



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 06:44 pm BST

PDB ID : 5KRQ
Title : Renalase in complex with NADPH
Authors : Silvaggi, N.R.; Moran, G.R.; Roman, J.V.
Deposited on : 2016-07-07
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

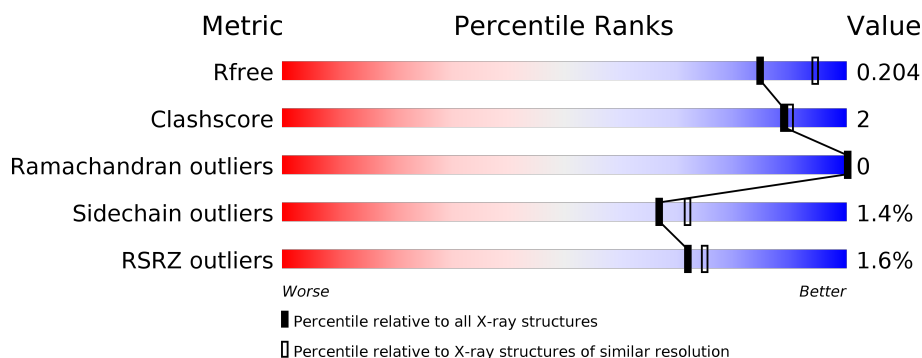
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	336	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 89%, yellow 89%, yellow 95%, green 95%, green 100%);"></div> <div style="position: absolute; right: 0; top: 0; width: 5%; height: 100%; background: linear-gradient(to right, yellow 0%, yellow 5%, green 5%, green 100%);"></div> </div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 89% 6% 5% </div> </div>
1	B	336	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 91%, yellow 91%, yellow 95%, green 95%, green 100%);"></div> <div style="position: absolute; right: 0; top: 0; width: 5%; height: 100%; background: linear-gradient(to right, yellow 0%, yellow 5%, green 5%, green 100%);"></div> </div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 2% 91% • 5% </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10195 atoms, of which 4822 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.

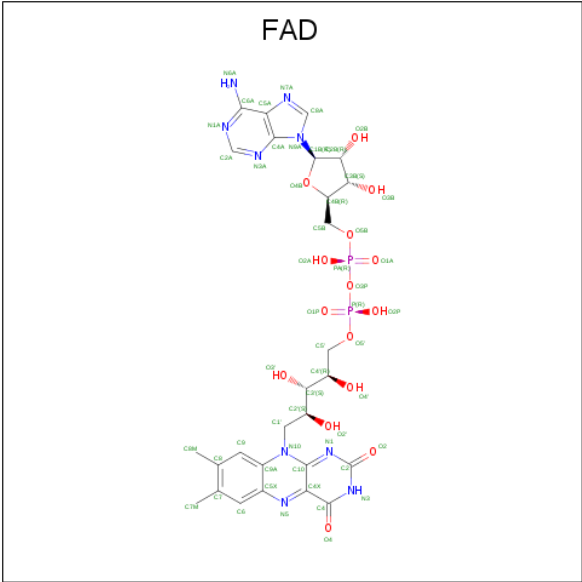
- Molecule 1 is a protein called Renalase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	H	N	O	S	0	0	0
			4828	1552	2365	449	450	12			
1	B	319	Total	C	H	N	O	S	0	0	0
			4828	1552	2369	448	447	12			

There are 18 discrepancies between the modelled and reference sequences:

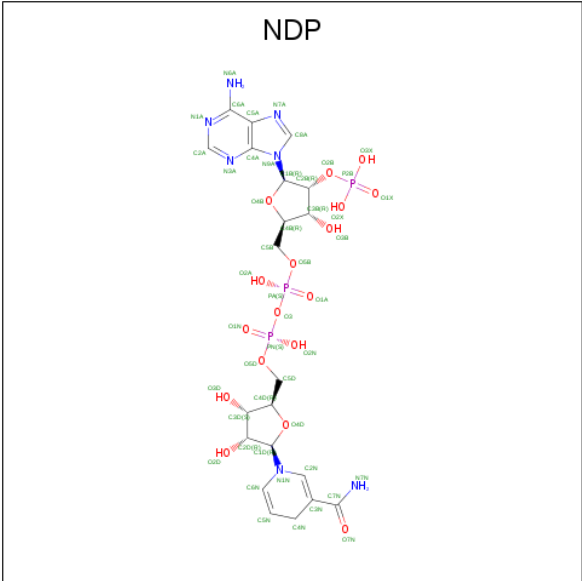
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	SER	GLY	engineered mutation	UNP A0A0P9WWR6
A	329	LEU	-	expression tag	UNP A0A0P9WWR6
A	330	GLU	-	expression tag	UNP A0A0P9WWR6
A	331	HIS	-	expression tag	UNP A0A0P9WWR6
A	332	HIS	-	expression tag	UNP A0A0P9WWR6
A	333	HIS	-	expression tag	UNP A0A0P9WWR6
A	334	HIS	-	expression tag	UNP A0A0P9WWR6
A	335	HIS	-	expression tag	UNP A0A0P9WWR6
A	336	HIS	-	expression tag	UNP A0A0P9WWR6
B	145	SER	GLY	engineered mutation	UNP A0A0P9WWR6
B	329	LEU	-	expression tag	UNP A0A0P9WWR6
B	330	GLU	-	expression tag	UNP A0A0P9WWR6
B	331	HIS	-	expression tag	UNP A0A0P9WWR6
B	332	HIS	-	expression tag	UNP A0A0P9WWR6
B	333	HIS	-	expression tag	UNP A0A0P9WWR6
B	334	HIS	-	expression tag	UNP A0A0P9WWR6
B	335	HIS	-	expression tag	UNP A0A0P9WWR6
B	336	HIS	-	expression tag	UNP A0A0P9WWR6

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			46	12	13	5	13	3		

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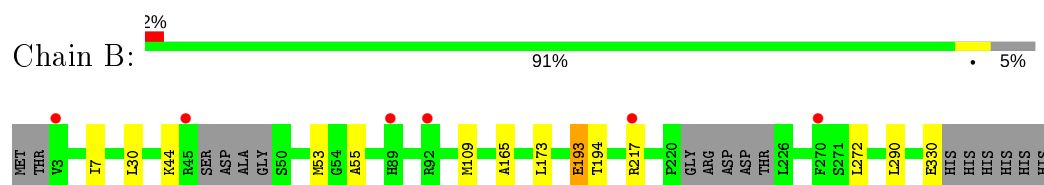
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	0	0
			46	12	13	5	13	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	138	Total	O	0	0
			138	138		

- Molecule 1: Renalase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.45Å 71.05Å 74.81Å 90.00° 107.79° 90.00°	Depositor
Resolution (Å)	46.02 – 2.09 46.02 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.02-2.09) 98.3 (46.02-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.08Å)	Xtriage
Refinement program	PHENIX (dev_2328: ???)	Depositor
R, R_{free}	0.157 , 0.203 0.159 , 0.204	Depositor DCC
R_{free} test set	1861 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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

5.1 Standard geometry

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

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	0.52	0/2531	0.69	0/3446
1	B	0.49	0/2526	0.64	0/3437
All	All	0.50	0/5057	0.67	0/6883

There are no bond length outliers.

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	2463	2365	2378	11	0
1	B	2459	2369	2381	9	0
2	A	53	31	31	1	0
2	B	53	31	31	0	0
3	A	33	13	13	0	0
3	B	33	13	13	0	0
4	A	141	0	0	3	1
4	B	138	0	0	3	1
All	All	5373	4822	4847	19	1

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 2.

The worst 5 of 19 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:B:330:GLU:O	4:B:501:HOH:O	2.11	0.68
1:A:266:PRO:O	4:A:501:HOH:O	2.15	0.64
1:B:194:THR:O	4:B:502:HOH:O	2.16	0.62
1:A:79:SER:OG	1:A:106:GLU:OE1	2.22	0.58
1:A:211:ASP:HB3	1:A:234:THR:HG22	1.91	0.52

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:637:HOH:O	4:B:632:HOH:O[1_556]	2.07	0.13

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	316/336 (94%)	312 (99%)	4 (1%)	0	100	100
1	B	313/336 (93%)	308 (98%)	5 (2%)	0	100	100
All	All	629/672 (94%)	620 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	252/266 (95%)	247 (98%)	5 (2%)	55	59
1	B	252/266 (95%)	250 (99%)	2 (1%)	81	85
All	All	504/532 (95%)	497 (99%)	7 (1%)	67	72

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	ILE
1	B	272	LEU
1	A	272	LEU
1	A	216	ASN
1	B	193	GLU

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

Mol	Chain	Res	Type
1	A	153	HIS
1	A	326	HIS
1	B	137	HIS
1	B	153	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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
3	NDP	A	401	-	29,35,52	2.59	5 (17%)	34,54,80	1.68	5 (14%)
3	NDP	B	401	-	29,35,52	2.59	6 (20%)	34,54,80	1.66	6 (17%)
2	FAD	A	400	-	51,58,58	1.66	6 (11%)	60,89,89	2.24	10 (16%)
2	FAD	B	400	-	51,58,58	1.60	9 (17%)	60,89,89	2.09	14 (23%)

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	NDP	A	401	-	-	6/21/41/77	0/3/3/5
3	NDP	B	401	-	-	8/21/41/77	0/3/3/5
2	FAD	A	400	-	-	2/30/50/50	0/6/6/6
2	FAD	B	400	-	-	6/30/50/50	0/6/6/6

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	NDP	P2B-O2B	10.80	1.79	1.59
3	A	401	NDP	P2B-O2B	10.32	1.78	1.59
2	A	400	FAD	C4X-C10	8.02	1.46	1.38
2	B	400	FAD	C4X-C10	7.36	1.46	1.38
3	A	401	NDP	PN-O5D	6.24	1.84	1.59

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	FAD	C4-N3-C2	10.11	123.68	115.14
2	B	400	FAD	C4-N3-C2	8.22	122.08	115.14
2	B	400	FAD	C1'-N10-C9A	7.05	123.84	118.29
2	A	400	FAD	C1'-N10-C9A	5.74	122.81	118.29
3	B	401	NDP	PN-O3-PA	-5.25	114.82	132.83

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

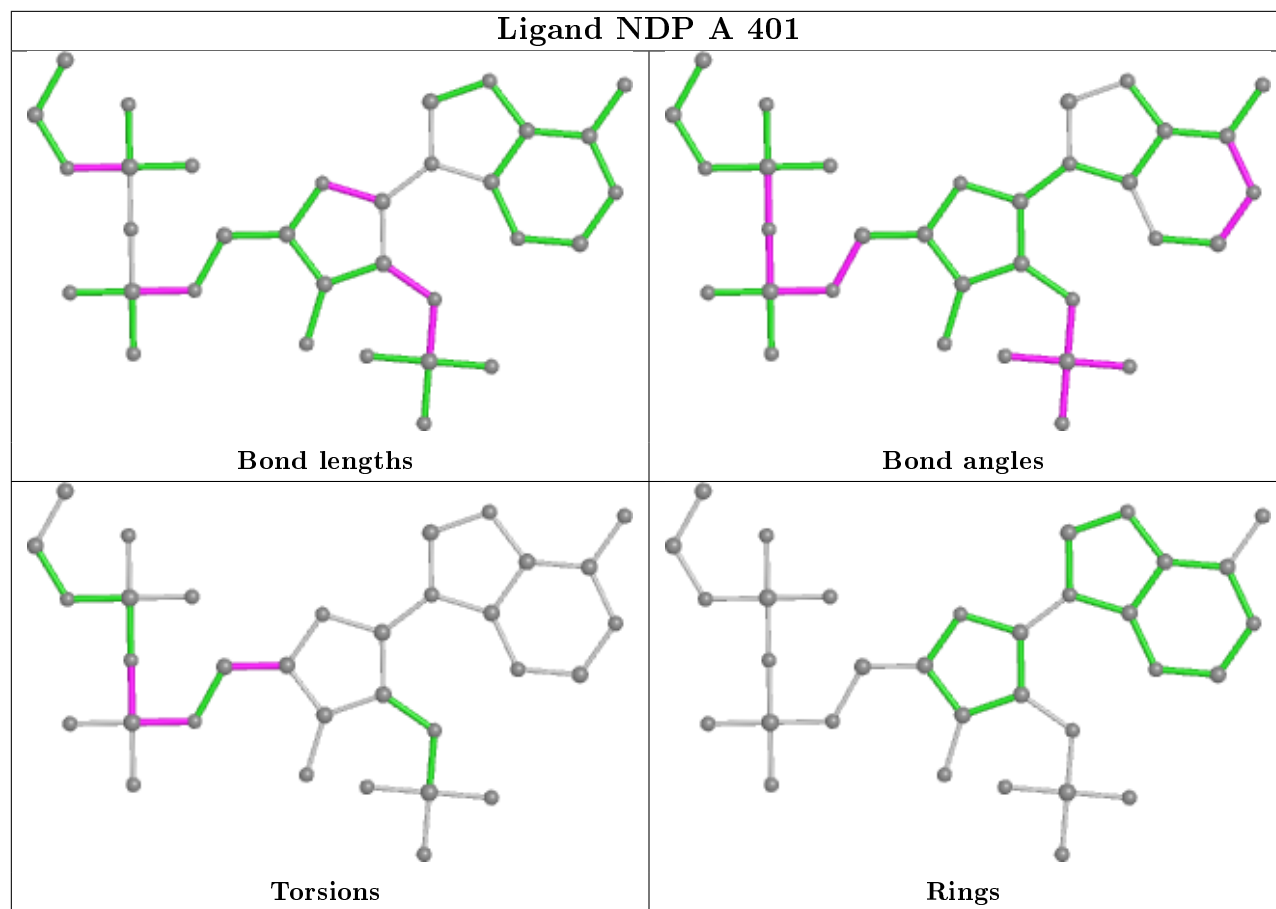
Mol	Chain	Res	Type	Atoms
3	A	401	NDP	C5B-O5B-PA-O1A
3	B	401	NDP	C5B-O5B-PA-O1A
3	B	401	NDP	C5D-O5D-PN-O3
3	B	401	NDP	C5D-O5D-PN-O1N
3	A	401	NDP	C3B-C4B-C5B-O5B

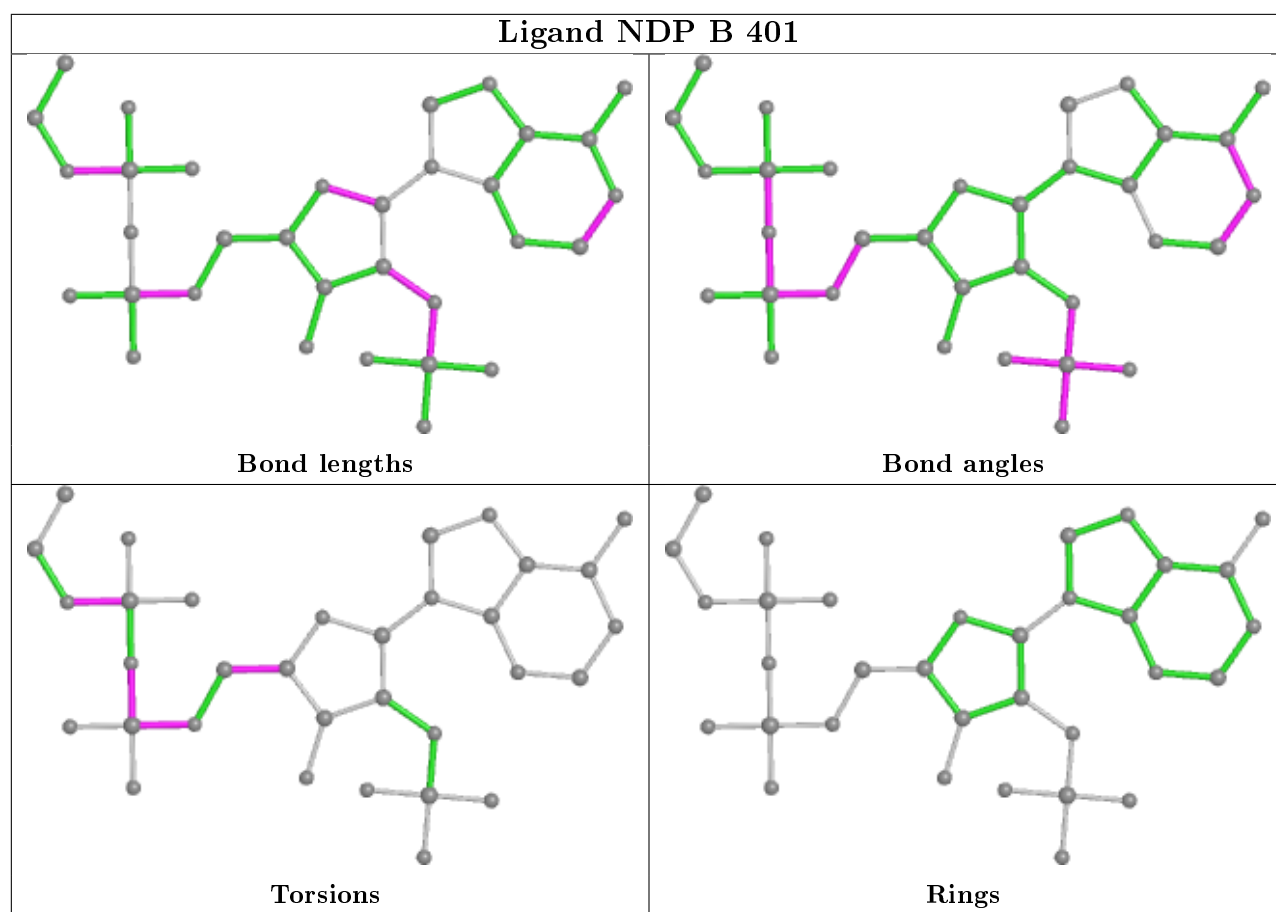
There are no ring outliers.

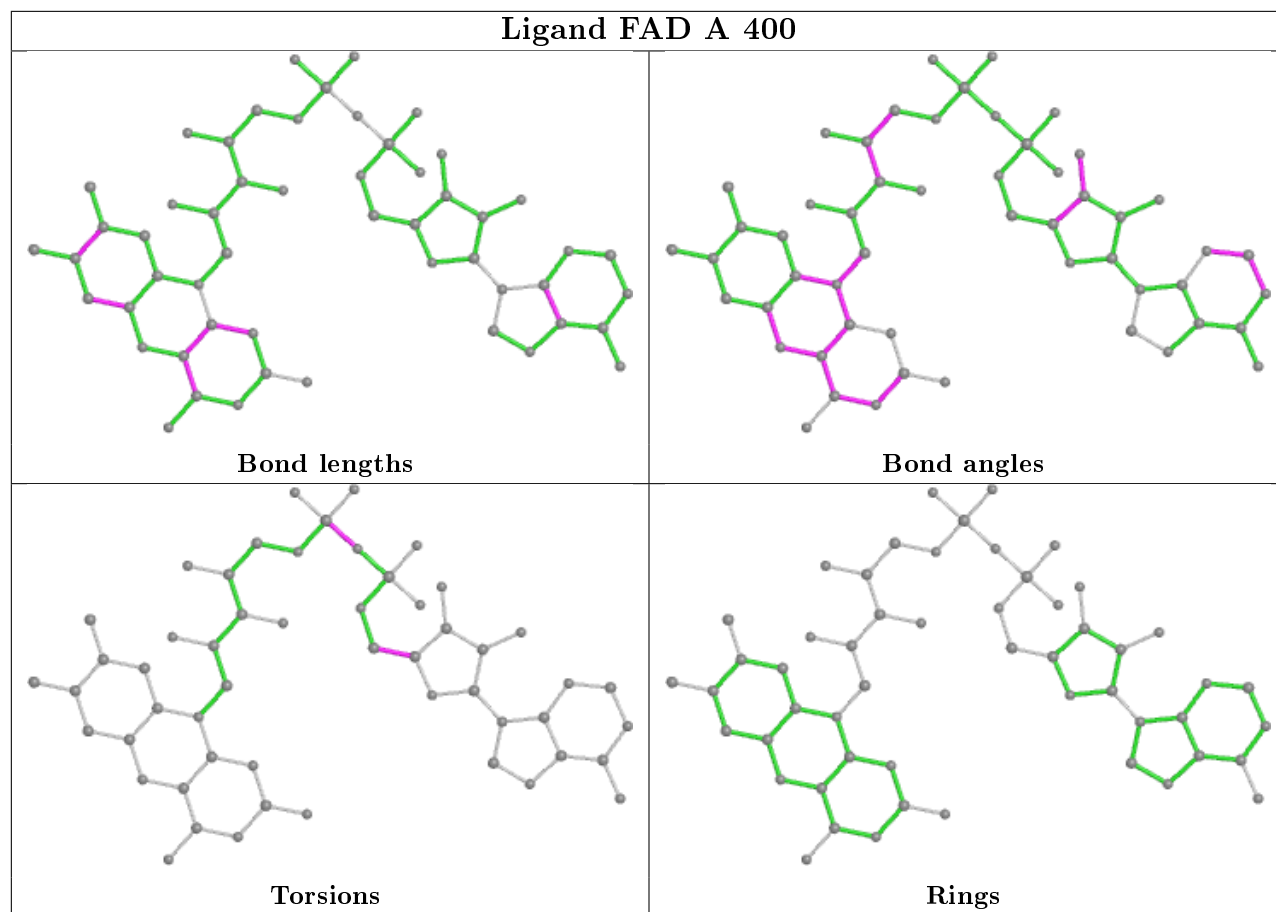
1 monomer is involved in 1 short contact:

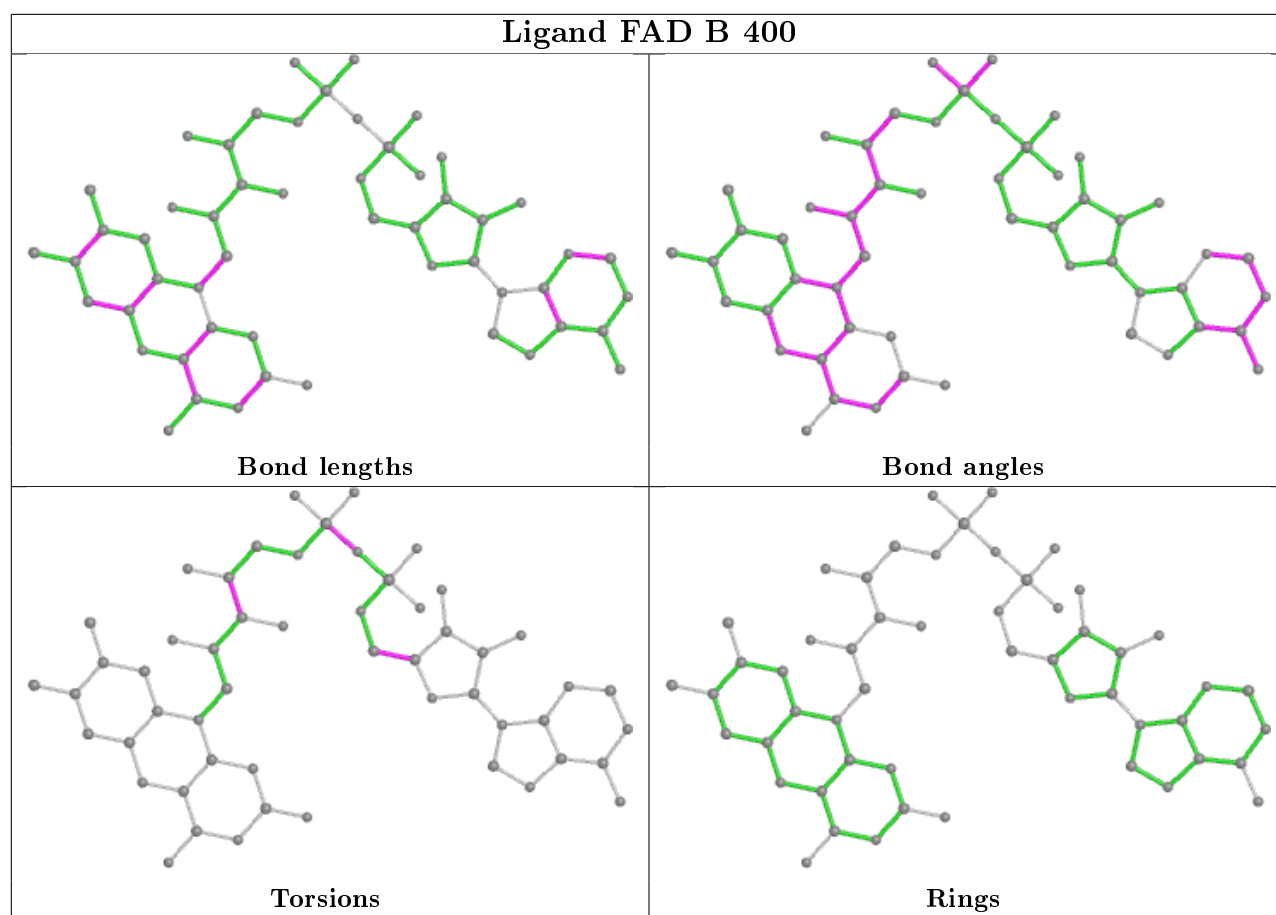
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	FAD	1	0

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 [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	320/336 (95%)	-0.18	4 (1%) 77 79	14, 26, 63, 94	0
1	B	319/336 (94%)	-0.16	6 (1%) 66 70	15, 31, 75, 98	0
All	All	639/672 (95%)	-0.17	10 (1%) 72 75	14, 28, 68, 98	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	ARG	3.2
1	B	89	HIS	3.0
1	A	51	LEU	3.0
1	A	89	HIS	2.9
1	A	90	GLY	2.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

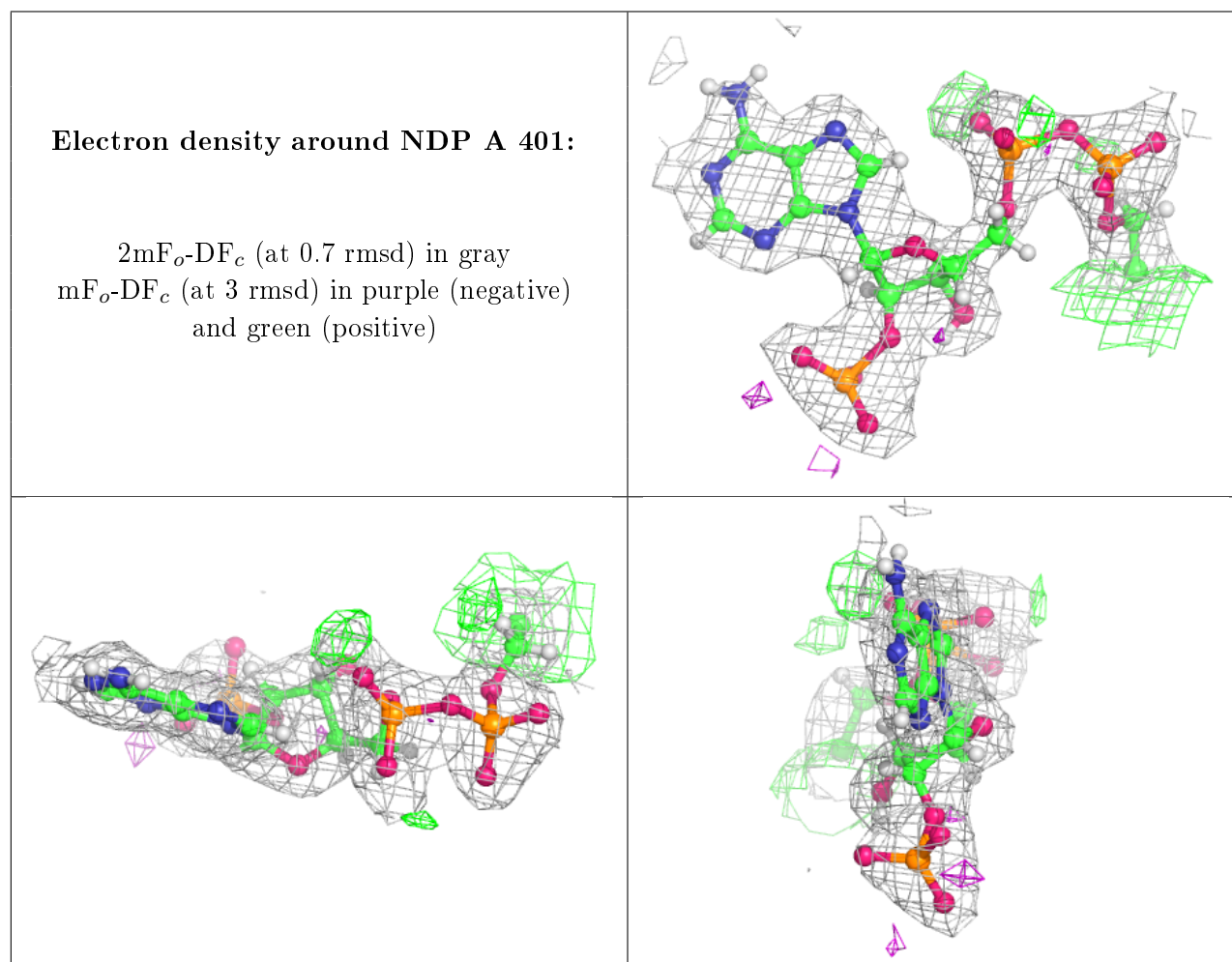
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

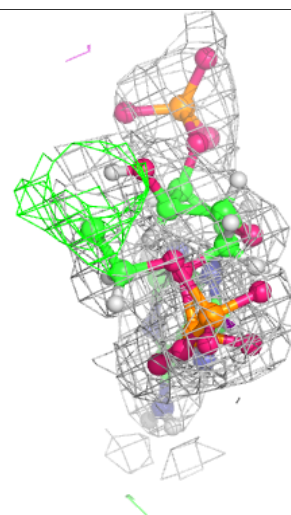
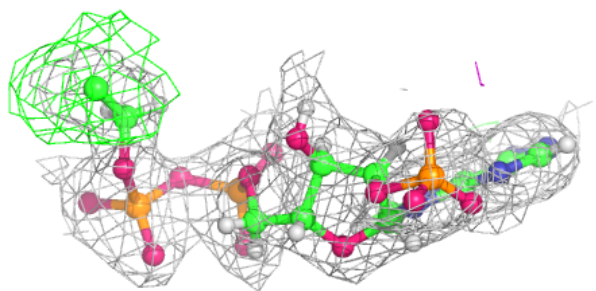
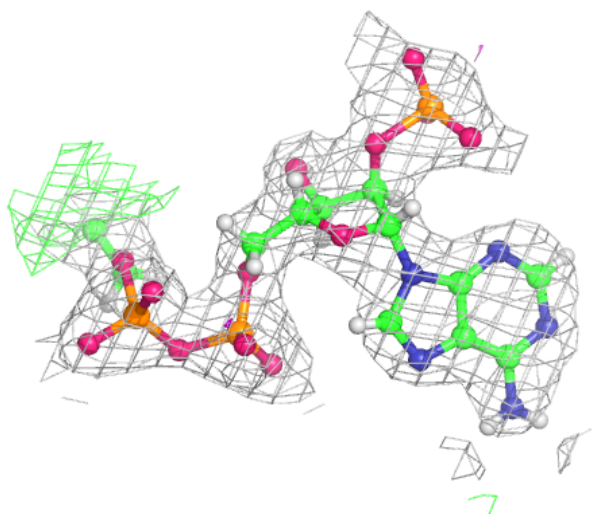
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NDP	A	401	33/48	0.91	0.14	20,43,65,92	0
3	NDP	B	401	33/48	0.93	0.14	25,44,66,78	0
2	FAD	A	400	53/53	0.97	0.12	8,19,26,33	0
2	FAD	B	400	53/53	0.98	0.10	7,19,30,33	0

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.



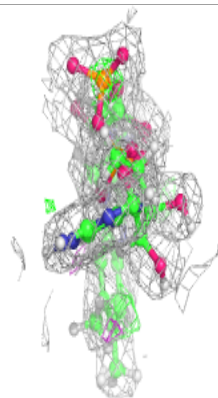
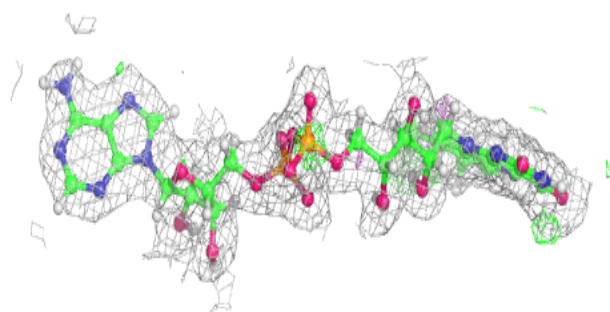
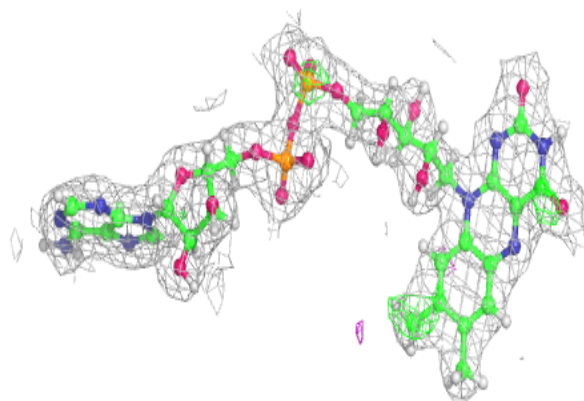
Electron density around NDP B 401:

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

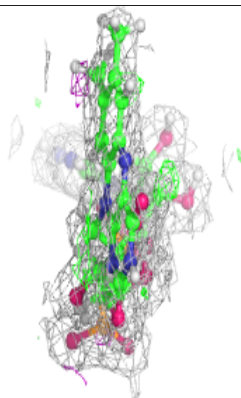
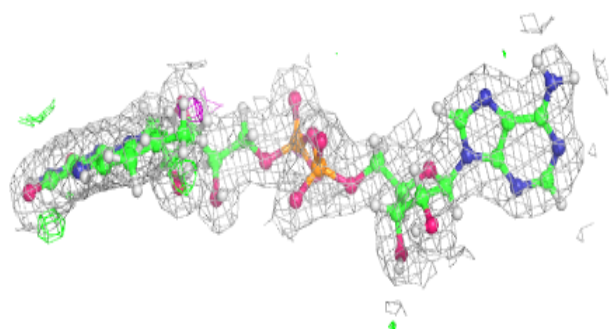
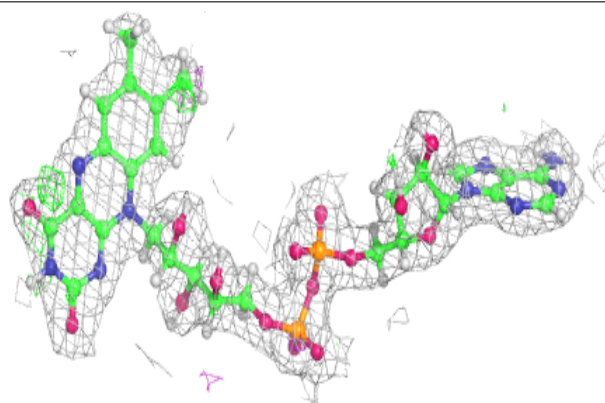


Electron density around FAD A 400:

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

**Electron density around FAD B 400:**

$2mF_o-DF_c$ (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.