WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2024 – 01:14 PM EST

PDB ID	:	3A73
Title	:	Crystal Structure Analysis of Human serum albumin complexed with delta 12-prostaglandin J2
Authors	:	Ito, S.
Deposited on	:	2009-09-11
Resolution	:	2.19 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

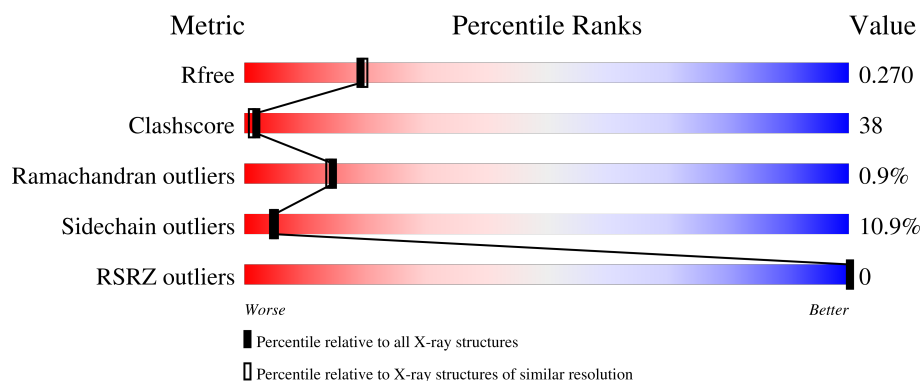|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.19 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	Percentile Ranks	Value
Rfree		0.270
Clashscore		38
Ramachandran outliers		0.9%
Sidechain outliers		10.9%
RSRZ outliers		0

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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	585	57% 35% 5% •
1	B	585	53% 38% 7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MYR	A	1004	-	-	X	-
2	MYR	B	1005	-	-	X	-
3	PJ2	A	1011	-	-	X	-
3	PJ2	A	1012	-	-	X	-
3	PJ2	B	1011	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9690 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 albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4580	2894	775	870	41			
1	B	576	Total	C	N	O	S	0	0	0
			4580	2894	775	870	41			

- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).
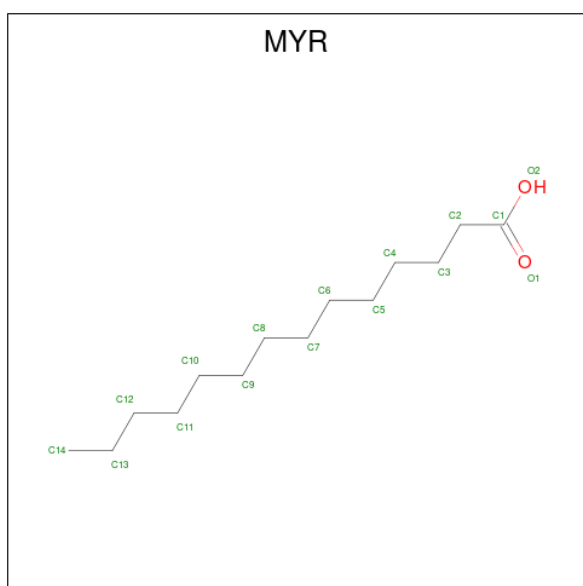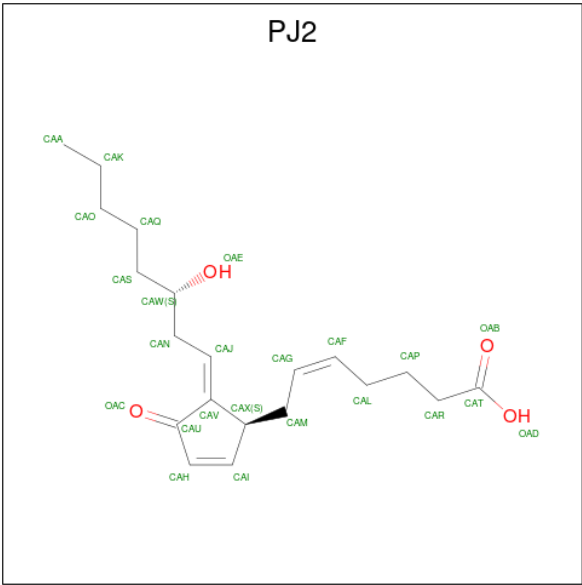

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		
2	A	1	Total	C	O	0	0
			16	14	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 16	C 14	O 2	0	0
2	A	1	Total 12	C 12		0	0
2	B	1	Total 16	C 14	O 2	0	0
2	B	1	Total 16	C 14	O 2	0	0
2	B	1	Total 16	C 14	O 2	0	0
2	B	1	Total 16	C 14	O 2	0	0
2	B	1	Total 16	C 14	O 2	0	0
2	B	1	Total 12	C 12		0	0

- Molecule 3 is (5Z,12Z,15S)-15-hydroxy-11-oxoprosta-5,9,12-trien-1-oic acid (three-letter code: PJ2) (formula: $C_{20}H_{30}O_4$).

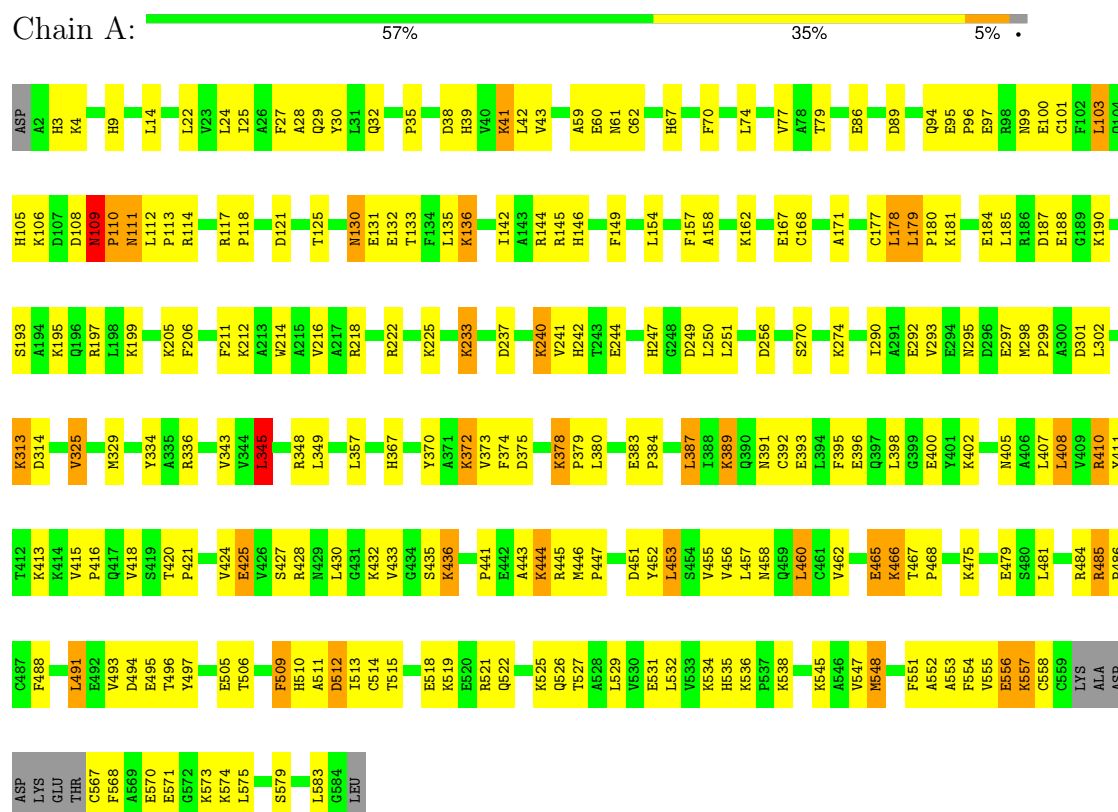| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 24	C 20	O 4	0	0
3	A	1	Total 24	C 20	O 4	0	0
3	B	1	Total 24	C 20	O 4	0	0

- Molecule 4 is water.

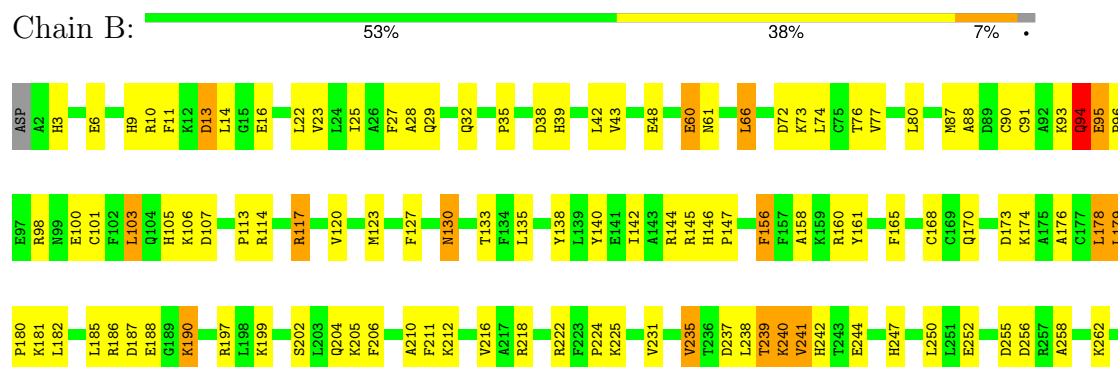| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total 135	O 135	0	0
4	B	139	Total 139	O 139	0	0

3 Residue-property plots ⓘ

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 albumin

Chain A:

• Molecule 1: Serum albumin

Chain B:

K274 L275 K276 E280 K281 P282 L283 L284 E285 K286 I290 A291 E294 N295 D296 E297 M298 P299 L302 S312 K313 D314 V315 Y334 R337 Y341 S342 L345 L346 L347 R348 K351 T352 Y353 T356 L357 A371 K372 V373 F374 D375 K378 P379 L380 V381 E382 E383

P384 Q385 N386 L387 Q390 N391 L394 Q397 L398 Y401 K402 F403 Q404 N405 A406 L407 L408 V409 R410 K413 K414 V415 P416 Q417 V418 S419 T420 P421 T422 L423 V424 E425 V426 S427 R428 N429 L430 V433 G434 S435 K439 H440 P441 K444 R445 M446 P447 C448 A449 E450 D451 Y452

L453 S454 V455 V456 L457 N458 Q459 L460 C461 V462 K466 T467 P468 V469 R472 L481 V482 N483 R484 R485 P486 C487 F488 L491 E492 V493 D494 E495 T496 Y497 V498 P499 K500 E501 F502 E505 T506 F507 T508 F509 H510 A511 D512 I513 C514 T515 L516 S517 E518 K519 E520 R521 Q522 I523 K524

K525 Q526 E531 L532 V533 K534 H535 K536 P537 K538 K541 K545 A546 V547 M548 D549 D550 F551 A552 A553 F554 V555 E556 K557 C558 C559 LYS ALA ASP ASP LYS GLU THR C567 F568 A569 E570 E571 G572 K573 K574 L575 V576 Q580 L583 G584 LEU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.06Å　92.05Å　94.66Å 74.80°　89.53°　80.21°	Depositor
Resolution (Å)	35.00　–　2.19 35.00　–　2.19	Depositor EDS
% Data completeness (in resolution range)	91.3 (35.00-2.19) 81.3 (35.00-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.55 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.229　,　0.291 0.240　,　0.270	Depositor DCC
R_{free} test set	2871 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.095 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9690	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, PJ2

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	0.91	1/4669 (0.0%)	0.91	4/6297 (0.1%)
1	B	0.89	4/4669 (0.1%)	0.88	3/6297 (0.0%)
All	All	0.90	5/9338 (0.1%)	0.89	7/12594 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	VAL	CB-CG2	5.47	1.64	1.52
1	B	371	ALA	CA-CB	5.46	1.64	1.52
1	B	348	ARG	C-N	-5.35	1.21	1.34
1	B	341	TYR	CD1-CE1	5.20	1.47	1.39
1	B	91	CYS	CB-SG	-5.18	1.73	1.81

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ALA	N-CA-C	5.90	126.94	111.00
1	A	336	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	171	ALA	N-CA-CB	-5.80	101.98	110.10
1	B	42	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	345	LEU	CB-CG-CD2	5.44	120.24	111.00

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	4580	0	4504	330	0
1	B	4580	0	4503	354	0
2	A	92	0	155	30	0
2	B	92	0	155	40	0
3	A	48	0	58	40	0
3	B	24	0	28	26	0
4	A	135	0	0	10	0
4	B	139	0	0	15	0
All	All	9690	0	9403	707	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 38.

The worst 5 of 707 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:A:146:HIS:CE1	3:A:1012:PJ2:HAI	1.39	1.57
1:A:146:HIS:NE2	3:A:1012:PJ2:CAI	1.71	1.50
1:A:146:HIS:CE1	3:A:1012:PJ2:CAI	2.01	1.40
1:A:142:ILE:CD1	3:A:1011:PJ2:HAAA	1.53	1.35
1:B:117:ARG:HD2	3:B:1011:PJ2:CAH	1.59	1.32

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	572/585 (98%)	532 (93%)	35 (6%)	5 (1%)	14	14
1	B	572/585 (98%)	532 (93%)	35 (6%)	5 (1%)	14	14

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1144/1170 (98%)	1064 (93%)	70 (6%)	10 (1%)	14 14

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	PRO
1	B	94	GLN
1	A	111	ASN
1	B	95	GLU
1	A	479	GLU

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	503/511 (98%)	452 (90%)	51 (10%)	6 6
1	B	503/511 (98%)	444 (88%)	59 (12%)	4 4
All	All	1006/1022 (98%)	896 (89%)	110 (11%)	5 5

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	107	ASP
1	B	239	THR
1	B	557	LYS
1	B	491	LEU
1	B	130	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	HIS
1	B	405	ASN
1	B	130	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	386	ASN
1	B	429	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	MYR	A	1005	-	15,15,15	0.51	0	15,15,15	1.55	2 (13%)
2	MYR	A	1007	-	11,11,15	0.35	0	10,10,15	0.73	0
3	PJ2	B	1011	-	21,24,24	2.37	6 (28%)	19,29,29	2.01	7 (36%)
3	PJ2	A	1012	-	21,24,24	2.24	7 (33%)	19,29,29	1.12	2 (10%)
2	MYR	B	1005	-	15,15,15	0.79	0	15,15,15	0.98	1 (6%)
2	MYR	A	1003	-	15,15,15	1.07	1 (6%)	15,15,15	1.55	4 (26%)
2	MYR	B	1006	-	15,15,15	0.85	0	15,15,15	1.07	1 (6%)
2	MYR	B	1002	-	15,15,15	0.62	0	15,15,15	0.82	0
2	MYR	A	1006	-	15,15,15	0.55	0	15,15,15	1.58	4 (26%)
2	MYR	B	1007	-	11,11,15	0.28	0	10,10,15	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	PJ2	A	1011	-	21,24,24	2.64	6 (28%)	19,29,29	2.04	6 (31%)
2	MYR	A	1002	-	15,15,15	0.70	0	15,15,15	0.88	0
2	MYR	B	1003	-	15,15,15	0.84	0	15,15,15	0.92	1 (6%)
2	MYR	A	1004	-	15,15,15	0.75	0	15,15,15	1.83	5 (33%)
2	MYR	B	1004	-	15,15,15	0.45	0	15,15,15	1.89	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	A	1005	-	-	5/13/13/13	-
2	MYR	A	1007	-	-	6/9/9/13	-
3	PJ2	B	1011	-	-	8/19/32/32	0/1/1/1
3	PJ2	A	1012	-	-	11/19/32/32	0/1/1/1
2	MYR	B	1005	-	-	7/13/13/13	-
2	MYR	A	1003	-	-	10/13/13/13	-
2	MYR	B	1006	-	-	4/13/13/13	-
2	MYR	B	1002	-	-	7/13/13/13	-
2	MYR	A	1006	-	-	7/13/13/13	-
2	MYR	B	1007	-	-	6/9/9/13	-
3	PJ2	A	1011	-	-	9/19/32/32	0/1/1/1
2	MYR	A	1002	-	-	8/13/13/13	-
2	MYR	B	1003	-	-	9/13/13/13	-
2	MYR	A	1004	-	-	9/13/13/13	-
2	MYR	B	1004	-	-	7/13/13/13	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1011	PJ2	CAJ-CAV	6.81	1.41	1.33
3	A	1011	PJ2	CAN-CAJ	-6.16	1.38	1.50
3	A	1012	PJ2	CAN-CAJ	-5.84	1.39	1.50
3	B	1011	PJ2	CAM-CAG	-5.44	1.34	1.50
3	A	1011	PJ2	CAH-CAU	-4.94	1.32	1.46

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1011	PJ2	CAN-CAJ-CAV	-5.92	119.12	126.45
3	B	1011	PJ2	CAP-CAR-CAT	-4.93	101.64	114.51
2	B	1004	MYR	O2-C1-C2	4.21	127.29	114.00
2	A	1005	MYR	O2-C1-C2	3.78	125.94	114.00
2	A	1004	MYR	C5-C4-C3	-3.46	96.89	114.37

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

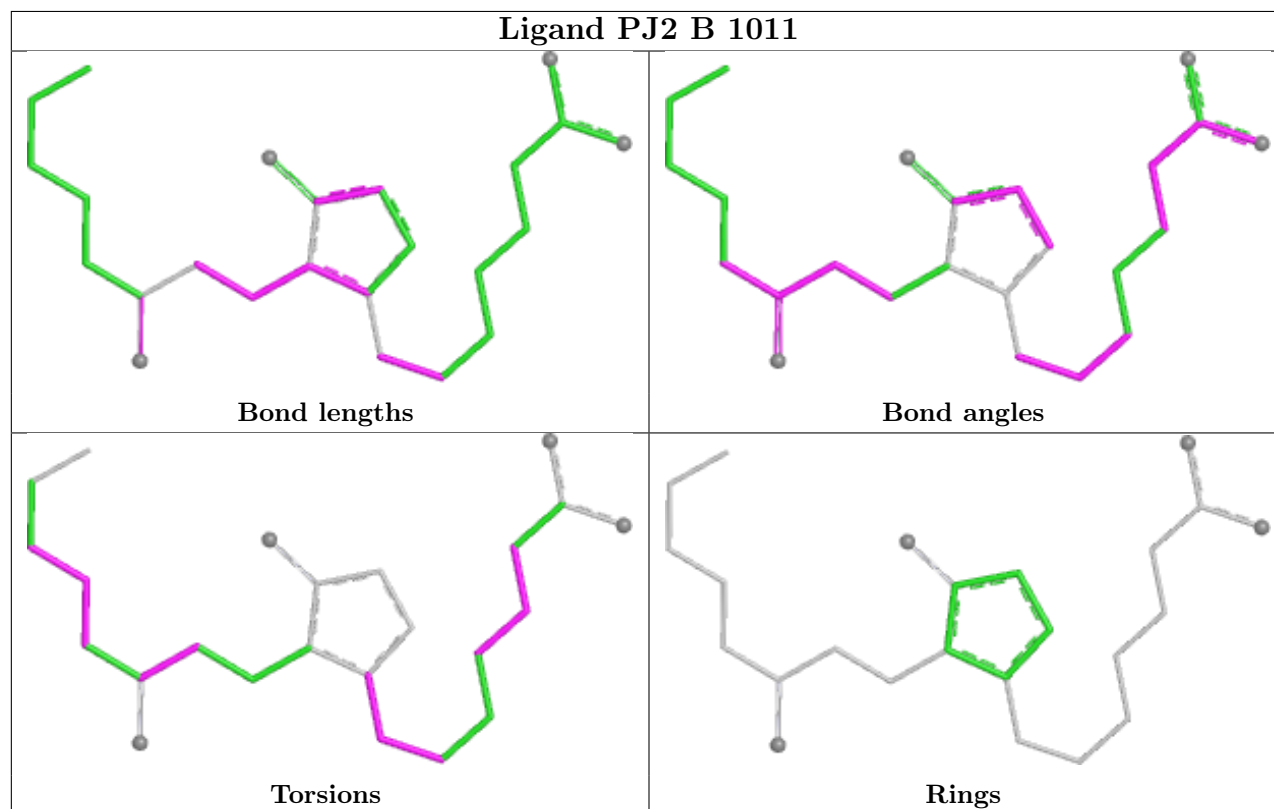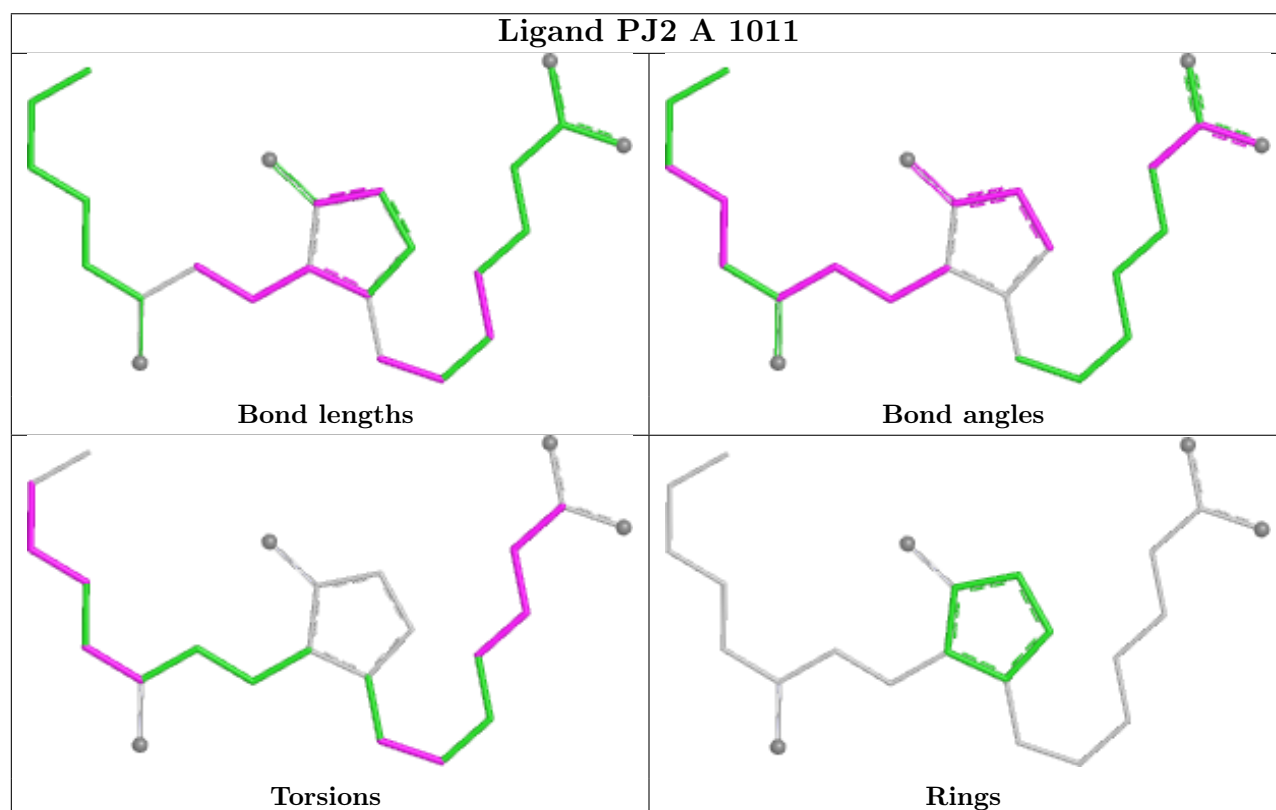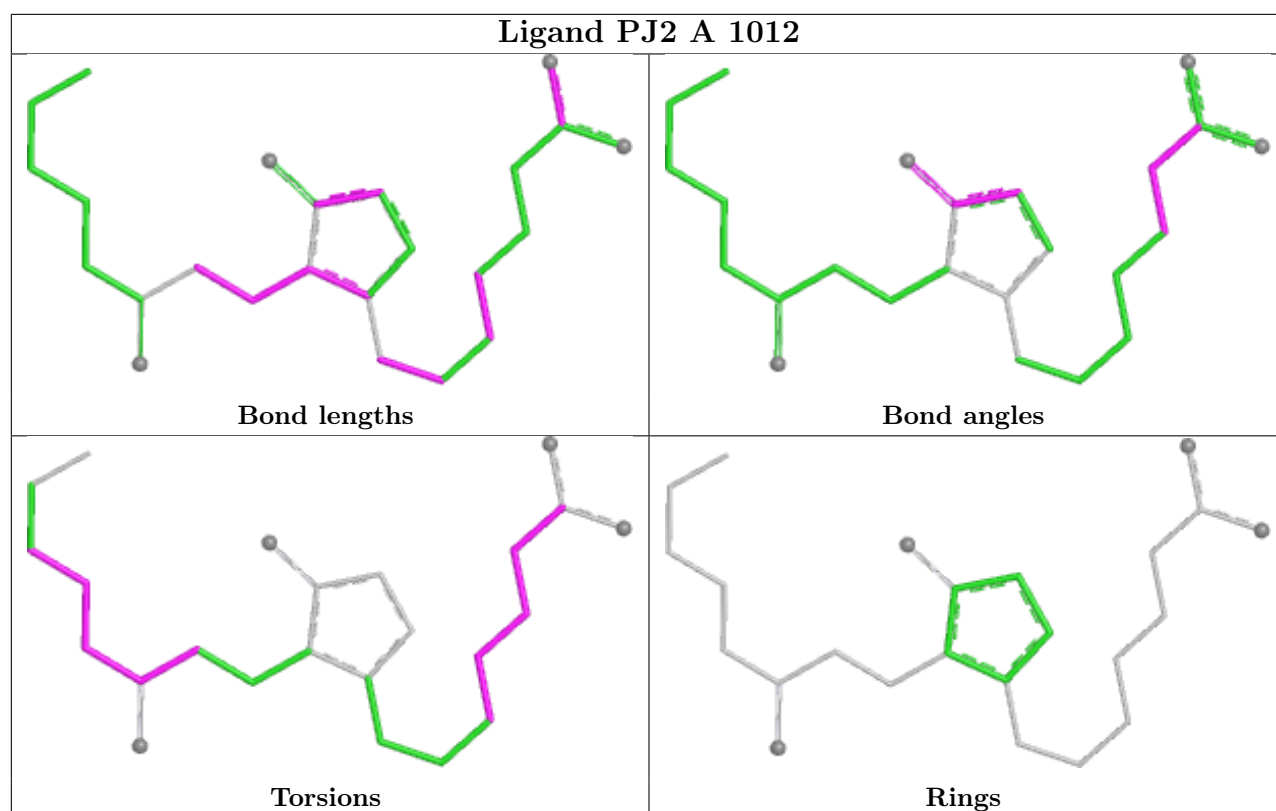| Mol	Chain	Res	Type	Atoms
3	A	1011	PJ2	CAQ-CAS-CAW-CAN
3	A	1012	PJ2	CAJ-CAN-CAW-OAE
3	A	1012	PJ2	CAQ-CAS-CAW-CAN
3	B	1011	PJ2	CAG-CAM-CAX-CAI
3	B	1011	PJ2	CAJ-CAN-CAW-OAE

There are no ring outliers.

15 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1005	MYR	6	0
2	A	1007	MYR	3	0
3	B	1011	PJ2	26	0
3	A	1012	PJ2	23	0
2	B	1005	MYR	11	0
2	A	1003	MYR	4	0
2	B	1006	MYR	5	0
2	B	1002	MYR	5	0
2	A	1006	MYR	1	0
2	B	1007	MYR	3	0
3	A	1011	PJ2	22	0
2	A	1002	MYR	4	0
2	B	1003	MYR	8	0
2	A	1004	MYR	12	0
2	B	1004	MYR	8	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 PJ2 B 1011

Ligand PJ2 A 1012

Bond lengths

Bond angles

Torsions

Rings

Ligand PJ2 A 1011

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	576/585 (98%)	-0.82	0	100	100	19, 29, 37, 44	0
1	B	576/585 (98%)	-0.85	0	100	100	19, 30, 38, 44	0
All	All	1152/1170 (98%)	-0.84	0	100	100	19, 29, 37, 44	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	MYR	A	1007	12/16	0.96	0.07	52,53,55,55	0
2	MYR	B	1005	16/16	0.96	0.07	52,56,56,57	0
3	PJ2	A	1012	24/24	0.96	0.08	65,74,78,79	0
3	PJ2	B	1011	24/24	0.96	0.07	46,61,65,65	0
2	MYR	A	1002	16/16	0.97	0.06	37,48,62,62	0
2	MYR	B	1002	16/16	0.97	0.06	40,49,56,56	0
2	MYR	B	1003	16/16	0.97	0.06	33,40,47,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MYR	B	1004	16/16	0.97	0.07	45,49,53,55	0
2	MYR	A	1003	16/16	0.97	0.07	37,50,58,59	0
2	MYR	B	1006	16/16	0.97	0.07	46,54,57,58	0
2	MYR	B	1007	12/16	0.97	0.06	49,55,59,60	0
3	PJ2	A	1011	24/24	0.97	0.07	50,65,71,72	0
2	MYR	A	1004	16/16	0.97	0.06	43,49,57,58	0
2	MYR	A	1006	16/16	0.97	0.08	44,53,59,60	0
2	MYR	A	1005	16/16	0.98	0.05	43,48,57,59	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.
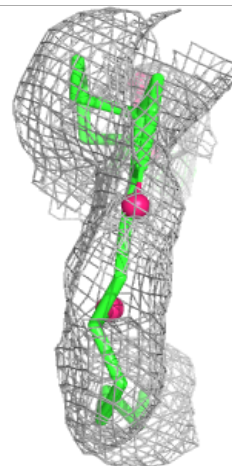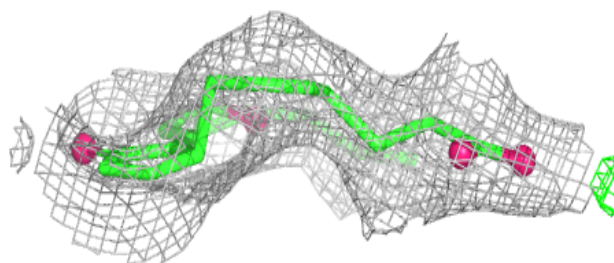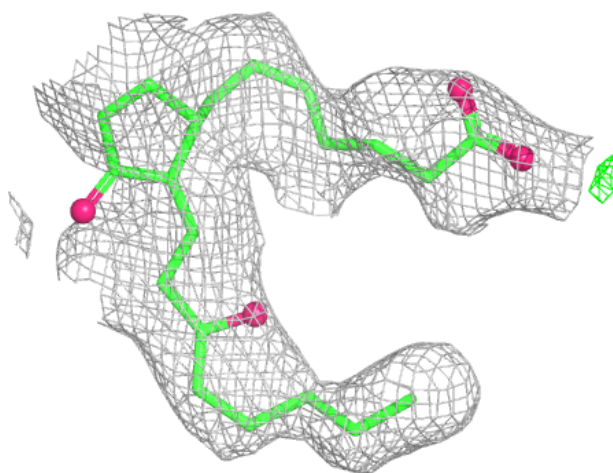
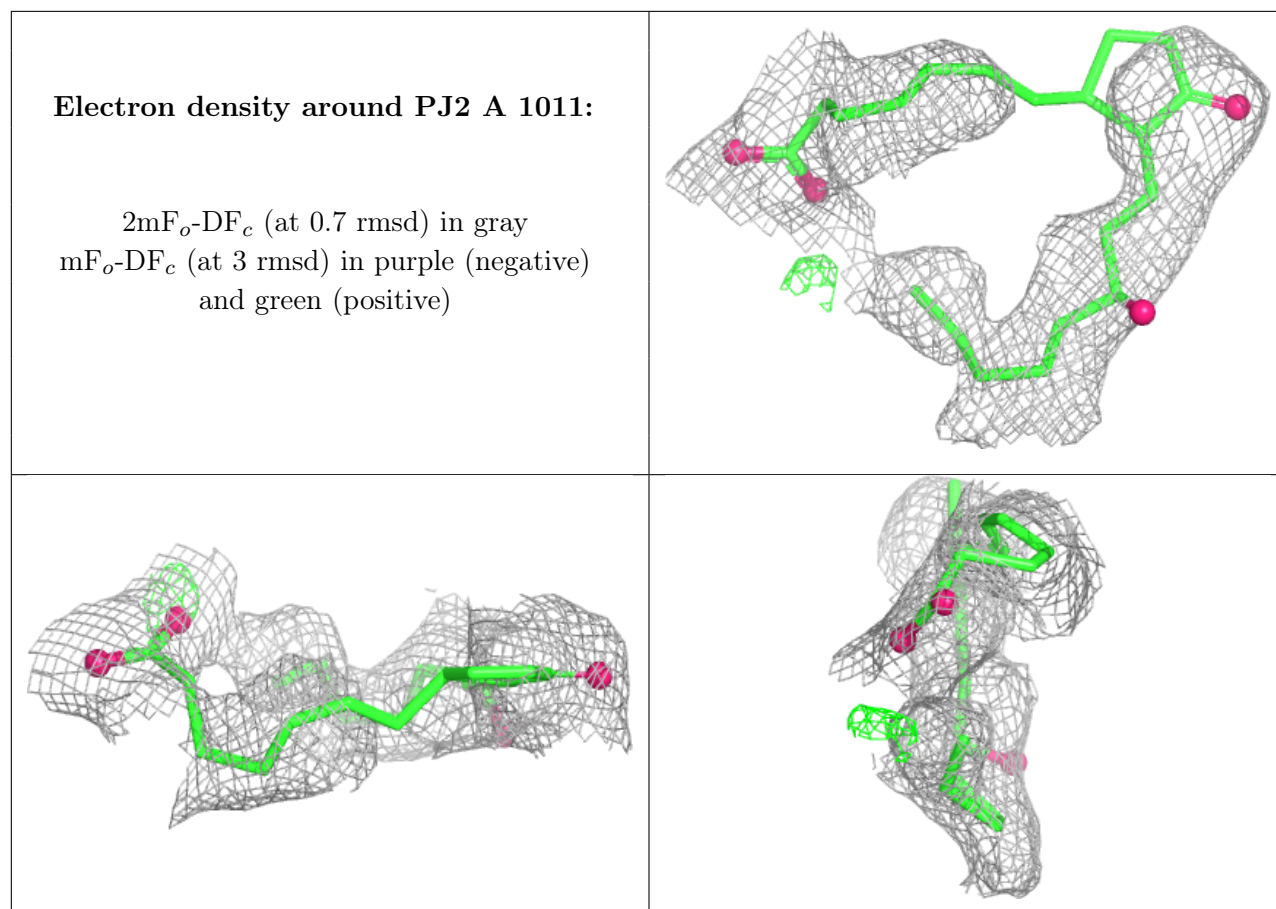**Electron density around PJ2 A 1012:**

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
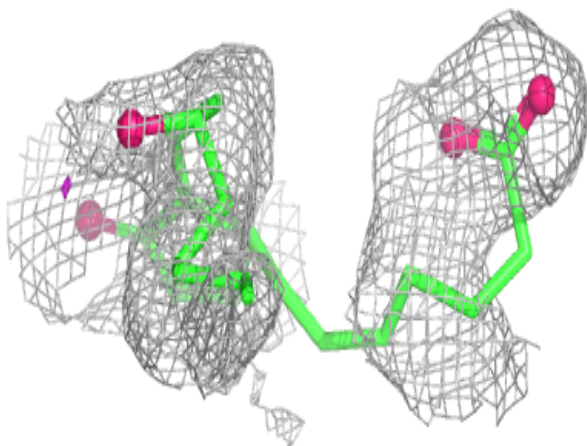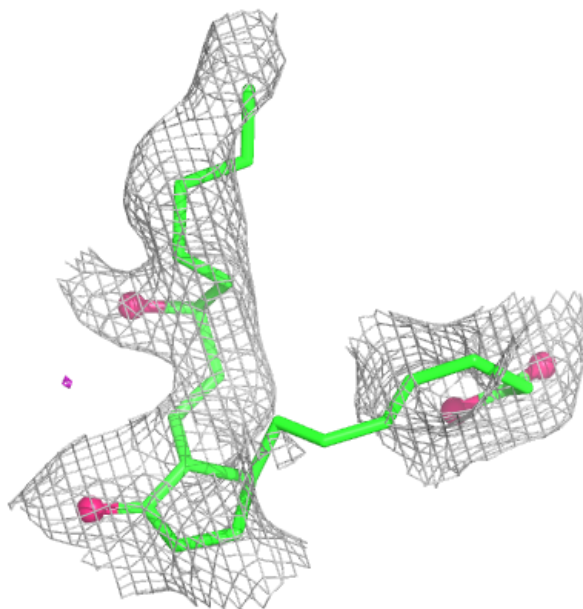
Electron density around PJ2 B 1011:

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

Electron density around PJ2 A 1011:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.