



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:47 PM UTC

PDB ID : 5ULS / pdb_00005uls
Title : Structure of GRP94 in the active conformation
Authors : Huck, J.D.; Que, N.L.S.; Gewirth, D.T.
Deposited on : 2017-01-25
Resolution : 2.62 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

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>.

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

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

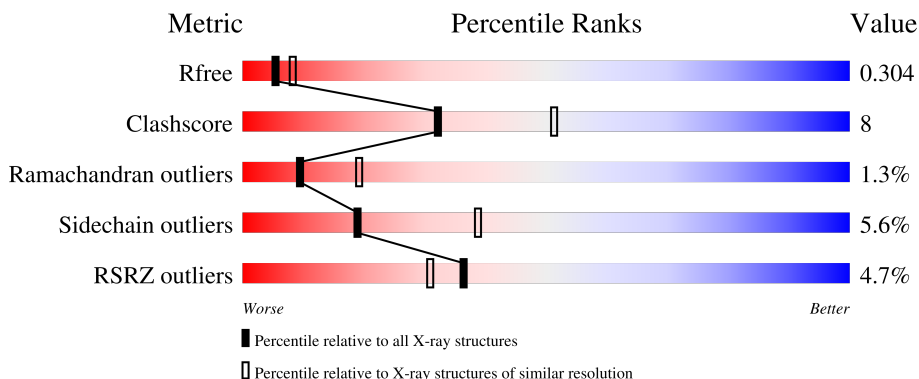
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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 $\leq 5\%$. 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	691	 5% 76% 16% • 6%
1	B	691	 4% 78% 14% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9869 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 Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			4805	3048	812	931	14			
1	B	642	Total	C	N	O	S	0	0	0
			4812	3059	792	944	17			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP P41148
A	28	GLY	-	expression tag	UNP P41148
A	29	SER	-	expression tag	UNP P41148
A	30	SER	-	expression tag	UNP P41148
A	31	HIS	-	expression tag	UNP P41148
A	32	HIS	-	expression tag	UNP P41148
A	33	HIS	-	expression tag	UNP P41148
A	34	HIS	-	expression tag	UNP P41148
A	35	HIS	-	expression tag	UNP P41148
A	36	HIS	-	expression tag	UNP P41148
A	37	SER	-	expression tag	UNP P41148
A	38	SER	-	expression tag	UNP P41148
A	39	GLY	-	expression tag	UNP P41148
A	40	LEU	-	expression tag	UNP P41148
A	41	VAL	-	expression tag	UNP P41148
A	42	PRO	-	expression tag	UNP P41148
A	43	ARG	-	expression tag	UNP P41148
A	44	GLY	-	expression tag	UNP P41148
A	45	SER	-	expression tag	UNP P41148
A	46	HIS	-	expression tag	UNP P41148
A	47	MET	-	expression tag	UNP P41148
A	287	GLY	-	linker	UNP P41148
A	288	GLY	-	linker	UNP P41148
A	326	GLY	-	linker	UNP P41148
A	327	GLY	-	linker	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	MET	-	initiating methionine	UNP P41148
B	28	GLY	-	expression tag	UNP P41148
B	29	SER	-	expression tag	UNP P41148
B	30	SER	-	expression tag	UNP P41148
B	31	HIS	-	expression tag	UNP P41148
B	32	HIS	-	expression tag	UNP P41148
B	33	HIS	-	expression tag	UNP P41148
B	34	HIS	-	expression tag	UNP P41148
B	35	HIS	-	expression tag	UNP P41148
B	36	HIS	-	expression tag	UNP P41148
B	37	SER	-	expression tag	UNP P41148
B	38	SER	-	expression tag	UNP P41148
B	39	GLY	-	expression tag	UNP P41148
B	40	LEU	-	expression tag	UNP P41148
B	41	VAL	-	expression tag	UNP P41148
B	42	PRO	-	expression tag	UNP P41148
B	43	ARG	-	expression tag	UNP P41148
B	44	GLY	-	expression tag	UNP P41148
B	45	SER	-	expression tag	UNP P41148
B	46	HIS	-	expression tag	UNP P41148
B	47	MET	-	expression tag	UNP P41148
B	324	GLY	-	linker	UNP P41148
B	325	GLY	-	linker	UNP P41148
B	326	GLY	-	linker	UNP P41148
B	327	GLY	-	linker	UNP P41148

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

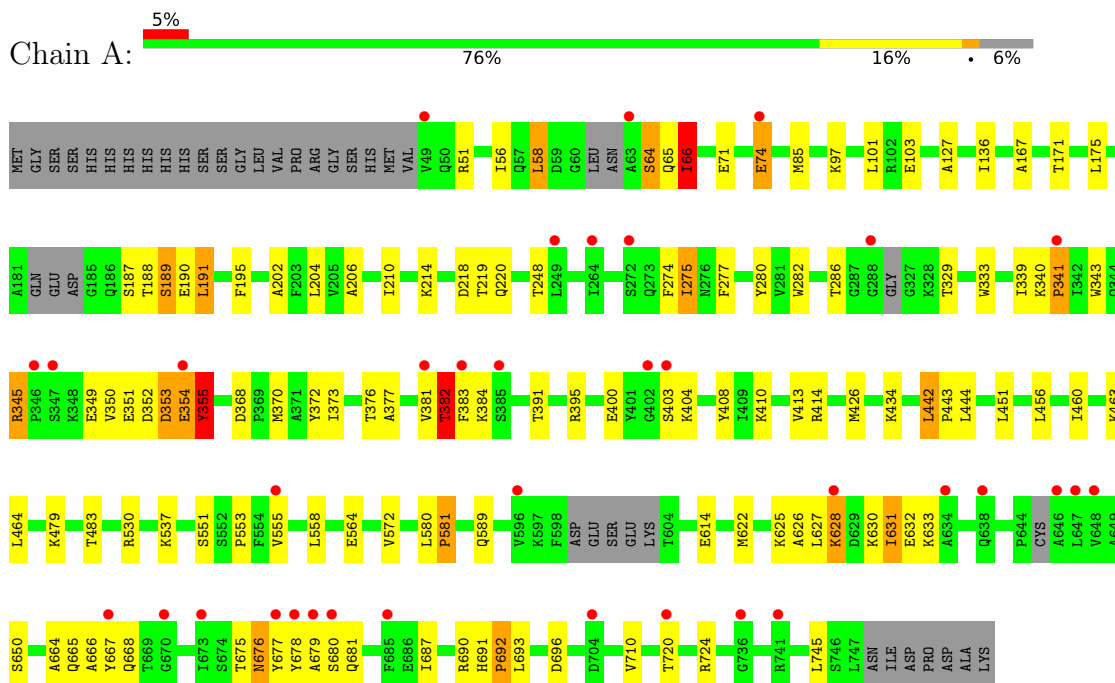
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	102	Total O 102 102	0	0
3	B	88	Total O 88 88	0	0

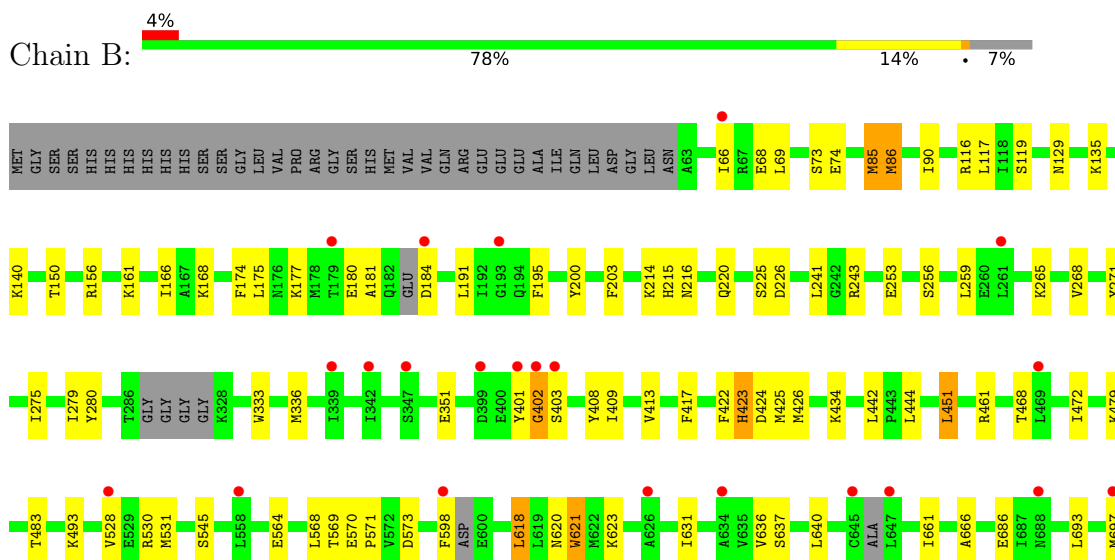
3 Residue-property plots [i](#)

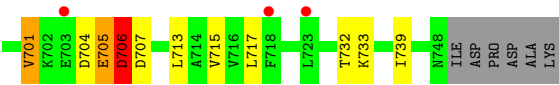
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Endoplasmic



• Molecule 1: Endoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.13Å 110.00Å 157.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.62 29.83 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.83-2.62) 98.6 (29.83-2.62)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.244 , 0.298 0.260 , 0.304	Depositor DCC
R_{free} test set	1998 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9869	wwPDB-VP
Average B, all atoms (Å ²)	78.0	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 30.27 % 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 1.3448e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.36	0/4892	0.80	9/6649 (0.1%)
1	B	0.33	0/4900	0.72	3/6664 (0.0%)
All	All	0.35	0/9792	0.76	12/13313 (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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	680	SER	N-CA-C	13.90	125.95	111.07
1	A	679	ALA	N-CA-C	10.06	122.33	111.36
1	A	64	SER	N-CA-C	9.59	122.90	110.53
1	B	706	ASP	N-CA-C	-9.28	101.91	113.23
1	A	625	LYS	N-CA-C	-6.62	104.14	111.36
1	A	345	ARG	CA-C-N	-5.81	114.77	120.52
1	A	345	ARG	C-N-CA	-5.81	114.77	120.52
1	A	678	TYR	CB-CA-C	-5.66	110.07	116.63
1	B	705	GLU	N-CA-C	-5.61	102.73	110.35
1	A	349	GLU	N-CA-C	-5.60	105.18	111.28
1	B	402	GLY	N-CA-C	-5.22	100.80	113.18
1	A	127	ALA	CB-CA-C	-5.19	110.17	117.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	ASP	Peptide

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	4805	0	4350	92	0
1	B	4812	0	4417	63	0
2	A	31	0	13	1	0
2	B	31	0	13	2	0
3	A	102	0	0	5	0
3	B	88	0	0	1	0
All	All	9869	0	8793	147	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 8.

All (147) 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:704:ASP:O	1:B:707:ASP:HB2	1.40	1.20
1:A:627:LEU:HB3	1:A:630:LYS:HG3	1.22	1.12
1:B:704:ASP:O	1:B:707:ASP:CB	2.07	1.02
1:A:345:ARG:NH2	1:A:350:VAL:CG2	2.35	0.90
1:A:345:ARG:NH2	1:A:350:VAL:HG21	1.93	0.84
1:A:681:GLN:NE2	3:A:901:HOH:O	2.09	0.84
1:A:627:LEU:CB	1:A:630:LYS:HG3	2.07	0.83
1:B:402:GLY:O	1:B:403:SER:OG	1.95	0.83
1:A:622:MET:O	1:A:626:ALA:CB	2.27	0.81
1:B:701:VAL:O	1:B:705:GLU:N	2.13	0.81
1:B:704:ASP:CB	1:B:707:ASP:HB2	2.11	0.81
1:A:74:GLU:OE1	1:B:156:ARG:NH2	2.15	0.79
1:A:627:LEU:HD23	1:A:628:LYS:N	1.97	0.79
1:A:691:HIS:HB2	1:A:692:PRO:HD2	1.63	0.79
1:A:627:LEU:HB3	1:A:630:LYS:CG	2.10	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ARG:NH2	1:A:350:VAL:HB	2.01	0.76
1:A:65:GLN:O	1:A:66:ILE:HD12	1.88	0.74
1:B:161:LYS:HD2	1:B:168:LYS:HE3	1.69	0.73
1:A:627:LEU:HD23	1:A:627:LEU:C	2.15	0.72
1:A:631:ILE:C	1:A:631:ILE:HD13	2.15	0.71
1:A:622:MET:O	1:A:626:ALA:HB3	1.90	0.71
1:A:58:LEU:O	1:A:58:LEU:HG	1.92	0.70
1:B:422:PHE:O	1:B:425:MET:N	2.17	0.69
1:A:345:ARG:NH2	1:A:350:VAL:CB	2.56	0.68
1:A:631:ILE:HD11	1:A:633:LYS:C	2.19	0.68
1:A:202:ALA:O	3:A:902:HOH:O	2.13	0.66
1:B:174:PHE:HA	1:B:177:LYS:HE2	1.78	0.66
1:A:691:HIS:O	1:A:693:LEU:N	2.29	0.65
1:A:345:ARG:HH21	1:A:350:VAL:HG21	1.61	0.65
2:B:801:ANP:N3B	2:B:801:ANP:O2A	2.30	0.65
1:A:195:PHE:O	2:A:801:ANP:O2B	2.14	0.63
1:B:402:GLY:C	1:B:403:SER:HG	2.02	0.63
1:A:555:VAL:HA	1:A:558:LEU:HD13	1.82	0.61
1:A:345:ARG:HH21	1:A:350:VAL:CG2	2.11	0.61
1:B:422:PHE:O	1:B:424:ASP:N	2.34	0.60
1:A:206:ALA:N	3:A:902:HOH:O	2.34	0.60
1:A:345:ARG:HH21	1:A:350:VAL:CB	2.14	0.60
1:B:620:ASN:OD1	1:B:623:LYS:NZ	2.35	0.59
1:A:666:ALA:HA	1:B:571:PRO:HG2	1.83	0.59
1:B:479:LYS:O	1:B:483:THR:OG1	2.20	0.59
1:A:65:GLN:C	1:A:66:ILE:HG13	2.27	0.58
1:A:404:LYS:NZ	3:A:904:HOH:O	2.35	0.58
1:A:408:TYR:HB3	1:A:434:LYS:HG2	1.84	0.58
1:B:493:LYS:NZ	1:B:570:GLU:OE1	2.36	0.58
1:A:400:GLU:HG3	1:A:404:LYS:HB2	1.85	0.57
1:A:622:MET:O	1:A:626:ALA:N	2.34	0.57
1:B:280:TYR:HB3	1:B:333:TRP:HB3	1.86	0.57
1:A:188:THR:O	1:A:190:GLU:N	2.38	0.56
1:B:705:GLU:O	1:B:706:ASP:HB2	2.04	0.56
1:A:403:SER:HA	1:B:403:SER:HB3	1.87	0.55
1:A:724:ARG:NH1	1:B:732:THR:OG1	2.39	0.55
1:A:214:LYS:HD3	1:A:220:GLN:HB2	1.87	0.55
1:A:353:ASP:O	1:A:355:TYR:HB2	2.07	0.55
1:A:372:TYR:CD1	1:A:372:TYR:C	2.85	0.55
1:A:442:LEU:HD13	1:A:443:PRO:HD2	1.89	0.55
1:A:286:THR:HA	1:A:329:THR:HA	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ARG:HH22	1:A:350:VAL:CG2	2.17	0.54
1:A:627:LEU:HD23	1:A:628:LYS:CB	2.38	0.54
1:B:413:VAL:HG21	1:B:444:LEU:HD21	1.89	0.54
1:B:214:LYS:HD3	1:B:220:GLN:HB2	1.90	0.53
1:A:622:MET:O	1:A:626:ALA:HB2	2.08	0.53
1:B:568:LEU:HD22	1:B:573:ASP:HB3	1.90	0.53
1:B:637:SER:HB2	1:B:686:GLU:HB3	1.90	0.53
1:B:704:ASP:C	1:B:707:ASP:HB2	2.25	0.53
1:B:175:LEU:HD13	1:B:191:LEU:HD12	1.92	0.52
1:A:572:VAL:HB	1:B:666:ALA:HB1	1.91	0.52
1:A:627:LEU:O	1:A:630:LYS:N	2.28	0.52
1:B:129:ASN:O	1:B:243:ARG:NH2	2.31	0.52
1:A:65:GLN:C	1:A:66:ILE:CG1	2.83	0.51
1:B:422:PHE:HA	1:B:425:MET:HE3	1.93	0.51
1:A:353:ASP:O	1:A:354:GLU:C	2.53	0.51
1:A:381:VAL:HG21	1:A:460:ILE:HG12	1.91	0.51
1:A:675:THR:O	1:A:676:ASN:HB2	2.11	0.50
1:B:90:ILE:HD12	1:B:203:PHE:HB2	1.93	0.50
2:B:801:ANP:O1G	2:B:801:ANP:O2B	2.29	0.50
1:A:551:SER:HB2	1:B:733:LYS:HD2	1.94	0.50
1:B:442:LEU:HD23	1:B:451:LEU:HD11	1.92	0.50
1:B:530:ARG:NH1	1:B:564:GLU:OE2	2.41	0.50
1:A:631:ILE:HD13	1:A:632:GLU:N	2.27	0.50
1:A:368:ASP:O	1:A:391:THR:OG1	2.24	0.50
1:A:274:PHE:CG	1:A:343:TRP:HH2	2.31	0.49
1:A:553:PRO:HG3	1:A:724:ARG:HG3	1.95	0.49
1:A:627:LEU:O	1:A:630:LYS:HB2	2.13	0.49
1:A:188:THR:C	1:A:190:GLU:H	2.21	0.49
1:B:425:MET:HA	1:B:461:ARG:HB2	1.95	0.49
1:B:135:LYS:NZ	3:B:910:HOH:O	2.44	0.49
1:B:140:LYS:HA	1:B:259:LEU:HG	1.94	0.49
1:B:265:LYS:HG3	1:B:336:MET:HE1	1.96	0.48
1:A:479:LYS:O	1:A:483:THR:OG1	2.27	0.48
1:A:426:MET:HE1	1:A:464:LEU:HB3	1.95	0.48
1:A:720:THR:HG21	1:B:739:ILE:HD13	1.96	0.47
1:B:181:ALA:O	1:B:184:ASP:N	2.47	0.47
1:B:225:SER:OG	1:B:226:ASP:O	2.31	0.47
1:B:545:SER:HA	1:B:569:THR:HG23	1.96	0.47
1:A:413:VAL:HG21	1:A:444:LEU:HD21	1.96	0.47
1:A:218:ASP:OD1	1:A:219:THR:N	2.48	0.47
1:A:626:ALA:HB1	1:A:631:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HA	1:A:204:LEU:HD13	1.95	0.47
1:A:627:LEU:C	1:A:627:LEU:CD2	2.85	0.47
1:B:116:ARG:O	1:B:119:SER:OG	2.27	0.47
1:B:697:MET:O	1:B:701:VAL:HG13	2.14	0.47
1:B:86:MET:HE1	1:B:200:TYR:HB3	1.97	0.47
1:B:705:GLU:HG2	1:B:706:ASP:N	2.30	0.46
1:A:442:LEU:HD12	1:A:451:LEU:HD22	1.97	0.46
1:B:271:TYR:HA	1:B:417:PHE:HB3	1.98	0.46
1:B:253:GLU:O	1:B:256:SER:OG	2.29	0.46
1:A:167:ALA:HB2	1:B:85:MET:HG2	1.97	0.46
1:A:65:GLN:O	1:A:66:ILE:CD1	2.62	0.46
1:A:456:LEU:O	1:A:460:ILE:HG13	2.17	0.45
1:B:86:MET:HG2	1:B:166:ILE:HD11	1.97	0.45
1:B:528:VAL:HA	1:B:531:MET:HG3	1.98	0.45
1:A:381:VAL:HG22	1:A:383:PHE:HD2	1.81	0.45
1:A:171:THR:HG23	1:A:191:LEU:HG	1.98	0.45
1:A:189:SER:HA	1:A:414:ARG:HH12	1.82	0.45
1:B:73:SER:HB3	1:B:74:GLU:H	1.64	0.45
1:B:86:MET:O	1:B:90:ILE:HG12	2.17	0.44
1:A:210:ILE:HB	1:A:248:THR:HB	1.98	0.44
1:A:345:ARG:HH21	1:A:350:VAL:HB	1.75	0.44
1:B:408:TYR:HB3	1:B:434:LYS:HG2	1.98	0.44
1:A:400:GLU:HB2	1:A:403:SER:OG	2.18	0.44
1:B:215:HIS:ND1	1:B:216:ASN:O	2.46	0.44
1:B:704:ASP:O	1:B:707:ASP:N	2.50	0.44
1:A:345:ARG:HH22	1:A:350:VAL:HG21	1.76	0.44
1:A:377:ALA:O	1:A:382:THR:HA	2.18	0.43
1:A:274:PHE:HE1	1:A:339:ILE:HB	1.83	0.43
1:A:280:TYR:HB3	1:A:333:TRP:HB3	2.00	0.43
1:B:704:ASP:CB	1:B:707:ASP:CB	2.90	0.43
1:A:664:ALA:HB1	1:B:661:ILE:HA	2.01	0.43
1:A:376:THR:HA	1:A:384:LYS:HA	1.99	0.43
1:A:580:LEU:HD12	1:A:581:PRO:HD2	1.99	0.43
1:B:275:ILE:HG21	1:B:279:ILE:HD11	2.01	0.43
1:A:530:ARG:NH1	1:A:564:GLU:OE2	2.52	0.43
1:A:676:ASN:O	1:A:677:TYR:CB	2.66	0.43
1:B:468:THR:O	1:B:472:ILE:HG12	2.19	0.42
1:A:410:LYS:NZ	3:A:913:HOH:O	2.51	0.42
1:A:340:LYS:HA	1:A:341:PRO:HD3	1.89	0.42
1:A:101:LEU:HD11	1:A:136:ILE:HD13	2.02	0.42
1:A:370:MET:HB2	1:A:391:THR:HA	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:PHE:CD1	1:A:343:TRP:HH2	2.39	0.41
1:A:275:ILE:HD12	1:A:277:PHE:HB2	2.03	0.41
1:A:345:ARG:CZ	1:A:350:VAL:HB	2.51	0.41
1:B:618:LEU:O	1:B:621:TRP:HD1	2.04	0.41
1:A:85:MET:SD	1:B:85:MET:HG3	2.61	0.40
1:B:259:LEU:HD12	1:B:259:LEU:HA	1.93	0.40
1:B:409:ILE:HD11	1:B:426:MET:HE2	2.03	0.40
1:A:537:LYS:HD2	1:A:589:GLN:HB2	2.03	0.40
1:B:423:HIS:CD2	1:B:423:HIS:C	3.00	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	638/691 (92%)	590 (92%)	34 (5%)	14 (2%)	5	9
1	B	632/691 (92%)	596 (94%)	33 (5%)	3 (0%)	24	44
All	All	1270/1382 (92%)	1186 (93%)	67 (5%)	17 (1%)	9	19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	SER
1	A	353	ASP
1	A	628	LYS
1	A	692	PRO
1	B	401	TYR
1	B	423	HIS
1	A	66	ILE
1	A	354	GLU
1	A	355	TYR

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Mol	Chain	Res	Type
1	A	382	THR
1	B	66	ILE
1	A	282	TRP
1	A	667	TYR
1	A	690	ARG
1	A	581	PRO
1	A	341	PRO
1	A	56	ILE

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	458/620 (74%)	430 (94%)	28 (6%)	17	35
1	B	478/620 (77%)	454 (95%)	24 (5%)	22	44
All	All	936/1240 (76%)	884 (94%)	52 (6%)	19	39

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	58	LEU
1	A	64	SER
1	A	66	ILE
1	A	71	GLU
1	A	74	GLU
1	A	103	GLU
1	A	175	LEU
1	A	187	SER
1	A	191	LEU
1	A	275	ILE
1	A	351	GLU
1	A	355	TYR
1	A	373	ILE
1	A	382	THR

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Mol	Chain	Res	Type
1	A	395	ARG
1	A	442	LEU
1	A	463	LYS
1	A	614	GLU
1	A	631	ILE
1	A	650	SER
1	A	665	GLN
1	A	668	GLN
1	A	676	ASN
1	A	687	ILE
1	A	696	ASP
1	A	710	VAL
1	A	745	LEU
1	B	68	GLU
1	B	69	LEU
1	B	85	MET
1	B	86	MET
1	B	117	LEU
1	B	150	THR
1	B	180	GLU
1	B	195	PHE
1	B	241	LEU
1	B	268	VAL
1	B	351	GLU
1	B	451	LEU
1	B	598	PHE
1	B	618	LEU
1	B	621	TRP
1	B	631	ILE
1	B	636	VAL
1	B	640	LEU
1	B	693	LEU
1	B	701	VAL
1	B	706	ASP
1	B	713	LEU
1	B	715	VAL
1	B	717	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	HIS

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Mol	Chain	Res	Type
1	A	454	HIS
1	A	668	GLN
1	B	454	HIS
1	B	502	ASN
1	B	516	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ANP	A	801	-	33,33,33	1.71	4 (12%)	45,52,52	0.64	0
2	ANP	B	801	-	33,33,33	2.07	7 (21%)	45,52,52	0.57	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
2	ANP	A	801	-	-	3/18/38/38	0/3/3/3
2	ANP	B	801	-	-	3/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PG-O1G	8.23	1.58	1.46
2	B	801	ANP	PG-O1G	8.22	1.58	1.46
2	B	801	ANP	PB-O1B	6.52	1.56	1.46
2	B	801	ANP	PG-O3G	-2.67	1.49	1.56
2	B	801	ANP	PB-O2B	-2.66	1.49	1.56
2	B	801	ANP	PG-N3B	2.61	1.70	1.63
2	A	801	ANP	PG-O3G	-2.55	1.50	1.56
2	A	801	ANP	PG-N3B	2.47	1.69	1.63
2	A	801	ANP	PB-O1B	2.25	1.49	1.46
2	B	801	ANP	PB-O3A	-2.21	1.56	1.59
2	B	801	ANP	PB-N3B	2.00	1.68	1.63

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PB-N3B-PG-O1G
2	B	801	ANP	PG-N3B-PB-O1B
2	A	801	ANP	O4'-C4'-C5'-O5'
2	A	801	ANP	C3'-C4'-C5'-O5'
2	B	801	ANP	PB-O3A-PA-O2A
2	B	801	ANP	PB-O3A-PA-O1A

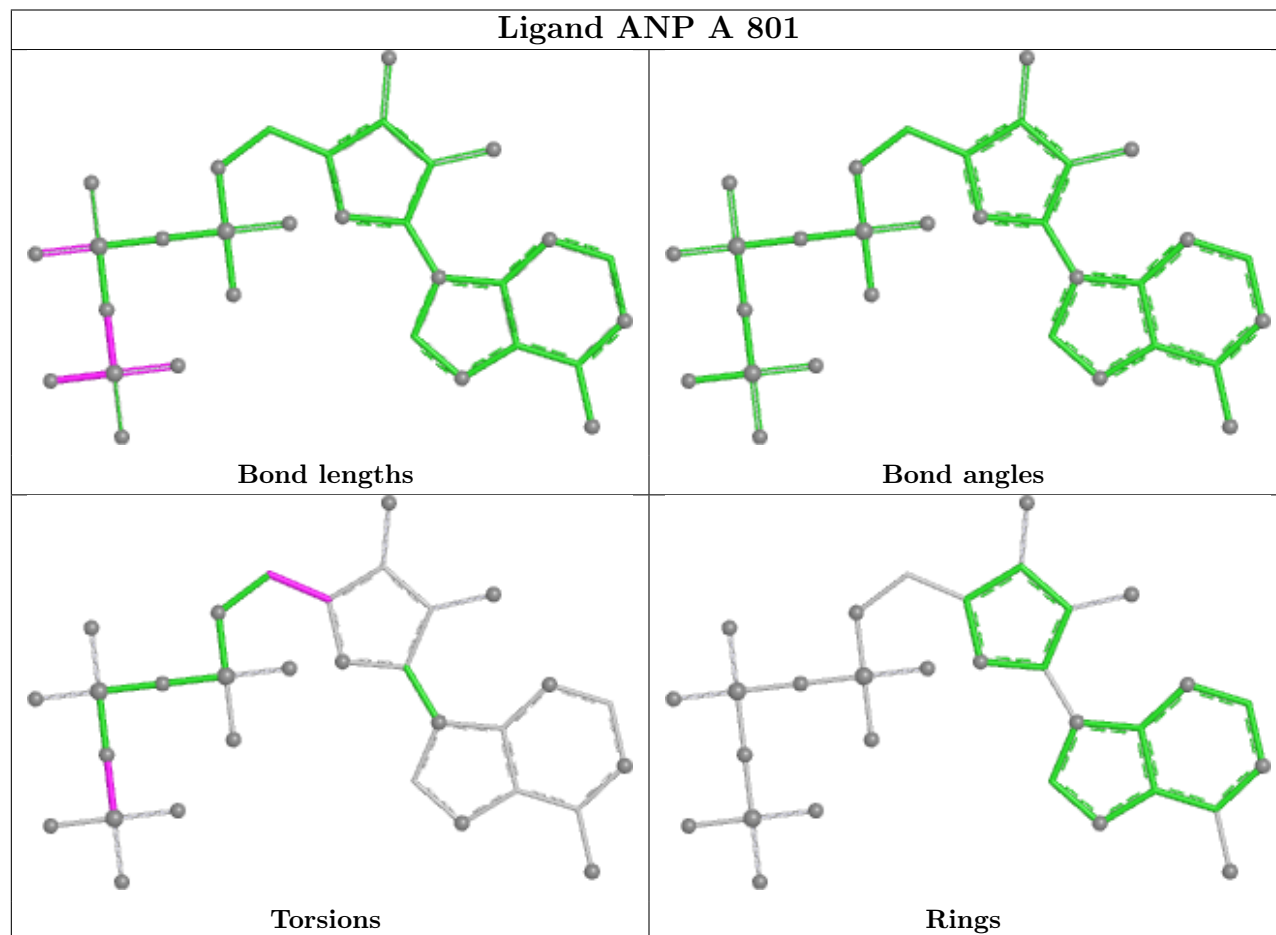
There are no ring outliers.

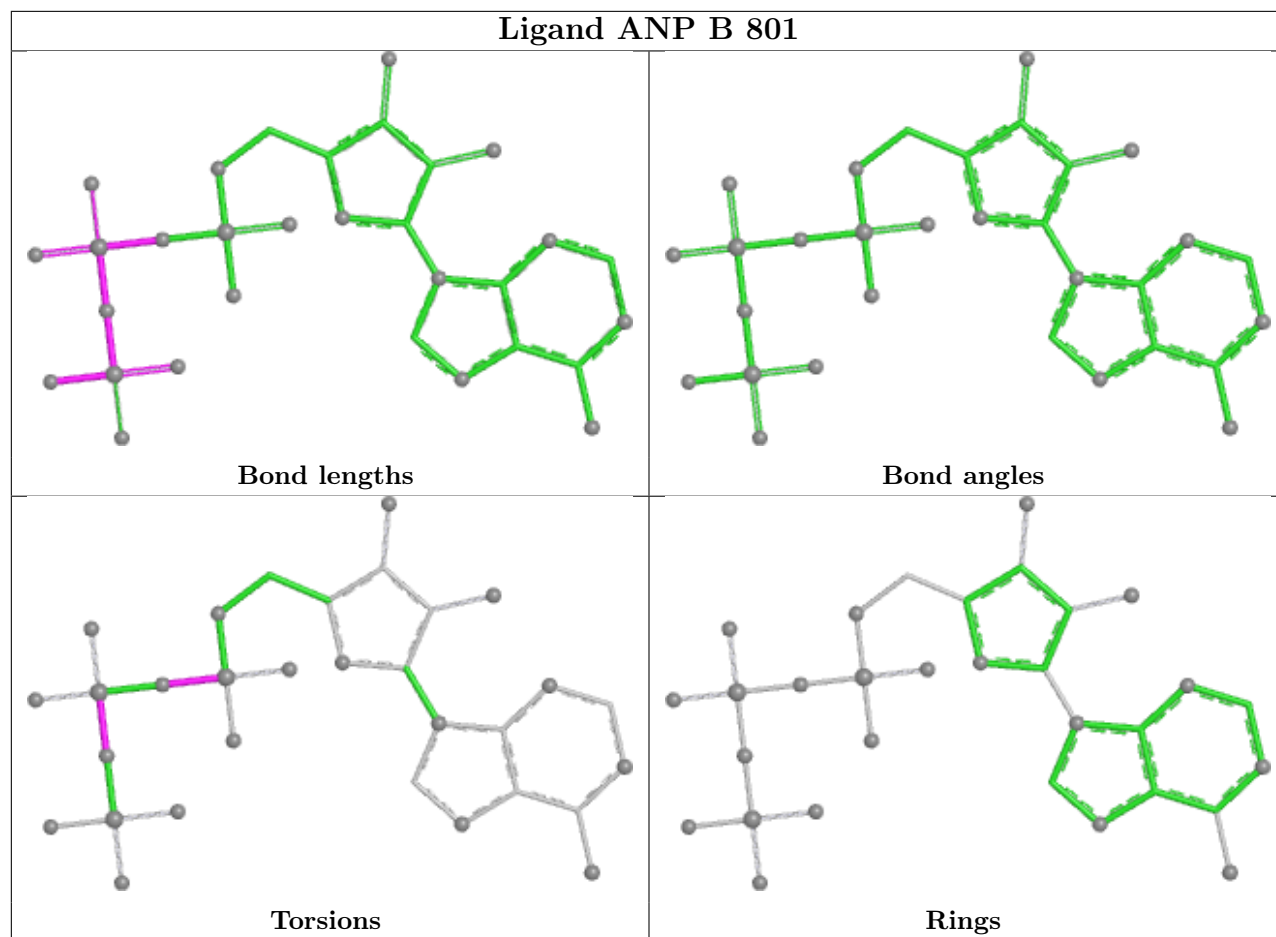
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ANP	1	0
2	B	801	ANP	2	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, 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	650/691 (94%)	0.58	36 (5%) 30 25	30, 76, 128, 148	0
1	B	642/691 (92%)	0.49	25 (3%) 43 38	30, 74, 124, 135	0
All	All	1292/1382 (93%)	0.53	61 (4%) 36 31	30, 75, 126, 148	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ASP	4.4
1	A	628	LYS	3.8
1	B	261	LEU	3.7
1	A	677	TYR	3.6
1	A	678	TYR	3.6
1	B	703	GLU	3.6
1	B	645	CYS	3.5
1	A	354	GLU	3.5
1	A	555	VAL	3.4
1	A	685	PHE	3.4
1	A	249	LEU	3.2
1	A	634	ALA	3.1
1	B	403	SER	3.1
1	B	193	GLY	3.0
1	A	638	GLN	2.9
1	A	63	ALA	2.8
1	B	339	ILE	2.7
1	A	736	GLY	2.7
1	B	626	ALA	2.7
1	B	401	TYR	2.7
1	A	704	ASP	2.7
1	B	647	LEU	2.6
1	B	723	LEU	2.6
1	A	381	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	646	ALA	2.5
1	A	402	GLY	2.5
1	A	49	VAL	2.5
1	A	648	VAL	2.5
1	B	342	ILE	2.4
1	A	596	VAL	2.4
1	A	667	TYR	2.4
1	A	383	PHE	2.4
1	A	347	SER	2.4
1	B	598	PHE	2.3
1	A	264	ILE	2.3
1	A	346	PRO	2.3
1	B	184	ASP	2.3
1	A	670	GLY	2.3
1	A	647	LEU	2.3
1	B	66	ILE	2.3
1	B	697	MET	2.3
1	A	680	SER	2.2
1	B	718	PHE	2.2
1	A	741	ARG	2.2
1	A	385	SER	2.2
1	A	403	SER	2.2
1	B	634	ALA	2.2
1	A	720	THR	2.2
1	A	288	GLY	2.2
1	B	558	LEU	2.2
1	A	272	SER	2.2
1	A	74	GLU	2.1
1	A	673	ILE	2.1
1	A	679	ALA	2.1
1	B	688	ASN	2.1
1	B	179	THR	2.1
1	A	341	PRO	2.1
1	B	347	SER	2.0
1	B	469	LEU	2.0
1	B	402	GLY	2.0
1	B	528	VAL	2.0

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 [i](#)

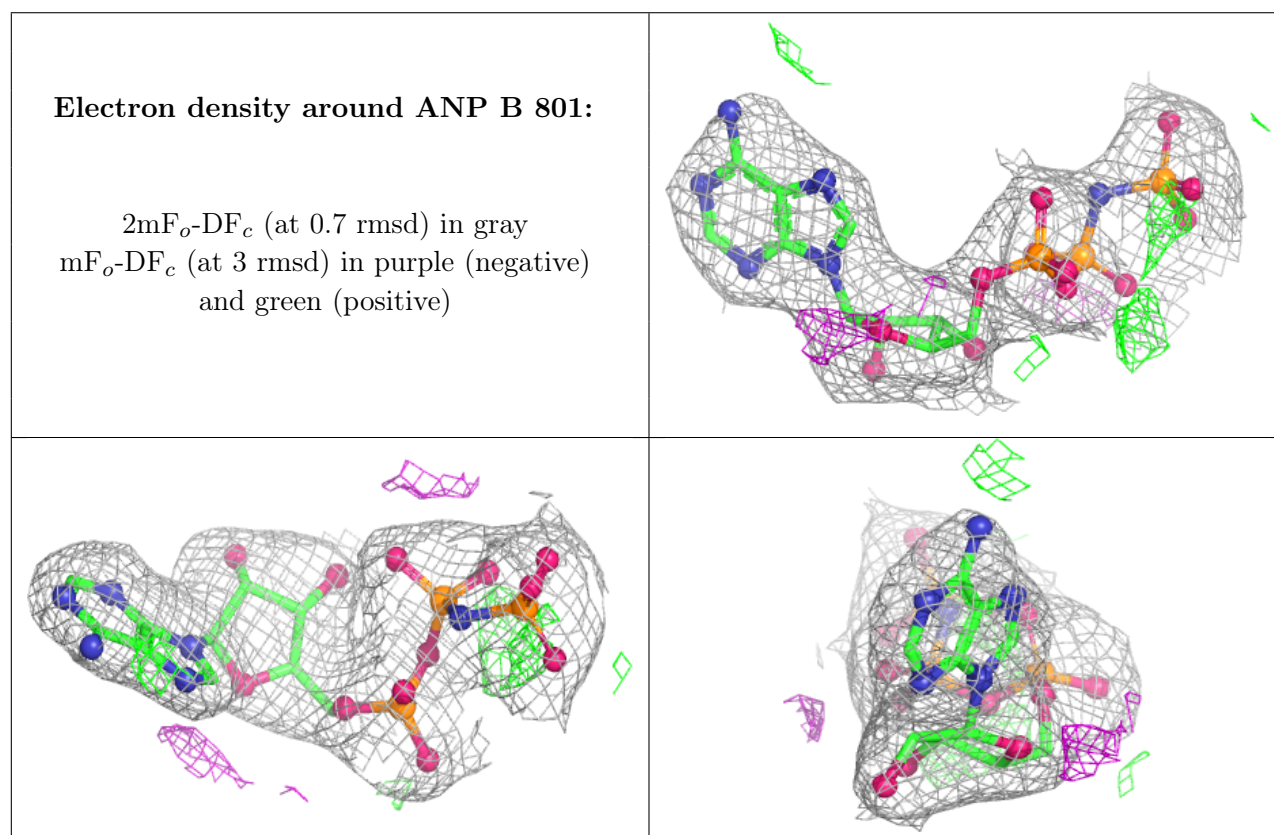
There are no oligosaccharides in this entry.

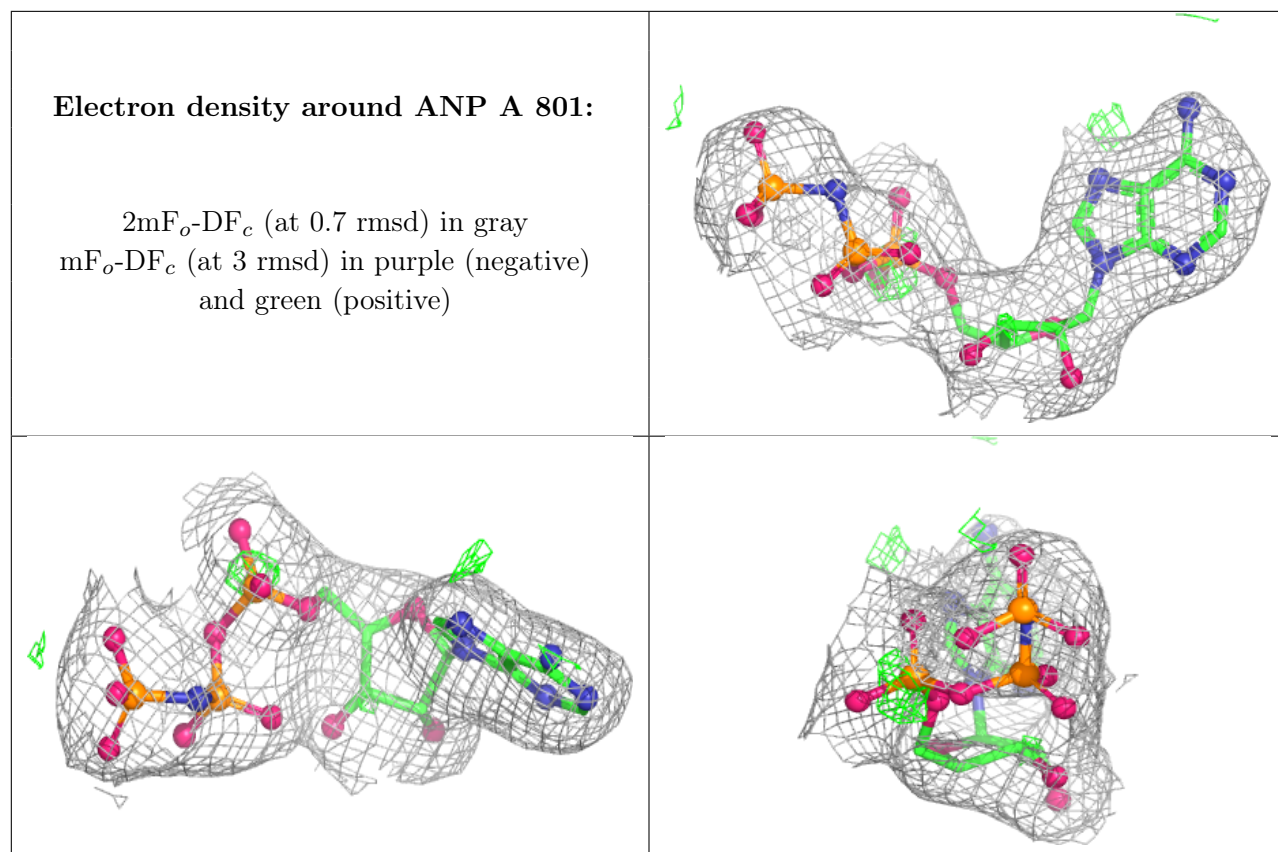
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	ANP	B	801	31/31	0.95	0.09	45,57,68,70	0
2	ANP	A	801	31/31	0.96	0.08	46,57,67,74	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.