



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 12:45 PM EST

PDB ID : 7M0E
Title : Pre-catalytic synaptic complex of DNA Polymerase Lambda with gapped DSB substrate and incoming dUMPNPP
Authors : Kaminski, A.M.; Bebenek, K.; Pedersen, L.C.; Kunkel, T.A.
Deposited on : 2021-03-10
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
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) : 2.27

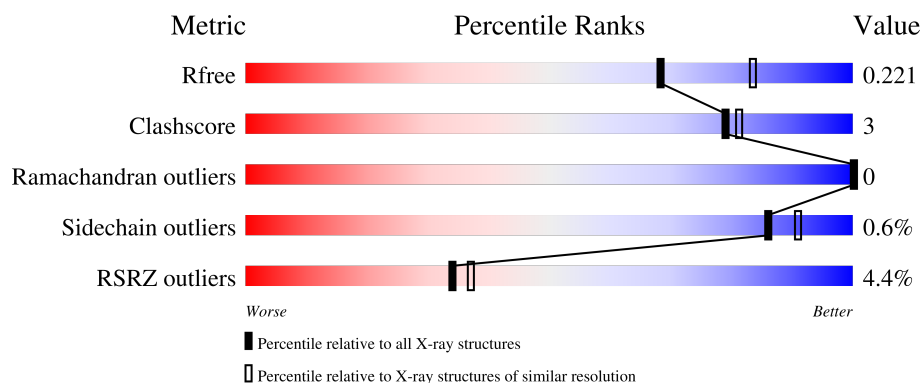
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	348	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> </div>
1	B	348	<div> <div style="width: 89%;"></div> <div style="width: 5%;"></div> <div style="width: 7%;"></div> </div>
1	C	348	<div> <div style="width: 86%;"></div> <div style="width: 7%;"></div> <div style="width: 6%;"></div> </div>
1	D	348	<div> <div style="width: 87%;"></div> <div style="width: 6%;"></div> <div style="width: 7%;"></div> </div>
2	G	7	<div> <div style="width: 71%;"></div> <div style="width: 29%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	K	7	 100%
2	O	7	 14% 71% 29%
2	T	7	 100%
3	F	6	 67% 33%
3	J	6	 100%
3	N	6	 83% 17%
3	R	6	 83% 17%
4	H	4	 25% 25% 75%
4	L	4	 100%
4	P	4	 75% 25%
4	U	4	 25% 75%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11774 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 DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	1	0
			2534	1598	457	467	12			
1	B	324	Total	C	N	O	S	0	0	0
			2446	1550	434	450	12			
1	C	326	Total	C	N	O	S	0	0	0
			2499	1576	451	460	12			
1	D	325	Total	C	N	O	S	0	2	0
			2415	1523	432	448	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	GLY	-	expression tag	UNP Q9UGP5
A	229	SER	-	expression tag	UNP Q9UGP5
A	230	ALA	-	expression tag	UNP Q9UGP5
A	231	ALA	-	expression tag	UNP Q9UGP5
B	228	GLY	-	expression tag	UNP Q9UGP5
B	229	SER	-	expression tag	UNP Q9UGP5
B	230	ALA	-	expression tag	UNP Q9UGP5
B	231	ALA	-	expression tag	UNP Q9UGP5
C	228	GLY	-	expression tag	UNP Q9UGP5
C	229	SER	-	expression tag	UNP Q9UGP5
C	230	ALA	-	expression tag	UNP Q9UGP5
C	231	ALA	-	expression tag	UNP Q9UGP5
D	228	GLY	-	expression tag	UNP Q9UGP5
D	229	SER	-	expression tag	UNP Q9UGP5
D	230	ALA	-	expression tag	UNP Q9UGP5
D	231	ALA	-	expression tag	UNP Q9UGP5

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*GP*GP*CP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total 141	C 67	N 29	O 39	P 6	0	1	0
2	K	7	Total 141	C 67	N 29	O 39	P 6	0	1	0
2	O	7	Total 141	C 67	N 29	O 39	P 6	0	1	0
2	T	7	Total 141	C 67	N 29	O 39	P 6	0	1	0

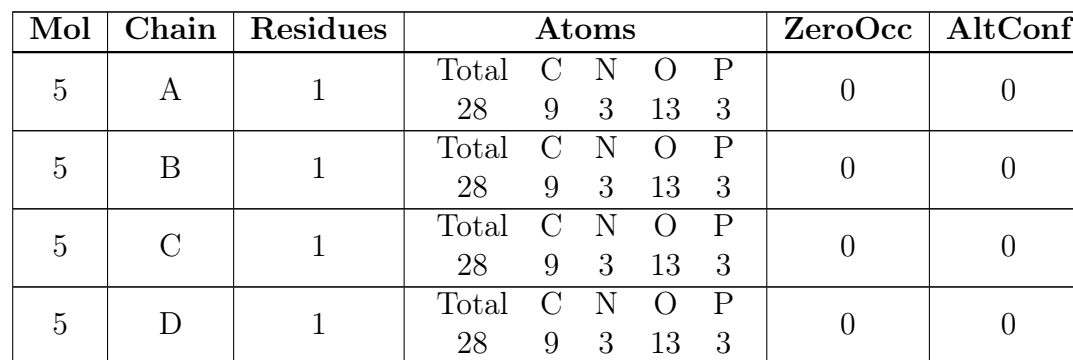
- Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	6	Total 120	C 58	N 23	O 34	P 5	0	0	0
3	J	6	Total 120	C 58	N 23	O 34	P 5	0	0	0
3	N	6	Total 120	C 58	N 23	O 34	P 5	0	0	0
3	R	6	Total 120	C 58	N 23	O 34	P 5	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	4	Total 83	C 38	N 16	O 25	P 4	0	1	0
4	L	4	Total 83	C 38	N 16	O 25	P 4	0	1	0
4	P	4	Total 83	C 38	N 16	O 25	P 4	0	1	0
4	U	4	Total 83	C 38	N 16	O 25	P 4	0	1	0

- Molecule 5 is 2'-DEOXYURIDINE 5'-ALPHA,BETA-IMIDO-TRIPHOSPHATE (three-letter code: DUP) (formula: C₉H₁₆N₃O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

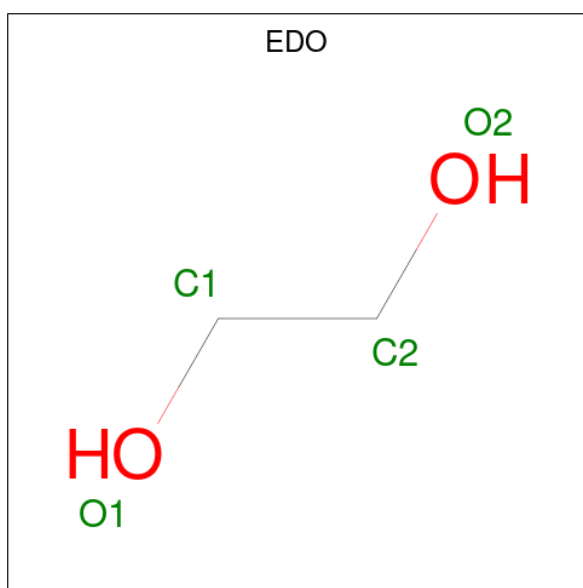


- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6 | A | 1 | Total Mg
1 1 | 0 | 0 |
| 6 | F | 1 | Total Mg
1 1 | 0 | 0 |
| 6 | B | 1 | Total Mg
1 1 | 0 | 0 |
| 6 | C | 1 | Total Mg
1 1 | 0 | 0 |
| 6 | N | 1 | Total Mg
1 1 | 0 | 0 |
| 6 | D | 1 | Total Mg
1 1 | 0 | 0 |

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0
7	D	1	Total Na 1 1	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	N	1	Total C O 4 2 2	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	O	S	0	1
			10	8	2		
9	N	1	Total	O	S	0	1
			10	8	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	111	Total	O	0	0
			111	111		
10	G	7	Total	O	0	0
			7	7		
10	F	19	Total	O	0	0
			19	19		
10	H	5	Total	O	0	0
			5	5		
10	B	70	Total	O	0	0
			70	70		
10	K	7	Total	O	0	0
			7	7		
10	J	16	Total	O	0	0
			16	16		
10	L	1	Total	O	0	0
			1	1		
10	C	51	Total	O	0	0
			51	51		
10	O	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	N	14	Total 14	O 14	0	0
10	D	36	Total 36	O 36	0	0
10	T	2	Total 2	O 2	0	0
10	R	11	Total 11	O 11	0	0
10	U	1	Total 1	O 1	0	0

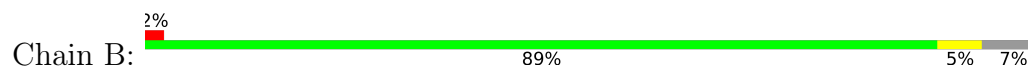
3 Residue-property plots [i](#)

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

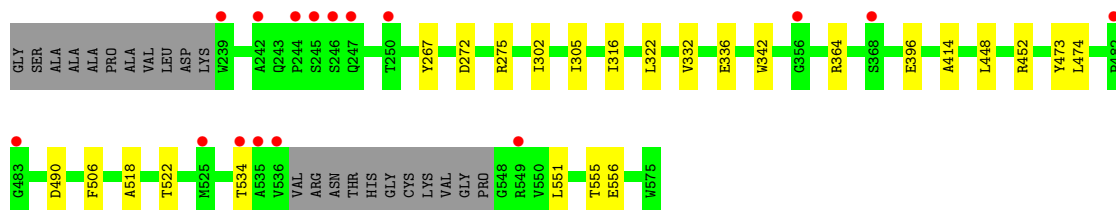
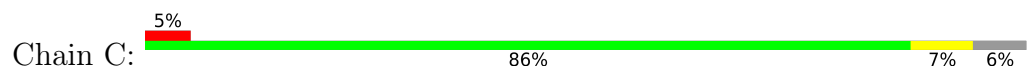
- Molecule 1: DNA polymerase lambda



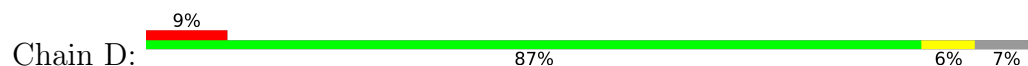
- Molecule 1: DNA polymerase lambda

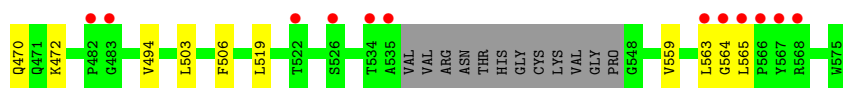


- Molecule 1: DNA polymerase lambda



- Molecule 1: DNA polymerase lambda





- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*AP*GP*C)-3')

Chain G: 71% 29%



- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*AP*GP*C)-3')

Chain K: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*AP*GP*C)-3')

Chain O: 14% 71% 29%



- Molecule 2: DNA (5'-D(*CP*GP*GP*CP*AP*GP*C)-3')

Chain T: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*GP*C)-3')

Chain F: 67% 33%



- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*GP*C)-3')

Chain J: 100%


There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*GP*C)-3')

Chain N: 83% 17%



- Molecule 3: DNA (5'-D(*CP*AP*GP*TP*GP*C)-3')

Chain R:  83% 17%



- Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain H:  25% 25% 75%




- Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain L:  100%



- Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain P:  75% 25%



- Molecule 4: DNA (5'-D(P*GP*CP*CP*G)-3')

Chain U:  25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.97Å 85.82Å 91.42Å 105.22° 92.58° 111.30°	Depositor
Resolution (Å)	38.16 – 2.25 38.16 – 2.25	Depositor EDS
% Data completeness (in resolution range)	91.5 (38.16-2.25) 88.7 (38.16-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.183 , 0.222 0.182 , 0.221	Depositor DCC
R_{free} test set	3809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11774	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DUP, NA, MG, EDO, SO4

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	0.28	0/2587	0.46	0/3493
1	B	0.33	0/2498	0.55	0/3382
1	C	0.31	0/2550	0.55	0/3445
1	D	0.30	0/2467	0.52	0/3348
2	G	0.67	0/158	0.78	0/242
2	K	0.57	0/158	0.87	0/242
2	O	0.56	0/158	0.77	0/242
2	T	0.60	0/158	0.74	0/242
3	F	0.63	0/134	0.88	0/205
3	J	0.57	0/134	0.87	0/205
3	N	0.55	0/134	0.84	0/205
3	R	0.57	0/134	0.81	0/205
4	H	1.24	1/92 (1.1%)	0.80	0/138
4	L	1.20	1/92 (1.1%)	0.76	0/138
4	P	1.22	1/92 (1.1%)	0.86	0/138
4	U	1.20	1/92 (1.1%)	0.65	0/138
All	All	0.40	4/11638 (0.0%)	0.57	0/16008

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	DG	OP3-P	-10.71	1.48	1.61
4	P	1	DG	OP3-P	-10.67	1.48	1.61
4	L	1	DG	OP3-P	-10.59	1.48	1.61
4	U	1	DG	OP3-P	-10.59	1.48	1.61

There are no bond angle outliers.

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	2534	0	2485	4	0
1	B	2446	0	2350	12	0
1	C	2499	0	2427	16	0
1	D	2415	0	2245	17	0
2	G	141	0	77	4	0
2	K	141	0	78	0	0
2	O	141	0	78	1	0
2	T	141	0	78	0	0
3	F	120	0	69	2	0
3	J	120	0	69	0	0
3	N	120	0	69	1	0
3	R	120	0	69	1	0
4	H	83	0	43	1	0
4	L	83	0	43	2	0
4	P	83	0	43	0	0
4	U	83	0	41	1	0
5	A	28	0	12	0	0
5	B	28	0	12	0	0
5	C	28	0	12	0	0
5	D	28	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	N	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	4	0	6	1	0
8	N	4	0	5	0	0
9	F	10	0	0	0	0
9	N	10	0	0	0	0
10	A	111	0	0	0	0
10	B	70	0	0	0	0
10	C	51	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	36	0	0	2	0
10	F	19	0	0	0	0
10	G	7	0	0	0	0
10	H	5	0	0	0	0
10	J	16	0	0	0	0
10	K	7	0	0	0	0
10	L	1	0	0	0	0
10	N	14	0	0	0	0
10	O	3	0	0	0	0
10	R	11	0	0	0	0
10	T	2	0	0	0	0
10	U	1	0	0	0	0
All	All	11774	0	10323	58	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 (58) 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:519:LEU:HD21	1:D:565:LEU:HD11	1.50	0.91
1:D:431:LEU:HD23	1:D:503:LEU:HD13	1.63	0.79
1:C:534:THR:HG23	1:C:551:LEU:HD21	1.68	0.76
1:D:559:VAL:O	1:D:563:LEU:HD12	1.95	0.66
1:D:519:LEU:CD2	1:D:565:LEU:HD11	2.26	0.64
1:B:269:VAL:HG21	1:B:336:GLU:CG	2.28	0.63
1:B:431:LEU:HD22	1:B:499:PHE:HE1	1.64	0.62
1:C:473:TYR:O	1:C:474:LEU:HD23	2.00	0.61
1:C:396:GLU:HG3	1:C:414:ALA:HB2	1.84	0.60
1:B:269:VAL:HG21	1:B:336:GLU:HG2	1.85	0.59
2:G:1[B]:DC:H2'	2:G:2:DG:N7	2.22	0.54
1:B:269:VAL:HG21	1:B:336:GLU:HG3	1.90	0.53
1:B:396:GLU:HG3	1:B:414:ALA:HB2	1.90	0.53
1:C:518:ALA:O	1:C:522:THR:HG23	2.08	0.53
2:G:1[B]:DC:C2'	2:G:2:DG:C8	2.93	0.52
1:D:434:HIS:ND1	1:D:435:PRO:HD2	2.25	0.52
1:C:534:THR:CG2	1:C:551:LEU:HD21	2.40	0.51
1:A:431:LEU:HD23	1:A:432:ILE:N	2.25	0.51
1:B:246:SER:O	1:B:249:ALA:HB2	2.11	0.51
1:D:564:GLY:C	1:D:565:LEU:HD12	2.31	0.51
1:B:525:MET:HG2	1:B:534:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:LEU:HD23	1:D:503:LEU:CD1	2.39	0.50
1:B:563:LEU:CB	1:B:565:LEU:HD23	2.43	0.49
1:D:312:LYS:NZ	10:D:704:HOH:O	2.39	0.49
1:C:267:TYR:CZ	1:C:275:ARG:HD3	2.48	0.49
4:L:3:DC:H2''	4:L:4[A]:DG:C8	2.48	0.49
4:H:3:DC:H2''	4:H:4[B]:DG:N7	2.29	0.47
1:C:302:ILE:HB	1:C:305:ILE:HD12	1.95	0.47
1:A:342:TRP:CZ2	3:F:5:DG:H4'	2.51	0.46
1:B:473:TYR:O	1:B:474:LEU:HD23	2.16	0.46
1:C:316:ILE:HD11	1:C:322:LEU:HD12	1.99	0.45
1:D:470:GLN:HG2	1:D:494:VAL:HG12	1.97	0.45
4:L:2:DC:H2'	4:L:3:DC:C6	2.53	0.43
1:D:472:LYS:NZ	10:D:709:HOH:O	2.51	0.43
2:G:1[B]:DC:H2'	2:G:2:DG:C5	2.53	0.43
1:D:312:LYS:HG2	1:D:322:LEU:HD11	2.00	0.43
1:B:431:LEU:C	1:B:431:LEU:HD23	2.40	0.43
1:C:474:LEU:HD22	1:C:490:ASP:CG	2.39	0.42
1:D:436:ASP:OD1	1:D:437:GLY:N	2.51	0.42
1:D:342:TRP:CZ2	3:R:5:DG:H4'	2.55	0.42
1:D:470:GLN:CG	1:D:494:VAL:HG12	2.50	0.42
2:G:1[B]:DC:H2'	2:G:2:DG:C8	2.54	0.42
1:C:332:VAL:O	1:C:336:GLU:HG3	2.18	0.42
2:O:1[A]:DC:H2''	2:O:2:DG:C8	2.54	0.42
1:A:474:LEU:HD22	1:A:490:ASP:CG	2.41	0.42
1:B:431:LEU:HD22	1:B:499:PHE:CE1	2.48	0.42
1:C:473:TYR:C	1:C:474:LEU:HD23	2.40	0.41
1:C:267:TYR:CE2	1:C:275:ARG:HD3	2.56	0.41
1:D:272:ASP:OD2	1:D:275:ARG:NH1	2.54	0.41
1:D:316:ILE:HD11	1:D:322:LEU:HD22	2.01	0.41
4:U:3:DC:H2''	4:U:4[B]:DG:C8	2.55	0.41
1:A:394:GLU:HB3	8:A:704:EDO:H12	2.02	0.41
1:C:448:LEU:O	1:C:452:ARG:HG3	2.21	0.41
1:C:555:THR:HG22	1:C:556:GLU:N	2.35	0.41
1:C:342:TRP:CZ2	3:N:5:DG:H4'	2.56	0.41
1:D:470:GLN:CD	1:D:494:VAL:HG12	2.42	0.40
1:C:272:ASP:OD2	1:C:275:ARG:NH1	2.51	0.40
3:F:1:DC:N3	1:B:465:GLU:OE2	2.55	0.40

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	323/348 (93%)	317 (98%)	6 (2%)	0	100	100
1	B	320/348 (92%)	310 (97%)	10 (3%)	0	100	100
1	C	322/348 (92%)	319 (99%)	3 (1%)	0	100	100
1	D	323/348 (93%)	313 (97%)	10 (3%)	0	100	100
All	All	1288/1392 (92%)	1259 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	260/289 (90%)	259 (100%)	1 (0%)	91	94
1	B	241/289 (83%)	240 (100%)	1 (0%)	91	94
1	C	250/289 (86%)	248 (99%)	2 (1%)	81	88
1	D	229/289 (79%)	227 (99%)	2 (1%)	78	86
All	All	980/1156 (85%)	974 (99%)	6 (1%)	86	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	506	PHE
1	B	506	PHE

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Mol	Chain	Res	Type
1	C	364	ARG
1	C	506	PHE
1	D	434	HIS
1	D	506	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 20 ligands modelled in this entry, 10 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	$\# Z > 2$
9	SO4	F	102[B]	-	4,4,4	0.14	0	6,6,6	0.28	0
5	DUP	A	701	6	28,29,29	2.14	5 (17%)	37,45,45	2.18	10 (27%)
5	DUP	D	603	6	28,29,29	2.15	6 (21%)	37,45,45	2.02	8 (21%)
8	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.35	0
5	DUP	B	603	6	28,29,29	2.14	6 (21%)	37,45,45	2.03	9 (24%)
9	SO4	N	102[A]	-	4,4,4	0.18	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	N	102[B]	-	4,4,4	0.16	0	6,6,6	0.19	0
5	DUP	C	603	6	28,29,29	2.19	7 (25%)	37,45,45	1.84	7 (18%)
9	SO4	F	102[A]	-	4,4,4	0.16	0	6,6,6	0.15	0
8	EDO	N	103	7	3,3,3	0.56	0	2,2,2	0.10	0

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
5	DUP	A	701	6	-	5/19/34/34	0/2/2/2
5	DUP	D	603	6	-	3/19/34/34	0/2/2/2
8	EDO	A	704	-	-	0/1/1/1	-
5	DUP	B	603	6	-	5/19/34/34	0/2/2/2
5	DUP	C	603	6	-	2/19/34/34	0/2/2/2
8	EDO	N	103	7	-	1/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	603	DUP	C6-C5	-6.44	1.35	1.52
5	B	603	DUP	C6-C5	-6.38	1.35	1.52
5	A	701	DUP	C6-C5	-6.38	1.35	1.52
5	C	603	DUP	C6-C5	-6.38	1.35	1.52
5	A	701	DUP	C6-N1	-5.65	1.37	1.47
5	C	603	DUP	C6-N1	-5.56	1.37	1.47
5	B	603	DUP	C6-N1	-5.43	1.37	1.47
5	D	603	DUP	C6-N1	-5.25	1.37	1.47
5	B	603	DUP	C5-C4	-3.47	1.42	1.50
5	C	603	DUP	C5-C4	-3.45	1.42	1.50
5	A	701	DUP	C5-C4	-3.45	1.42	1.50
5	D	603	DUP	C5-C4	-3.41	1.42	1.50
5	A	701	DUP	PB-O2B	-3.25	1.48	1.56
5	C	603	DUP	PA-O2A	-3.08	1.48	1.56
5	A	701	DUP	PA-O2A	-3.08	1.48	1.56
5	B	603	DUP	PB-O2B	-3.01	1.48	1.56
5	D	603	DUP	PB-O2B	-2.98	1.48	1.56
5	D	603	DUP	PA-O2A	-2.94	1.48	1.56
5	C	603	DUP	PB-O2B	-2.82	1.49	1.56
5	B	603	DUP	PA-O2A	-2.68	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	603	DUP	PA-N3A	2.27	1.69	1.63
5	B	603	DUP	PB-N3A	2.21	1.69	1.63
5	C	603	DUP	PA-O1A	2.08	1.49	1.46
5	D	603	DUP	PA-N3A	2.00	1.68	1.63

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	DUP	C2'-C1'-N1	-7.10	106.93	115.61
5	A	701	DUP	C4-N3-C2	-6.68	120.25	125.79
5	D	603	DUP	C4-N3-C2	-6.65	120.27	125.79
5	B	603	DUP	C4-N3-C2	-6.65	120.28	125.79
5	C	603	DUP	C4-N3-C2	-6.58	120.34	125.79
5	B	603	DUP	C2'-C1'-N1	-6.16	108.08	115.61
5	D	603	DUP	C2'-C1'-N1	-6.11	108.14	115.61
5	C	603	DUP	C2'-C1'-N1	-4.99	109.50	115.61
5	D	603	DUP	N3-C2-N1	3.99	120.87	116.65
5	C	603	DUP	N3-C2-N1	3.92	120.80	116.65
5	A	701	DUP	N3-C2-N1	3.91	120.78	116.65
5	B	603	DUP	N3-C2-N1	3.81	120.69	116.65
5	A	701	DUP	O1B-PB-N3A	-3.13	107.17	111.77
5	A	701	DUP	O2B-PB-O1B	2.93	116.06	109.92
5	B	603	DUP	C5-C4-N3	2.80	119.80	116.65
5	B	603	DUP	O2B-PB-O1B	2.74	115.67	109.92
5	A	701	DUP	O2-C2-N1	-2.73	119.67	123.11
5	A	701	DUP	O1A-PA-N3A	-2.73	107.75	111.77
5	D	603	DUP	C5-C4-N3	2.67	119.64	116.65
5	D	603	DUP	O2B-PB-O1B	2.58	115.33	109.92
5	C	603	DUP	C5-C4-N3	2.54	119.50	116.65
5	A	701	DUP	C5-C4-N3	2.50	119.46	116.65
5	D	603	DUP	O2-C2-N1	-2.47	120.01	123.11
5	D	603	DUP	O2A-PA-O1A	2.45	115.07	109.92
5	C	603	DUP	C5-C6-N1	2.45	119.68	111.61
5	A	701	DUP	C5-C6-N1	2.45	119.68	111.61
5	C	603	DUP	O2-C2-N1	-2.42	120.07	123.11
5	D	603	DUP	C5-C6-N1	2.40	119.52	111.61
5	B	603	DUP	C5-C6-N1	2.39	119.47	111.61
5	A	701	DUP	O4'-C1'-N1	2.38	111.44	108.41
5	B	603	DUP	O2-C2-N1	-2.37	120.13	123.11
5	B	603	DUP	O1A-PA-N3A	-2.20	108.53	111.77
5	C	603	DUP	O2B-PB-O1B	2.08	114.29	109.92
5	B	603	DUP	O1B-PB-N3A	-2.01	108.82	111.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

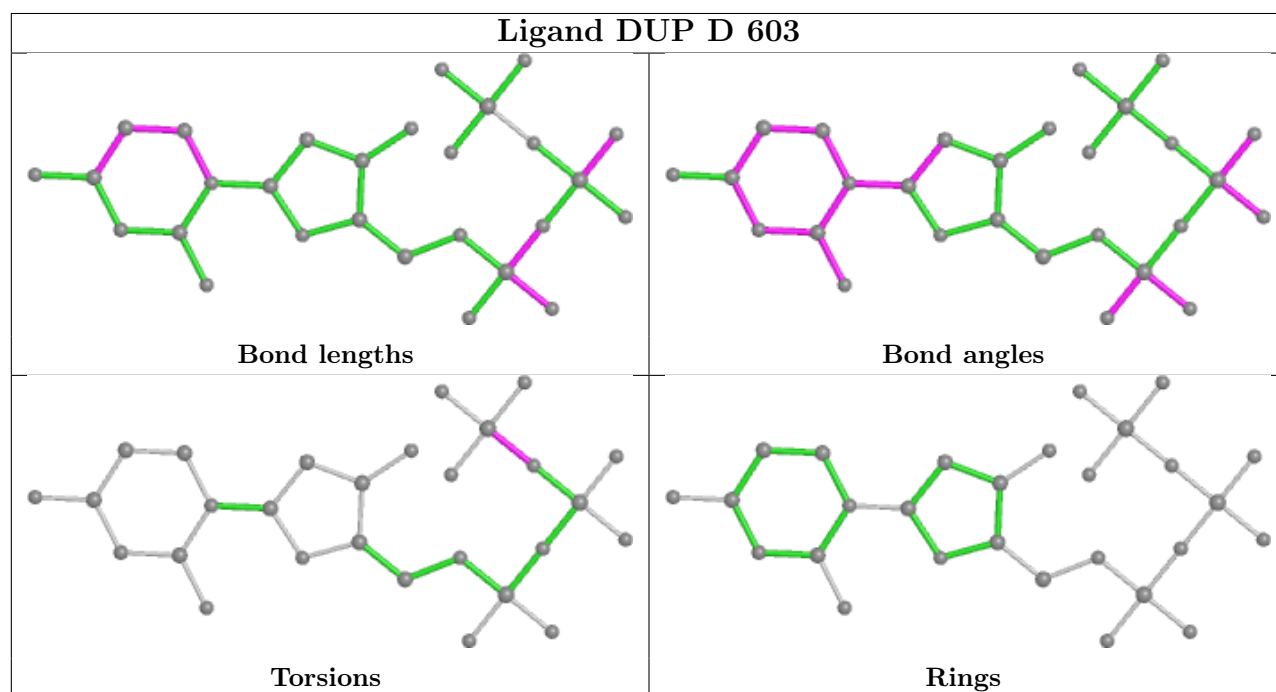
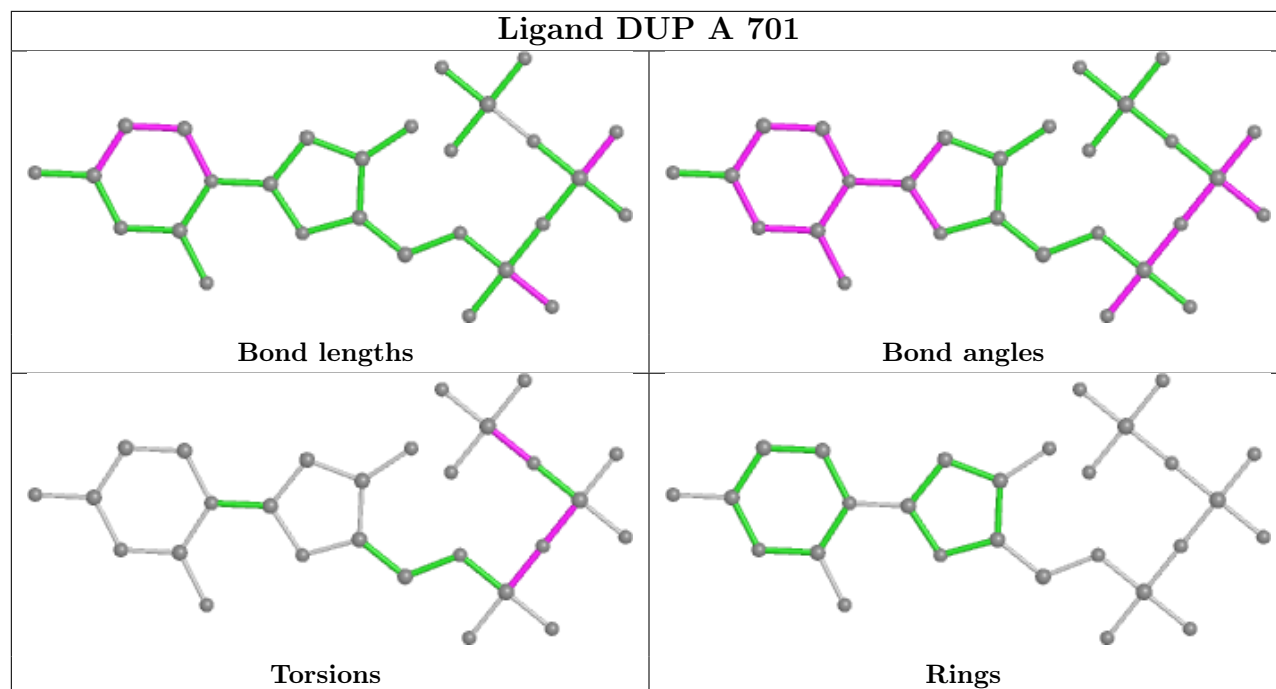
Mol	Chain	Res	Type	Atoms
5	A	701	DUP	PB-N3A-PA-O1A
5	A	701	DUP	PA-N3A-PB-O1B
5	B	603	DUP	PB-N3A-PA-O1A
5	B	603	DUP	PA-N3A-PB-O1B
5	B	603	DUP	PB-O3B-PG-O1G
5	D	603	DUP	PB-O3B-PG-O3G
5	A	701	DUP	PB-O3B-PG-O2G
5	B	603	DUP	PB-O3B-PG-O3G
5	B	603	DUP	PB-N3A-PA-O5'
5	C	603	DUP	PB-O3B-PG-O2G
5	A	701	DUP	PB-O3B-PG-O1G
5	A	701	DUP	PB-O3B-PG-O3G
5	C	603	DUP	PB-O3B-PG-O1G
5	D	603	DUP	PB-O3B-PG-O1G
8	N	103	EDO	O1-C1-C2-O2
5	D	603	DUP	PB-O3B-PG-O2G

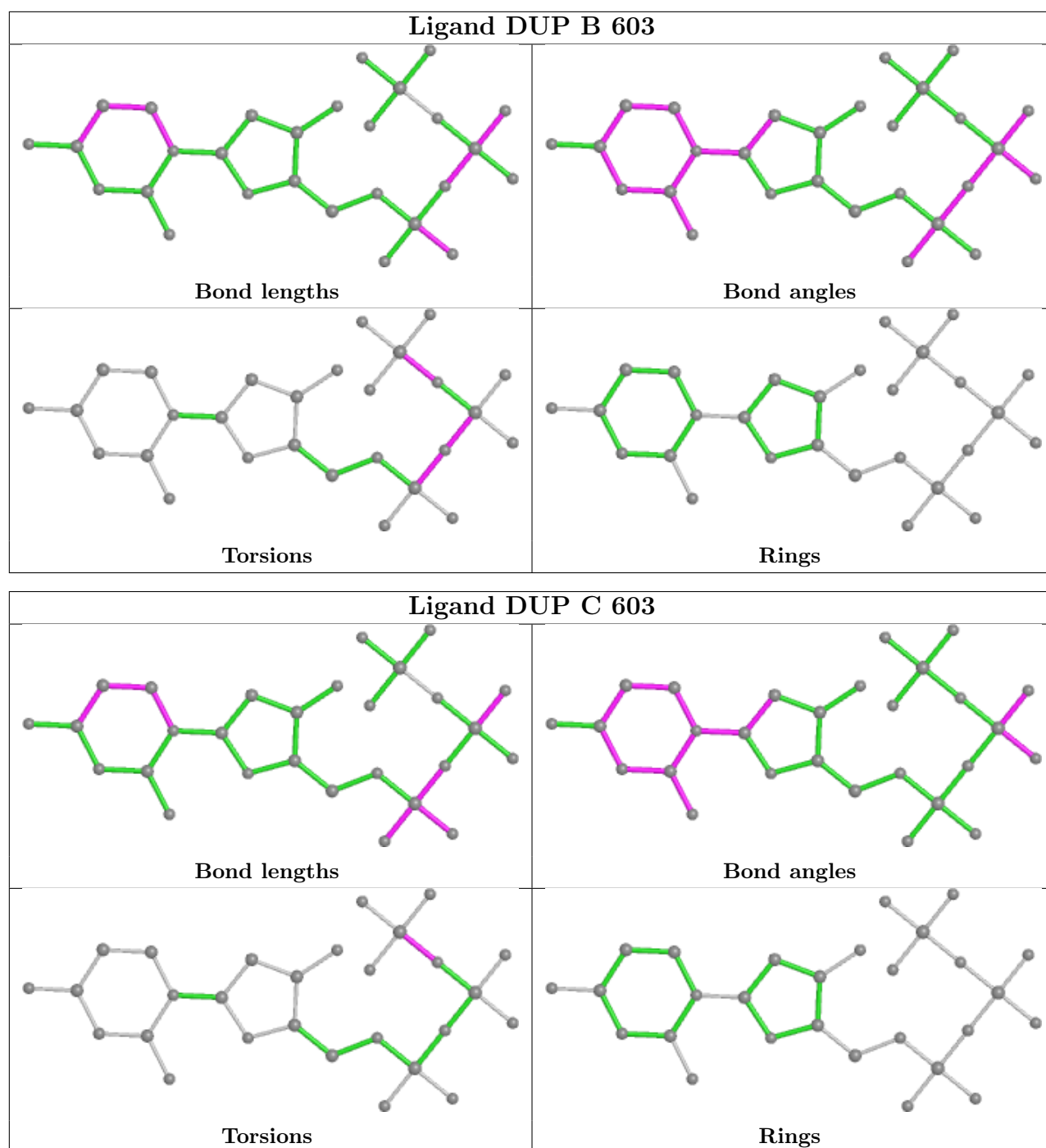
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	704	EDO	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/348 (93%)	-0.27	3 (0%) 84 85	23, 37, 56, 87	0
1	B	324/348 (93%)	-0.13	6 (1%) 66 69	27, 44, 71, 97	0
1	C	326/348 (93%)	0.09	16 (4%) 29 32	29, 48, 75, 103	0
1	D	325/348 (93%)	0.30	33 (10%) 6 6	34, 62, 105, 122	0
2	G	7/7 (100%)	-0.09	0 100 100	28, 32, 60, 61	1 (14%)
2	K	7/7 (100%)	0.03	0 100 100	31, 33, 72, 77	1 (14%)
2	O	7/7 (100%)	0.11	1 (14%) 2 2	39, 43, 62, 64	1 (14%)
2	T	7/7 (100%)	0.04	0 100 100	55, 56, 83, 84	1 (14%)
3	F	6/6 (100%)	-0.30	0 100 100	25, 26, 27, 29	0
3	J	6/6 (100%)	-0.22	0 100 100	25, 26, 28, 31	0
3	N	6/6 (100%)	-0.33	0 100 100	35, 36, 38, 39	0
3	R	6/6 (100%)	-0.49	0 100 100	33, 34, 40, 46	0
4	H	4/4 (100%)	0.24	1 (25%) 0 0	39, 43, 49, 59	1 (25%)
4	L	4/4 (100%)	-0.39	0 100 100	48, 49, 58, 72	1 (25%)
4	P	4/4 (100%)	-0.63	0 100 100	45, 45, 51, 56	1 (25%)
4	U	4/4 (100%)	0.08	0 100 100	53, 54, 63, 71	1 (25%)
All	All	1369/1460 (93%)	-0.01	60 (4%) 34 37	23, 46, 86, 122	8 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	PRO	6.1
1	C	535	ALA	4.9
1	D	535	ALA	4.8
1	C	242	ALA	4.4
1	D	239	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	442	GLY	4.2
1	D	406	PHE	4.0
1	C	250	THR	4.0
1	B	549	ARG	3.9
1	B	247	GLN	3.8
1	D	242	ALA	3.8
1	D	565	LEU	3.8
1	D	247	GLN	3.8
1	B	246	SER	3.7
1	D	568	ARG	3.6
1	D	483	GLY	3.6
1	C	536	VAL	3.6
1	C	483	GLY	3.6
1	B	245	SER	3.5
4	H	4[B]	DG	3.5
1	C	534	THR	3.4
1	C	239	TRP	3.3
1	D	522	THR	3.3
1	D	421	GLY	3.2
1	D	566	PRO	3.2
1	A	548	GLY	3.1
1	D	405	ALA	3.1
1	C	482	PRO	3.1
1	D	246	SER	3.0
1	D	563	LEU	2.9
1	D	245	SER	2.9
1	D	564	GLY	2.8
1	D	409	GLY	2.8
1	C	525	MET	2.7
1	C	247	GLN	2.7
1	C	246	SER	2.6
1	C	244	PRO	2.5
1	D	440	HIS	2.5
1	D	443	ILE	2.4
1	D	441	ARG	2.4
1	D	411	LEU	2.4
1	C	549	ARG	2.4
1	D	534	THR	2.4
1	B	239	TRP	2.3
1	D	408	SER	2.3
1	D	327	HIS	2.3
1	D	482	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	404	GLN	2.2
1	A	242	ALA	2.2
1	C	245	SER	2.2
1	C	368	SER	2.2
1	D	526	SER	2.2
1	B	362	ASP	2.1
1	D	241	CYS	2.1
1	D	436	ASP	2.1
1	D	567	TYR	2.1
1	D	452	ARG	2.1
1	A	327	HIS	2.1
2	O	1[A]	DC	2.0
1	C	356	GLY	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.

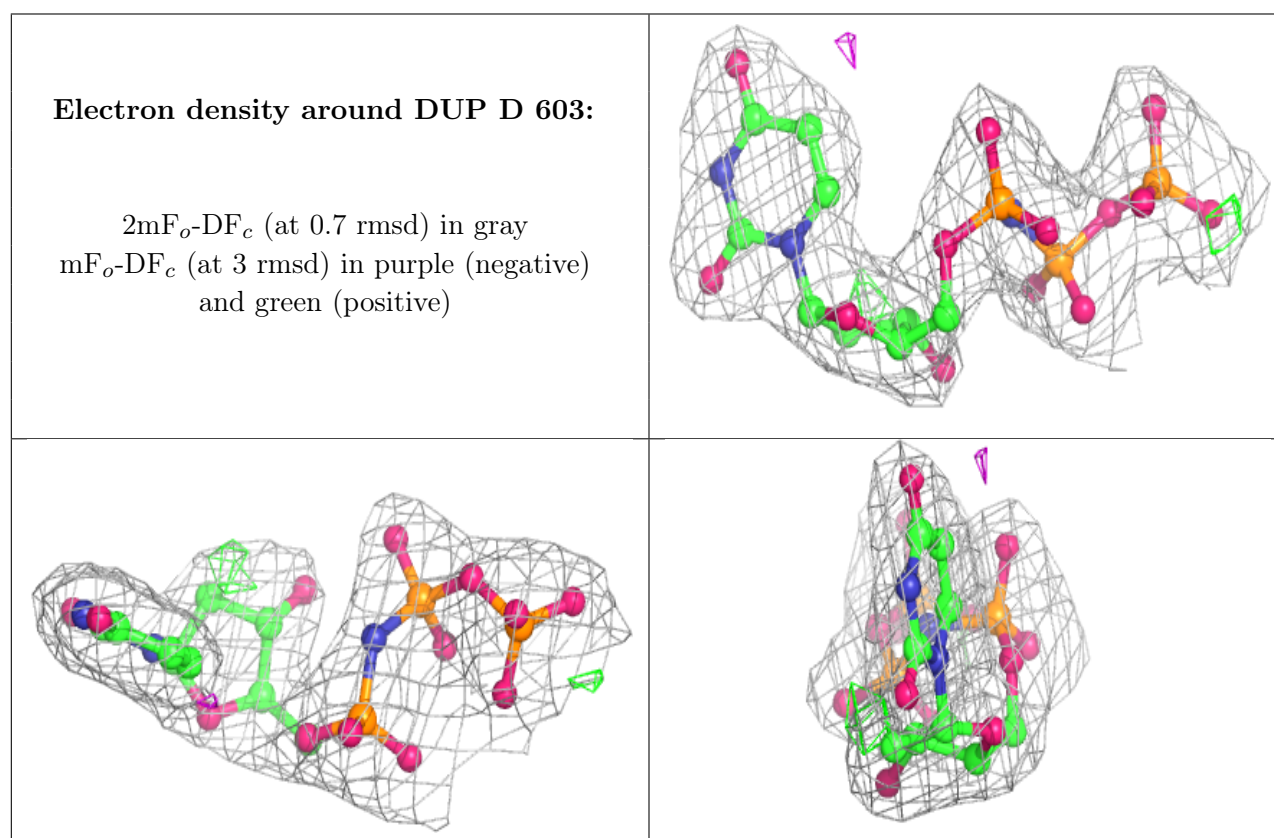
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	601	1/1	0.84	0.14	48,48,48,48	0
8	EDO	N	103	4/4	0.89	0.15	34,40,48,58	0
7	NA	B	602	1/1	0.92	0.13	29,29,29,29	0
6	MG	C	601	1/1	0.95	0.10	37,37,37,37	0
7	NA	A	703	1/1	0.95	0.08	28,28,28,28	0
6	MG	F	101	1/1	0.96	0.15	27,27,27,27	0
8	EDO	A	704	4/4	0.96	0.11	40,43,50,51	0
6	MG	A	702	1/1	0.96	0.07	24,24,24,24	0
9	SO4	N	102[A]	5/5	0.96	0.27	29,32,36,39	5
9	SO4	N	102[B]	5/5	0.96	0.27	30,34,38,40	5

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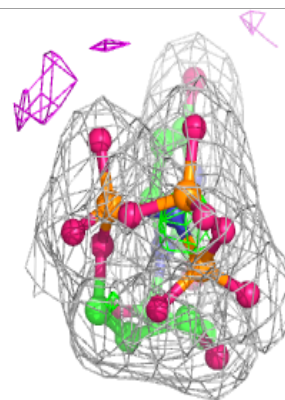
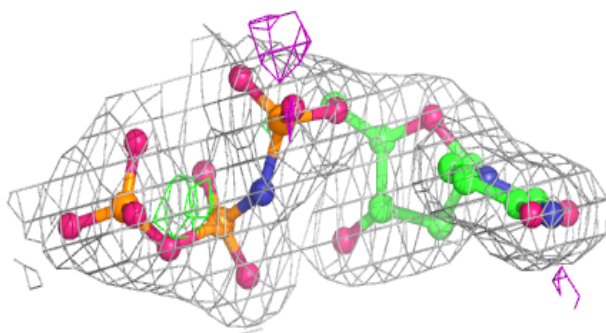
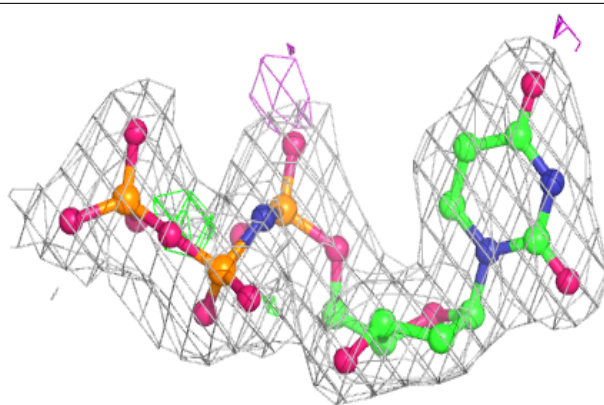
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	N	101	1/1	0.97	0.13	36,36,36,36	0
5	DUP	D	603	28/28	0.97	0.13	28,43,52,53	0
9	SO4	F	102[A]	5/5	0.98	0.29	23,28,30,32	5
9	SO4	F	102[B]	5/5	0.98	0.29	23,27,31,33	5
7	NA	C	602	1/1	0.98	0.08	31,31,31,31	0
7	NA	D	602	1/1	0.98	0.06	33,33,33,33	0
5	DUP	B	603	28/28	0.99	0.14	23,25,32,33	0
5	DUP	C	603	28/28	0.99	0.15	27,33,38,41	0
6	MG	B	601	1/1	0.99	0.08	30,30,30,30	0
5	DUP	A	701	28/28	0.99	0.13	23,23,26,35	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.

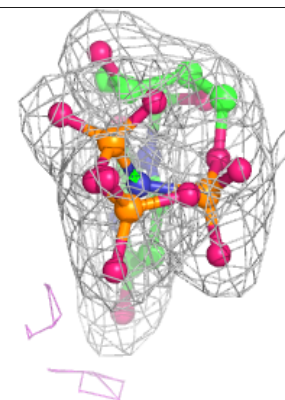
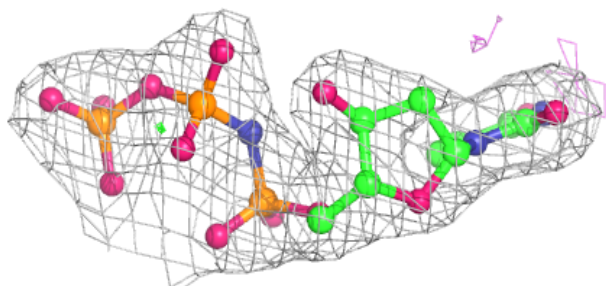
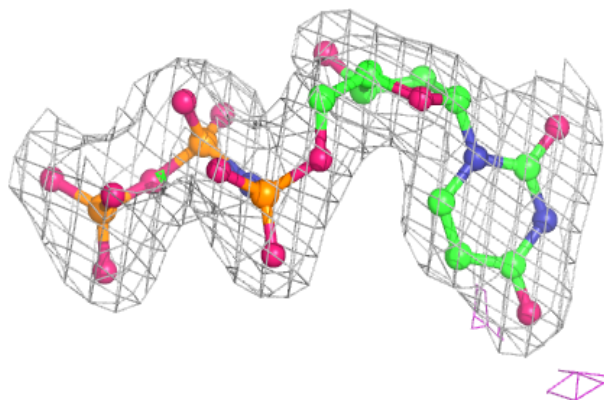


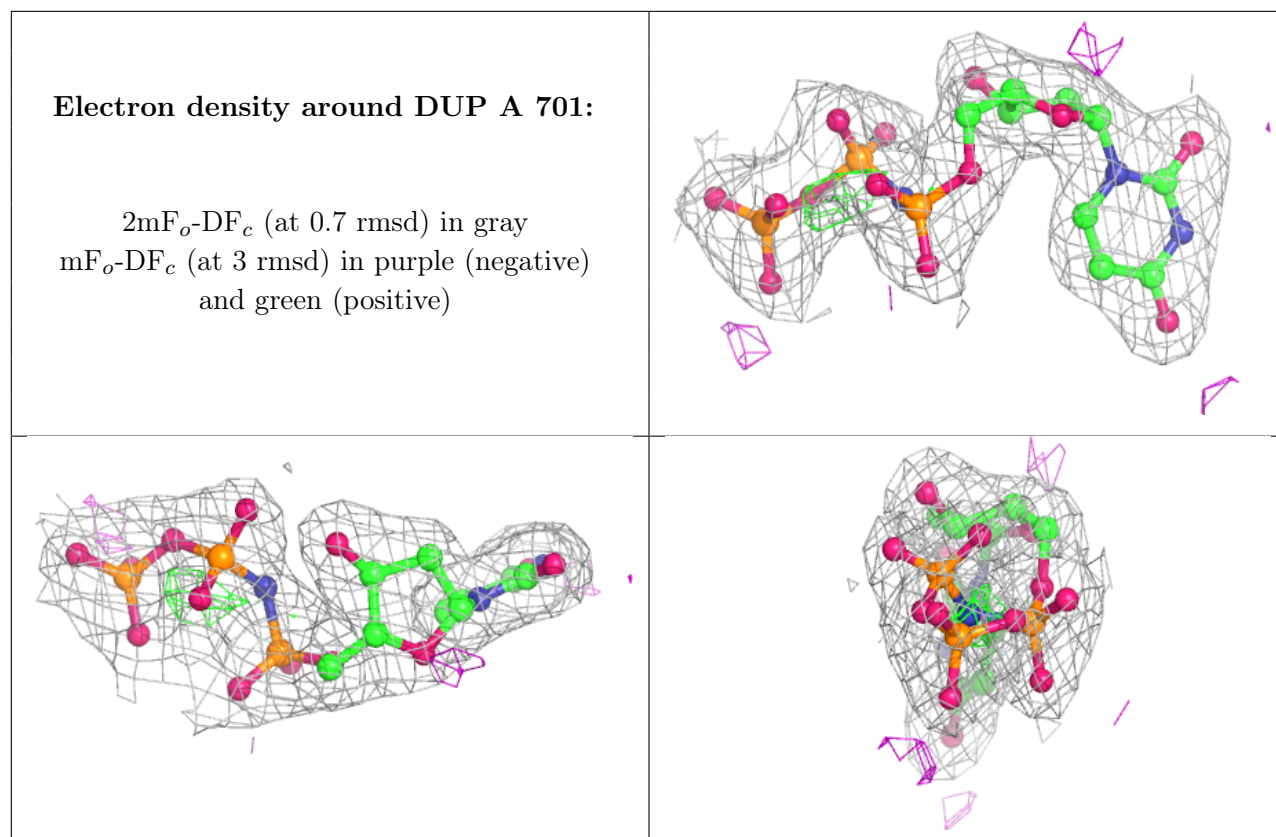
Electron density around DUP B 603:

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

**Electron density around DUP C 603:**

$2mF_o-DF_c$ (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.