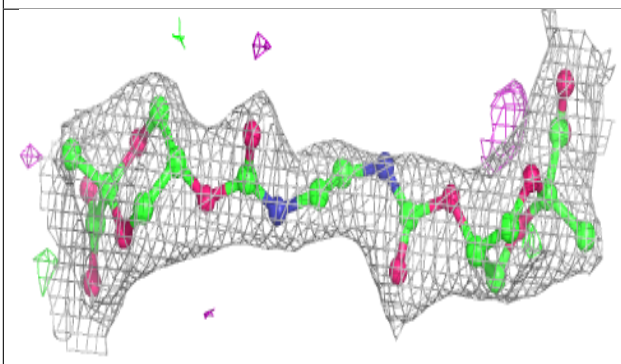
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

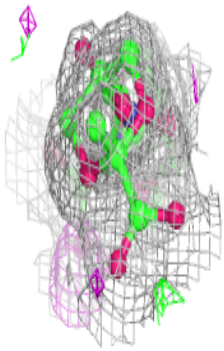


Electron density around CPJ B 342:

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

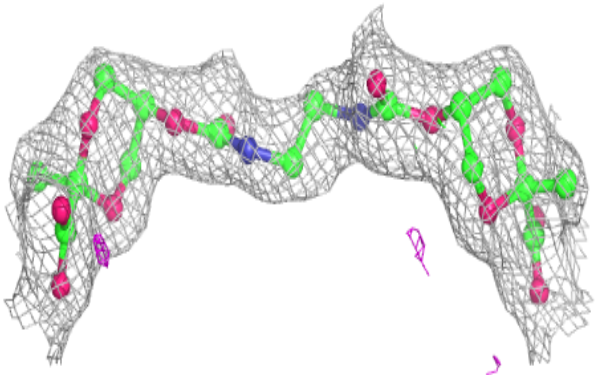


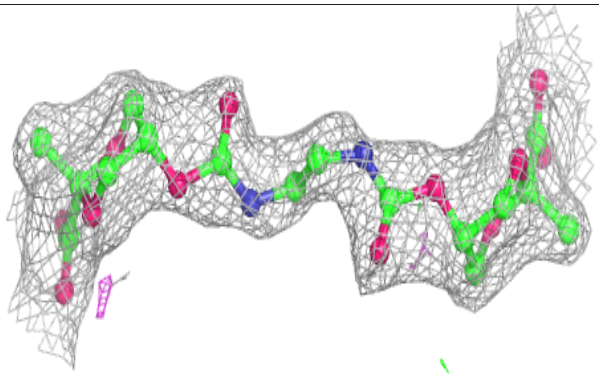


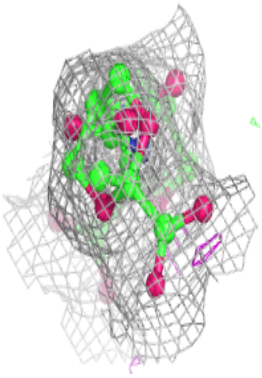


Electron density around CPJ D 344:

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

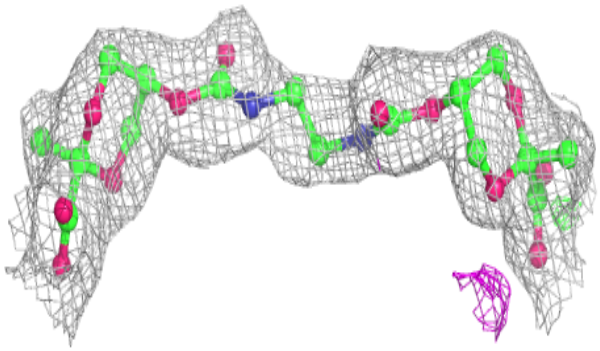


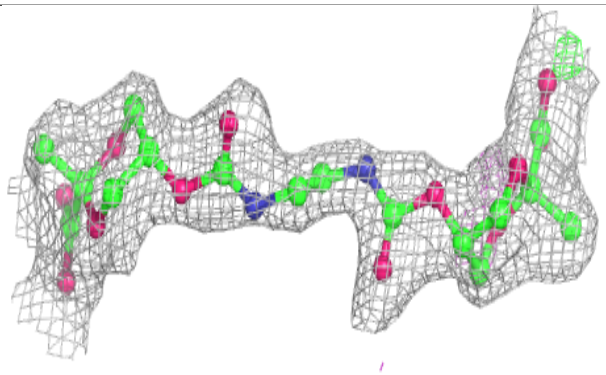


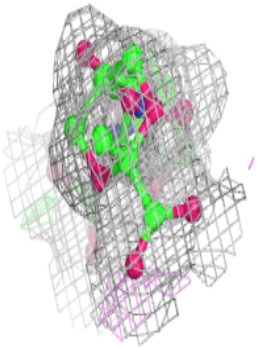


Electron density around CPJ C 343:

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

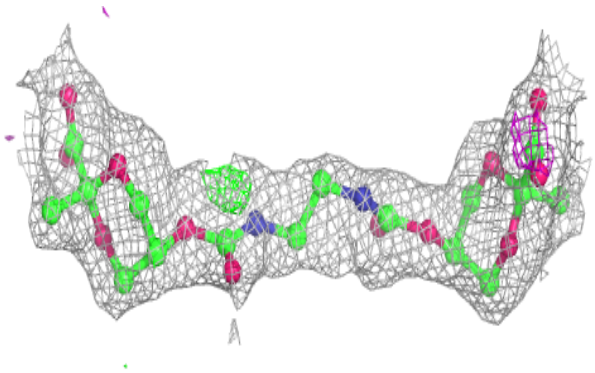


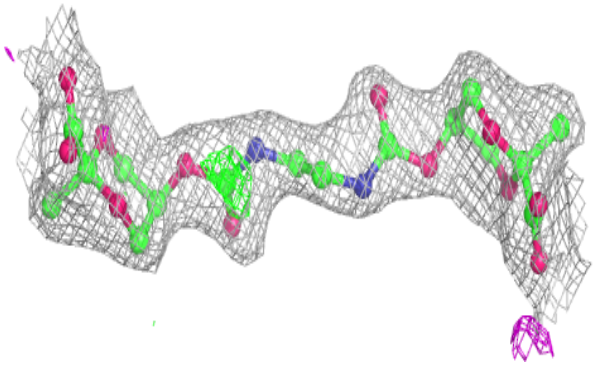


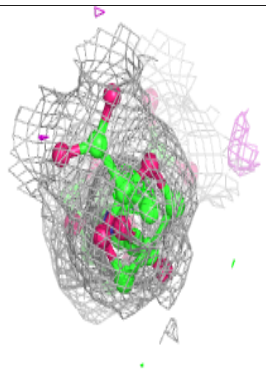


Electron density around CPJ A 341:

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

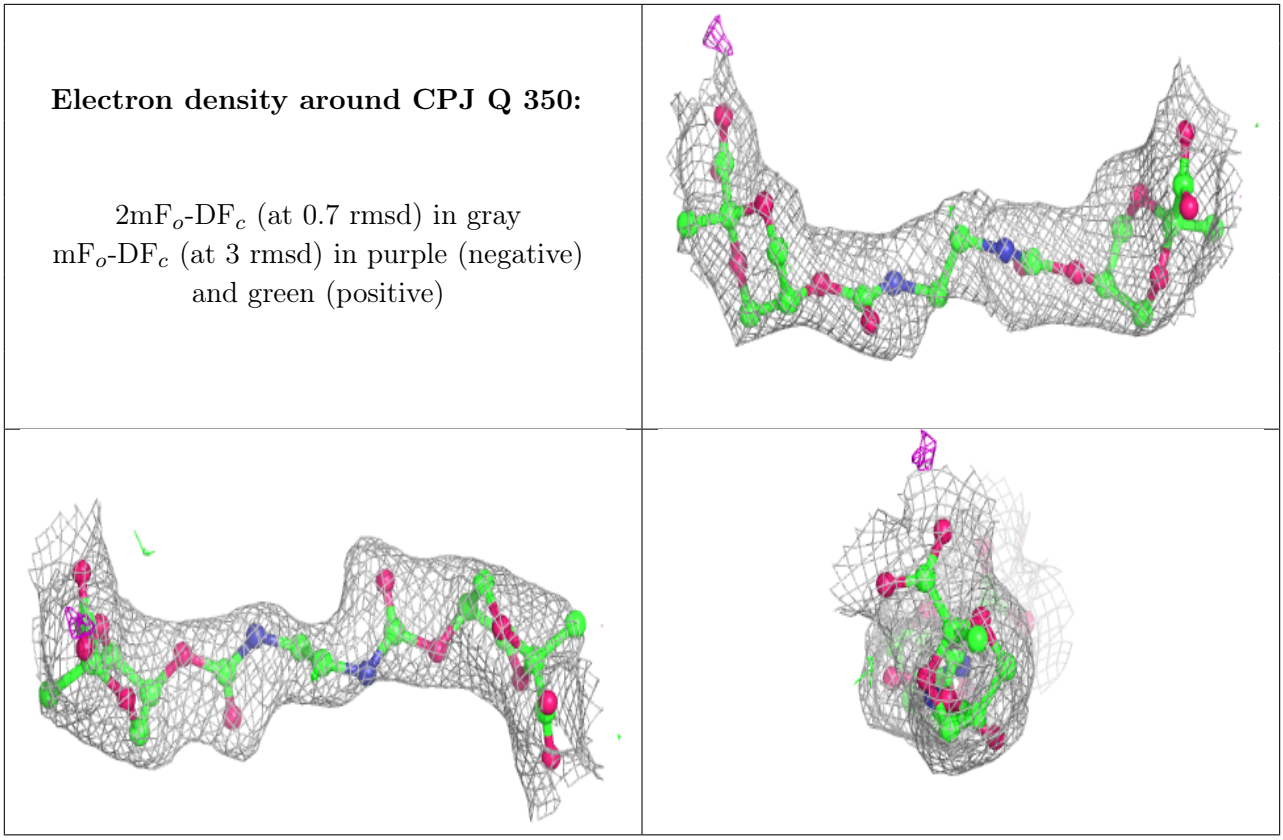






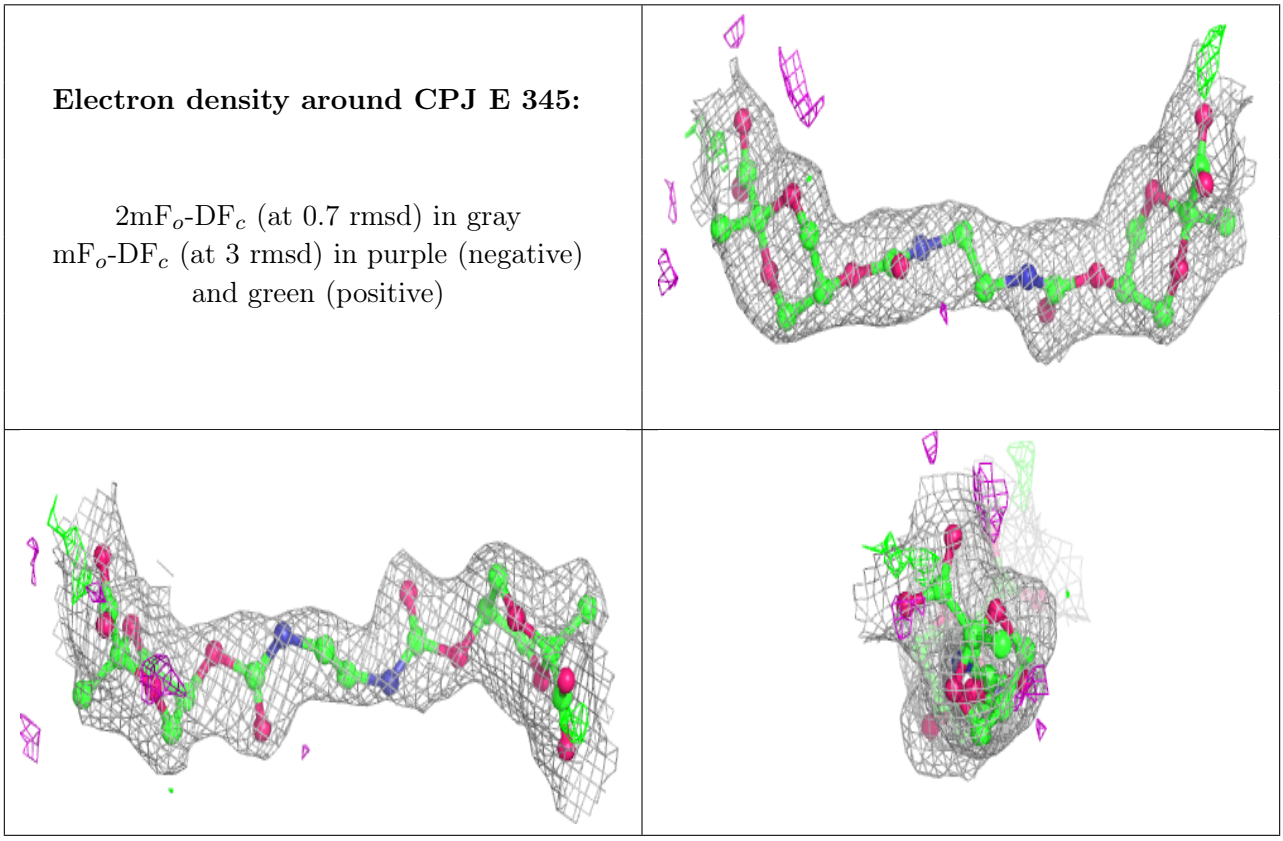
Electron density around CPJ Q 350:

$2mF_o$-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 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.