



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:14 PM UTC

PDB ID : 5HV3 / pdb_00005hv3
Title : Rifampin phosphotransferase G527Y mutant in complex with AMPPNP from *Listeria monocytogenes*
Authors : Zhang, P.; Qi, X.
Deposited on : 2016-01-28
Resolution : 3.12 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

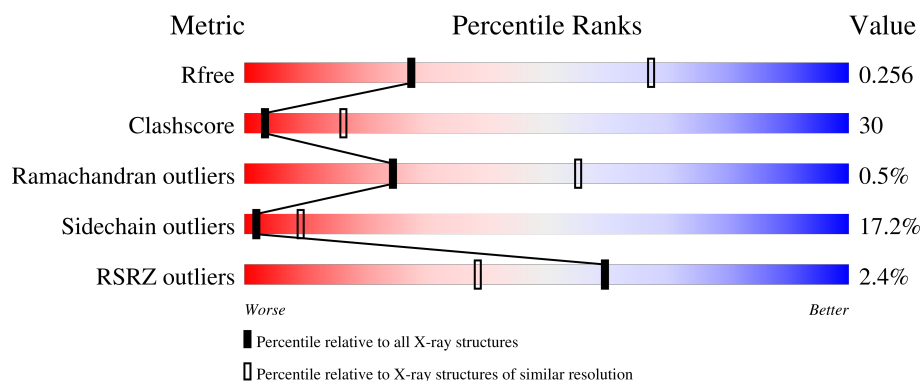
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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 ≥ 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	879	2% 46% 36% 12% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6691 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 Phosphoenolpyruvate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	846	Total	C	N	O	S	0	0	0
			6659	4227	1125	1277	30			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP A0A0S2YLC8
A	-10	ARG	-	expression tag	UNP A0A0S2YLC8
A	-9	GLY	-	expression tag	UNP A0A0S2YLC8
A	-8	SER	-	expression tag	UNP A0A0S2YLC8
A	-7	HIS	-	expression tag	UNP A0A0S2YLC8
A	-6	HIS	-	expression tag	UNP A0A0S2YLC8
A	-5	HIS	-	expression tag	UNP A0A0S2YLC8
A	-4	HIS	-	expression tag	UNP A0A0S2YLC8
A	-3	HIS	-	expression tag	UNP A0A0S2YLC8
A	-2	HIS	-	expression tag	UNP A0A0S2YLC8
A	-1	GLY	-	expression tag	UNP A0A0S2YLC8
A	0	SER	-	expression tag	UNP A0A0S2YLC8
A	527	TYR	GLY	engineered mutation	UNP A0A0S2YLC8

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

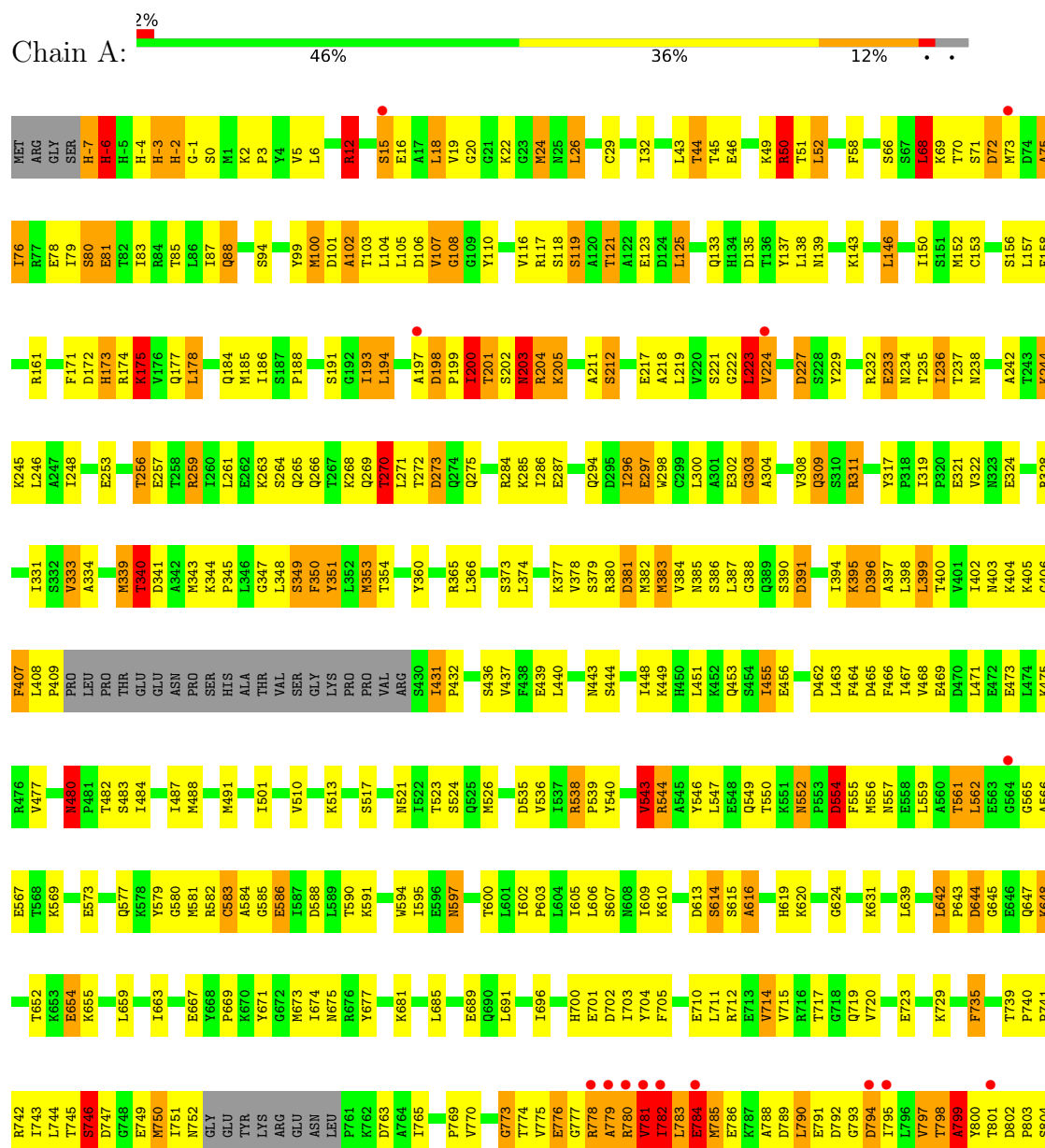
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

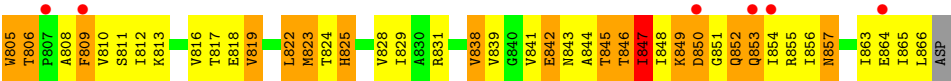
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

3 Residue-property plots

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: Phosphoenolpyruvate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.69Å 127.99Å 140.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.51 – 3.12 34.51 – 3.12	Depositor EDS
% Data completeness (in resolution range)	88.2 (34.51-3.12) 88.2 (34.51-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.202 , 0.254 0.223 , 0.256	Depositor DCC
R_{free} test set	1821 reflections (9.29%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6691	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.98	2/6782 (0.0%)	1.59	124/9173 (1.4%)

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	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	ILE	CA-C	-7.38	1.47	1.52
1	A	583	CYS	C-O	-5.54	1.18	1.24

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	PHE	N-CA-C	31.15	153.38	112.26
1	A	735	PHE	CA-C-N	25.77	170.76	121.54
1	A	735	PHE	C-N-CA	25.77	170.76	121.54
1	A	735	PHE	CB-CA-C	-24.65	71.45	111.13
1	A	567	GLU	N-CA-C	-18.99	89.62	113.55
1	A	15	SER	N-CA-C	-17.44	78.24	108.23
1	A	431	ILE	N-CA-C	17.28	146.20	108.88
1	A	584	ALA	N-CA-C	-17.08	85.21	110.48
1	A	197	ALA	CB-CA-C	16.30	143.12	111.17
1	A	799	ALA	N-CA-C	15.93	133.03	113.12
1	A	311	ARG	CB-CA-C	14.81	130.32	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ALA	N-CA-C	-14.47	87.48	108.60
1	A	-6	HIS	CB-CA-C	-14.43	82.69	110.10
1	A	794	ASP	N-CA-C	13.14	131.18	109.24
1	A	739	THR	CA-C-N	12.68	128.91	119.66
1	A	739	THR	C-N-CA	12.68	128.91	119.66
1	A	799	ALA	CB-CA-C	-12.48	88.97	109.56
1	A	799	ALA	CA-C-N	12.39	139.22	121.50
1	A	799	ALA	C-N-CA	12.39	139.22	121.50
1	A	431	ILE	CB-CA-C	-12.31	88.95	111.36
1	A	340	THR	CB-CA-C	-11.83	86.88	110.42
1	A	801	THR	N-CA-C	-11.46	89.16	108.75
1	A	779	ALA	N-CA-C	11.14	127.62	110.36
1	A	270	THR	CB-CA-C	-10.84	88.85	110.42
1	A	852	GLN	N-CA-C	10.81	133.83	110.80
1	A	778	ARG	N-CA-C	10.66	125.06	110.35
1	A	554	ASP	N-CA-C	-10.49	86.59	107.69
1	A	15	SER	CA-C-N	10.41	140.27	122.36
1	A	15	SER	C-N-CA	10.41	140.27	122.36
1	A	52	LEU	N-CA-C	10.38	126.92	114.04
1	A	311	ARG	N-CA-C	-10.20	98.95	108.13
1	A	806	THR	CA-C-N	9.89	132.21	119.84
1	A	806	THR	C-N-CA	9.89	132.21	119.84
1	A	171	PHE	N-CA-C	-9.88	97.48	110.53
1	A	801	THR	CB-CA-C	9.82	129.13	109.68
1	A	52	LEU	CB-CA-C	-9.39	92.44	109.15
1	A	50	ARG	N-CA-C	9.18	121.06	111.14
1	A	846	THR	N-CA-C	-9.04	96.13	110.14
1	A	102	ALA	N-CA-C	8.79	120.47	111.07
1	A	238	ASN	CB-CA-C	8.75	124.08	109.99
1	A	-7	HIS	CA-C-N	8.56	137.10	121.70
1	A	-7	HIS	C-N-CA	8.56	137.10	121.70
1	A	158	PHE	N-CA-C	8.46	123.42	112.26
1	A	224	VAL	CB-CA-C	-8.25	95.73	111.40
1	A	842	GLU	N-CA-C	8.11	119.74	111.07
1	A	50	ARG	CB-CA-C	-8.03	98.22	110.90
1	A	864	GLU	N-CA-C	7.99	121.05	109.14
1	A	236	ILE	N-CA-C	-7.82	99.49	109.58
1	A	223	LEU	CA-C-N	7.82	135.77	121.70
1	A	223	LEU	C-N-CA	7.82	135.77	121.70
1	A	173	HIS	N-CA-C	-7.60	100.50	110.53
1	A	714	VAL	N-CA-C	-7.60	105.36	112.96
1	A	849	LYS	N-CA-C	7.59	121.51	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASN	N-CA-C	7.46	121.92	111.92
1	A	809	PHE	N-CA-C	7.42	122.39	112.30
1	A	12	ARG	CA-C-N	-7.41	110.58	119.84
1	A	12	ARG	C-N-CA	-7.41	110.58	119.84
1	A	585	GLY	N-CA-C	7.29	126.59	114.48
1	A	270	THR	N-CA-C	7.26	126.26	110.80
1	A	340	THR	CA-C-N	7.05	134.12	122.07
1	A	340	THR	C-N-CA	7.05	134.12	122.07
1	A	233	GLU	N-CA-C	-6.89	97.80	108.00
1	A	75	ALA	N-CA-C	-6.75	103.92	111.28
1	A	351	TYR	N-CA-C	-6.72	104.03	111.36
1	A	201	THR	CB-CA-C	-6.72	97.52	110.35
1	A	68	LEU	N-CA-C	6.67	119.34	110.53
1	A	73	MET	N-CA-C	6.67	118.21	111.07
1	A	-2	HIS	N-CA-C	6.60	120.64	112.59
1	A	198	ASP	CA-C-N	6.59	126.37	119.05
1	A	198	ASP	C-N-CA	6.59	126.37	119.05
1	A	852	GLN	CB-CA-C	-6.47	97.54	110.42
1	A	203	ASN	N-CA-C	6.45	118.31	111.28
1	A	-6	HIS	CA-C-N	6.42	133.80	121.54
1	A	-6	HIS	C-N-CA	6.42	133.80	121.54
1	A	848	ILE	N-CA-C	-6.41	96.02	109.34
1	A	808	ALA	CB-CA-C	6.40	118.95	109.29
1	A	266	GLN	N-CA-C	6.39	120.54	112.87
1	A	543	VAL	CB-CA-C	-6.31	103.81	111.88
1	A	696	ILE	N-CA-C	6.29	117.07	110.72
1	A	223	LEU	N-CA-C	-6.25	97.61	107.93
1	A	224	VAL	N-CA-C	6.22	128.41	111.00
1	A	644	ASP	N-CA-C	-6.22	105.28	112.86
1	A	238	ASN	N-CA-C	-6.19	99.11	108.52
1	A	102	ALA	CB-CA-C	-6.08	101.33	110.88
1	A	717	THR	N-CA-C	-6.07	99.00	108.90
1	A	794	ASP	N-CA-CB	-6.00	100.15	111.00
1	A	850	ASP	N-CA-C	6.00	119.69	111.54
1	A	200	ILE	CB-CA-C	-5.89	102.05	110.83
1	A	556	MET	N-CA-C	5.88	117.69	111.28
1	A	108	GLY	N-CA-C	-5.83	96.39	113.30
1	A	334	ALA	N-CA-C	-5.63	105.06	111.14
1	A	852	GLN	CA-C-N	5.60	132.23	121.54
1	A	852	GLN	C-N-CA	5.60	132.23	121.54
1	A	616	ALA	N-CA-C	-5.58	106.30	114.39
1	A	800	TYR	N-CA-C	5.58	118.63	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ILE	CB-CA-C	-5.54	104.76	110.13
1	A	350	PHE	N-CA-C	5.49	117.27	111.28
1	A	784	GLU	N-CA-C	-5.49	98.02	108.17
1	A	631	LYS	N-CA-C	-5.46	106.46	113.23
1	A	781	VAL	N-CA-C	-5.43	100.30	108.12
1	A	790	LEU	CB-CA-C	-5.40	102.12	112.43
1	A	480	ASN	CA-C-N	-5.35	114.31	119.87
1	A	480	ASN	C-N-CA	-5.35	114.31	119.87
1	A	51	THR	N-CA-C	5.35	116.91	111.14
1	A	407	PHE	N-CA-C	5.34	117.91	111.40
1	A	200	ILE	N-CA-C	-5.33	100.70	108.17
1	A	782	ILE	N-CA-C	5.32	116.04	110.62
1	A	552	ASN	CA-C-N	5.30	124.97	119.56
1	A	552	ASN	C-N-CA	5.30	124.97	119.56
1	A	554	ASP	CA-C-N	5.28	131.05	121.92
1	A	554	ASP	C-N-CA	5.28	131.05	121.92
1	A	303	GLY	CA-C-N	5.21	128.27	120.87
1	A	303	GLY	C-N-CA	5.21	128.27	120.87
1	A	773	GLY	N-CA-C	5.20	117.45	110.43
1	A	175	LYS	N-CA-C	-5.20	105.82	113.61
1	A	-6	HIS	N-CA-C	5.18	125.51	111.00
1	A	296	ILE	N-CA-C	5.17	115.56	108.12
1	A	597	ASN	CA-C-N	5.17	126.30	119.84
1	A	597	ASN	C-N-CA	5.17	126.30	119.84
1	A	689	GLU	N-CA-C	-5.13	105.58	111.07
1	A	309	GLN	CB-CA-C	5.05	118.92	110.43
1	A	78	GLU	N-CA-C	5.04	116.46	111.07
1	A	333	VAL	N-CA-C	-5.03	107.02	112.80
1	A	298	TRP	N-CA-C	5.01	117.28	109.52

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-6	HIS	Peptide
1	A	107	VAL	Peptide
1	A	15	SER	Peptide
1	A	340	THR	Peptide
1	A	554	ASP	Peptide
1	A	735	PHE	Peptide
1	A	799	ALA	Peptide

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	6659	0	6678	403	1
2	A	31	0	13	1	0
3	A	1	0	0	0	0
All	All	6691	0	6691	404	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 30.

All (404) 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:779:ALA:HB1	1:A:851:GLY:CA	1.53	1.37
1:A:431:ILE:O	1:A:431:ILE:CG2	1.63	1.33
1:A:779:ALA:HB2	1:A:851:GLY:C	1.52	1.33
1:A:799:ALA:O	1:A:819:VAL:HG13	1.16	1.31
1:A:779:ALA:CB	1:A:851:GLY:CA	2.07	1.30
1:A:779:ALA:CB	1:A:851:GLY:HA2	1.68	1.20
1:A:777:GLY:O	1:A:853:GLN:HB3	1.40	1.20
1:A:790:LEU:O	1:A:791:GLU:HG3	1.47	1.14
1:A:294:GLN:OE1	1:A:311:ARG:O	1.73	1.07
1:A:172:ASP:OD2	1:A:174:ARG:NH2	1.88	1.05
1:A:781:VAL:HG11	1:A:783:LEU:HD22	1.40	1.04
1:A:778:ARG:HB2	1:A:794:ASP:HB2	1.39	1.03
1:A:779:ALA:CB	1:A:851:GLY:C	2.28	1.03
1:A:783:LEU:HD11	1:A:788:ALA:CB	1.89	1.03
1:A:841:VAL:HG21	1:A:844:ALA:HB2	1.40	1.02
1:A:778:ARG:HD2	1:A:794:ASP:HB3	1.34	1.02
1:A:843:ASN:O	1:A:846:THR:O	1.78	1.02
1:A:783:LEU:HD12	1:A:784:GLU:N	1.79	0.97
1:A:780:ARG:NH2	1:A:845:THR:HB	1.79	0.97
1:A:52:LEU:O	1:A:58:PHE:CD2	2.17	0.97
1:A:799:ALA:O	1:A:819:VAL:CG1	2.12	0.96
1:A:552:ASN:CG	1:A:554:ASP:O	2.09	0.96
1:A:781:VAL:HG12	1:A:783:LEU:HB2	1.45	0.95
1:A:779:ALA:HB1	1:A:851:GLY:HA2	0.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:ARG:HA	1:A:797:VAL:HG23	1.49	0.94
1:A:76:ILE:O	1:A:80:SER:OG	1.85	0.94
1:A:854:ILE:HD11	1:A:863:ILE:HG23	1.49	0.93
1:A:270:THR:HG22	1:A:270:THR:O	1.65	0.93
1:A:783:LEU:HD11	1:A:788:ALA:HB2	1.49	0.92
1:A:644:ASP:OD1	1:A:647:GLN:HB3	1.70	0.92
1:A:217:GLU:O	1:A:221:SER:HB2	1.70	0.92
1:A:745:THR:HG22	1:A:747:ASP:H	1.34	0.91
1:A:340:THR:O	1:A:340:THR:OG1	1.75	0.90
1:A:778:ARG:HB2	1:A:794:ASP:CB	2.01	0.90
1:A:257:GLU:OE2	1:A:259:ARG:NH2	2.04	0.90
1:A:552:ASN:OD1	1:A:554:ASP:O	1.90	0.90
1:A:841:VAL:CG2	1:A:844:ALA:HB2	2.01	0.90
1:A:802:ASP:OD1	1:A:804:SER:OG	1.90	0.88
1:A:781:VAL:CG1	1:A:783:LEU:HB2	2.03	0.88
1:A:397:ALA:HB1	1:A:751:ILE:HG22	1.56	0.87
1:A:781:VAL:CG1	1:A:783:LEU:HD22	2.05	0.87
1:A:227:ASP:OD1	1:A:229:TYR:OH	1.93	0.86
1:A:777:GLY:O	1:A:853:GLN:CB	2.24	0.86
1:A:118:SER:HB2	1:A:178:LEU:HD21	1.59	0.85
1:A:201:THR:HG22	1:A:201:THR:O	1.74	0.83
1:A:72:ASP:O	1:A:76:ILE:HG13	1.77	0.83
1:A:198:ASP:OD2	1:A:199:PRO:HD2	1.78	0.83
1:A:779:ALA:HB2	1:A:851:GLY:O	1.78	0.82
1:A:781:VAL:CB	1:A:783:LEU:HB2	2.10	0.82
1:A:852:GLN:C	1:A:853:GLN:HG3	2.02	0.82
1:A:782:ILE:HG22	1:A:783:LEU:HA	1.61	0.81
1:A:107:VAL:O	1:A:184:GLN:NE2	2.11	0.81
1:A:790:LEU:O	1:A:791:GLU:CG	2.29	0.80
1:A:387:LEU:O	1:A:390:SER:O	2.01	0.79
1:A:779:ALA:HB1	1:A:851:GLY:HA3	1.58	0.77
1:A:802:ASP:HB2	1:A:803:PRO:HD3	1.66	0.77
1:A:818:GLU:OE2	1:A:845:THR:OG1	2.02	0.77
1:A:172:ASP:CG	1:A:174:ARG:HH21	1.93	0.77
1:A:779:ALA:CB	1:A:851:GLY:HA3	2.11	0.77
1:A:778:ARG:CD	1:A:794:ASP:HB3	2.14	0.76
1:A:790:LEU:C	1:A:791:GLU:CG	2.57	0.76
1:A:790:LEU:CA	1:A:791:GLU:OE2	2.32	0.76
1:A:224:VAL:CG1	1:A:246:LEU:HB2	2.16	0.75
1:A:242:ALA:O	1:A:244:LYS:NZ	2.20	0.75
1:A:253:GLU:N	1:A:253:GLU:OE1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:MET:HA	1:A:788:ALA:HB2	1.69	0.75
1:A:792:ASP:OD1	1:A:793:GLY:N	2.20	0.74
1:A:270:THR:O	1:A:270:THR:CG2	2.35	0.74
1:A:431:ILE:O	1:A:431:ILE:HG22	0.82	0.74
1:A:-2:HIS:N	1:A:-1:GLY:HA3	2.03	0.73
1:A:22:LYS:HB3	1:A:119:SER:HB2	1.68	0.73
1:A:526:MET:HE1	1:A:582:ARG:HD3	1.71	0.73
1:A:849:LYS:HD2	1:A:850:ASP:H	1.53	0.73
1:A:3:PRO:HG2	1:A:6:LEU:HD11	1.70	0.73
1:A:799:ALA:C	1:A:819:VAL:HG13	2.10	0.72
1:A:802:ASP:CG	1:A:803:PRO:HD2	2.14	0.72
1:A:852:GLN:O	1:A:853:GLN:HG3	1.88	0.72
1:A:790:LEU:C	1:A:791:GLU:CD	2.59	0.71
1:A:790:LEU:C	1:A:791:GLU:OE2	2.34	0.70
1:A:783:LEU:HD12	1:A:784:GLU:C	2.16	0.70
1:A:284:ARG:NH2	1:A:287:GLU:OE1	2.24	0.70
1:A:379:SER:HA	1:A:382:MET:HB3	1.72	0.70
1:A:790:LEU:C	1:A:791:GLU:HG3	2.15	0.69
1:A:44:THR:HG22	1:A:46:GLU:H	1.58	0.69
1:A:331:ILE:HD11	1:A:394:ILE:HG21	1.75	0.68
1:A:388:GLY:HA2	1:A:395:LYS:HD3	1.74	0.68
1:A:825:HIS:HD1	1:A:825:HIS:C	2.01	0.68
1:A:802:ASP:CB	1:A:803:PRO:CD	2.72	0.68
1:A:700:HIS:CD2	1:A:701:GLU:HG3	2.29	0.68
1:A:391:ASP:HB3	1:A:394:ILE:HG13	1.76	0.67
1:A:138:LEU:HD22	1:A:185:MET:HE1	1.77	0.67
1:A:203:ASN:O	1:A:203:ASN:ND2	2.25	0.67
1:A:783:LEU:HD12	1:A:783:LEU:C	2.20	0.66
1:A:783:LEU:HD11	1:A:788:ALA:HB1	1.72	0.66
1:A:224:VAL:HG11	1:A:246:LEU:O	1.95	0.66
1:A:20:GLY:HA2	1:A:121:THR:HG23	1.78	0.66
1:A:52:LEU:O	1:A:58:PHE:HD2	1.77	0.66
1:A:345:PRO:HD2	1:A:705:PHE:HA	1.79	0.65
1:A:224:VAL:HG12	1:A:246:LEU:HB2	1.77	0.65
1:A:642:LEU:CB	1:A:643:PRO:HD2	2.26	0.65
1:A:790:LEU:HA	1:A:791:GLU:OE2	1.95	0.65
1:A:198:ASP:OD2	1:A:199:PRO:CD	2.45	0.65
1:A:186:ILE:O	1:A:188:PRO:HD3	1.97	0.65
1:A:217:GLU:O	1:A:217:GLU:HG3	1.96	0.65
1:A:339:MET:HE2	1:A:341:ASP:HB2	1.79	0.65
1:A:782:ILE:HG22	1:A:783:LEU:CA	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:PHE:HB2	1:A:812:ILE:HD13	1.78	0.64
1:A:654:GLU:OE2	1:A:654:GLU:N	2.30	0.64
1:A:784:GLU:O	1:A:788:ALA:HB2	1.97	0.63
1:A:846:THR:O	1:A:847:ILE:HG22	1.98	0.63
1:A:789:ASP:O	1:A:791:GLU:OE2	2.17	0.62
1:A:203:ASN:C	1:A:203:ASN:HD22	2.02	0.62
1:A:781:VAL:HG12	1:A:783:LEU:CB	2.25	0.62
1:A:222:GLY:O	1:A:819:VAL:HG11	1.99	0.62
1:A:849:LYS:HD2	1:A:850:ASP:N	2.15	0.62
1:A:79:ILE:O	1:A:83:ILE:HG13	2.00	0.62
1:A:68:LEU:HD22	1:A:75:ALA:HB3	1.81	0.62
1:A:749:GLU:HG2	1:A:751:ILE:HD11	1.81	0.61
1:A:-2:HIS:O	1:A:-2:HIS:ND1	2.33	0.61
1:A:397:ALA:HB2	1:A:752:ASN:HB3	1.83	0.61
1:A:809:PHE:O	1:A:812:ILE:HD13	2.01	0.61
1:A:806:THR:HA	1:A:809:PHE:HE2	1.65	0.61
1:A:544:ARG:HB3	1:A:544:ARG:CZ	2.31	0.61
1:A:841:VAL:HG11	1:A:863:ILE:HD12	1.82	0.61
1:A:552:ASN:ND2	1:A:554:ASP:O	2.33	0.60
1:A:790:LEU:HD11	1:A:812:ILE:HD11	1.84	0.60
1:A:199:PRO:HG2	1:A:822:LEU:HD21	1.82	0.60
1:A:365:ARG:HD3	1:A:740:PRO:HG3	1.84	0.60
1:A:557:ASN:HA	1:A:569:LYS:NZ	2.17	0.60
1:A:797:VAL:HA	1:A:816:VAL:O	2.02	0.59
1:A:223:LEU:O	1:A:223:LEU:HD23	2.02	0.59
1:A:381:ASP:O	1:A:385:ASN:ND2	2.31	0.59
1:A:431:ILE:O	1:A:432:PRO:O	2.20	0.59
1:A:802:ASP:C	1:A:825:HIS:HD2	2.10	0.59
1:A:235:THR:HG22	1:A:236:ILE:O	2.03	0.59
1:A:805:TRP:O	1:A:809:PHE:CD2	2.55	0.59
1:A:856:ILE:HG22	1:A:863:ILE:HG12	1.83	0.59
1:A:344:LYS:HD2	1:A:704:TYR:HB3	1.83	0.58
1:A:223:LEU:HD23	1:A:223:LEU:N	2.18	0.58
1:A:741:PRO:HD3	1:A:750:MET:HE1	1.86	0.58
1:A:487:ILE:HD11	1:A:669:PRO:HG2	1.85	0.58
1:A:642:LEU:HB2	1:A:643:PRO:HD2	1.85	0.58
1:A:172:ASP:HB3	1:A:175:LYS:HG3	1.84	0.58
1:A:201:THR:CG2	1:A:749:GLU:HG3	2.34	0.58
1:A:272:THR:O	1:A:275:GLN:N	2.37	0.58
1:A:782:ILE:CG2	1:A:783:LEU:HA	2.33	0.58
1:A:455:ILE:HG12	1:A:466:PHE:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:VAL:HG21	1:A:844:ALA:CB	2.26	0.57
1:A:852:GLN:O	1:A:853:GLN:CG	2.52	0.57
1:A:193:ILE:HD11	1:A:219:LEU:HD22	1.86	0.57
1:A:300:LEU:CD1	1:A:303:GLY:O	2.53	0.57
1:A:805:TRP:N	1:A:805:TRP:CD1	2.72	0.57
1:A:557:ASN:HA	1:A:569:LYS:HZ2	1.67	0.57
1:A:394:ILE:HD13	1:A:742:ARG:HG2	1.87	0.57
1:A:780:ARG:CA	1:A:797:VAL:HG23	2.31	0.56
1:A:538:ARG:NH2	1:A:609:ILE:HA	2.20	0.56
1:A:540:TYR:O	1:A:543:VAL:HG23	2.06	0.56
1:A:785:MET:CA	1:A:788:ALA:HB2	2.35	0.56
1:A:157:LEU:HB2	1:A:178:LEU:HD13	1.88	0.56
1:A:471:LEU:O	1:A:475:LYS:HG3	2.06	0.56
1:A:803:PRO:N	1:A:825:HIS:HD2	2.03	0.56
1:A:573:GLU:O	1:A:577:GLN:HG2	2.06	0.55
1:A:778:ARG:HD2	1:A:794:ASP:CB	2.22	0.55
1:A:464:PHE:O	1:A:468:VAL:HG23	2.07	0.55
1:A:-7:HIS:HB3	1:A:-6:HIS:HB2	1.87	0.55
1:A:439:GLU:O	1:A:443:ASN:ND2	2.40	0.55
1:A:535:ASP:OD1	1:A:538:ARG:NH1	2.40	0.55
1:A:294:GLN:OE1	1:A:311:ARG:C	2.47	0.55
1:A:841:VAL:HG11	1:A:863:ILE:CD1	2.37	0.55
1:A:333:VAL:HG12	1:A:366:LEU:O	2.07	0.55
1:A:223:LEU:HD23	1:A:223:LEU:H	1.71	0.55
1:A:380:ARG:HD3	1:A:402:ILE:HD12	1.89	0.54
1:A:104:LEU:O	1:A:108:GLY:HA2	2.07	0.54
1:A:201:THR:O	1:A:201:THR:CG2	2.47	0.54
1:A:588:ASP:OD1	1:A:590:THR:OG1	2.19	0.54
1:A:782:ILE:CG2	1:A:783:LEU:CA	2.85	0.54
1:A:849:LYS:HG3	1:A:850:ASP:HB2	1.90	0.54
1:A:464:PHE:HE1	1:A:711:LEU:HG	1.72	0.54
1:A:673:MET:HE3	1:A:677:TYR:CZ	2.43	0.54
1:A:782:ILE:N	1:A:783:LEU:HA	2.21	0.54
1:A:18:LEU:O	1:A:45:THR:HG23	2.07	0.54
1:A:16:GLU:HG3	1:A:24:MET:SD	2.48	0.54
1:A:781:VAL:HB	1:A:783:LEU:CB	2.37	0.54
1:A:81:GLU:O	1:A:85:THR:HG23	2.08	0.53
1:A:805:TRP:O	1:A:809:PHE:CE2	2.62	0.53
1:A:88:GLN:HE21	1:A:152:MET:HG2	1.72	0.53
1:A:465:ASP:OD1	1:A:712:ARG:NH2	2.38	0.53
1:A:780:ARG:HG2	1:A:781:VAL:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LYS:H	1:A:244:LYS:HZ3	1.56	0.53
1:A:536:VAL:O	1:A:539:PRO:HD2	2.08	0.53
1:A:779:ALA:CB	1:A:851:GLY:O	2.47	0.53
1:A:781:VAL:CB	1:A:783:LEU:HD22	2.39	0.53
1:A:781:VAL:C	1:A:783:LEU:HB2	2.34	0.53
1:A:2:LYS:HB2	1:A:46:GLU:HG3	1.89	0.53
1:A:782:ILE:N	1:A:783:LEU:CA	2.72	0.53
1:A:781:VAL:HG12	1:A:783:LEU:HD13	1.91	0.53
1:A:404:LYS:O	1:A:406:GLY:N	2.39	0.53
1:A:583:CYS:O	1:A:586:GLU:HG3	2.10	0.52
1:A:123:GLU:O	1:A:125:LEU:HD12	2.08	0.52
1:A:223:LEU:N	1:A:223:LEU:CD2	2.72	0.52
1:A:648:LYS:O	1:A:652:THR:HG23	2.10	0.52
1:A:841:VAL:CG2	1:A:844:ALA:CB	2.82	0.52
1:A:451:LEU:O	1:A:455:ILE:HG13	2.10	0.52
1:A:137:TYR:CZ	1:A:152:MET:HE2	2.45	0.52
1:A:198:ASP:CG	1:A:200:ILE:O	2.53	0.52
1:A:212:SER:OG	1:A:219:LEU:HD12	2.10	0.52
1:A:269:GLN:HG2	1:A:271:LEU:O	2.09	0.52
1:A:544:ARG:HD3	1:A:610:LYS:NZ	2.25	0.52
1:A:351:TYR:CD2	1:A:366:LEU:HD13	2.45	0.51
1:A:583:CYS:H	1:A:586:GLU:HG2	1.75	0.51
1:A:227:ASP:OD1	1:A:229:TYR:CZ	2.63	0.51
1:A:269:GLN:NE2	1:A:273:ASP:OD2	2.42	0.51
1:A:749:GLU:HG2	1:A:751:ILE:CD1	2.40	0.51
1:A:803:PRO:HA	1:A:825:HIS:CD2	2.45	0.51
1:A:328:ARG:H	1:A:746:SER:HB3	1.76	0.51
1:A:526:MET:HE2	1:A:594:TRP:HZ3	1.74	0.51
2:A:901:ANP:H5'1	2:A:901:ANP:H8	1.92	0.51
1:A:642:LEU:HB3	1:A:643:PRO:HD2	1.93	0.51
1:A:224:VAL:HG13	1:A:246:LEU:HB2	1.90	0.51
1:A:781:VAL:HB	1:A:783:LEU:HB2	1.87	0.51
1:A:173:HIS:O	1:A:174:ARG:HB2	2.11	0.50
1:A:201:THR:O	1:A:202:SER:C	2.54	0.50
1:A:218:ALA:HB2	1:A:248:ILE:HD12	1.94	0.50
1:A:440:LEU:HD11	1:A:483:SER:HA	1.93	0.50
1:A:783:LEU:CD1	1:A:784:GLU:C	2.85	0.50
1:A:273:ASP:OD2	1:A:273:ASP:N	2.44	0.50
1:A:565:GLY:O	1:A:566:ALA:HB3	2.12	0.50
1:A:822:LEU:HD23	1:A:823:MET:SD	2.51	0.50
1:A:333:VAL:HG22	1:A:333:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:HIS:C	1:A:825:HIS:ND1	2.62	0.50
1:A:449:LYS:O	1:A:453:GLN:HG3	2.12	0.50
1:A:803:PRO:HD2	1:A:804:SER:H	1.76	0.50
1:A:546:TYR:CE1	1:A:550:THR:HB	2.47	0.49
1:A:606:LEU:O	1:A:610:LYS:HG2	2.11	0.49
1:A:781:VAL:C	1:A:783:LEU:CB	2.85	0.49
1:A:809:PHE:HZ	1:A:829:ILE:HG21	1.77	0.49
1:A:552:ASN:OD1	1:A:554:ASP:C	2.55	0.49
1:A:300:LEU:HD11	1:A:303:GLY:O	2.13	0.49
1:A:642:LEU:CB	1:A:643:PRO:CD	2.89	0.49
1:A:615:SER:O	1:A:619:HIS:ND1	2.46	0.49
1:A:343:MET:HB3	1:A:348:LEU:HG	1.93	0.49
1:A:535:ASP:O	1:A:538:ARG:HG3	2.13	0.48
1:A:395:LYS:HG2	1:A:399:LEU:HD12	1.95	0.48
1:A:521:ASN:HB3	1:A:524:SER:HB3	1.95	0.48
1:A:194:LEU:HD22	1:A:296:ILE:HD12	1.96	0.48
1:A:350:PHE:HA	1:A:353:MET:HG3	1.95	0.48
1:A:802:ASP:CG	1:A:803:PRO:CD	2.86	0.48
1:A:805:TRP:O	1:A:809:PHE:HD2	1.97	0.48
1:A:790:LEU:HD13	1:A:811:SER:OG	2.14	0.48
1:A:157:LEU:HD13	1:A:178:LEU:HD12	1.96	0.48
1:A:173:HIS:C	1:A:175:LYS:H	2.22	0.47
1:A:383:MET:O	1:A:386:SER:N	2.43	0.47
1:A:103:THR:O	1:A:106:ASP:N	2.31	0.47
1:A:802:ASP:C	1:A:825:HIS:CD2	2.91	0.47
1:A:842:GLU:HG3	1:A:843:ASN:N	2.30	0.47
1:A:781:VAL:CG1	1:A:783:LEU:CD2	2.85	0.47
1:A:68:LEU:CD2	1:A:75:ALA:CB	2.92	0.47
1:A:431:ILE:O	1:A:432:PRO:C	2.57	0.47
1:A:710:GLU:O	1:A:714:VAL:HG23	2.14	0.47
1:A:802:ASP:O	1:A:804:SER:N	2.47	0.47
1:A:70:THR:HG22	1:A:70:THR:O	2.14	0.47
1:A:642:LEU:HB2	1:A:643:PRO:CD	2.40	0.47
1:A:841:VAL:HG23	1:A:844:ALA:HB2	1.92	0.47
1:A:374:LEU:O	1:A:380:ARG:NH2	2.42	0.47
1:A:261:LEU:HD22	1:A:265:GLN:HG2	1.97	0.47
1:A:652:THR:O	1:A:655:LYS:HB2	2.15	0.47
1:A:780:ARG:HH22	1:A:845:THR:HB	1.75	0.47
1:A:806:THR:HA	1:A:809:PHE:CE2	2.47	0.47
1:A:-7:HIS:HB3	1:A:-6:HIS:CB	2.45	0.46
1:A:809:PHE:O	1:A:810:VAL:C	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:OD1	1:A:110:TYR:OH	2.23	0.46
1:A:616:ALA:O	1:A:620:LYS:HB2	2.14	0.46
1:A:349:SER:O	1:A:353:MET:HG2	2.16	0.46
1:A:643:PRO:C	1:A:645:GLY:N	2.70	0.46
1:A:775:VAL:HG21	1:A:813:LYS:O	2.15	0.46
1:A:265:GLN:OE1	1:A:265:GLN:HA	2.16	0.46
1:A:380:ARG:O	1:A:383:MET:HB3	2.16	0.46
1:A:396:ASP:OD2	1:A:396:ASP:N	2.48	0.46
1:A:354:THR:HA	1:A:475:LYS:HE2	1.97	0.46
1:A:16:GLU:O	1:A:121:THR:HG21	2.16	0.46
1:A:463:LEU:O	1:A:466:PHE:HB3	2.15	0.46
1:A:591:LYS:O	1:A:681:LYS:NZ	2.48	0.46
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.82	0.46
1:A:146:LEU:O	1:A:150:ILE:HG13	2.15	0.46
1:A:218:ALA:O	1:A:221:SER:HB3	2.16	0.46
1:A:802:ASP:HB2	1:A:803:PRO:CD	2.32	0.46
1:A:263:LYS:O	1:A:264:SER:C	2.56	0.46
1:A:605:ILE:O	1:A:609:ILE:HG13	2.16	0.46
1:A:659:LEU:O	1:A:663:ILE:HB	2.16	0.46
1:A:339:MET:HG3	1:A:341:ASP:H	1.81	0.45
1:A:602:ILE:N	1:A:603:PRO:HD2	2.30	0.45
1:A:828:VAL:HG12	1:A:831:ARG:HH22	1.81	0.45
1:A:68:LEU:HD22	1:A:75:ALA:CB	2.45	0.45
1:A:580:GLY:HA3	1:A:595:ILE:HB	1.97	0.45
1:A:770:VAL:HG21	1:A:839:VAL:HG22	1.98	0.45
1:A:639:LEU:HD23	1:A:639:LEU:HA	1.81	0.45
1:A:774:THR:OG1	1:A:857:ASN:HB2	2.17	0.45
1:A:803:PRO:CD	1:A:804:SER:H	2.30	0.45
1:A:26:LEU:HD13	1:A:26:LEU:HA	1.73	0.45
1:A:193:ILE:HD11	1:A:219:LEU:CD2	2.46	0.45
1:A:805:TRP:CD1	1:A:805:TRP:H	2.34	0.45
1:A:244:LYS:HZ2	1:A:244:LYS:HG3	1.68	0.45
1:A:203:ASN:C	1:A:205:LYS:H	2.23	0.45
1:A:780:ARG:HH11	1:A:782:ILE:HA	1.82	0.45
1:A:377:LYS:C	1:A:379:SER:N	2.75	0.45
1:A:297:GLU:HB2	1:A:309:GLN:HB3	1.99	0.44
1:A:703:ILE:C	1:A:705:PHE:N	2.73	0.44
1:A:804:SER:OG	1:A:805:TRP:CD1	2.70	0.44
1:A:345:PRO:HD2	1:A:704:TYR:O	2.18	0.44
1:A:397:ALA:HB1	1:A:751:ILE:CG2	2.37	0.44
1:A:744:LEU:HD13	1:A:750:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:THR:HG22	1:A:46:GLU:N	2.30	0.44
1:A:153:CYS:O	1:A:156:SER:OG	2.25	0.44
1:A:775:VAL:C	1:A:776:GLU:HG2	2.42	0.44
1:A:268:LYS:HA	1:A:268:LYS:HD3	1.70	0.44
1:A:523:THR:OG1	1:A:667:GLU:HG2	2.18	0.44
1:A:742:ARG:HD2	1:A:752:ASN:ND2	2.33	0.44
1:A:100:MET:HE2	1:A:100:MET:HB3	1.70	0.44
1:A:444:SER:O	1:A:448:ILE:HG13	2.18	0.44
1:A:484:ILE:O	1:A:488:MET:HG2	2.17	0.44
1:A:816:VAL:HA	1:A:838:VAL:O	2.18	0.44
1:A:854:ILE:HG12	1:A:855:ARG:N	2.32	0.44
1:A:464:PHE:CE1	1:A:711:LEU:HG	2.51	0.43
1:A:526:MET:HB2	1:A:579:TYR:CE1	2.53	0.43
1:A:555:PHE:CZ	1:A:602:ILE:HD11	2.53	0.43
1:A:703:ILE:C	1:A:705:PHE:H	2.25	0.43
1:A:822:LEU:O	1:A:822:LEU:HG	2.18	0.43
1:A:5:VAL:C	1:A:6:LEU:HD12	2.43	0.43
1:A:22:LYS:HB3	1:A:119:SER:CB	2.45	0.43
1:A:349:SER:O	1:A:353:MET:CG	2.66	0.43
1:A:378:VAL:O	1:A:382:MET:HB2	2.17	0.43
1:A:480:ASN:OD1	1:A:480:ASN:N	2.50	0.43
1:A:745:THR:HB	1:A:749:GLU:HB3	2.00	0.43
1:A:780:ARG:NH1	1:A:782:ILE:HD13	2.33	0.43
1:A:198:ASP:HA	1:A:199:PRO:HD3	1.60	0.43
1:A:135:ASP:H	1:A:156:SER:HB2	1.81	0.43
1:A:211:ALA:O	1:A:227:ASP:HB2	2.18	0.43
1:A:235:THR:O	1:A:237:THR:HG23	2.16	0.43
1:A:354:THR:HG22	1:A:471:LEU:HD22	2.01	0.43
1:A:517:SER:OG	1:A:624:GLY:HA3	2.19	0.43
1:A:773:GLY:C	1:A:774:THR:HG1	2.27	0.43
1:A:561:THR:HG23	1:A:562:LEU:HG	2.01	0.43
1:A:805:TRP:H	1:A:805:TRP:HD1	1.66	0.43
1:A:43:LEU:HD12	1:A:43:LEU:HA	1.90	0.43
1:A:778:ARG:CG	1:A:794:ASP:HB3	2.47	0.43
1:A:101:ASP:OD1	1:A:143:LYS:HD2	2.19	0.42
1:A:172:ASP:O	1:A:175:LYS:HB2	2.19	0.42
1:A:343:MET:HE3	1:A:343:MET:HB2	1.69	0.42
1:A:317:TYR:HB3	1:A:750:MET:HE3	2.01	0.42
1:A:395:LYS:O	1:A:398:LEU:HB3	2.20	0.42
1:A:743:ILE:HB	1:A:751:ILE:HB	2.00	0.42
1:A:347:GLY:HA3	1:A:588:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:PHE:CZ	1:A:829:ILE:HG21	2.54	0.42
1:A:286:ILE:HD12	1:A:296:ILE:HD13	2.01	0.42
1:A:597:ASN:ND2	1:A:600:THR:HG23	2.35	0.42
1:A:804:SER:OG	1:A:805:TRP:HD1	2.03	0.42
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.85	0.42
1:A:49:LYS:HE3	1:A:177:GLN:CD	2.45	0.42
1:A:285:LYS:HB2	1:A:285:LYS:HE2	1.90	0.42
1:A:462:ASP:O	1:A:466:PHE:N	2.41	0.42
1:A:785:MET:HA	1:A:788:ALA:CB	2.46	0.42
1:A:50:ARG:O	1:A:50:ARG:HG3	2.12	0.42
1:A:781:VAL:HG11	1:A:783:LEU:CD2	2.29	0.42
1:A:405:LYS:HD3	1:A:405:LYS:HA	1.89	0.41
1:A:778:ARG:CB	1:A:794:ASP:CB	2.86	0.41
1:A:322:VAL:HG22	1:A:360:TYR:CE1	2.55	0.41
1:A:-3:HIS:C	1:A:-1:GLY:HA3	2.44	0.41
1:A:702:ASP:OD1	1:A:729:LYS:NZ	2.29	0.41
1:A:765:ILE:HD12	1:A:863:ILE:HG22	2.01	0.41
1:A:857:ASN:OD1	1:A:857:ASN:C	2.63	0.41
1:A:19:VAL:O	1:A:119:SER:OG	2.38	0.41
1:A:248:ILE:CG2	1:A:256:THR:HG23	2.49	0.41
1:A:582:ARG:HG2	1:A:674:ILE:HD11	2.01	0.41
1:A:778:ARG:O	1:A:795:ILE:HG12	2.20	0.41
1:A:68:LEU:HD21	1:A:75:ALA:HB1	2.03	0.41
1:A:333:VAL:HG12	1:A:366:LEU:C	2.46	0.41
1:A:353:MET:HB3	1:A:353:MET:HE2	1.83	0.41
1:A:407:PHE:CZ	1:A:745:THR:HG23	2.55	0.41
1:A:781:VAL:CA	1:A:783:LEU:HB2	2.49	0.41
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.76	0.41
1:A:83:ILE:O	1:A:87:ILE:HG13	2.21	0.41
1:A:436:SER:OG	1:A:437:VAL:N	2.52	0.41
1:A:741:PRO:HG3	1:A:750:MET:HE2	2.02	0.41
1:A:798:THR:HG22	1:A:799:ALA:H	1.86	0.41
1:A:663:ILE:HD12	1:A:663:ILE:HA	1.87	0.41
1:A:781:VAL:CG1	1:A:783:LEU:HD13	2.50	0.41
1:A:805:TRP:N	1:A:805:TRP:HD1	2.16	0.41
1:A:769:PRO:O	1:A:770:VAL:HB	2.20	0.41
1:A:248:ILE:HG23	1:A:256:THR:HG23	2.01	0.40
1:A:302:GLU:C	1:A:304:ALA:H	2.29	0.40
1:A:671:TYR:O	1:A:675:ASN:HB2	2.21	0.40
1:A:803:PRO:CA	1:A:825:HIS:HD2	2.33	0.40
1:A:-7:HIS:CB	1:A:-6:HIS:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:GLU:O	1:A:794:ASP:CG	2.65	0.40
1:A:203:ASN:O	1:A:204:ARG:CB	2.70	0.40
1:A:408:LEU:HA	1:A:409:PRO:C	2.46	0.40
1:A:408:LEU:HA	1:A:409:PRO:O	2.21	0.40
1:A:547:LEU:H	1:A:547:LEU:HG	1.77	0.40
1:A:782:ILE:CD1	1:A:782:ILE:O	2.70	0.40
1:A:99:TYR:O	1:A:102:ALA:HB3	2.21	0.40
1:A:203:ASN:O	1:A:747:ASP:O	2.39	0.40
1:A:339:MET:O	1:A:340:THR:C	2.65	0.40
1:A:501:ILE:HD12	1:A:510:VAL:HG11	2.04	0.40
1:A:798:THR:O	1:A:817:THR:HA	2.22	0.40

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)
1:A:324:GLU:OE2	1:A:614:SER:OG[1_455]	1.99	0.21

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	840/879 (96%)	746 (89%)	90 (11%)	4 (0%)	24 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	847	ILE
1	A	270	THR
1	A	746	SER
1	A	12	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	726/757 (96%)	601 (83%)	125 (17%)	2	9

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	HIS
1	A	-4	HIS
1	A	-3	HIS
1	A	0	SER
1	A	12	ARG
1	A	18	LEU
1	A	24	MET
1	A	26	LEU
1	A	29	CYS
1	A	32	ILE
1	A	44	THR
1	A	50	ARG
1	A	66	SER
1	A	68	LEU
1	A	69	LYS
1	A	71	SER
1	A	72	ASP
1	A	76	ILE
1	A	80	SER
1	A	81	GLU
1	A	88	GLN
1	A	94	SER
1	A	100	MET
1	A	105	LEU
1	A	116	VAL
1	A	117	ARG
1	A	119	SER
1	A	121	THR
1	A	125	LEU
1	A	133	GLN

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Mol	Chain	Res	Type
1	A	146	LEU
1	A	161	ARG
1	A	175	LYS
1	A	178	LEU
1	A	191	SER
1	A	193	ILE
1	A	194	LEU
1	A	200	ILE
1	A	203	ASN
1	A	204	ARG
1	A	205	LYS
1	A	212	SER
1	A	223	LEU
1	A	227	ASP
1	A	232	ARG
1	A	233	GLU
1	A	234	ASN
1	A	244	LYS
1	A	245	LYS
1	A	256	THR
1	A	259	ARG
1	A	273	ASP
1	A	297	GLU
1	A	308	VAL
1	A	321	GLU
1	A	339	MET
1	A	349	SER
1	A	353	MET
1	A	373	SER
1	A	381	ASP
1	A	383	MET
1	A	384	VAL
1	A	391	ASP
1	A	395	LYS
1	A	396	ASP
1	A	399	LEU
1	A	400	THR
1	A	403	ASN
1	A	455	ILE
1	A	456	GLU
1	A	467	ILE
1	A	469	GLU

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Mol	Chain	Res	Type
1	A	473	GLU
1	A	477	VAL
1	A	480	ASN
1	A	482	THR
1	A	491	MET
1	A	513	LYS
1	A	538	ARG
1	A	543	VAL
1	A	544	ARG
1	A	549	GLN
1	A	554	ASP
1	A	559	LEU
1	A	561	THR
1	A	562	LEU
1	A	581	MET
1	A	586	GLU
1	A	607	SER
1	A	613	ASP
1	A	614	SER
1	A	642	LEU
1	A	648	LYS
1	A	654	GLU
1	A	691	LEU
1	A	715	VAL
1	A	719	GLN
1	A	720	VAL
1	A	723	GLU
1	A	746	SER
1	A	750	MET
1	A	763	ASP
1	A	776	GLU
1	A	780	ARG
1	A	781	VAL
1	A	782	ILE
1	A	783	LEU
1	A	784	GLU
1	A	785	MET
1	A	786	GLU
1	A	797	VAL
1	A	798	THR
1	A	805	TRP
1	A	819	VAL

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Mol	Chain	Res	Type
1	A	822	LEU
1	A	823	MET
1	A	824	THR
1	A	825	HIS
1	A	838	VAL
1	A	845	THR
1	A	847	ILE
1	A	853	GLN
1	A	857	ASN
1	A	865	ILE
1	A	866	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	89	HIS
1	A	139	ASN
1	A	597	ASN
1	A	752	ASN
1	A	825	HIS
1	A	857	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
2	ANP	A	901	3	33,33,33	1.14	5 (15%)	45,52,52	0.90	3 (6%)

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	901	3	-	5/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ANP	PG-N3B	3.04	1.71	1.63
2	A	901	ANP	PB-O1B	2.84	1.50	1.46
2	A	901	ANP	PA-O3A	-2.61	1.56	1.59
2	A	901	ANP	PB-N3B	2.31	1.69	1.63
2	A	901	ANP	PG-O1G	2.03	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ANP	O3G-PG-O1G	-2.10	108.19	113.45
2	A	901	ANP	O2B-PB-O3A	2.02	111.37	104.64
2	A	901	ANP	O2A-PA-O3A	-2.01	101.83	107.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ANP	PG-N3B-PB-O1B
2	A	901	ANP	C5'-O5'-PA-O1A
2	A	901	ANP	C5'-O5'-PA-O3A

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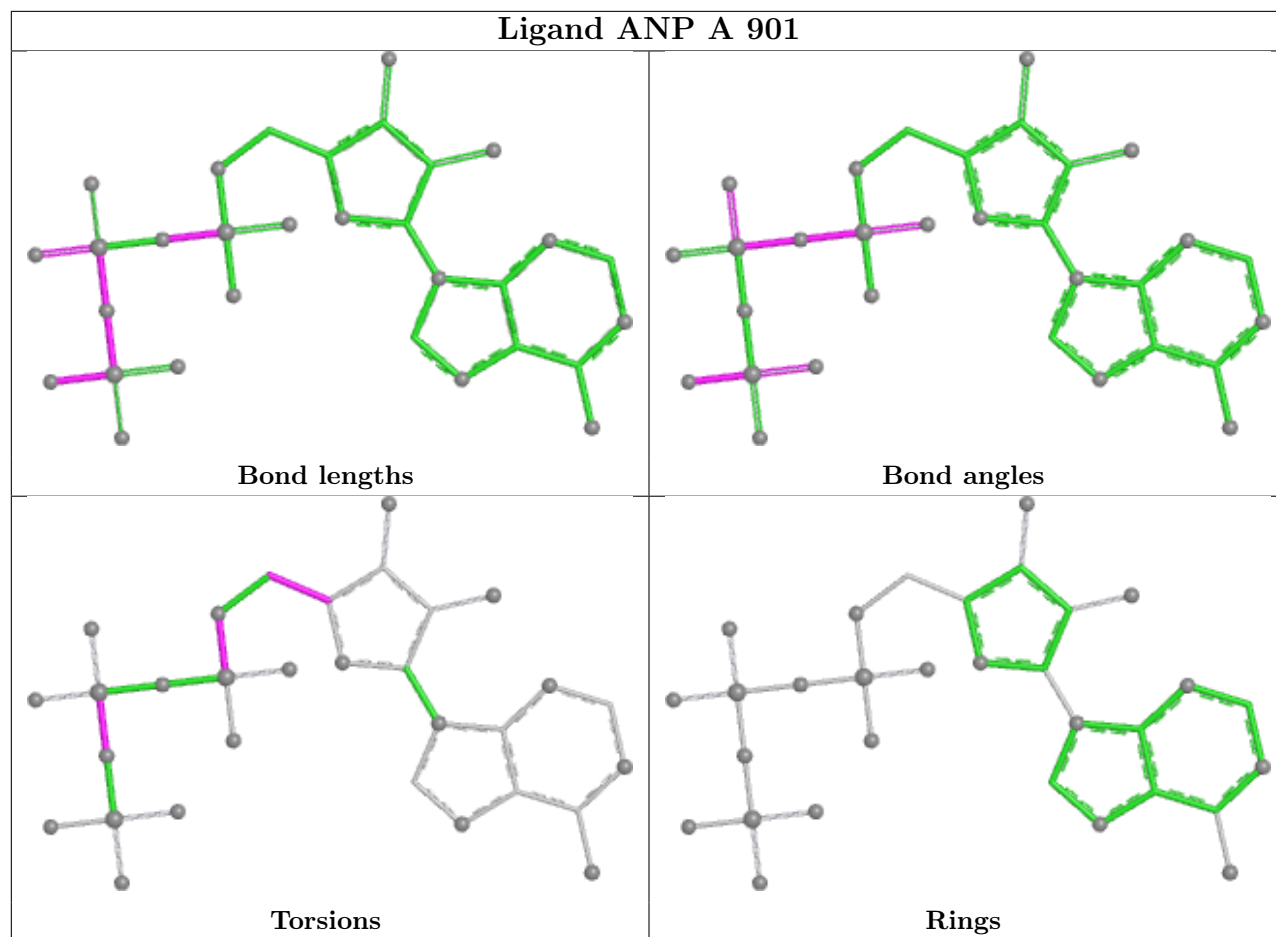
Mol	Chain	Res	Type	Atoms
2	A	901	ANP	C5'-O5'-PA-O2A
2	A	901	ANP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	846/879 (96%)	-0.11	20 (2%) 59 38	27, 53, 89, 147	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	794	ASP	7.7
1	A	780	ARG	4.8
1	A	850	ASP	4.8
1	A	801	THR	3.9
1	A	807	PRO	3.6
1	A	795	ILE	3.3
1	A	853	GLN	3.1
1	A	15	SER	3.1
1	A	864	GLU	3.0
1	A	854	ILE	2.9
1	A	73	MET	2.8
1	A	779	ALA	2.7
1	A	809	PHE	2.6
1	A	197	ALA	2.6
1	A	784	GLU	2.5
1	A	564	GLY	2.2
1	A	224	VAL	2.2
1	A	781	VAL	2.1
1	A	782	ILE	2.0
1	A	778	ARG	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](#)

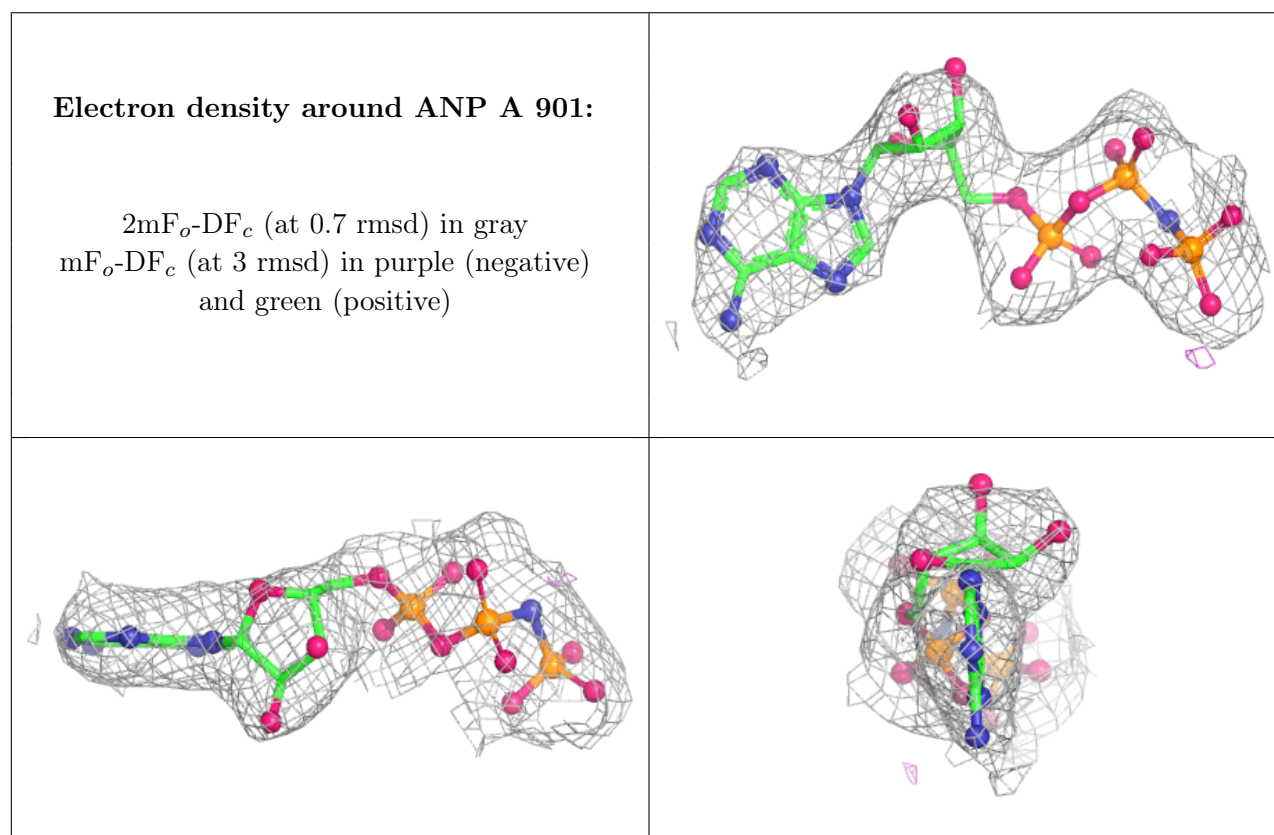
There are no oligosaccharides in this entry.

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	A	901	31/31	0.94	0.07	46,59,77,82	0
3	MG	A	902	1/1	0.96	0.05	65,65,65,65	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.