WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 10, 2023 – 12:07 pm GMT

PDB ID	:	1E94
Title	:	HslV-HslU from E.coli
Authors	:	Song, H.K.; Hartmann, C.; Ravishankar, R.; Bochtler, M.
Deposited on	:	2000-10-07
Resolution	:	2.80 Å(reported)

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

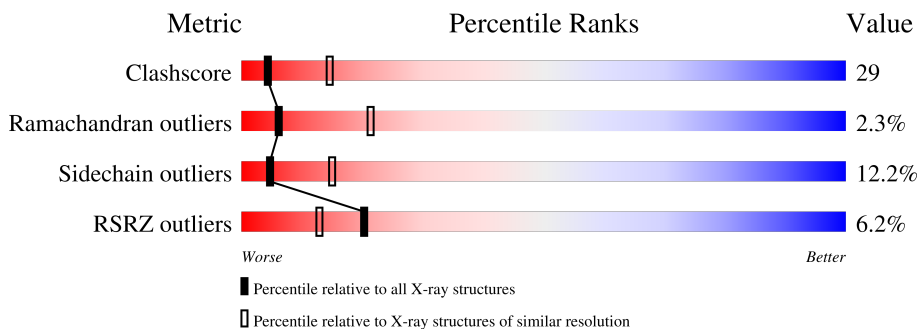|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	Percentile Ranks	Value
Clashscore		29
Ramachandran outliers		2.3%
Sidechain outliers		12.2%
RSRZ outliers		6.2%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	175	66% 31% ••
1	B	175	3% 53% 41% 6% •
1	C	175	6% 57% 37% 5% ••
1	D	175	6% 46% 47% 6% •
2	E	449	7% 46% 39% 6% 9%
2	F	449	7% 50% 34% 7% 9%

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
3	ANP	F	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12028 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 HEAT SHOCK PROTEIN HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	25	0	0
			1328	834	237	253	4			
1	B	174	Total	C	N	O	S	24	0	0
			1328	834	237	253	4			
1	C	174	Total	C	N	O	S	18	0	0
			1328	834	237	253	4			
1	D	174	Total	C	N	O	S	24	0	0
			1328	834	237	253	4			

- Molecule 2 is a protein called HEAT SHOCK PROTEIN HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	408	Total	C	N	O	S	220	1	0
			3184	1989	570	615	10			
2	F	409	Total	C	N	O	S	443	0	1
			3184	1989	571	614	10			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

ANP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	29	Total	O	0	0
			29	29		
4	C	33	Total	O	0	0
			33	33		
4	D	31	Total	O	0	0
			31	31		
4	E	94	Total	O	0	0
			94	94		
4	F	68	Total	O	0	0
			68	68		

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.
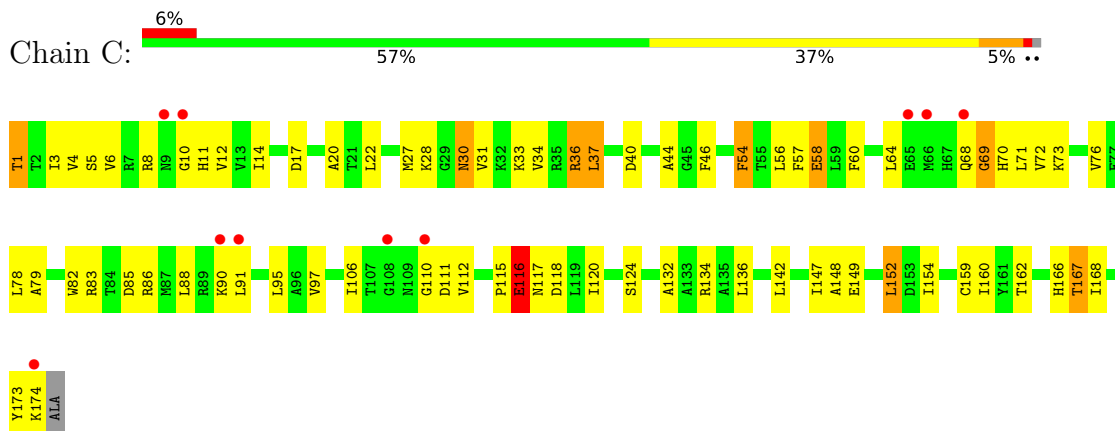
• Molecule 1: HEAT SHOCK PROTEIN HSLV
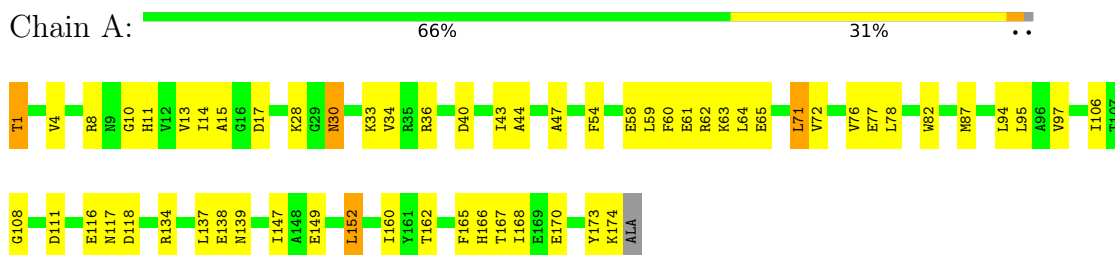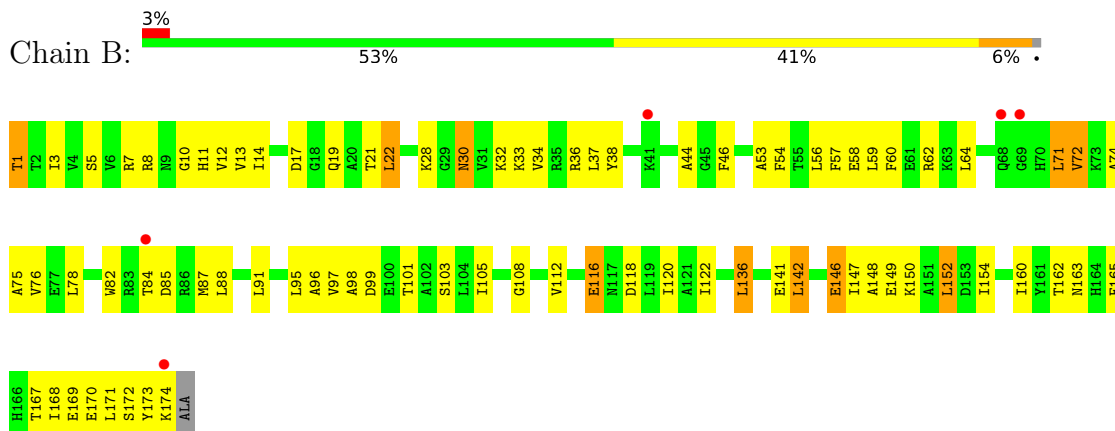
Chain A:

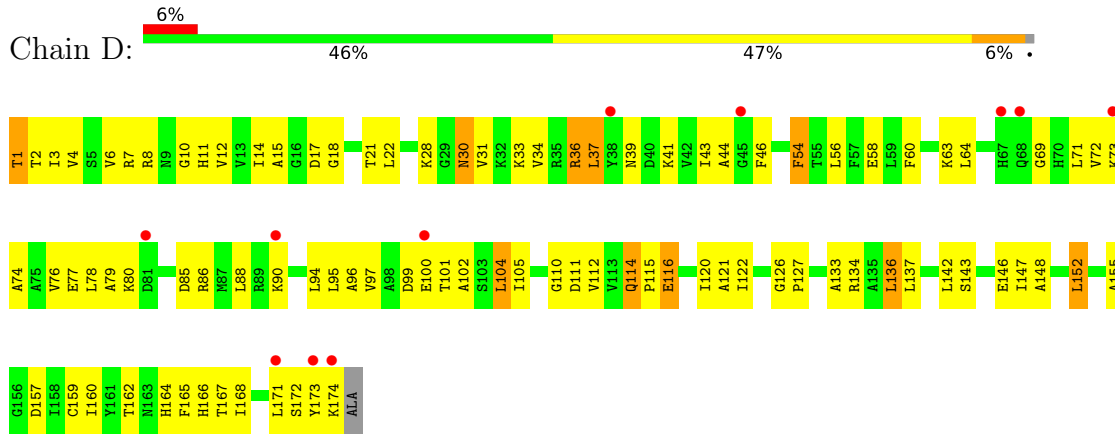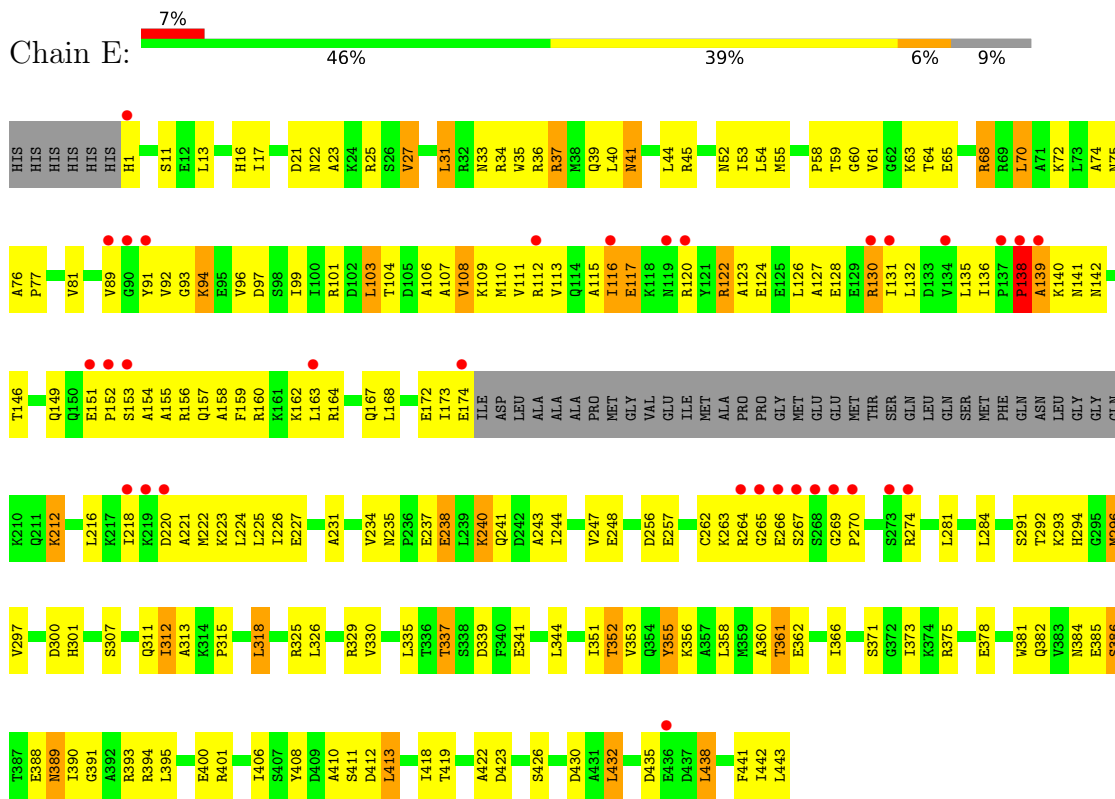• Molecule 1: HEAT SHOCK PROTEIN HSLV

Chain B:

• Molecule 1: HEAT SHOCK PROTEIN HSLV

Chain C:

• Molecule 1: HEAT SHOCK PROTEIN HSLV

Chain D:

• Molecule 2: HEAT SHOCK PROTEIN HSLU

Chain E:

• Molecule 2: HEAT SHOCK PROTEIN HSLU

Chain F:
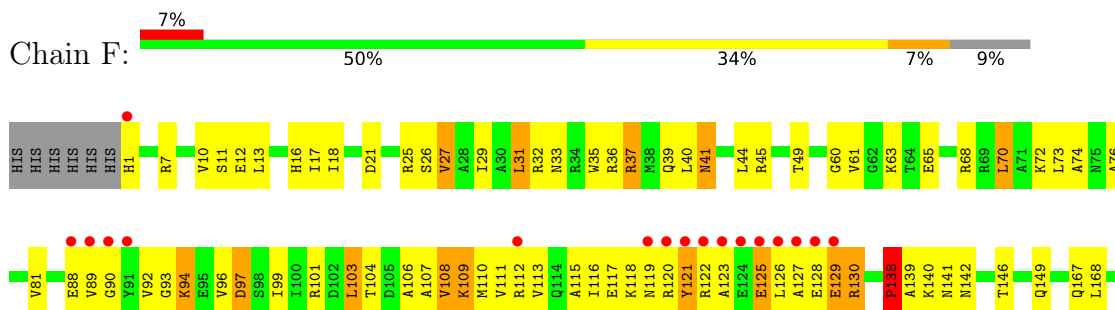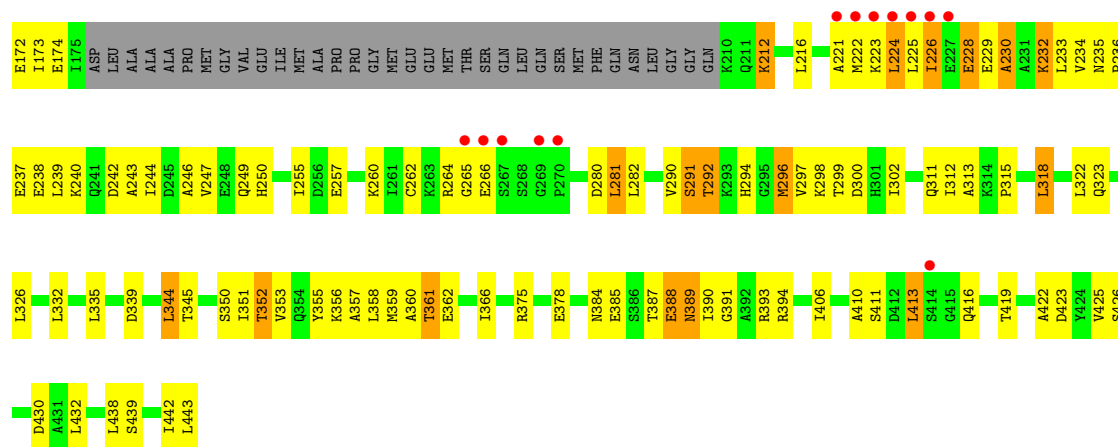
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	172.02Å 172.02Å 276.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80 29.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (15.00-2.80) 92.3 (29.62-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	4.48 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.254 , 0.304 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	68.0	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 88.5	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12028	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3856e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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: ANP

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	0.59	0/1345	0.80	1/1817 (0.1%)
1	B	0.59	0/1345	0.80	2/1817 (0.1%)
1	C	0.48	0/1345	0.74	1/1817 (0.1%)
1	D	0.53	0/1345	0.71	0/1817
2	E	0.59	1/3228 (0.0%)	0.80	1/4352 (0.0%)
2	F	0.63	3/3221 (0.1%)	1.01	7/4345 (0.2%)
All	All	0.58	4/11829 (0.0%)	0.85	12/15965 (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
2	E	0	1
2	F	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	224	LEU	C-N	12.55	1.62	1.34
2	F	129	GLU	C-N	-8.55	1.14	1.34
2	F	138	PRO	C-N	-6.77	1.18	1.34
2	E	138	PRO	C-N	-6.77	1.18	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	129	GLU	O-C-N	-25.89	81.27	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	224	LEU	O-C-N	20.97	156.26	122.70
2	E	138	PRO	O-C-N	-18.12	93.71	122.70
2	F	138	PRO	O-C-N	-18.10	93.75	122.70
2	F	224	LEU	CA-C-N	-15.95	82.11	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	138	PRO	Mainchain
2	F	129	GLU	Mainchain
2	F	138	PRO	Mainchain

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	1328	0	1348	49	0
1	B	1328	0	1347	64	0
1	C	1328	0	1348	57	0
1	D	1328	0	1348	78	0
2	E	3184	0	3205	223	0
2	F	3184	0	3207	174	0
3	E	31	0	12	6	0
3	F	31	0	12	9	0
4	A	31	0	0	3	0
4	B	29	0	0	1	0
4	C	33	0	0	5	0
4	D	31	0	0	5	0
4	E	94	0	0	11	0
4	F	68	0	0	11	0
All	All	12028	0	11827	640	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.

The worst 5 of 640 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:E:153:SER:CA	2:E:156:ARG:HB3	1.47	1.44
2:E:153:SER:HB3	2:E:157:GLN:CG	1.52	1.37
2:E:131:ILE:HD11	2:E:218:ILE:CD1	1.57	1.34
2:E:151:GLU:O	2:E:154:ALA:N	1.57	1.32
2:F:224:LEU:O	2:F:228:GLU:HB2	1.14	1.29

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/175 (98%)	158 (92%)	13 (8%)	1 (1%)	25	56
1	B	172/175 (98%)	144 (84%)	23 (13%)	5 (3%)	4	15
1	C	172/175 (98%)	153 (89%)	16 (9%)	3 (2%)	9	29
1	D	172/175 (98%)	148 (86%)	22 (13%)	2 (1%)	13	39
2	E	398/449 (89%)	348 (87%)	41 (10%)	9 (2%)	6	21
2	F	399/449 (89%)	342 (86%)	43 (11%)	14 (4%)	3	12
All	All	1485/1598 (93%)	1293 (87%)	158 (11%)	34 (2%)	6	21

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	GLU
2	E	92	VAL
2	E	139	ALA
2	F	92	VAL
2	F	130	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/136 (100%)	129 (95%)	7 (5%)	24	55
1	B	136/136 (100%)	127 (93%)	9 (7%)	16	44
1	C	136/136 (100%)	123 (90%)	13 (10%)	8	24
1	D	136/136 (100%)	122 (90%)	14 (10%)	7	21
2	E	340/383 (89%)	285 (84%)	55 (16%)	2	7
2	F	339/383 (88%)	287 (85%)	52 (15%)	2	8
All	All	1223/1310 (93%)	1073 (88%)	150 (12%)	5	15

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	140	LYS
2	F	389	ASN
2	F	167	GLN
2	F	281	LEU
2	E	37	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	416	GLN
2	F	301	HIS
2	F	22	ASN
2	F	75	ASN
2	F	348	ASN

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	#$|Z| > 2$
3	ANP	E	500	-	29,33,33	5.17	19 (65%)	31,52,52	2.40	11 (35%)
3	ANP	F	501	-	29,33,33	4.51	22 (75%)	31,52,52	2.68	13 (41%)

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	ANP	E	500	-	-	6/14/38/38	0/3/3/3
3	ANP	F	501	-	-	7/14/38/38	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	500	ANP	PG-O1G	17.26	1.73	1.46
3	F	501	ANP	PG-O1G	13.67	1.67	1.46
3	E	500	ANP	PG-N3B	9.24	1.87	1.63
3	F	501	ANP	C2-N1	8.84	1.50	1.33
3	E	500	ANP	C2-N1	7.88	1.48	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	500	ANP	C4-C5-N7	8.20	117.95	109.40
3	F	501	ANP	C4-C5-N7	7.58	117.30	109.40
3	F	501	ANP	O1G-PG-N3B	-6.80	101.76	111.77
3	E	500	ANP	O2B-PB-O1B	4.41	119.17	109.92
3	F	501	ANP	C2'-C3'-C4'	4.37	111.12	102.64

There are no chirality outliers.
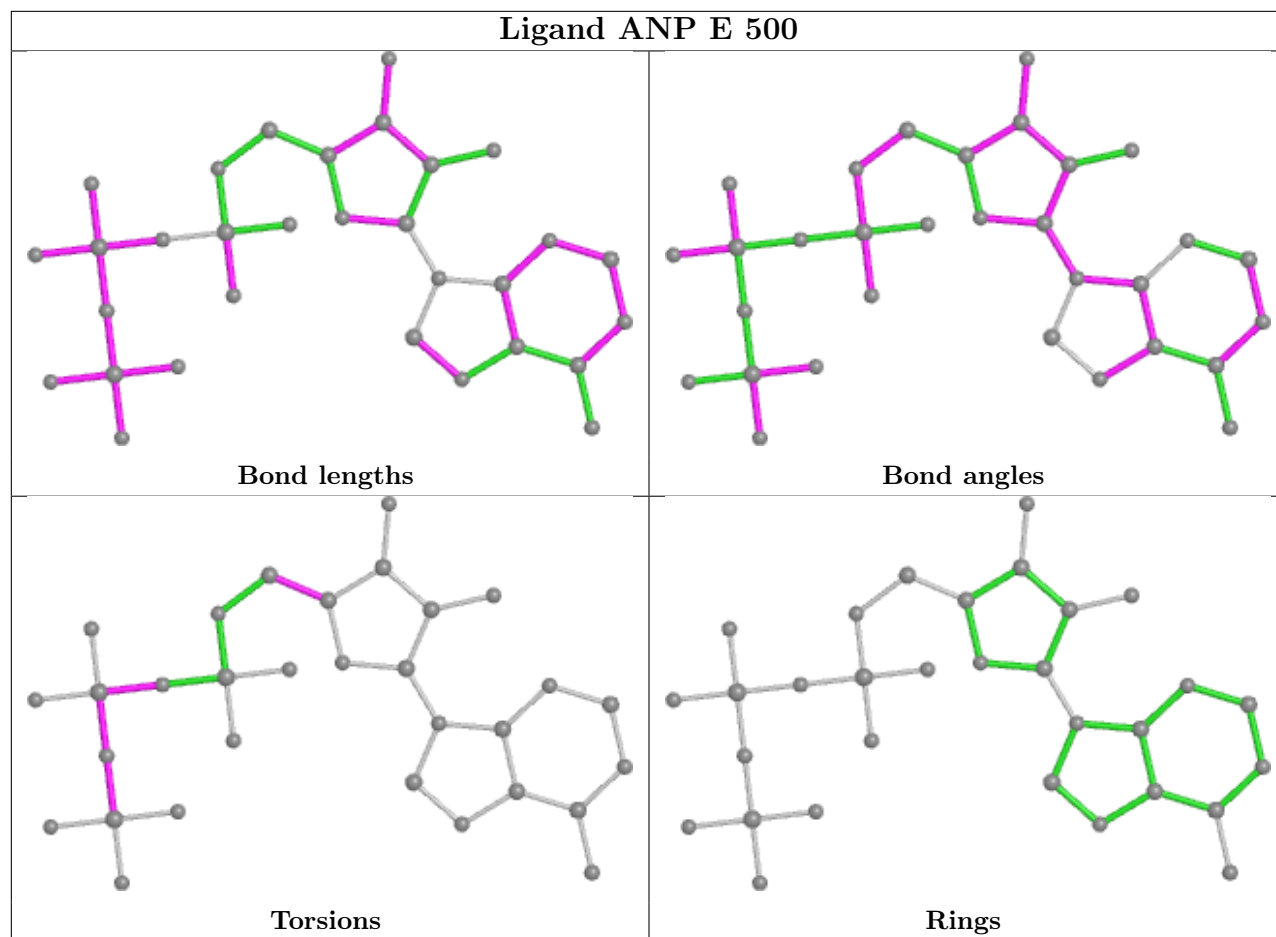
5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	500	ANP	PB-N3B-PG-O1G
3	E	500	ANP	PG-N3B-PB-O1B
3	E	500	ANP	PG-N3B-PB-O3A
3	E	500	ANP	PA-O3A-PB-O1B
3	F	501	ANP	PB-N3B-PG-O1G

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	500	ANP	6	0
3	F	501	ANP	9	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 ANP E 500

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP F 501

Bond lengths

Bond angles

Torsions

Rings
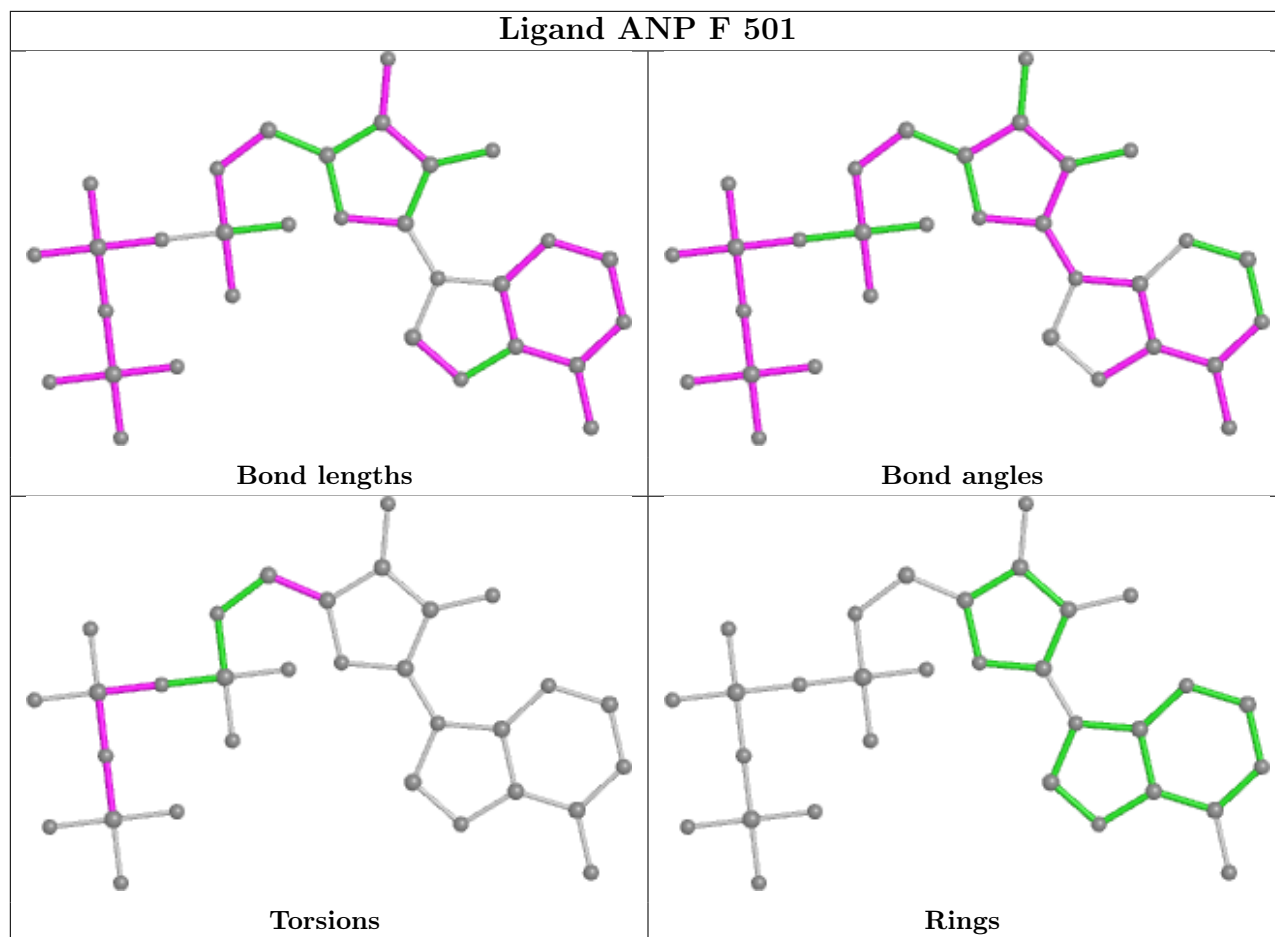
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	6
2	E	4

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	153:SER	C	154:ALA	N	2.67
1	F	153:SER	C	154:ALA	N	2.67
1	E	220:ASP	C	221:ALA	N	2.60
1	F	220:ASP	C	221:ALA	N	2.60

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	165:GLU	C	166:GLY	N	2.22

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	174/175 (99%)	-0.00	0	100	100	36, 64, 101, 108	4 (2%)
1	B	174/175 (99%)	0.06	5 (2%)	51	41	39, 68, 102, 108	4 (2%)
1	C	174/175 (99%)	0.24	10 (5%)	23	15	56, 80, 107, 113	3 (1%)
1	D	174/175 (99%)	0.48	11 (6%)	20	12	56, 82, 108, 114	4 (2%)
2	E	382/449 (85%)	0.36	32 (8%)	11	5	0, 60, 116, 124	6 (1%)
2	F	352/449 (78%)	0.33	30 (8%)	10	5	35, 58, 123, 132	4 (1%)
All	All	1430/1598 (89%)	0.27	88 (6%)	20	13	0, 66, 113, 132	25 (1%)

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	90	GLY	10.8
2	E	91	TYR	10.2
2	F	90	GLY	9.0
2	F	91	TYR	8.6
2	F	123	ALA	8.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.
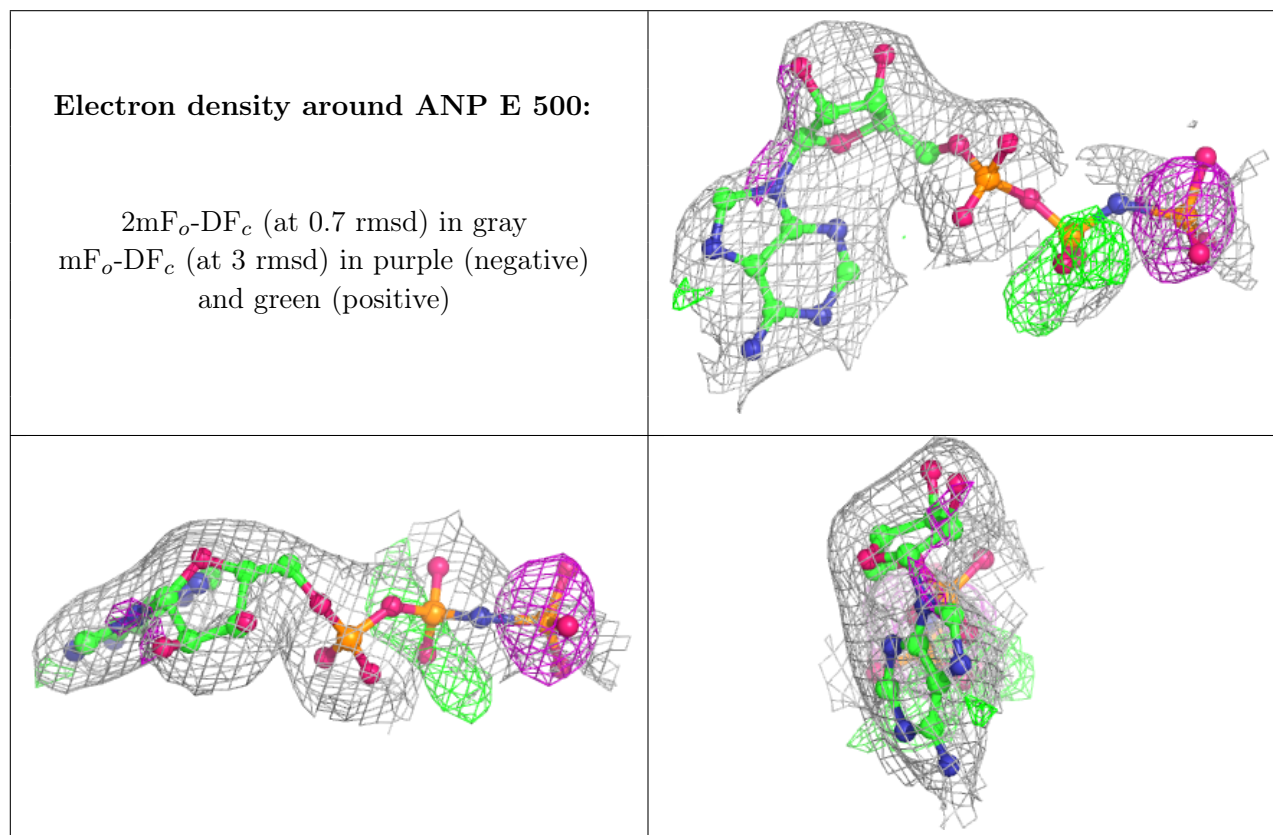
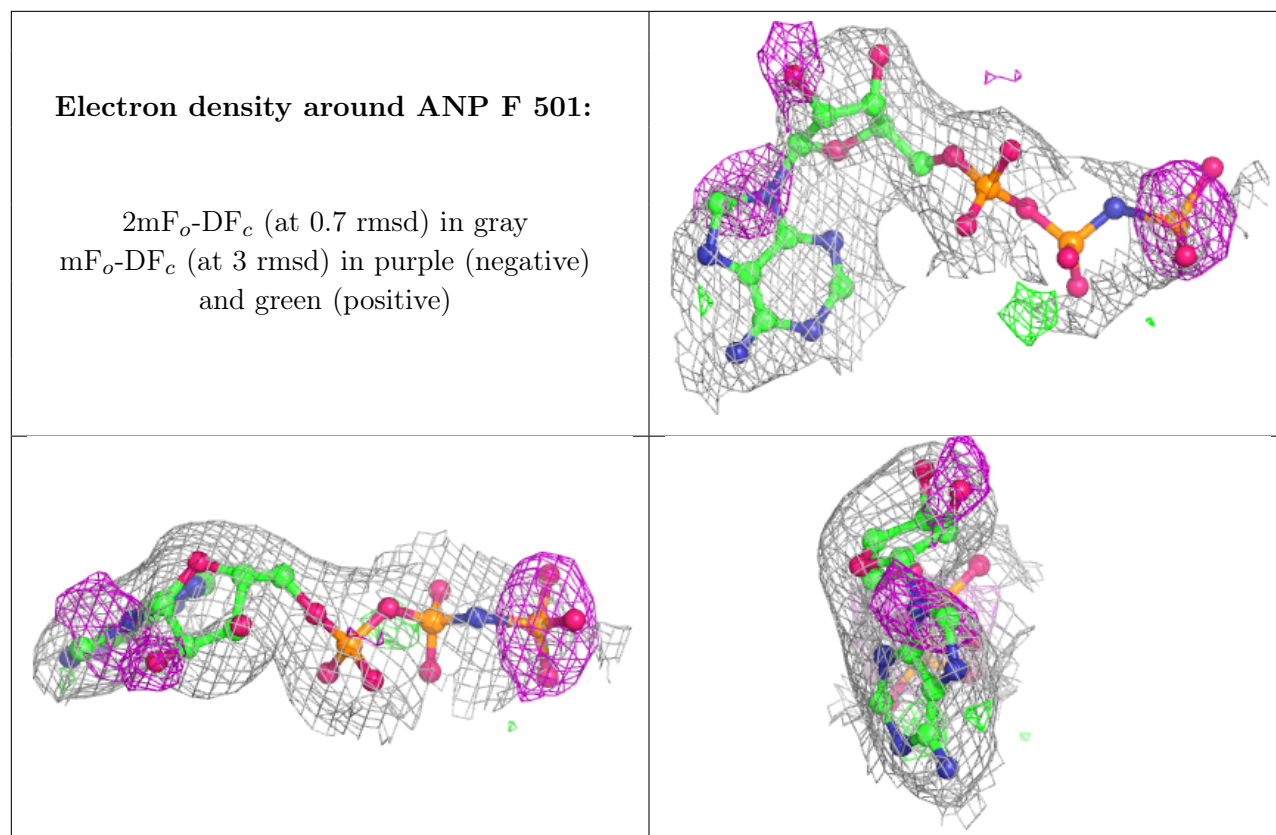## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ANP	E	500	31/31	0.89	0.27	41,46,77,78	0
3	ANP	F	501	31/31	0.91	0.24	47,50,79,80	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 ANP E 500:

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

Electron density around ANP F 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.