



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 01:22 PM EDT

PDB ID : 2AFH  
Title : Crystal Structure of Nucleotide-Free Av2-Av1 Complex  
Authors : Tezcan, F.A.; Kaiser, J.T.; Mustafi, D.; Walton, M.Y.; Howard, J.B.; Rees, D.C.  
Deposited on : 2005-07-25  
Resolution : 2.10 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](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 : 2.35  
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) : 2.35

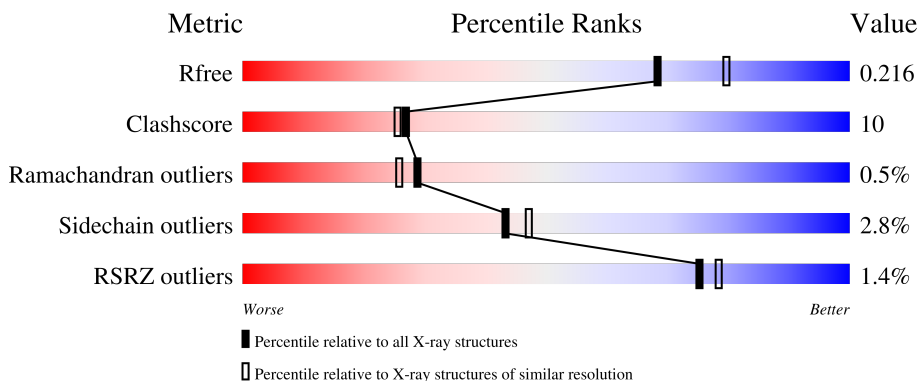
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



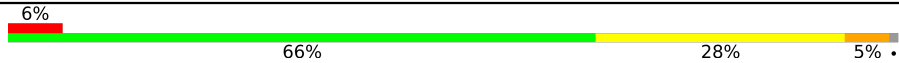
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	491	 81% 15% .
1	C	491	 81% 14% ..
2	B	522	 87% 12% .
2	D	522	 87% 12% .
3	E	289	 5% 62% 36% .

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Mol	Chain	Length	Quality of chain
3	F	289	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	PG4	E	5007	-	-	X	-
12	1PE	B	5017	-	-	X	-
12	1PE	C	5013	-	-	X	-
13	PEG	D	5020	-	-	X	-
14	P6G	D	5009	-	X	-	-
6	PGE	A	5015	-	-	X	-
6	PGE	D	5010	-	X	-	-

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 22638 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 Nitrogenase molybdenum-iron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	Total	C	N	O	S	8	0	0
			3782	2405	645	708	24			
1	C	477	Total	C	N	O	S	0	0	0
			3790	2410	646	709	25			

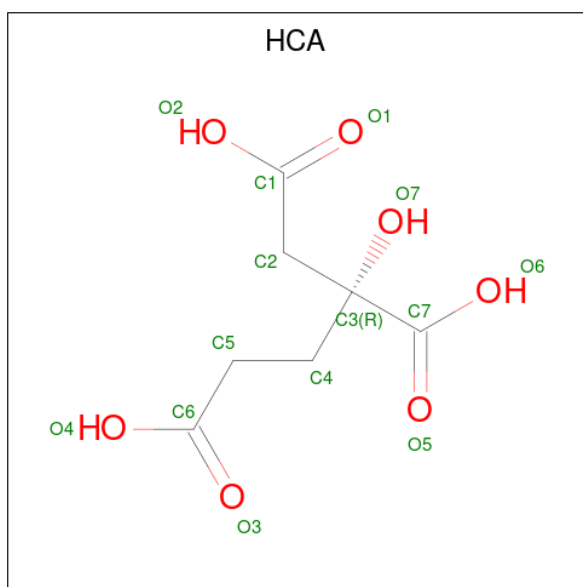
- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	522	Total	C	N	O	S	6	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called Nitrogenase iron protein 1.

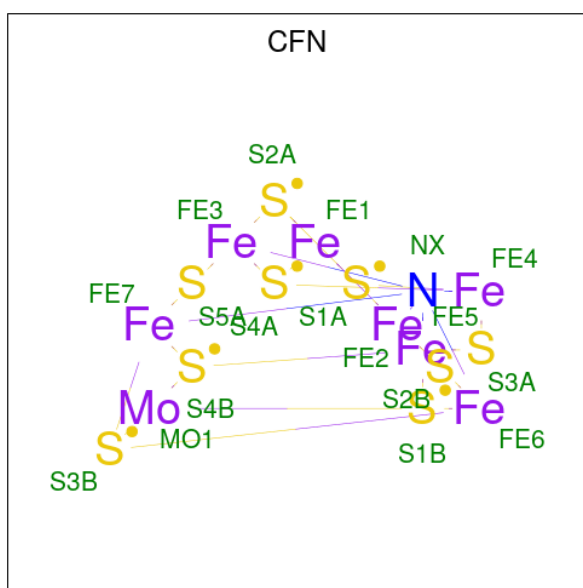
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	289	Total	C	N	O	S	0	0	0
			2187	1364	369	433	21			
3	F	286	Total	C	N	O	S	4	0	0
			2161	1349	366	425	21			

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>7</sub>).



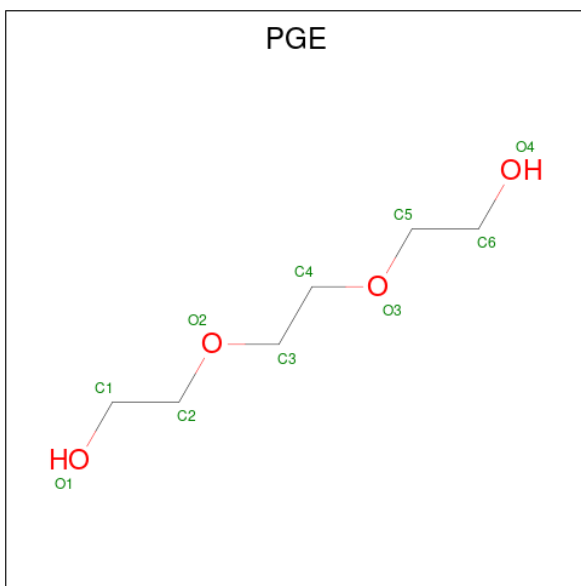
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 14 7 7	0	0
4	C	1	Total C O 14 7 7	0	0

- Molecule 5 is FE(7)-MO-S(9)-N CLUSTER (three-letter code: CFN) (formula: Fe<sub>7</sub>MoNS<sub>9</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Fe Mo N S 18 7 1 1 9	0	0
5	C	1	Total Fe Mo N S 18 7 1 1 9	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 6 4	0	0
6	A	1	Total C O 10 6 4	0	0
6	B	1	Total C O 10 6 4	0	0
6	C	1	Total C O 10 6 4	0	0
6	C	1	Total C O 10 6 4	0	0
6	D	1	Total C O 10 6 4	0	0
6	D	1	Total C O 10 6 4	0	0
6	D	1	Total C O 10 6 4	0	0

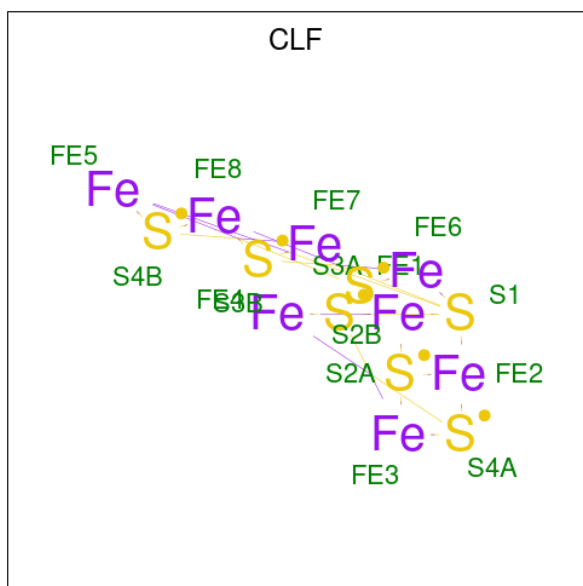
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Na 1 1	0	0

- Molecule 9 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe<sub>8</sub>S<sub>7</sub>).



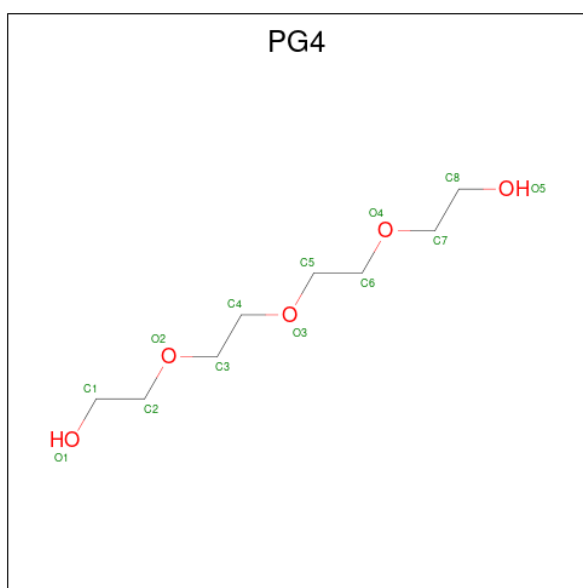
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 15 8 7	0	0
9	C	1	Total Fe S 15 8 7	0	0

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
10	B	1	Total	C	N	O	0	0
			8	4	1	3		
10	C	1	Total	C	N	O	0	0
			8	4	1	3		

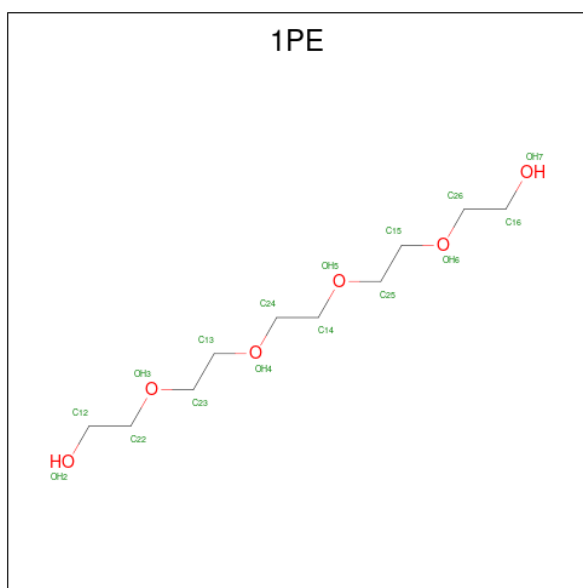
- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			13	8	5		
11	E	1	Total	C	O	0	0
			13	8	5		

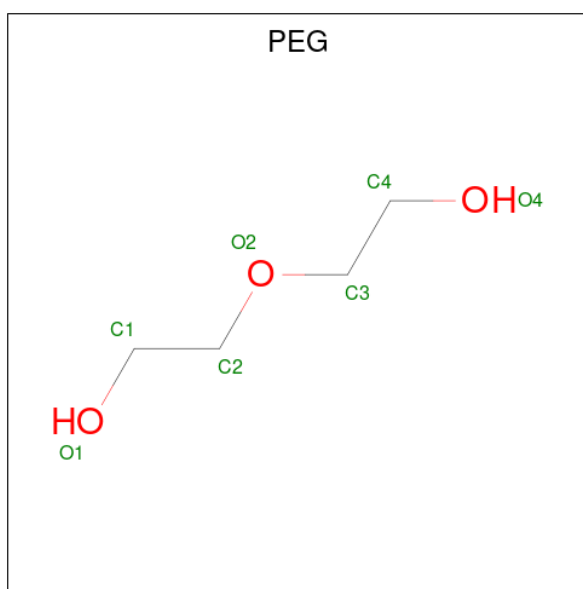


- Molecule 12 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



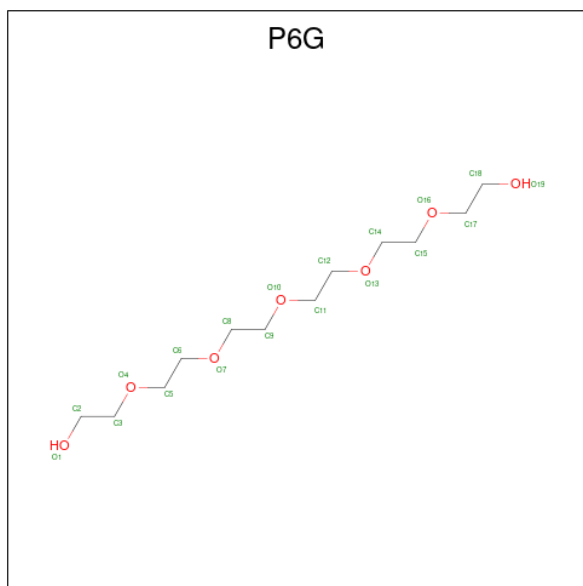
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	C O	0	0
			16	10 6		
12	C	1	Total	C O	0	0
			16	10 6		

- Molecule 13 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



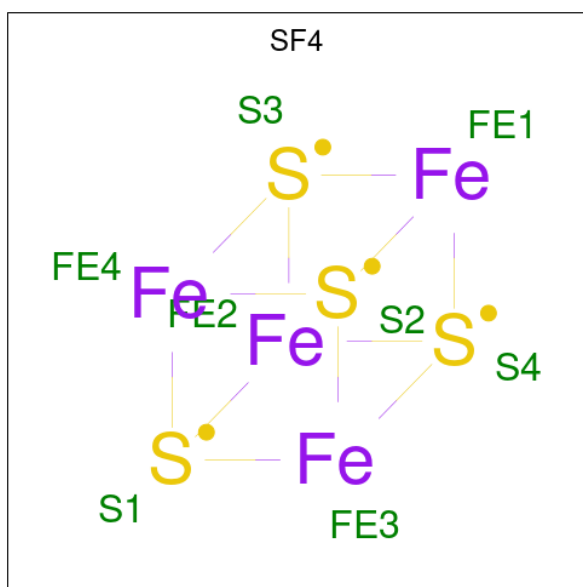
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			7	4	3		
13	D	1	Total	C	O	0	0
			7	4	3		
13	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 14 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	C	O	0	0
			19	12	7		

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	E	1	Total	Fe S	0	0
			8	4 4		

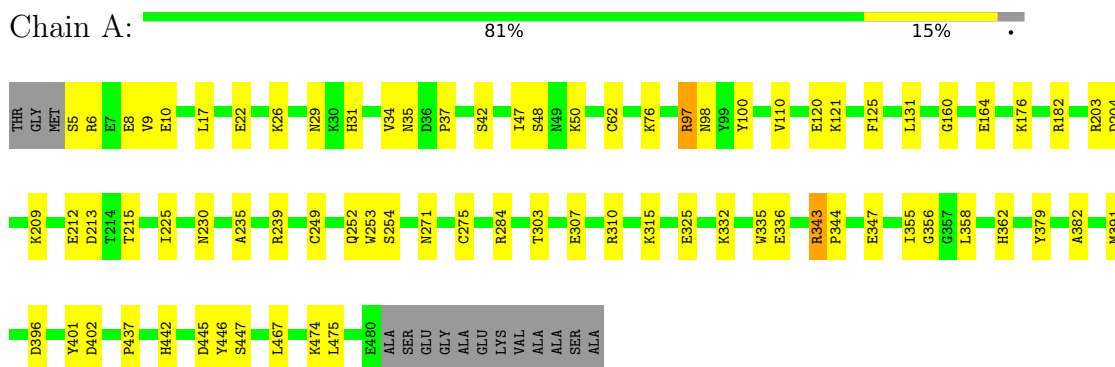
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	355	Total	O	0	0
			355	355		
16	B	594	Total	O	0	0
			594	594		
16	C	362	Total	O	0	0
			362	362		
16	D	527	Total	O	0	0
			527	527		
16	E	115	Total	O	0	0
			115	115		
16	F	118	Total	O	0	0
			118	118		

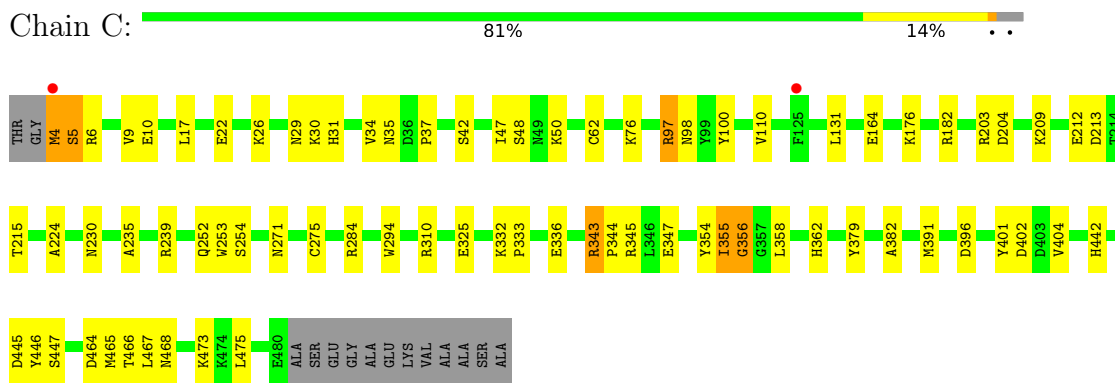
### 3 Residue-property plots [i](#)

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.

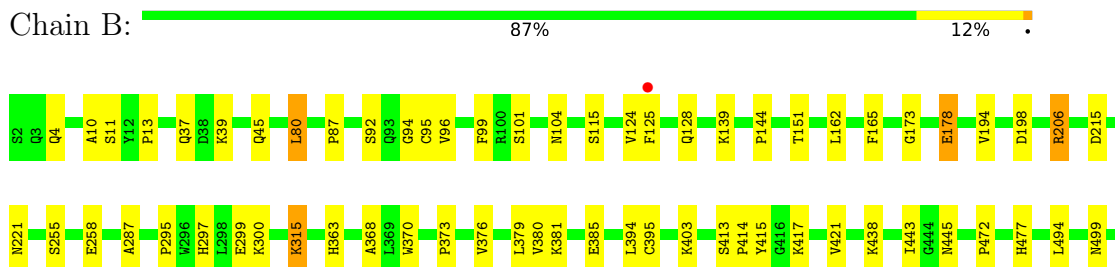
- Molecule 1: Nitrogenase molybdenum-iron protein



- Molecule 1: Nitrogenase molybdenum-iron protein

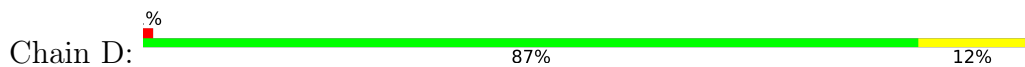


- Molecule 2: Nitrogenase molybdenum-iron protein





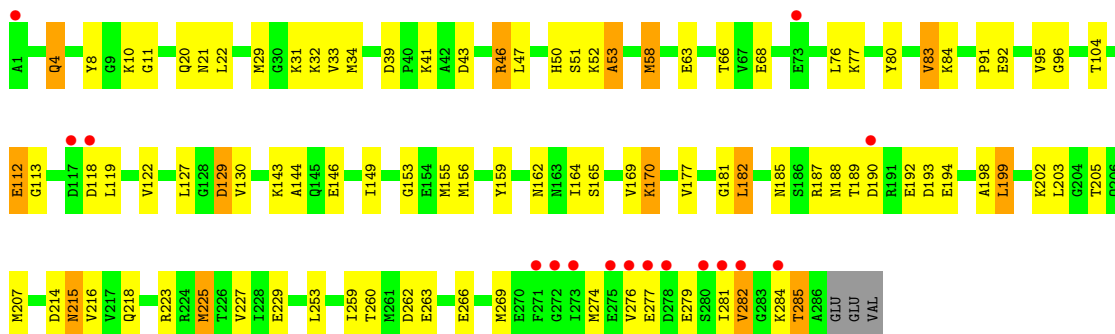
• Molecule 2: Nitrogenase molybdenum-iron protein



• Molecule 3: Nitrogenase iron protein 1



• Molecule 3: Nitrogenase iron protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.91Å 75.89Å 223.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.28 – 2.10 43.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (43.28-2.10) 95.6 (43.28-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.172 , 0.221 0.167 , 0.216	Depositor DCC
$R_{free}$ test set	8399 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtrriage
Anisotropy	0.342	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22638	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: SF4, 1PE, CLF, HCA, PEG, PG4, CA, TRS, NA, CFN, P6G, PGE

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	0.55	0/3870	0.80	4/5219 (0.1%)
1	C	0.55	0/3878	0.80	4/5229 (0.1%)
2	B	0.63	0/4280	0.83	5/5786 (0.1%)
2	D	0.60	0/4280	0.83	5/5786 (0.1%)
3	E	0.48	0/2211	0.74	1/2977 (0.0%)
3	F	0.48	0/2185	0.76	1/2943 (0.0%)
All	All	0.57	0/20704	0.80	20/27940 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	206	ARG	NE-CZ-NH1	-17.03	111.78	120.30
2	B	206	ARG	NE-CZ-NH2	-16.77	111.92	120.30
2	B	206	ARG	NE-CZ-NH1	14.63	127.62	120.30
2	D	206	ARG	NE-CZ-NH2	14.33	127.47	120.30
1	C	97	ARG	NE-CZ-NH2	-9.99	115.30	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	TYR	Sidechain
1	C	446	TYR	Sidechain

## 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	3782	0	3720	66	0
1	C	3790	0	3729	63	0
2	B	4174	0	4088	60	0
2	D	4174	0	4088	59	0
3	E	2187	0	2197	106	0
3	F	2161	0	2176	81	0
4	A	14	0	6	2	0
4	C	14	0	6	1	0
5	A	18	0	0	1	0
5	C	18	0	0	0	0
6	A	20	0	28	8	0
6	B	10	0	14	5	0
6	C	20	0	28	4	0
6	D	30	0	42	8	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	1	0	0	0	0
9	B	15	0	0	0	0
9	C	15	0	0	0	0
10	B	8	0	12	0	0
10	C	8	0	12	2	0
11	B	13	0	18	0	0
11	E	13	0	18	7	0
12	B	16	0	22	7	0
12	C	16	0	22	22	0
13	B	7	0	10	0	0
13	D	14	0	20	5	0
14	D	19	0	26	1	0
15	E	8	0	0	0	0
16	A	355	0	0	11	0
16	B	594	0	0	8	0
16	C	362	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	D	527	0	0	11	1
16	E	115	0	0	9	0
16	F	118	0	0	5	0
All	All	22638	0	20282	415	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 10.

The worst 5 of 415 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:160:GLY:HA3	3:E:140:ARG:HH21	1.16	1.06
1:A:303:THR:HG23	6:A:5015:PGE:H22	1.39	1.01
2:B:295:PRO:HB2	6:B:5005:PGE:H4	1.46	0.96
3:F:21:ASN:HD21	3:F:227:VAL:H	1.05	0.95
1:A:249:CYS:HB3	16:A:5292:HOH:O	1.65	0.94

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)
16:D:5299:HOH:O	16:D:5382:HOH:O[3_545]	2.19	0.01

## 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	474/491 (96%)	450 (95%)	23 (5%)	1 (0%)	47 49
1	C	475/491 (97%)	447 (94%)	26 (6%)	2 (0%)	34 32
2	B	520/522 (100%)	504 (97%)	15 (3%)	1 (0%)	47 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	520/522 (100%)	504 (97%)	15 (3%)	1 (0%)	47	49
3	E	287/289 (99%)	267 (93%)	17 (6%)	3 (1%)	15	11
3	F	284/289 (98%)	265 (93%)	14 (5%)	5 (2%)	8	4
All	All	2560/2604 (98%)	2437 (95%)	110 (4%)	13 (0%)	29	26

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	64	ALA
3	F	190	ASP
3	F	282	VAL
2	B	255	SER
2	D	255	SER

### 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	406/414 (98%)	398 (98%)	8 (2%)	55	60
1	C	407/414 (98%)	399 (98%)	8 (2%)	55	60
2	B	454/454 (100%)	445 (98%)	9 (2%)	55	60
2	D	454/454 (100%)	447 (98%)	7 (2%)	65	71
3	E	233/233 (100%)	218 (94%)	15 (6%)	17	14
3	F	230/233 (99%)	216 (94%)	14 (6%)	18	16
All	All	2184/2202 (99%)	2123 (97%)	61 (3%)	43	47

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	215	ASP
3	F	182	LEU
3	E	83	VAL
3	F	170	LYS

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Mol	Chain	Res	Type
3	F	225	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	20	GLN
3	E	201	ASN
3	E	21	ASN
3	E	55	ASN
3	E	218	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 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
14	P6G	D	5009	-	18,18,18	1.76	10 (55%)	17,17,17	0.68	0
4	HCA	A	2494	-	13,13,13	1.42	1 (7%)	14,18,18	1.50	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CFN	A	2496	1	18,30,30	1.61	3 (16%)	-		
9	CLF	B	2498	1,2	0,24,24	-	-	-		
10	TRS	B	5003	-	7,7,7	0.52	0	9,9,9	1.24	1 (11%)
12	1PE	B	5017	-	15,15,15	1.78	7 (46%)	14,14,14	0.60	0
15	SF4	E	3290	3	0,12,12	-	-	-		
6	PGE	C	5011	-	9,9,9	1.53	4 (44%)	8,8,8	0.49	0
9	CLF	C	3498	1,2	0,24,24	-	-	-		
6	PGE	B	5005	-	9,9,9	1.16	0	8,8,8	0.57	0
13	PEG	B	5018	-	6,6,6	1.07	1 (16%)	5,5,5	0.36	0
13	PEG	D	5020	-	6,6,6	1.37	2 (33%)	5,5,5	0.38	0
6	PGE	D	5010	-	9,9,9	1.58	4 (44%)	8,8,8	0.56	0
13	PEG	D	5019	-	6,6,6	1.03	0	5,5,5	0.32	0
6	PGE	A	5012	-	9,9,9	1.22	0	8,8,8	0.32	0
6	PGE	D	5008	-	9,9,9	1.21	0	8,8,8	0.35	0
4	HCA	C	3494	-	13,13,13	1.40	1 (7%)	14,18,18	2.11	4 (28%)
5	CFN	C	3496	1	18,30,30	1.90	6 (33%)	-		
12	1PE	C	5013	-	15,15,15	1.69	6 (40%)	14,14,14	0.65	0
10	TRS	C	5004	-	7,7,7	0.37	0	9,9,9	1.32	0
11	PG4	B	5014	-	12,12,12	1.35	1 (8%)	11,11,11	0.36	0
6	PGE	D	5006	-	9,9,9	1.09	0	8,8,8	0.45	0
11	PG4	E	5007	-	12,12,12	1.45	2 (16%)	11,11,11	0.55	0
6	PGE	C	5016	-	9,9,9	1.49	4 (44%)	8,8,8	0.49	0
6	PGE	A	5015	-	9,9,9	1.65	4 (44%)	8,8,8	0.52	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
14	P6G	D	5009	-	-	15/16/16/16	-
4	HCA	A	2494	-	-	2/17/17/17	-
10	TRS	B	5003	-	-	2/9/9/9	-
9	CLF	B	2498	1,2	-	-	0/12/10/10
12	1PE	B	5017	-	-	8/13/13/13	-
15	SF4	E	3290	3	-	-	0/6/5/5
6	PGE	C	5011	-	-	1/7/7/7	-
9	CLF	C	3498	1,2	-	-	0/12/10/10

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGE	B	5005	-	-	2/7/7/7	-
13	PEG	B	5018	-	-	3/4/4/4	-
13	PEG	D	5020	-	-	2/4/4/4	-
6	PGE	D	5010	-	-	6/7/7/7	-
13	PEG	D	5019	-	-	3/4/4/4	-
6	PGE	A	5012	-	-	3/7/7/7	-
6	PGE	D	5008	-	-	4/7/7/7	-
4	HCA	C	3494	-	-	3/17/17/17	-
12	1PE	C	5013	-	-	8/13/13/13	-
10	TRS	C	5004	-	-	8/9/9/9	-
11	PG4	B	5014	-	-	1/10/10/10	-
6	PGE	D	5006	-	-	5/7/7/7	-
11	PG4	E	5007	-	-	5/10/10/10	-
6	PGE	C	5016	-	-	2/7/7/7	-
6	PGE	A	5015	-	-	4/7/7/7	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2494	HCA	O7-C3	3.32	1.49	1.43
5	C	3496	CFN	S1B-FE6	-3.30	2.23	2.29
5	C	3496	CFN	S2A-FE2	-3.26	2.23	2.29
5	A	2496	CFN	S1B-FE6	-3.13	2.23	2.29
4	C	3494	HCA	O7-C3	3.06	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3494	HCA	O7-C3-C7	-4.41	102.68	108.86
4	C	3494	HCA	O6-C7-C3	3.73	119.53	113.05
4	C	3494	HCA	O5-C7-C3	-3.35	117.51	122.25
4	A	2494	HCA	O6-C7-C3	3.12	118.47	113.05
4	A	2494	HCA	O5-C7-C3	-3.08	117.90	122.25

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

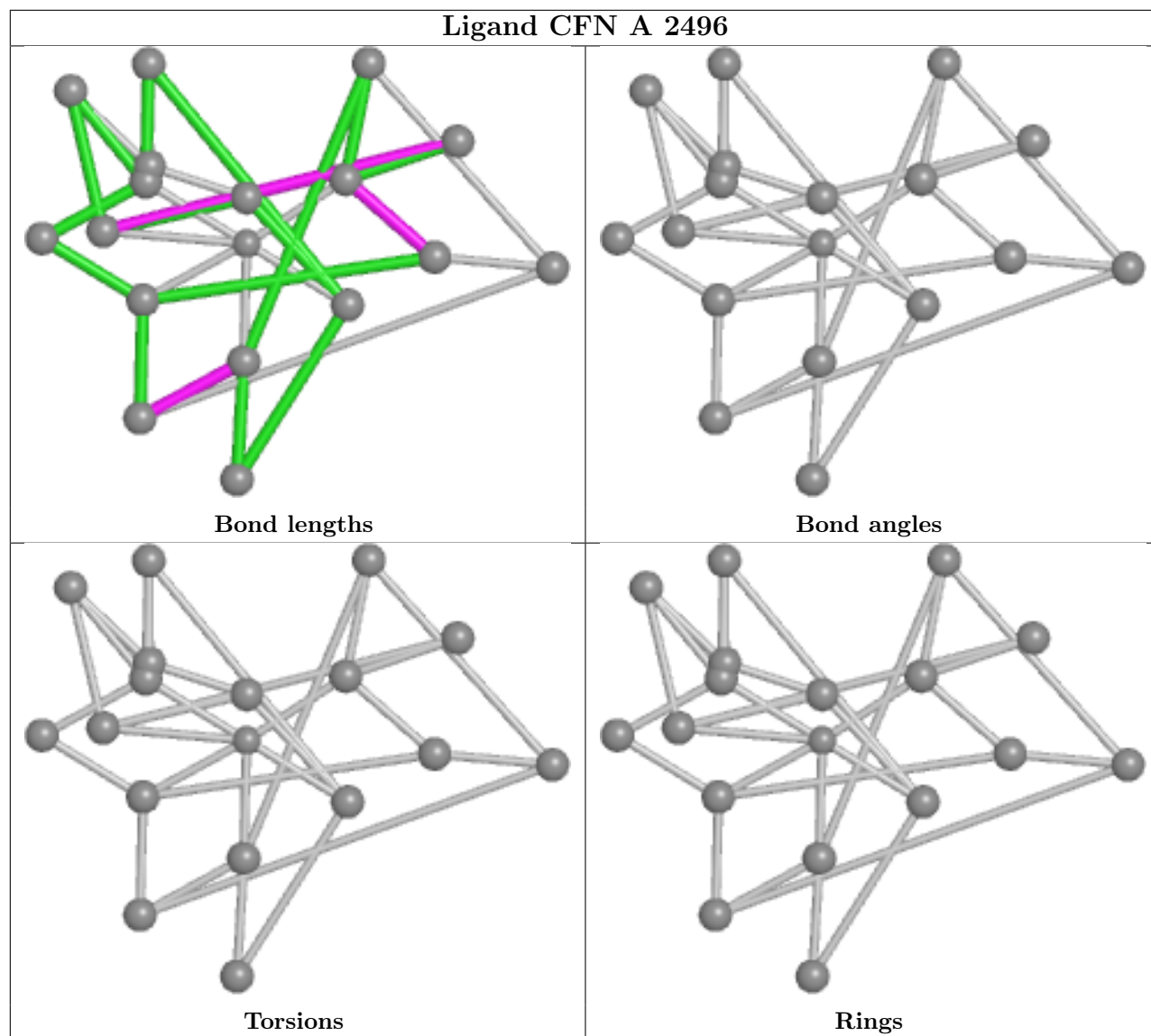
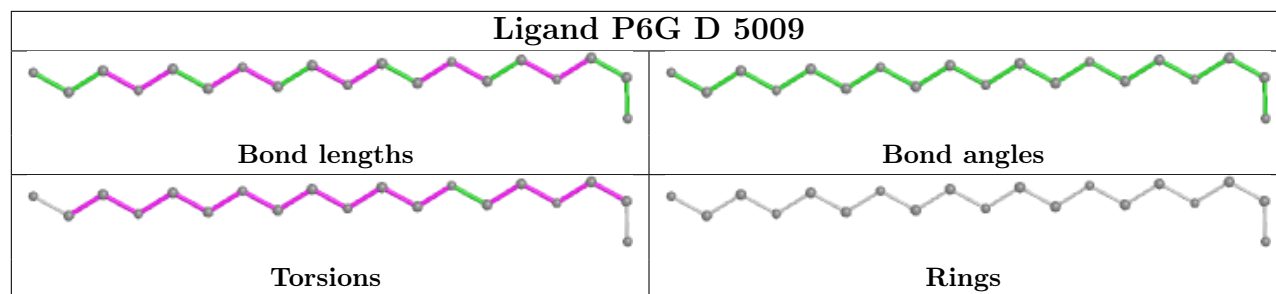
Mol	Chain	Res	Type	Atoms
10	C	5004	TRS	C1-C-C2-O2
10	C	5004	TRS	C3-C-C2-O2
10	C	5004	TRS	N-C-C2-O2
10	C	5004	TRS	C2-C-C3-O3
14	D	5009	P6G	C15-C14-O13-C12

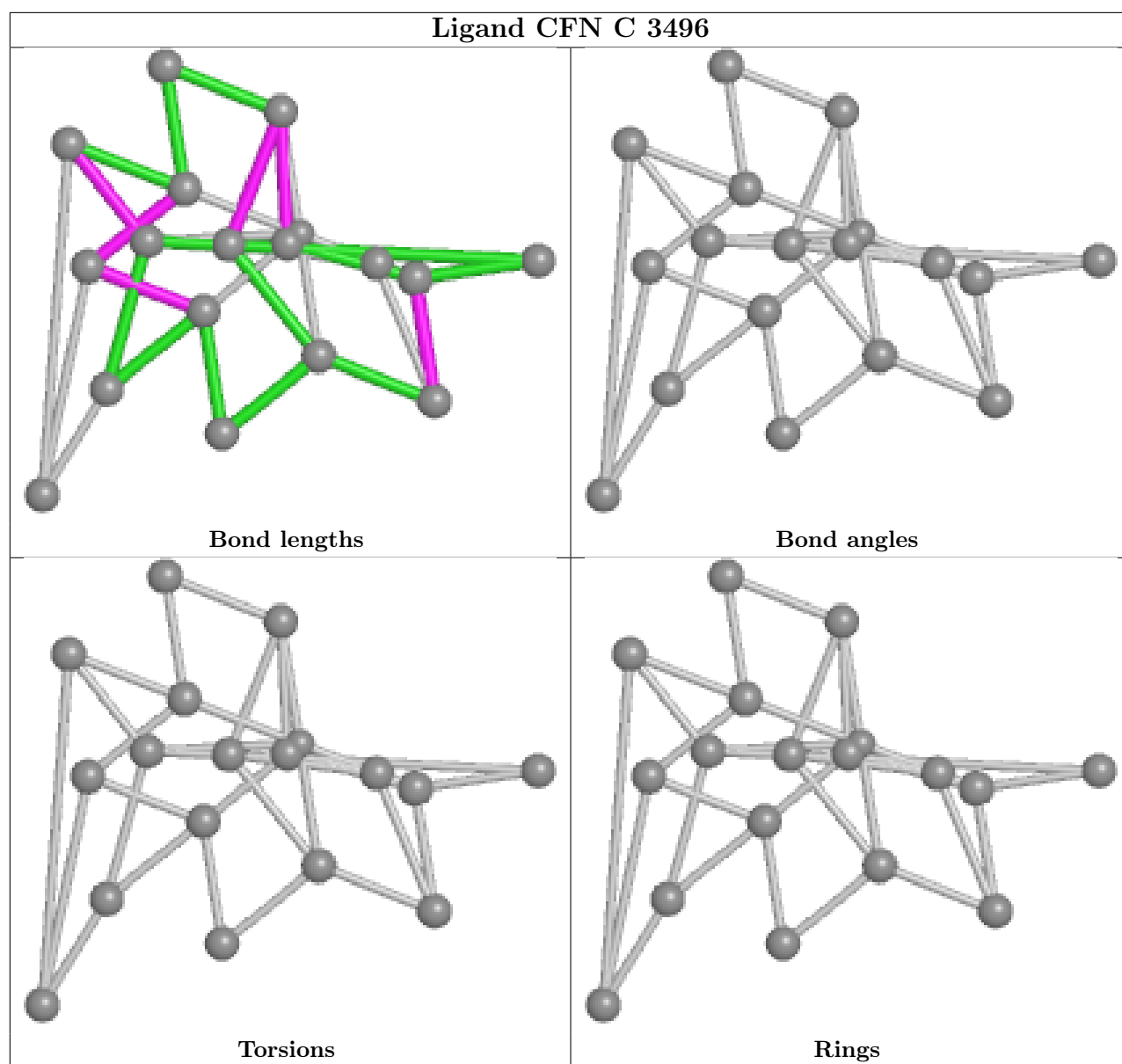
There are no ring outliers.

17 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	5009	P6G	1	0
4	A	2494	HCA	2	0
5	A	2496	CFN	1	0
12	B	5017	1PE	7	0
6	C	5011	PGE	4	0
6	B	5005	PGE	5	0
13	D	5020	PEG	4	0
6	D	5010	PGE	4	0
13	D	5019	PEG	1	0
6	A	5012	PGE	1	0
6	D	5008	PGE	2	0
4	C	3494	HCA	1	0
12	C	5013	1PE	22	0
10	C	5004	TRS	2	0
6	D	5006	PGE	2	0
11	E	5007	PG4	7	0
6	A	5015	PGE	7	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, 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	476/491 (96%)	-0.44	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	12, 22, 40, 66	2 (0%)
1	C	477/491 (97%)	-0.43	2 (0%) <span style="border: 1px solid blue; padding: 2px;">92</span> <span style="border: 1px solid blue; padding: 2px;">93</span>	12, 22, 41, 64	0
2	B	522/522 (100%)	-0.60	1 (0%) <span style="border: 1px solid blue; padding: 2px;">95</span> <span style="border: 1px solid blue; padding: 2px;">95</span>	10, 16, 32, 55	1 (0%)
2	D	522/522 (100%)	-0.56	3 (0%) <span style="border: 1px solid blue; padding: 2px;">89</span> <span style="border: 1px solid blue; padding: 2px;">91</span>	10, 18, 35, 53	0
3	E	289/289 (100%)	0.02	14 (4%) <span style="border: 1px solid red; padding: 2px;">30</span> <span style="border: 1px solid red; padding: 2px;">36</span>	20, 35, 65, 85	0
3	F	286/289 (98%)	-0.05	16 (5%) <span style="border: 1px solid red; padding: 2px;">24</span> <span style="border: 1px solid red; padding: 2px;">29</span>	19, 35, 67, 84	1 (0%)
All	All	2572/2604 (98%)	-0.40	36 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">78</span>	10, 22, 49, 85	4 (0%)

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	66	THR	7.6
2	B	125	PHE	6.4
3	E	42	ALA	5.6
3	F	276	VAL	4.8
3	E	65	GLY	4.7

### 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](#)

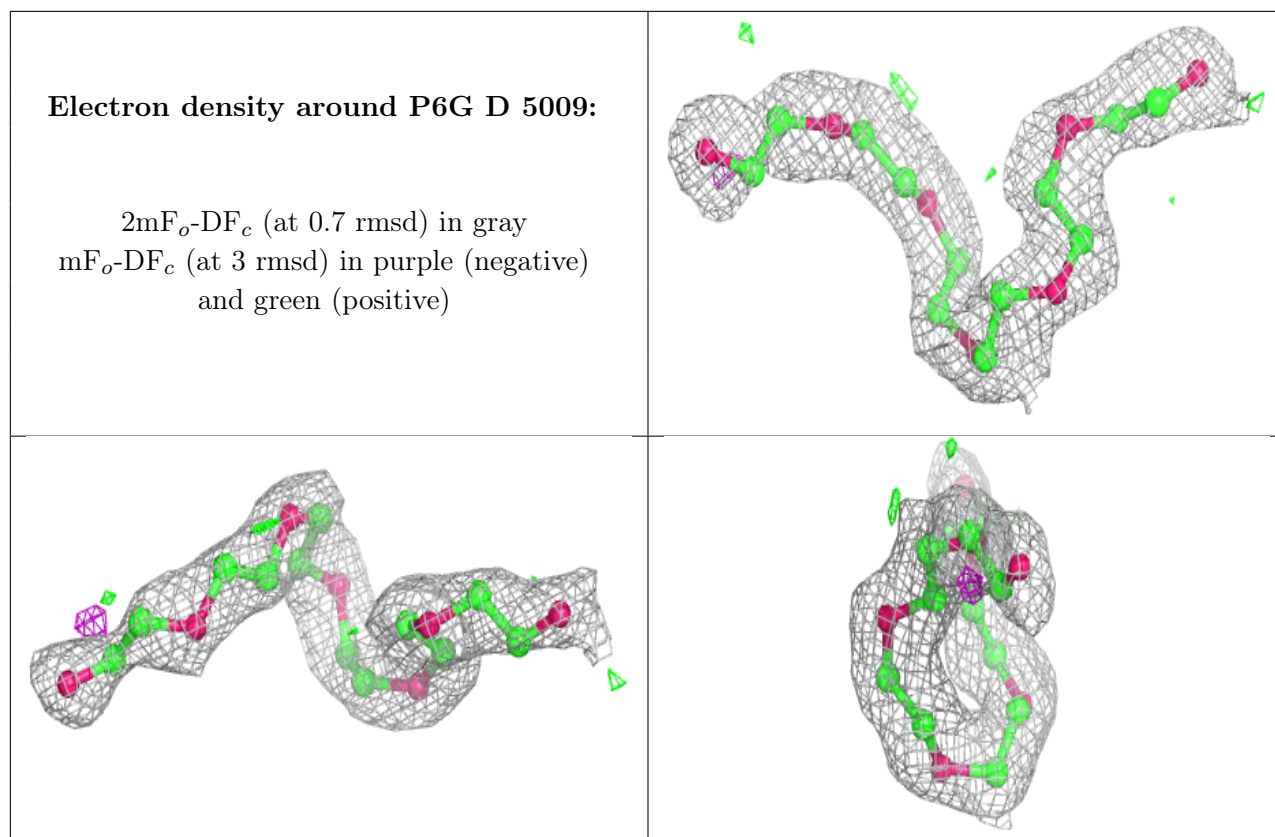
There are no monosaccharides in this entry.

## 6.4 Ligands

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.

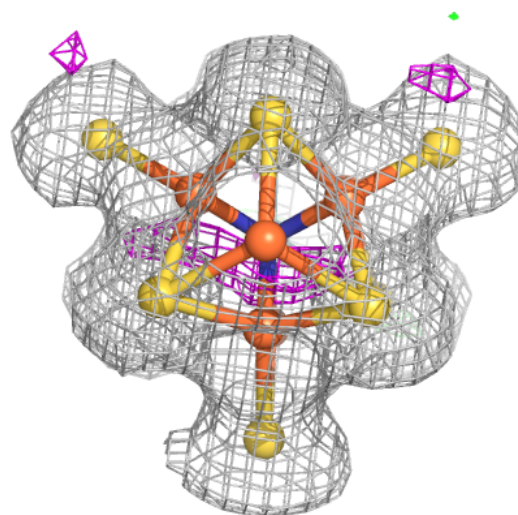
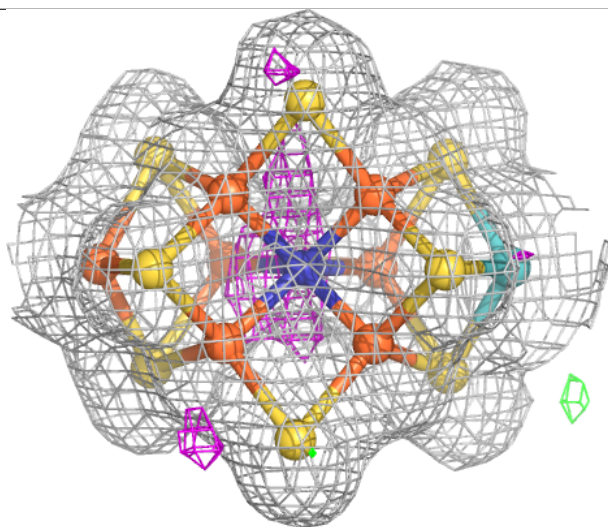
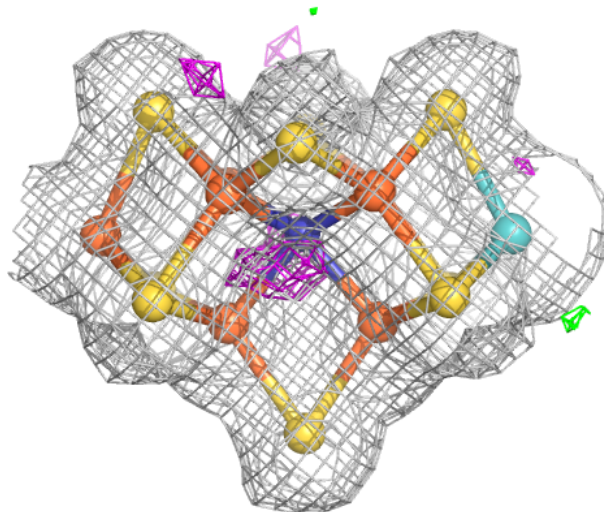
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NA	B	2492	1/1	0.43	0.13	40,40,40,40	0
6	PGE	A	5015	10/10	0.76	0.33	44,48,52,61	0
11	PG4	E	5007	13/13	0.79	0.21	43,48,56,57	0
6	PGE	D	5010	10/10	0.81	0.28	39,46,53,58	0
10	TRS	C	5004	8/8	0.82	0.27	44,47,50,50	0
6	PGE	C	5016	10/10	0.83	0.34	40,49,53,62	0
12	1PE	C	5013	16/16	0.84	0.24	36,45,50,55	0
6	PGE	A	5012	10/10	0.86	0.33	40,47,58,58	0
13	PEG	D	5020	7/7	0.86	0.29	33,38,45,50	0
13	PEG	D	5019	7/7	0.87	0.16	46,52,59,65	0
6	PGE	C	5011	10/10	0.88	0.20	37,46,52,56	0
12	1PE	B	5017	16/16	0.89	0.31	22,44,51,57	0
6	PGE	D	5006	10/10	0.90	0.13	29,41,45,47	0
14	P6G	D	5009	19/19	0.90	0.12	24,38,48,51	0
13	PEG	B	5018	7/7	0.93	0.10	28,30,46,49	0
6	PGE	D	5008	10/10	0.93	0.15	29,44,51,62	0
11	PG4	B	5014	13/13	0.94	0.10	26,34,40,47	0
6	PGE	B	5005	10/10	0.94	0.11	26,30,45,48	0
10	TRS	B	5003	8/8	0.95	0.16	22,28,37,45	0
4	HCA	A	2494	14/14	0.96	0.16	12,17,22,23	0
9	CLF	B	2498	15/15	0.96	0.09	3,15,16,36	2
9	CLF	C	3498	15/15	0.97	0.07	18,21,24,38	0
4	HCA	C	3494	14/14	0.98	0.14	15,17,21,21	0
15	SF4	E	3290	8/8	0.98	0.05	25,27,28,30	0
7	CA	B	2491	1/1	0.99	0.05	25,25,25,25	0
7	CA	D	2490	1/1	0.99	0.03	24,24,24,24	0
5	CFN	A	2496	18/18	0.99	0.08	15,18,19,20	0
5	CFN	C	3496	18/18	0.99	0.10	14,18,22,22	0

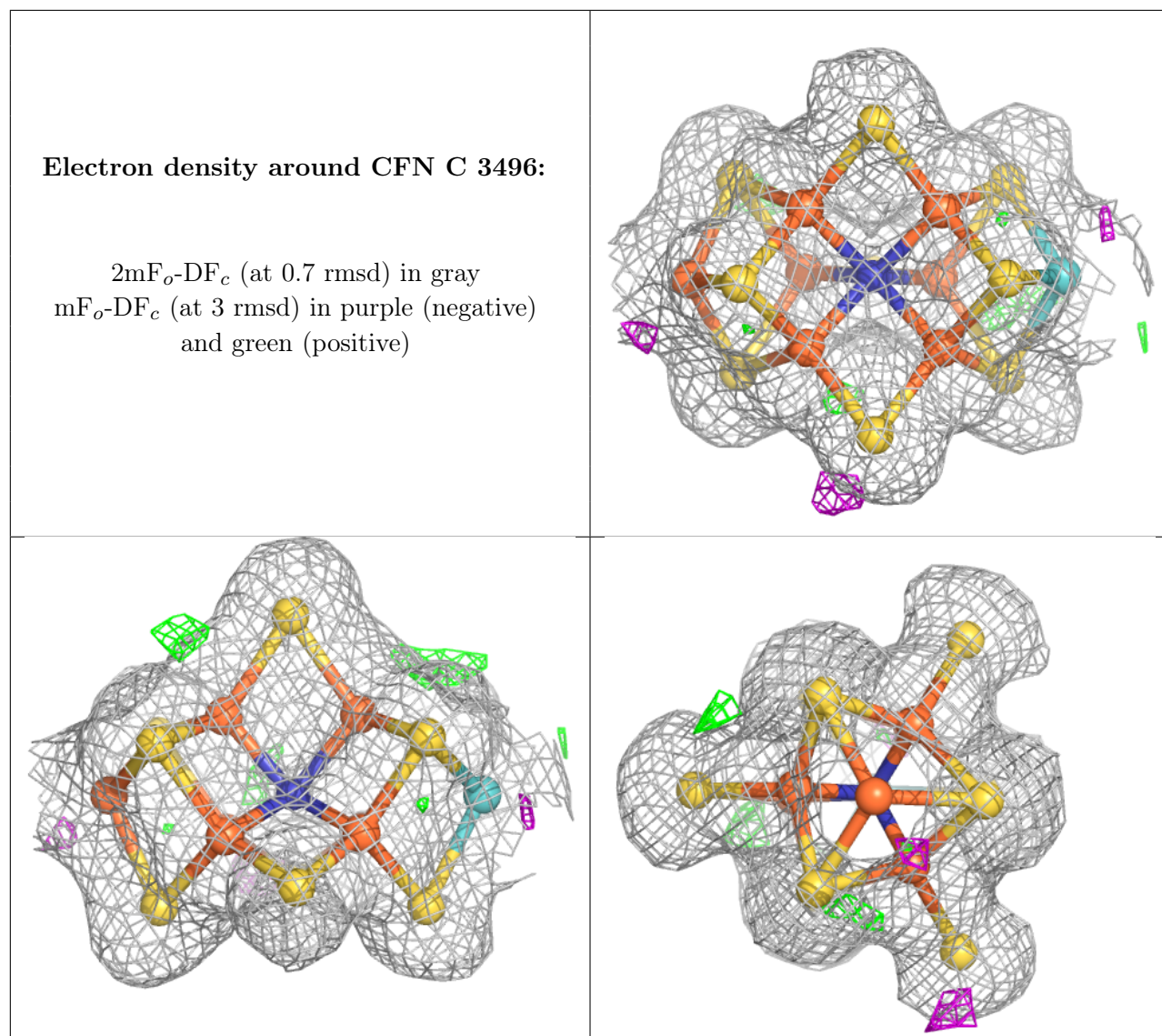
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around CFN A 2496:**

$2mF_o-DF_c$  (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.