wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2026 – 08:26 AM UTC

PDB ID	:	4LX0 / pdb_00004lx0
Title	:	Crystal structure of Myo5b globular tail domain in complex with active Rab11a
Authors	:	Pylypenko, O.; Attanda, W.; Gauquelin, C.; Houdusse, A.
Deposited on	:	2013-07-29
Resolution	:	2.19 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

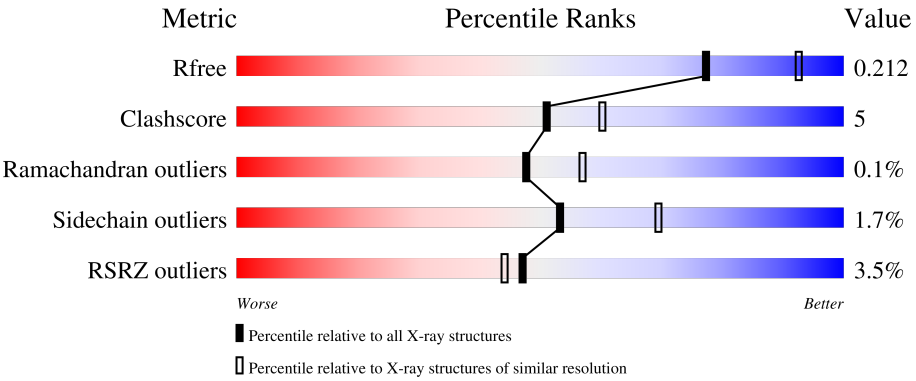
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.19 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	177	90% 6%
1	C	177	7% 81% 15%
2	B	427	4% 81% 8% 11%
2	D	427	3% 76% 12% 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9344 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 Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1352	856	232	263	1			
1	C	171	Total	C	N	O	S	0	0	0
			1317	835	223	258	1			

- Molecule 2 is a protein called Unconventional myosin-Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	382	Total	C	N	O	S	0	1	0
			2979	1892	509	553	25			
2	D	380	Total	C	N	O	S	0	2	0
			2973	1888	501	559	25			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1423	MET	-	expression tag	UNP Q9ULV0
B	1424	ARG	-	expression tag	UNP Q9ULV0
B	1425	SER	-	expression tag	UNP Q9ULV0
B	1426	GLU	-	expression tag	UNP Q9ULV0
B	1427	THR	-	expression tag	UNP Q9ULV0
B	1428	MET	-	expression tag	UNP Q9ULV0
B	1429	SER	-	expression tag	UNP Q9ULV0
B	1430	TYR	-	expression tag	UNP Q9ULV0
B	1431	TYR	-	expression tag	UNP Q9ULV0
B	1432	HIS	-	expression tag	UNP Q9ULV0
B	1433	HIS	-	expression tag	UNP Q9ULV0
B	1434	HIS	-	expression tag	UNP Q9ULV0
B	1435	HIS	-	expression tag	UNP Q9ULV0
B	1436	HIS	-	expression tag	UNP Q9ULV0
B	1437	HIS	-	expression tag	UNP Q9ULV0
B	1438	ASP	-	expression tag	UNP Q9ULV0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1439	TYR	-	expression tag	UNP Q9ULV0
B	1440	ASP	-	expression tag	UNP Q9ULV0
B	1441	ILE	-	expression tag	UNP Q9ULV0
B	1442	PRO	-	expression tag	UNP Q9ULV0
B	1443	THR	-	expression tag	UNP Q9ULV0
B	1444	THR	-	expression tag	UNP Q9ULV0
B	1445	GLU	-	expression tag	UNP Q9ULV0
B	1446	ASN	-	expression tag	UNP Q9ULV0
B	1447	LEU	-	expression tag	UNP Q9ULV0
B	1448	TYR	-	expression tag	UNP Q9ULV0
B	1449	PHE	-	expression tag	UNP Q9ULV0
B	1450	GLN	-	expression tag	UNP Q9ULV0
B	1451	GLY	-	expression tag	UNP Q9ULV0
B	1452	ALA	-	expression tag	UNP Q9ULV0
B	1452A	MET	-	expression tag	UNP Q9ULV0
B	1452B	GLY	-	expression tag	UNP Q9ULV0
B	1452C	SER	-	expression tag	UNP Q9ULV0
B	1455	MET	-	expression tag	UNP Q9ULV0
D	1420	MET	-	expression tag	UNP Q9ULV0
D	1421	ARG	-	expression tag	UNP Q9ULV0
D	1422	SER	-	expression tag	UNP Q9ULV0
D	1423	GLU	-	expression tag	UNP Q9ULV0
D	1424	THR	-	expression tag	UNP Q9ULV0
D	1425	MET	-	expression tag	UNP Q9ULV0
D	1426	SER	-	expression tag	UNP Q9ULV0
D	1427	TYR	-	expression tag	UNP Q9ULV0
D	1428	TYR	-	expression tag	UNP Q9ULV0
D	1429	HIS	-	expression tag	UNP Q9ULV0
D	1430	HIS	-	expression tag	UNP Q9ULV0
D	1431	HIS	-	expression tag	UNP Q9ULV0
D	1432	HIS	-	expression tag	UNP Q9ULV0
D	1433	HIS	-	expression tag	UNP Q9ULV0
D	1434	HIS	-	expression tag	UNP Q9ULV0
D	1435	ASP	-	expression tag	UNP Q9ULV0
D	1436	TYR	-	expression tag	UNP Q9ULV0
D	1437	ASP	-	expression tag	UNP Q9ULV0
D	1438	ILE	-	expression tag	UNP Q9ULV0
D	1439	PRO	-	expression tag	UNP Q9ULV0
D	1440	THR	-	expression tag	UNP Q9ULV0
D	1441	THR	-	expression tag	UNP Q9ULV0
D	1442	GLU	-	expression tag	UNP Q9ULV0
D	1443	ASN	-	expression tag	UNP Q9ULV0

Continued on next page...

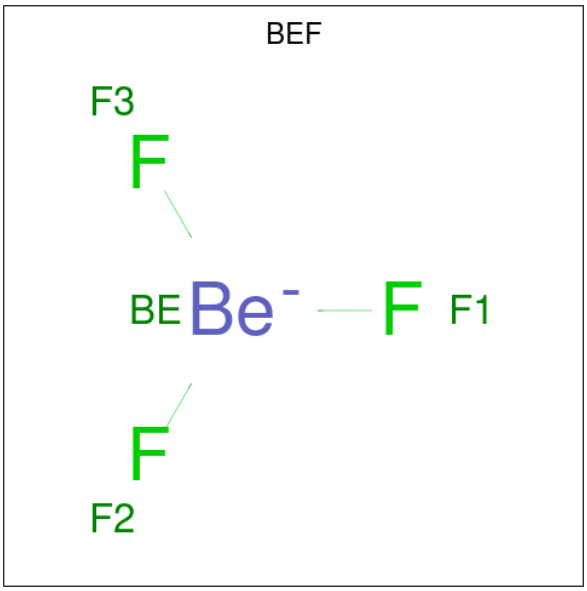
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1444	LEU	-	expression tag	UNP Q9ULV0
D	1445	TYR	-	expression tag	UNP Q9ULV0
D	1446	PHE	-	expression tag	UNP Q9ULV0
D	1447	GLN	-	expression tag	UNP Q9ULV0
D	1448	GLY	-	expression tag	UNP Q9ULV0
D	1449	ALA	-	expression tag	UNP Q9ULV0
D	1450	MET	-	expression tag	UNP Q9ULV0
D	1451	GLY	-	expression tag	UNP Q9ULV0
D	1454	SER	-	expression tag	UNP Q9ULV0
D	1455	MET	-	expression tag	UNP Q9ULV0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

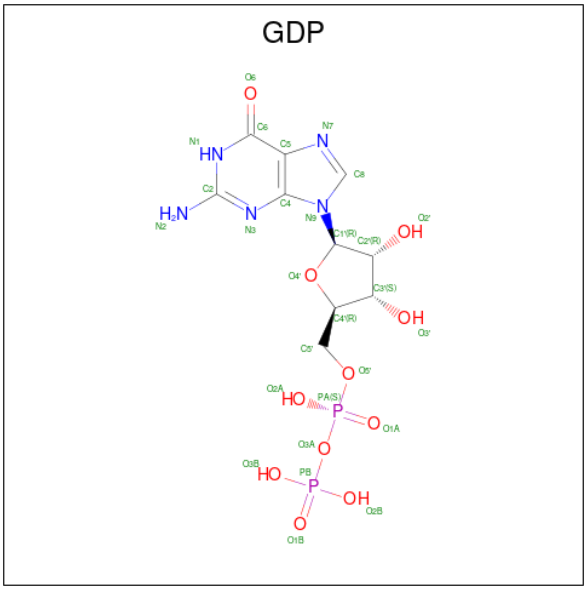
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



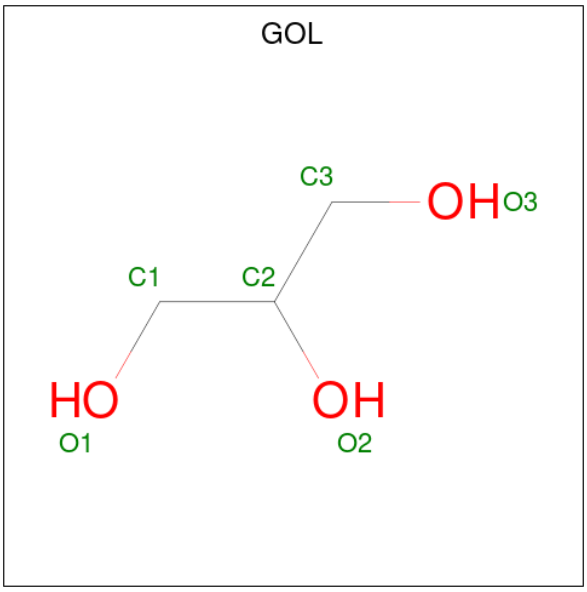
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Be F 4 1 3	0	0
4	C	1	Total Be F 4 1 3	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
5	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			6	3	3			

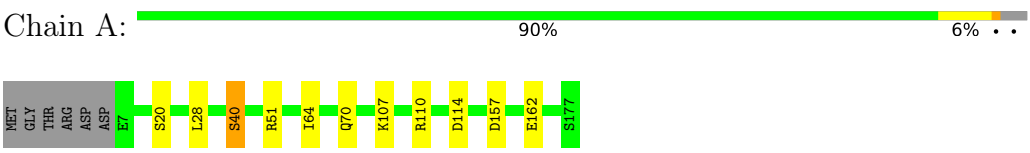
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	187	Total O 187 187	0	0
7	B	225	Total O 225 225	0	0
7	C	51	Total O 51 51	0	0
7	D	188	Total O 188 188	0	0

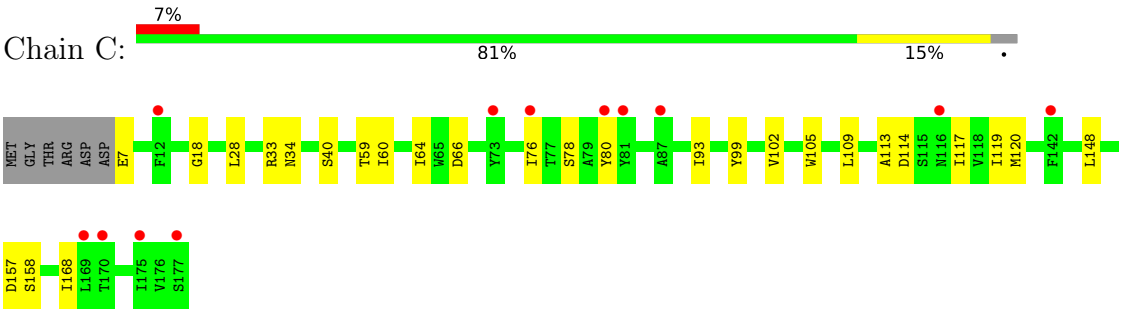
3 Residue-property plots (i)

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.

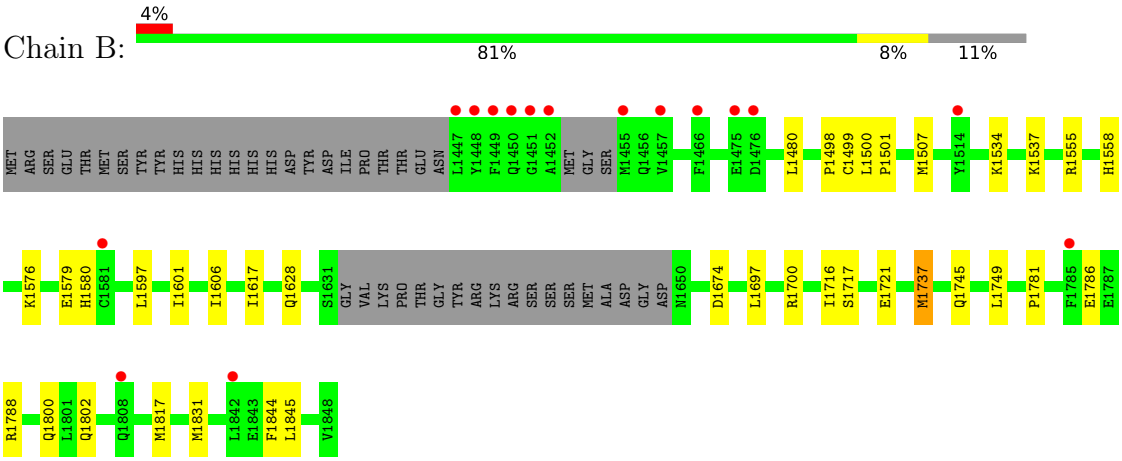
• Molecule 1: Ras-related protein Rab-11A



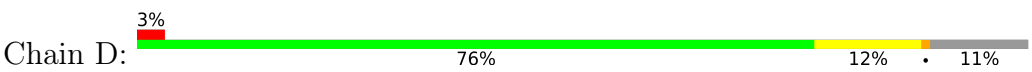
• Molecule 1: Ras-related protein Rab-11A

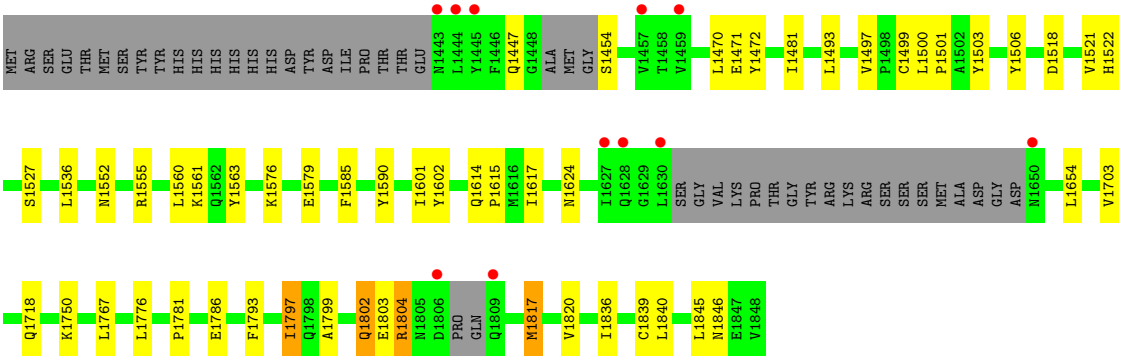


• Molecule 2: Unconventional myosin-Vb



• Molecule 2: Unconventional myosin-Vb




MET ARG SER GLU THR MET SER TYR TYR HIS HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU N1443 L1444 Y1445 F1446 Q1447 G1448 ALA MET GLY S1454 V1457 T1458 V1459 L1470 E1471 Y1472 I1481 L1493 V1497 P1498 C1499 L1500 P1501 A1502 Y1503 Y1506 D1518 V1521 H1522
S1527 L1536 N1552 R1555 L1560 K1561 Q1562 Y1563 K1576 E1579 F1585 Y1590 I1601 Y1602 Q1614 P1615 M1616 I1617 N1624 I1627 Q1628 G1629 L1630 SER GLY VAL LYS PRO THR GLY TYR ARG LYS ARG SER SER SER MET ALA ASP GLY ASP N1650 L1654 V1703
Q1718 K1750 L1767 L1776 P1781 E1786 F1793 I1797 Q1798 A1799 Q1802 E1803 R1804 N1805 D1806 PRO GLN Q1809 M1817 V1820 I1836 C1839 L1840 L1845 N1846 E1847 V1848

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.10Å 125.92Å 157.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 2.19 31.50 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.50-2.19) 99.9 (31.50-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.181 , 0.218 0.175 , 0.212	Depositor DCC
R_{free} test set	4890 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	51.8	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9344	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: BEF, GOL, GDP, MG

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	0.93	0/1374	0.95	0/1859
1	C	0.62	0/1338	0.84	0/1815
2	B	0.79	0/3032	0.90	3/4112 (0.1%)
2	D	0.77	0/3026	0.87	2/4101 (0.0%)
All	All	0.78	0/8770	0.89	5/11887 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1802	GLN	N-CA-C	6.39	119.06	111.33
2	D	1617	ILE	N-CA-C	5.53	115.66	110.30
2	B	1617	ILE	N-CA-C	5.37	115.57	110.42
2	B	1700	ARG	N-CA-C	5.20	116.87	108.34
2	D	1521	VAL	N-CA-C	-5.15	105.69	110.53

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	1352	0	1333	8	0
1	C	1317	0	1268	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2979	0	2928	23	0
2	D	2973	0	2913	43	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
5	A	28	0	12	1	0
5	C	28	0	12	0	0
6	A	6	0	8	0	0
7	A	187	0	0	3	0
7	B	225	0	0	2	0
7	C	51	0	0	1	0
7	D	188	0	0	2	0
All	All	9344	0	8474	89	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 5.

The worst 5 of 89 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1767:LEU:O	2:D:1804:ARG:NH2	2.24	0.69
2:D:1776:LEU:CD1	2:D:1797:ILE:HD13	2.23	0.69
1:C:117:ILE:HD11	7:C:312:HOH:O	1.95	0.67
2:D:1839:CYS:SG	2:D:1840:LEU:HD12	2.35	0.67
2:D:1776:LEU:HD11	2:D:1797:ILE:HD13	1.76	0.66

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	169/177 (96%)	164 (97%)	5 (3%)	0	100 100
1	C	169/177 (96%)	162 (96%)	6 (4%)	1 (1%)	21 23
2	B	377/427 (88%)	368 (98%)	9 (2%)	0	100 100
2	D	374/427 (88%)	367 (98%)	7 (2%)	0	100 100
All	All	1089/1208 (90%)	1061 (97%)	27 (2%)	1 (0%)	48 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	ASN

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	143/150 (95%)	140 (98%)	3 (2%)	47 63
1	C	134/150 (89%)	129 (96%)	5 (4%)	30 41
2	B	323/391 (83%)	321 (99%)	2 (1%)	78 89
2	D	324/391 (83%)	318 (98%)	6 (2%)	50 66
All	All	924/1082 (85%)	908 (98%)	16 (2%)	53 69

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	1804	ARG
2	D	1802	GLN
1	C	93	ILE
2	D	1797	ILE
1	C	40	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1511	HIS
2	B	1600	GLN
2	D	1718	GLN
2	D	1802	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	BEF	A	202	5	0,3,3	-	-	-		
5	GDP	C	203	3,4	29,30,30	1.16	4 (13%)	45,47,47	2.10	11 (24%)
6	GOL	A	204	-	5,5,5	0.34	0	5,5,5	0.44	0
4	BEF	C	202	5	0,3,3	-	-	-		
5	GDP	A	203	3,4	29,30,30	1.20	3 (10%)	45,47,47	1.81	11 (24%)

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
6	GOL	A	204	-	-	3/4/4/4	-
5	GDP	A	203	3,4	-	1/16/32/32	0/3/3/3
5	GDP	C	203	3,4	-	1/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	203	GDP	C6-N1	-2.91	1.33	1.38
5	A	203	GDP	C5-C4	2.82	1.46	1.38
5	C	203	GDP	C5-C4	2.50	1.45	1.38
5	C	203	GDP	C5-N7	-2.29	1.34	1.39
5	A	203	GDP	C6-N1	-2.29	1.34	1.38

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	203	GDP	C5-C4-N3	-6.17	118.57	128.39
5	C	203	GDP	O4'-C1'-N9	5.64	121.14	108.36
5	C	203	GDP	N9-C4-N3	5.24	136.44	125.95
5	C	203	GDP	C2-N3-C4	5.02	120.95	112.30
5	A	203	GDP	C5-C4-N3	-4.46	121.29	128.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	203	GDP	PA-O3A-PB-O2B
5	C	203	GDP	PA-O3A-PB-O2B
6	A	204	GOL	O1-C1-C2-C3
6	A	204	GOL	O1-C1-C2-O2
6	A	204	GOL	O2-C2-C3-O3

There are no ring outliers.

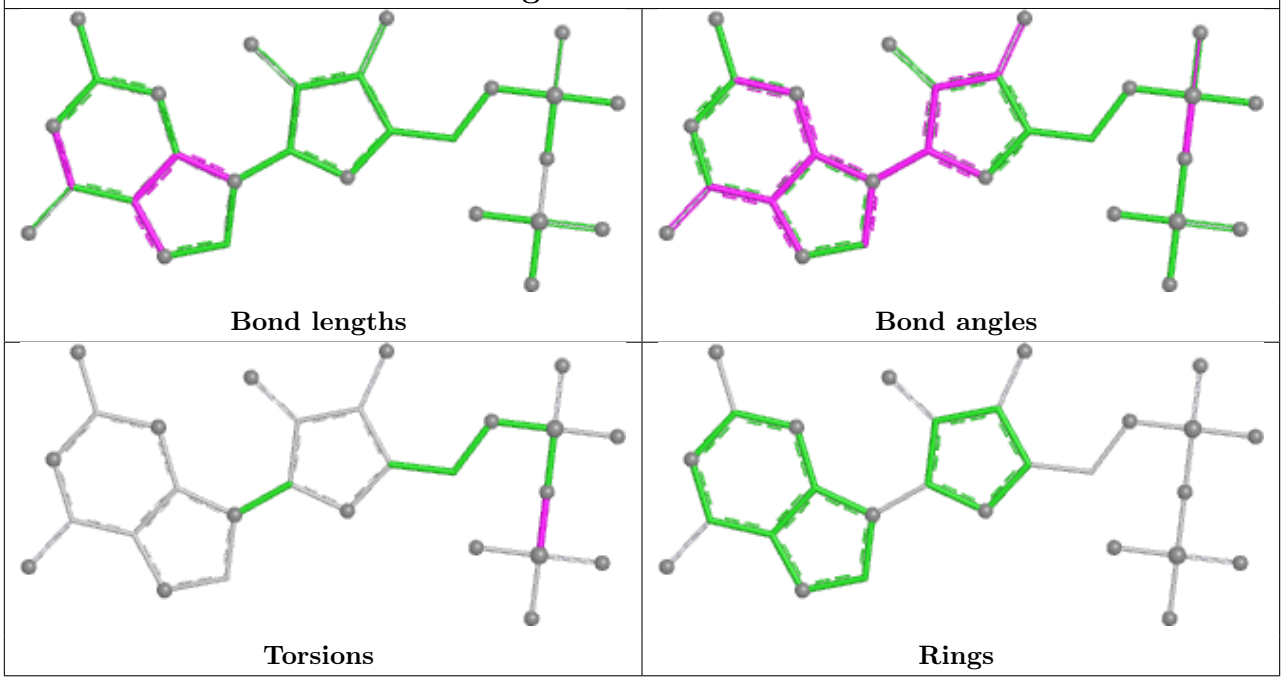
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	203	GDP	1	0

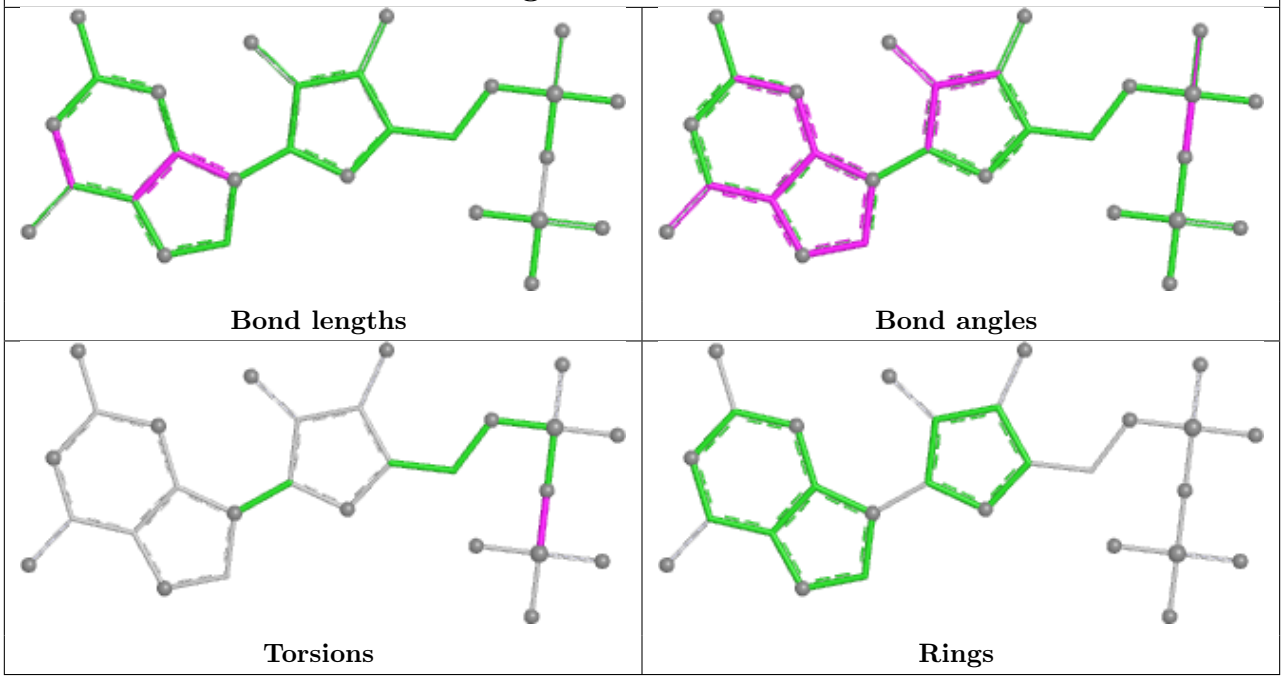
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GDP C 203



Ligand GDP A 203



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, 95^{th} 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	171/177 (96%)	-0.29	0	100	100	36, 49, 75, 113	0
1	C	171/177 (96%)	0.62	12 (7%)	22	19	47, 89, 143, 168	0
2	B	382/427 (89%)	0.05	16 (4%)	40	37	34, 67, 120, 173	1 (0%)
2	D	380/427 (88%)	0.10	11 (2%)	53	50	34, 68, 120, 154	2 (0%)
All	All	1104/1208 (91%)	0.10	39 (3%)	47	44	34, 67, 124, 173	3 (0%)

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1809	GLN	5.1
2	B	1449	PHE	4.2
2	B	1476	ASP	4.1
2	B	1447	LEU	4.0
2	B	1452	ALA	3.8

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 oligosaccharides in this entry.

6.4 Ligands

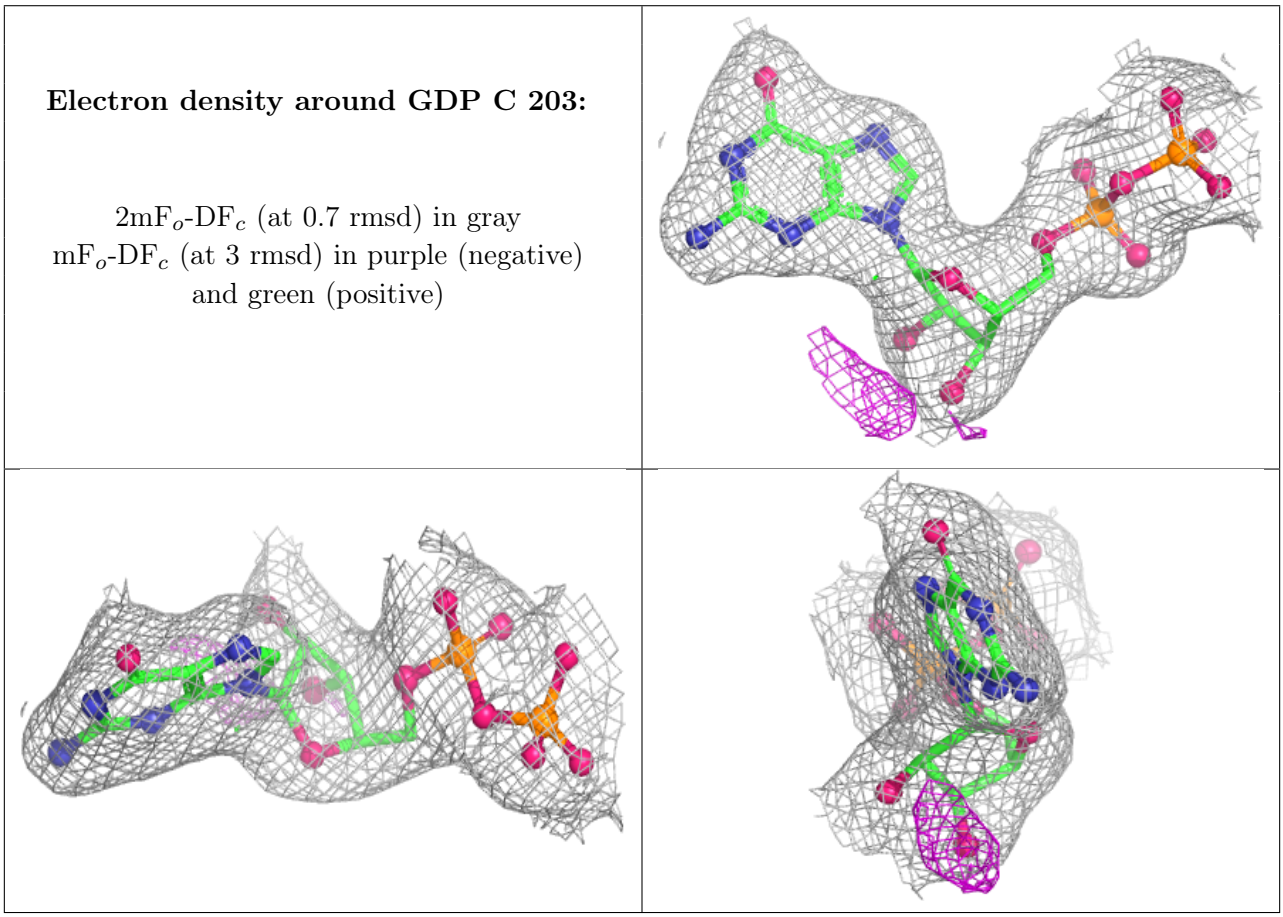
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	BEF	C	202	4/4	0.94	0.07	49,50,52,54	0
6	GOL	A	204	6/6	0.94	0.08	57,67,71,80	0
4	BEF	A	202	4/4	0.95	0.07	42,43,44,45	0
5	GDP	C	203	28/28	0.98	0.05	43,50,62,65	0
5	GDP	A	203	28/28	0.99	0.04	37,43,52,55	0
3	MG	A	201	1/1	0.99	0.06	42,42,42,42	0
3	MG	C	201	1/1	0.99	0.07	58,58,58,58	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.

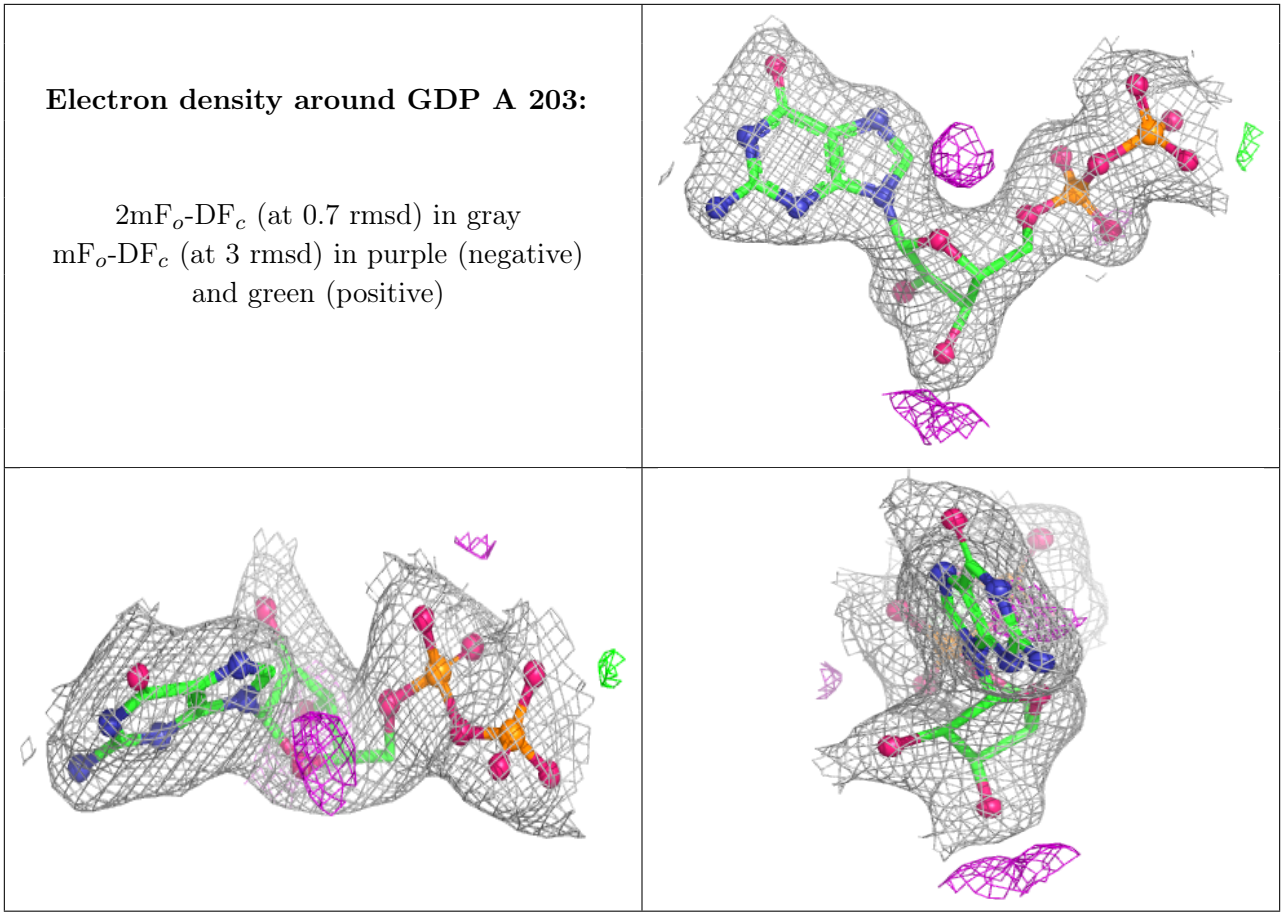
Electron density around GDP C 203:

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



Electron density around GDP A 203:

$2mF_o$-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.