



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2022 – 02:45 PM EDT

PDB ID : 7SV0  
Title : NADPH-dependent cytochrome P450 reductase 2b from Sorghum bicolor (SbCPR2b) -oxidized form of NADP<sup>+</sup> complex  
Authors : Zhang, B.; Kang, C.  
Deposited on : 2021-11-18  
Resolution : 2.70 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](mailto: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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.29
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)	:	2.29

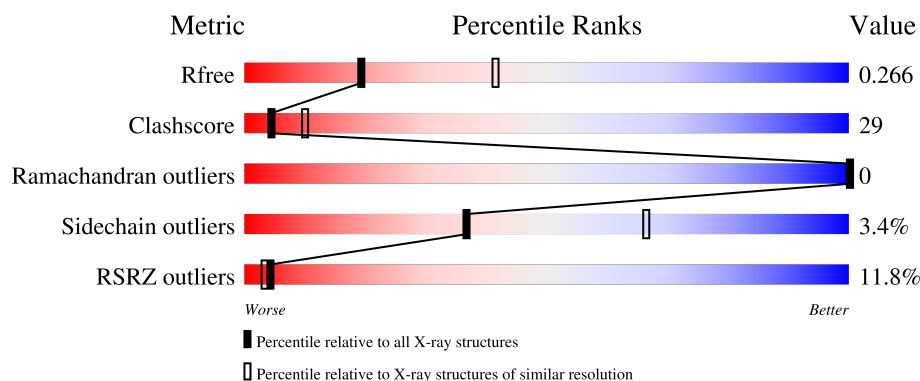
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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	706	<div> <div>7%</div> <div>34%</div> <div>20%</div> <div>•</div> <div>45%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3200 atoms, of which 56 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 NADPH–cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	3026	1913	526	571	16	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O P		
2	A	1	73	21	25	7	17 3	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.95Å 69.16Å 150.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.83 – 2.70 44.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.83-2.70) 99.9 (44.83-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.221 , 0.265 0.221 , 0.266	Depositor DCC
$R_{free}$ test set	1411 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FAD, NAP

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	0.44	1/3101 (0.0%)	0.63	0/4209

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	503	CYS	CB-SG	-5.58	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3026	0	2950	174	0
2	A	48	25	25	6	0
3	A	53	31	31	4	0
4	A	17	0	0	5	0
All	All	3144	56	3006	176	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 29.

All (176) 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:519:VAL:N	3:A:802:FAD:O2P	1.56	1.34
1:A:626:SER:HB2	2:A:801:NAP:O3B	1.63	0.96
1:A:643:ALA:HA	1:A:676:ILE:HD11	1.56	0.88
1:A:654:ALA:O	1:A:700:ARG:NH1	2.10	0.85
1:A:603:PHE:CD1	1:A:606:GLU:HG3	2.14	0.83
1:A:518:GLY:C	3:A:802:FAD:O2P	2.18	0.83
1:A:557:PRO:HB3	1:A:589:PRO:HG2	1.62	0.82
1:A:581:LYS:HB2	1:A:587:LEU:HD21	1.64	0.80
1:A:490:SER:HB3	1:A:500:HIS:HB2	1.64	0.80
1:A:456:LEU:HD11	1:A:477:VAL:HG12	1.66	0.78
1:A:455:SER:OG	4:A:902:HOH:O	1.97	0.75
1:A:560:MET:CE	1:A:570:PHE:HB3	2.16	0.75
1:A:624:ALA:HB1	1:A:633:GLU:HB3	1.66	0.74
1:A:494:MET:HG3	1:A:575:GLN:HB3	1.69	0.74
1:A:636:GLN:HB2	1:A:672:VAL:HG21	1.70	0.74
1:A:677:VAL:HG21	1:A:691:PHE:CD2	2.23	0.73
1:A:413:LYS:HE3	1:A:414:LYS:H	1.54	0.73
1:A:665:MET:O	1:A:669:VAL:HG23	1.89	0.73
2:A:801:NAP:O2A	2:A:801:NAP:O3D	2.05	0.72
1:A:316:LEU:HD21	1:A:605:TYR:CE1	2.25	0.72
1:A:349:THR:HG21	1:A:520:CYS:SG	2.30	0.71
1:A:557:PRO:HG2	1:A:654:ALA:HB2	1.71	0.71
1:A:306:CYS:HB3	1:A:337:LEU:HD11	1.74	0.70
1:A:622:VAL:HG12	1:A:638:LYS:HD2	1.74	0.70
1:A:345:VAL:HB	1:A:488:ILE:HD11	1.76	0.68
1:A:626:SER:CB	2:A:801:NAP:O3B	2.40	0.68
1:A:613:LEU:HD13	1:A:618:LEU:HD23	1.76	0.68
1:A:673:LEU:HA	1:A:676:ILE:HG22	1.75	0.68
1:A:557:PRO:CB	1:A:589:PRO:HG2	2.25	0.67
1:A:561:ILE:HD13	1:A:639:MET:SD	2.35	0.67
1:A:577:ARG:NH1	1:A:590:SER:OG	2.28	0.67
1:A:603:PHE:CG	1:A:606:GLU:HG3	2.30	0.66
1:A:557:PRO:HB3	1:A:589:PRO:CG	2.25	0.66
1:A:345:VAL:HB	1:A:488:ILE:CD1	2.26	0.66
1:A:626:SER:HB2	2:A:801:NAP:HO3A	1.56	0.66
1:A:305:PRO:HG3	1:A:348:TYR:CE2	2.31	0.66
1:A:490:SER:HB3	1:A:500:HIS:CG	2.31	0.65
1:A:597:ARG:HA	1:A:626:SER:HB3	1.78	0.65
1:A:530:SER:HA	1:A:533:SER:O	1.97	0.65
1:A:622:VAL:CG1	1:A:638:LYS:HD2	2.27	0.65
1:A:677:VAL:HG21	1:A:691:PHE:HD2	1.58	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ILE:HG13	1:A:604:ILE:O	1.96	0.64
1:A:328:LEU:HB3	1:A:501:VAL:HG13	1.80	0.64
1:A:643:ALA:HB1	1:A:676:ILE:HG13	1.79	0.64
1:A:681:GLY:C	1:A:683:LEU:HD12	2.19	0.63
1:A:557:PRO:HG2	1:A:654:ALA:CA	2.27	0.63
1:A:594:PHE:O	1:A:623:LEU:HA	1.98	0.63
1:A:306:CYS:CB	1:A:337:LEU:HD11	2.29	0.62
1:A:352:CYS:HB3	1:A:354:GLU:OE1	1.99	0.62
1:A:313:ARG:O	1:A:313:ARG:HD2	2.00	0.62
1:A:647:TRP:CD1	1:A:680:GLN:HB3	2.35	0.62
1:A:557:PRO:HG2	1:A:654:ALA:CB	2.29	0.61
1:A:576:GLU:OE2	1:A:580:GLN:NE2	2.31	0.61
1:A:490:SER:HB3	1:A:500:HIS:CB	2.29	0.61
1:A:598:ASN:HA	1:A:628:GLN:HB2	1.82	0.61
1:A:305:PRO:HG3	1:A:348:TYR:HE2	1.64	0.60
1:A:534:LYS:HD2	1:A:534:LYS:O	2.01	0.60
1:A:491:SER:OG	1:A:576:GLU:OE1	2.21	0.59
1:A:613:LEU:HD12	1:A:618:LEU:O	2.02	0.58
1:A:591:VAL:HG22	1:A:593:PHE:CE1	2.39	0.58
1:A:454:ARG:HH11	1:A:454:ARG:HG3	1.70	0.57
1:A:665:MET:SD	1:A:669:VAL:HG21	2.44	0.57
1:A:679:GLU:OE2	1:A:680:GLN:HB2	2.05	0.57
1:A:458:GLU:HG3	4:A:902:HOH:O	2.05	0.57
1:A:557:PRO:HG3	1:A:652:GLN:HG3	1.87	0.56
1:A:349:THR:CG2	1:A:520:CYS:SG	2.93	0.55
1:A:591:VAL:CG2	1:A:593:PHE:HE1	2.19	0.55
1:A:597:ARG:CZ	1:A:627:ARG:HH21	2.20	0.55
1:A:624:ALA:HB2	1:A:638:LYS:HG3	1.87	0.55
2:A:801:NAP:H2N	2:A:801:NAP:H51N	1.87	0.55
1:A:643:ALA:CA	1:A:676:ILE:HD11	2.32	0.55
1:A:645:GLU:O	1:A:649:MET:HG3	2.07	0.55
1:A:677:VAL:O	1:A:681:GLY:N	2.30	0.54
1:A:354:GLU:HG2	1:A:355:VAL:N	2.22	0.54
1:A:309:ASN:HB3	1:A:536:CYS:SG	2.47	0.54
1:A:591:VAL:HG22	1:A:593:PHE:HE1	1.73	0.53
1:A:580:GLN:O	1:A:584:GLY:N	2.41	0.53
1:A:413:LYS:HE3	1:A:413:LYS:CA	2.38	0.53
1:A:313:ARG:HB3	1:A:529:PRO:HG3	1.91	0.53
1:A:557:PRO:HG2	1:A:654:ALA:HA	1.90	0.53
1:A:639:MET:CE	1:A:672:VAL:HG11	2.38	0.53
1:A:639:MET:HE2	1:A:672:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:ASP:HB3	1:A:556:VAL:HG23	1.91	0.52
1:A:557:PRO:O	1:A:654:ALA:HA	2.10	0.52
1:A:413:LYS:HE3	1:A:414:LYS:N	2.22	0.52
1:A:414:LYS:NZ	4:A:901:HOH:O	1.96	0.52
1:A:683:LEU:HD23	1:A:687:LYS:HB3	1.92	0.52
1:A:454:ARG:HA	1:A:458:GLU:OE1	2.10	0.52
1:A:673:LEU:HA	1:A:676:ILE:CG2	2.40	0.52
1:A:674:HIS:O	1:A:677:VAL:HG12	2.10	0.51
1:A:312:VAL:CG2	1:A:314:ARG:HG3	2.41	0.51
1:A:569:PRO:HG3	1:A:659:CYS:SG	2.50	0.51
1:A:656:ILE:HG23	1:A:701:TYR:HA	1.93	0.51
1:A:414:LYS:HE2	1:A:445:TYR:CD2	2.46	0.50
1:A:593:PHE:HB3	1:A:635:VAL:HG23	1.93	0.50
1:A:570:PHE:O	1:A:574:LEU:HD13	2.11	0.50
1:A:643:ALA:HB1	1:A:676:ILE:CG1	2.42	0.50
1:A:342:GLY:HA3	1:A:548:PHE:O	2.12	0.49
1:A:673:LEU:O	1:A:676:ILE:HG22	2.12	0.49
1:A:673:LEU:CA	1:A:676:ILE:HG22	2.42	0.49
1:A:520:CYS:O	1:A:524:ILE:HG13	2.11	0.49
1:A:633:GLU:OE2	1:A:638:LYS:HE2	2.12	0.49
1:A:539:ALA:O	1:A:541:ILE:HG23	2.11	0.49
1:A:305:PRO:CG	1:A:348:TYR:CE2	2.95	0.49
1:A:694:ASN:O	1:A:698:GLU:HG3	2.13	0.49
1:A:312:VAL:HG22	1:A:314:ARG:HG3	1.93	0.49
1:A:593:PHE:HB3	1:A:635:VAL:CG2	2.43	0.48
1:A:494:MET:HE3	1:A:575:GLN:HG2	1.95	0.48
1:A:354:GLU:OE2	1:A:517:LYS:HE2	2.14	0.48
1:A:599:SER:CB	1:A:628:GLN:OE1	2.62	0.48
1:A:636:GLN:OE1	1:A:636:GLN:N	2.36	0.48
1:A:639:MET:CE	1:A:672:VAL:CG1	2.92	0.48
1:A:301:ASP:OD1	1:A:306:CYS:HB2	2.14	0.48
1:A:590:SER:O	1:A:619:SER:HB3	2.14	0.48
1:A:321:SER:HB2	1:A:601:MET:HB3	1.95	0.48
1:A:328:LEU:HB3	1:A:501:VAL:CG1	2.44	0.48
1:A:600:LYS:HG3	1:A:601:MET:HG3	1.96	0.47
1:A:342:GLY:O	1:A:546:SER:OG	2.29	0.47
1:A:623:LEU:O	1:A:638:LYS:HE3	2.15	0.47
1:A:676:ILE:O	1:A:679:GLU:HG3	2.15	0.47
1:A:621:LEU:HD12	1:A:622:VAL:N	2.30	0.46
1:A:656:ILE:HD11	1:A:673:LEU:HD11	1.97	0.46
1:A:557:PRO:HG3	1:A:652:GLN:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:PHE:CE1	1:A:704:ASP:HB2	2.51	0.46
1:A:594:PHE:CE1	1:A:596:CYS:HB3	2.52	0.45
1:A:673:LEU:HA	1:A:673:LEU:HD23	1.77	0.45
1:A:591:VAL:CG2	1:A:593:PHE:CE1	3.00	0.45
1:A:618:LEU:HD21	1:A:620:GLU:O	2.17	0.45
1:A:677:VAL:HG21	1:A:691:PHE:CE2	2.52	0.45
1:A:352:CYS:SG	4:A:911:HOH:O	2.61	0.45
1:A:518:GLY:O	1:A:522:THR:OG1	2.27	0.45
1:A:313:ARG:HD2	1:A:313:ARG:C	2.37	0.45
1:A:349:THR:HG21	1:A:520:CYS:HA	1.99	0.45
1:A:363:LEU:HD21	1:A:473:PHE:CD1	2.52	0.44
1:A:674:HIS:HE1	1:A:692:VAL:HB	1.82	0.44
1:A:312:VAL:HG12	1:A:329:GLU:HB2	1.98	0.44
1:A:599:SER:HB2	1:A:628:GLN:OE1	2.18	0.44
1:A:456:LEU:HD23	1:A:456:LEU:O	2.18	0.44
1:A:681:GLY:HA3	1:A:683:LEU:CD1	2.47	0.44
1:A:693:LYS:HA	1:A:693:LYS:HD3	1.80	0.44
1:A:581:LYS:HD2	1:A:587:LEU:HG	2.00	0.44
1:A:647:TRP:CD1	1:A:680:GLN:CB	3.01	0.44
1:A:636:GLN:HE22	2:A:801:NAP:C2A	2.31	0.43
1:A:489:SER:HA	1:A:568:ALA:O	2.18	0.43
1:A:322:ASP:OD1	1:A:322:ASP:C	2.57	0.43
1:A:413:LYS:HE3	1:A:413:LYS:HA	1.99	0.43
1:A:643:ALA:CB	1:A:676:ILE:HG13	2.46	0.43
1:A:590:SER:H	1:A:619:SER:HB2	1.84	0.43
1:A:593:PHE:CD2	1:A:639:MET:HG3	2.53	0.43
1:A:351:ASN:HA	4:A:906:HOH:O	2.19	0.43
1:A:328:LEU:HD13	1:A:524:ILE:HG23	2.01	0.43
1:A:516:HIS:CD2	3:A:802:FAD:H8A	2.53	0.42
1:A:674:HIS:CE1	1:A:692:VAL:HB	2.54	0.42
1:A:592:PHE:CZ	1:A:594:PHE:HB2	2.54	0.42
1:A:560:MET:HB3	1:A:560:MET:HE2	1.96	0.42
1:A:561:ILE:HG22	1:A:561:ILE:O	2.20	0.41
1:A:568:ALA:N	1:A:569:PRO:HD2	2.35	0.41
1:A:354:GLU:HG2	1:A:355:VAL:H	1.84	0.41
1:A:562:GLY:N	1:A:570:PHE:HE2	2.17	0.41
1:A:656:ILE:CD1	1:A:673:LEU:HD11	2.50	0.41
1:A:352:CYS:SG	1:A:517:LYS:HE3	2.61	0.41
1:A:454:ARG:HG3	1:A:454:ARG:NH1	2.35	0.41
1:A:534:LYS:C	1:A:536:CYS:H	2.24	0.41
1:A:633:GLU:OE2	1:A:638:LYS:CE	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:TRP:CD1	1:A:680:GLN:HG2	2.56	0.41
1:A:675:THR:O	1:A:678:GLN:HG2	2.21	0.41
1:A:560:MET:HE3	1:A:570:PHE:HB3	1.99	0.41
1:A:405:TYR:O	1:A:480:ARG:HA	2.21	0.40
1:A:516:HIS:CG	3:A:802:FAD:H8A	2.56	0.40
1:A:610:ASN:O	1:A:614:GLU:HB2	2.21	0.40
1:A:634:TYR:HB3	1:A:636:GLN:OE1	2.21	0.40
1:A:581:LYS:HB2	1:A:587:LEU:HD11	2.02	0.40
1:A:636:GLN:HB2	1:A:672:VAL:CG2	2.43	0.40
1:A:636:GLN:HG2	1:A:637:HIS:N	2.37	0.40
1:A:488:ILE:H	1:A:488:ILE:HG12	1.70	0.40
1:A:494:MET:HE1	1:A:578:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/706 (54%)	363 (94%)	22 (6%)	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	324/560 (58%)	313 (97%)	11 (3%)	37	66

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	HIS
1	A	416	SER
1	A	432	ARG
1	A	547	ASN
1	A	563	PRO
1	A	582	GLU
1	A	603	PHE
1	A	623	LEU
1	A	631	THR
1	A	680	GLN
1	A	701	TYR

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

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	NAP	A	801	-	45,52,52	0.86	0	56,80,80	1.27	6 (10%)
3	FAD	A	802	-	53,58,58	1.41	9 (16%)	68,89,89	1.49	14 (20%)

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	NAP	A	801	-	-	9/31/67/67	0/5/5/5
3	FAD	A	802	-	-	2/30/50/50	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	FAD	C9A-C5X	3.71	1.47	1.41
3	A	802	FAD	C2B-C1B	-3.49	1.48	1.53
3	A	802	FAD	C4-N3	-3.03	1.33	1.38
3	A	802	FAD	C5X-N5	-2.87	1.33	1.39
3	A	802	FAD	C8-C7	2.36	1.46	1.40
3	A	802	FAD	C2-N3	-2.30	1.33	1.39
3	A	802	FAD	C5A-N7A	-2.10	1.32	1.39
3	A	802	FAD	O4B-C4B	-2.06	1.40	1.45
3	A	802	FAD	C4A-N3A	-2.01	1.32	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAP	PN-O3-PA	-4.75	116.52	132.83
2	A	801	NAP	N3A-C2A-N1A	-3.77	122.79	128.68
3	A	802	FAD	N3A-C2A-N1A	-3.58	123.09	128.68
3	A	802	FAD	C4-C4X-N5	3.19	122.77	118.23
3	A	802	FAD	C10-N1-C2	2.77	122.44	116.90
3	A	802	FAD	C4X-C10-N10	2.69	120.41	116.48
3	A	802	FAD	O4B-C1B-C2B	-2.65	103.06	106.93
3	A	802	FAD	C4X-C10-N1	-2.57	118.78	124.73
3	A	802	FAD	O4-C4-C4X	-2.53	119.88	126.60
3	A	802	FAD	O2-C2-N1	-2.52	117.65	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	FAD	C4X-C4-N3	2.44	119.39	113.19
3	A	802	FAD	C4-N3-C2	-2.38	121.24	125.64
2	A	801	NAP	O3X-P2B-O2X	2.36	116.67	107.64
2	A	801	NAP	C4A-C5A-N7A	-2.31	106.99	109.40
2	A	801	NAP	C3D-C2D-C1D	2.28	104.42	100.98
3	A	802	FAD	C2A-N1A-C6A	2.24	122.58	118.75
2	A	801	NAP	C2A-N1A-C6A	2.15	122.43	118.75
3	A	802	FAD	O2P-P-O5'	2.11	117.53	107.75
3	A	802	FAD	O5'-C5'-C4'	2.07	114.90	109.36
3	A	802	FAD	C4A-C5A-N7A	-2.07	107.25	109.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAP	C5D-O5D-PN-O1N
3	A	802	FAD	C3'-C4'-C5'-O5'
3	A	802	FAD	O4'-C4'-C5'-O5'
2	A	801	NAP	O4D-C4D-C5D-O5D
2	A	801	NAP	O4B-C4B-C5B-O5B
2	A	801	NAP	C3B-C4B-C5B-O5B
2	A	801	NAP	C3D-C4D-C5D-O5D
2	A	801	NAP	PA-O3-PN-O1N
2	A	801	NAP	PA-O3-PN-O5D
2	A	801	NAP	C2B-O2B-P2B-O1X
2	A	801	NAP	C2B-O2B-P2B-O2X

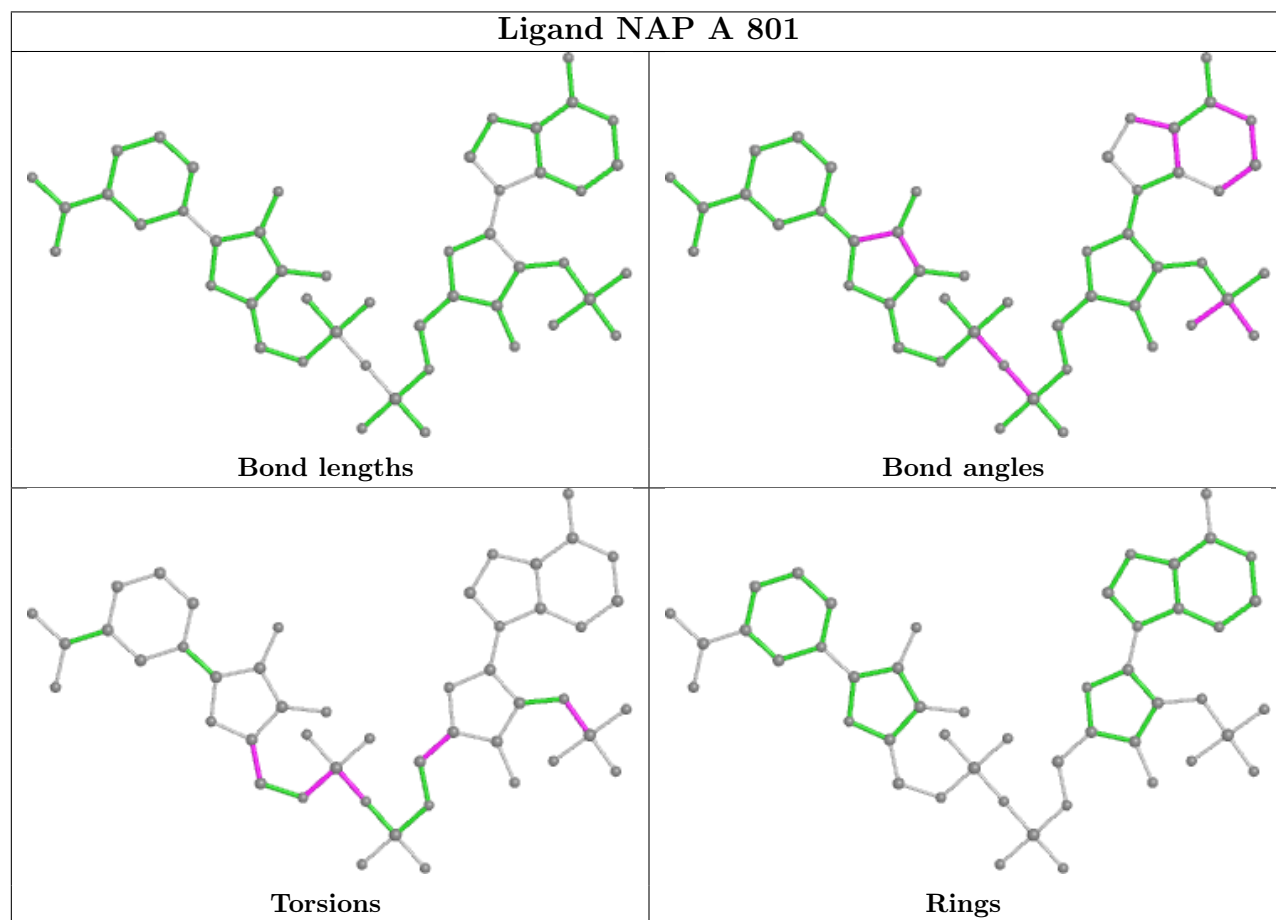
There are no ring outliers.

2 monomers are involved in 10 short contacts:

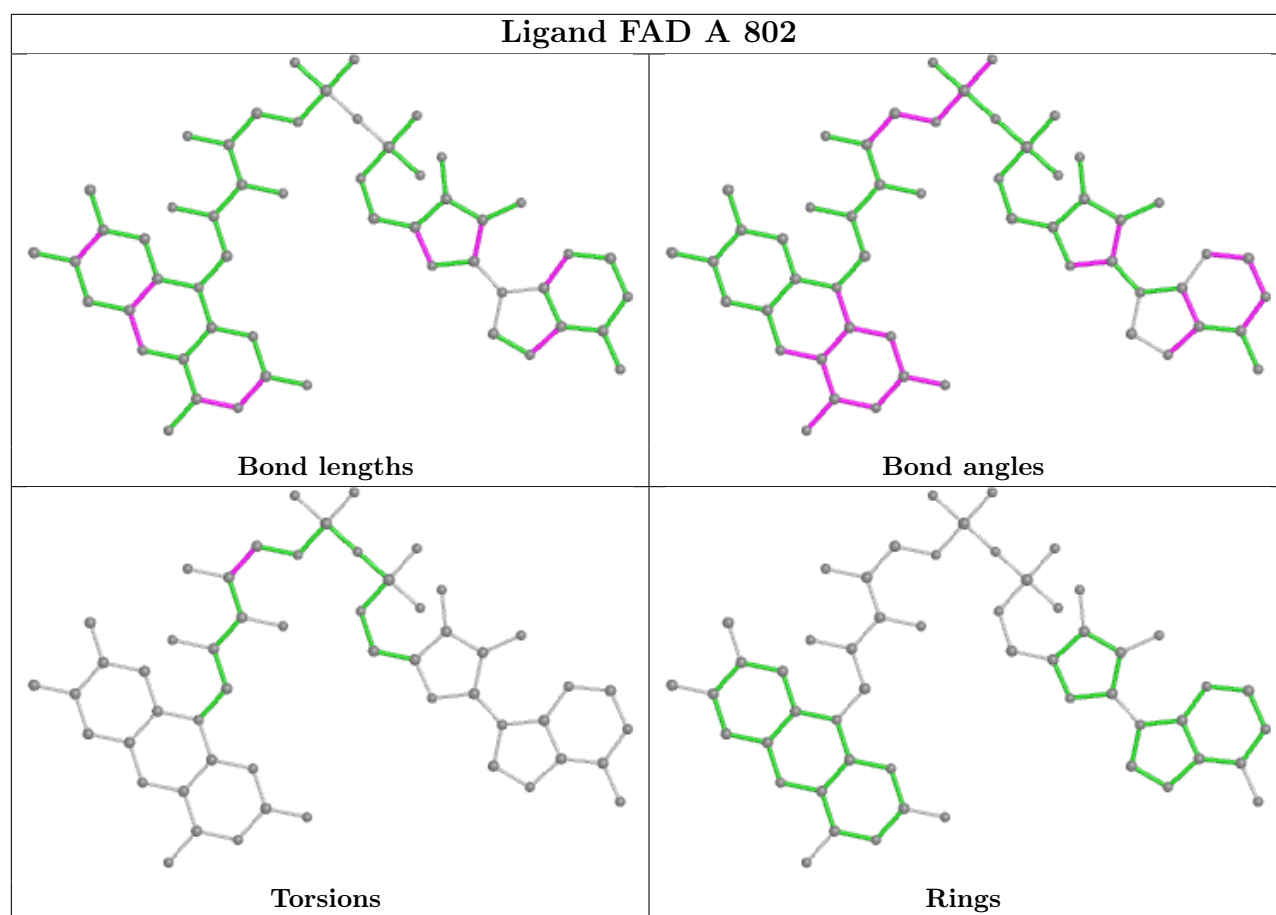
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAP	6	0
3	A	802	FAD	4	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	389/706 (55%)	0.68	46 (11%) 4 3	43, 85, 129, 148	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	650	ILE	7.5
1	A	559	ILE	6.4
1	A	655	TYR	4.8
1	A	646	ILE	4.4
1	A	651	SER	4.4
1	A	652	GLN	4.4
1	A	573	PHE	4.3
1	A	621	LEU	4.1
1	A	561	ILE	3.8
1	A	692	VAL	3.7
1	A	616	GLY	3.7
1	A	647	TRP	3.6
1	A	593	PHE	3.6
1	A	558	ILE	3.4
1	A	300	HIS	3.3
1	A	362	LEU	3.3
1	A	701	TYR	3.2
1	A	620	GLU	3.2
1	A	587	LEU	3.1
1	A	653	GLY	3.1
1	A	499	ILE	3.1
1	A	609	LEU	3.1
1	A	681	GLY	3.0
1	A	649	MET	2.9
1	A	618	LEU	2.9
1	A	639	MET	2.9
1	A	631	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	393	PRO	2.7
1	A	680	GLN	2.7
1	A	501	VAL	2.7
1	A	702	LEU	2.7
1	A	604	ILE	2.6
1	A	657	TYR	2.6
1	A	617	ALA	2.6
1	A	673	LEU	2.5
1	A	630	PRO	2.5
1	A	328	LEU	2.5
1	A	557	PRO	2.4
1	A	402	LEU	2.4
1	A	643	ALA	2.4
1	A	306	CYS	2.3
1	A	578	LEU	2.3
1	A	648	ASP	2.3
1	A	590	SER	2.3
1	A	550	LEU	2.2
1	A	591	VAL	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, 95<sup>th</sup> 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.

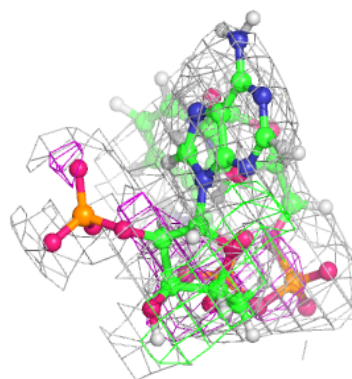
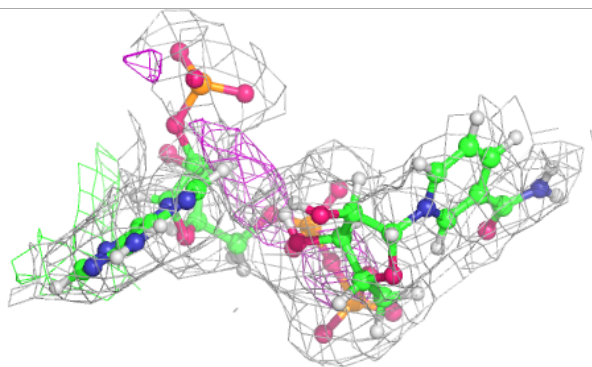
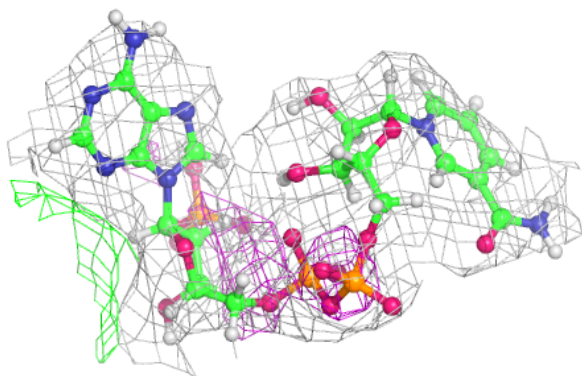
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	A	801	48/48	0.87	0.14	83,108,145,157	0
3	FAD	A	802	53/53	0.94	0.16	47,67,84,90	0

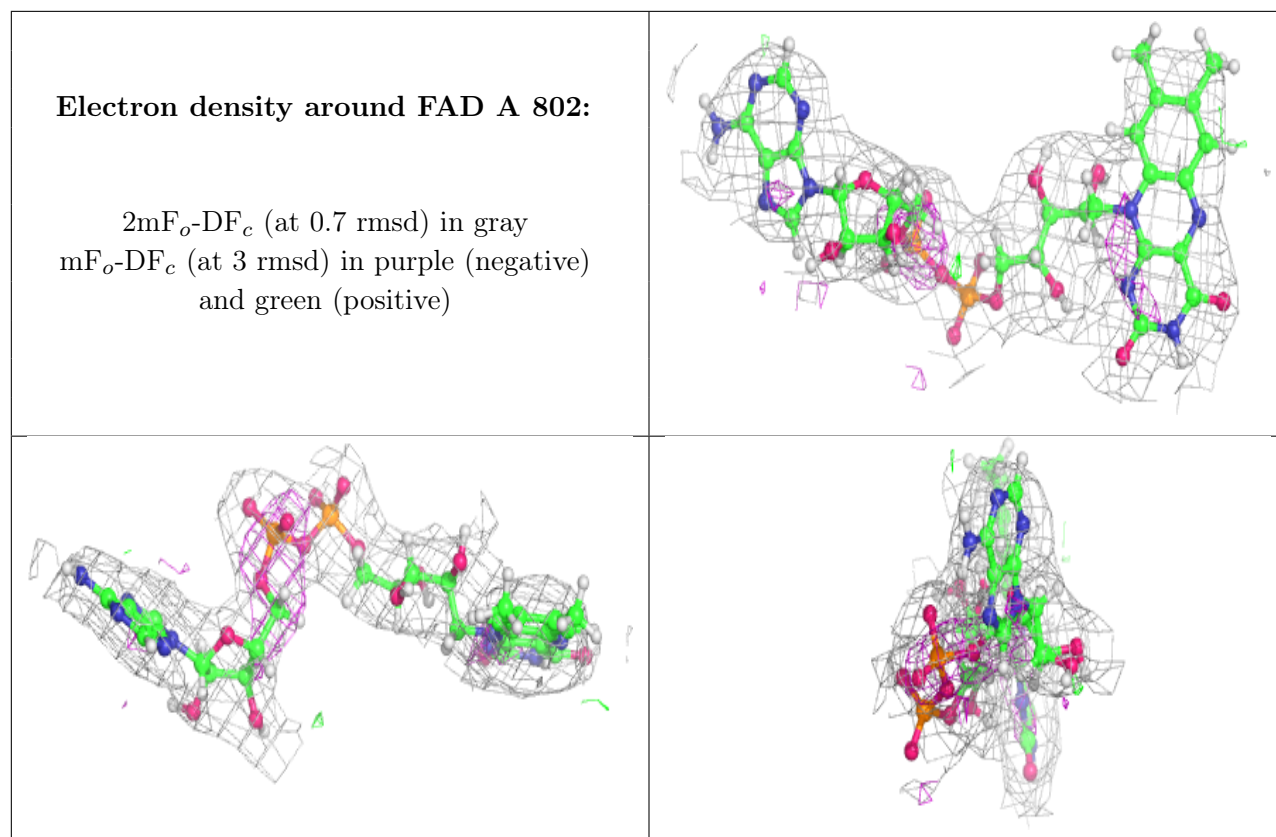
The following is a graphical depiction of the model fit to experimental electron density of all

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 NAP A 801:**

$2mF_o-DF_c$  (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.