



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:59 AM UTC

PDB ID : 1H72 / pdb_00001h72
Title : CRYSTAL STRUCTURE OF HOMOSERINE KINASE COMPLEXED WITH HSE
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Deposited on : 2001-07-02
Resolution : 1.80 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

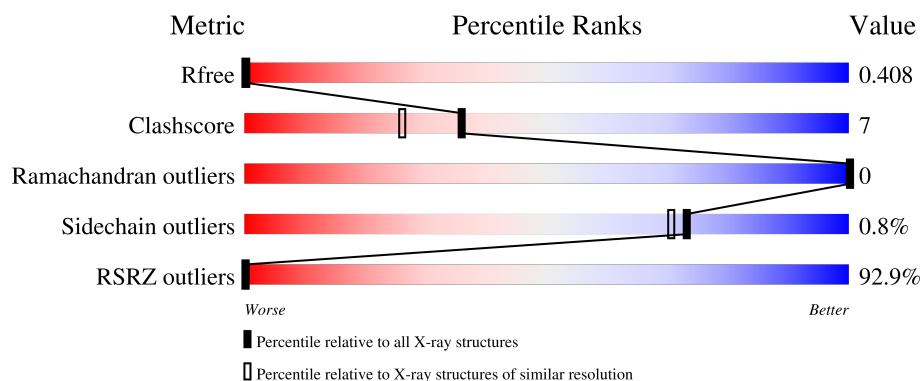
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	C	296	93% 84%16%

2 Entry composition [i](#)

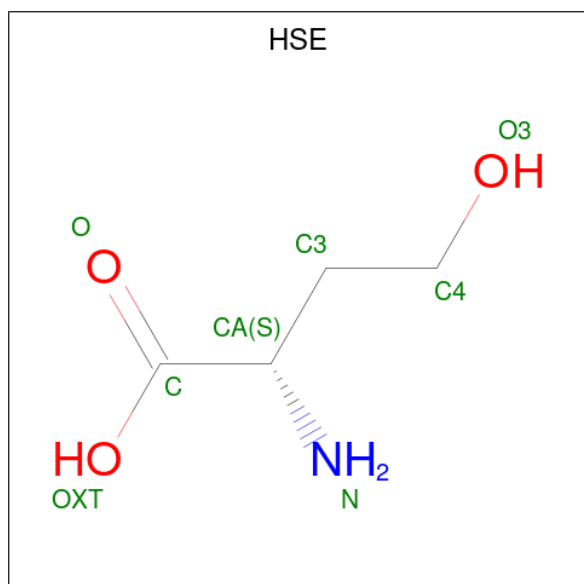
There are 5 unique types of molecules in this entry. The entry contains 2669 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HOMOSERINE KINASE.

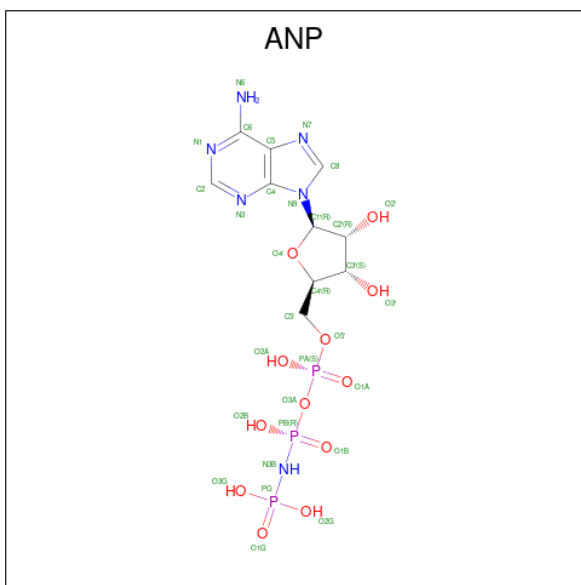
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	296	2314	1484	373	448	9	0	7	0

- Molecule 2 is L-HOMOSERINE (CCD ID: HSE) (formula: $C_4H_9NO_3$).



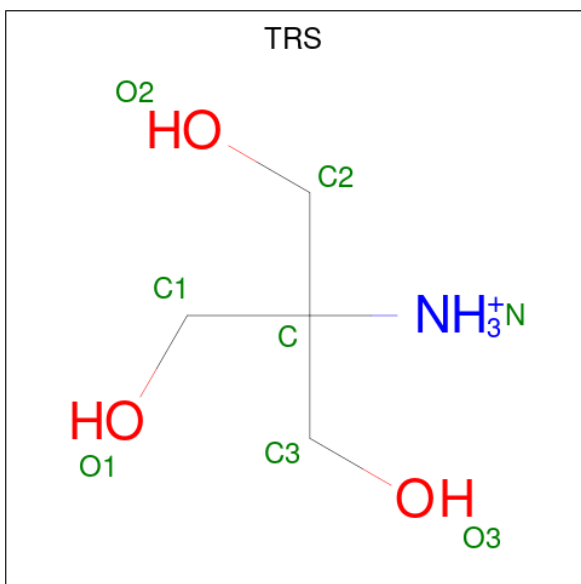
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	8	4	1	3	0	0

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



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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

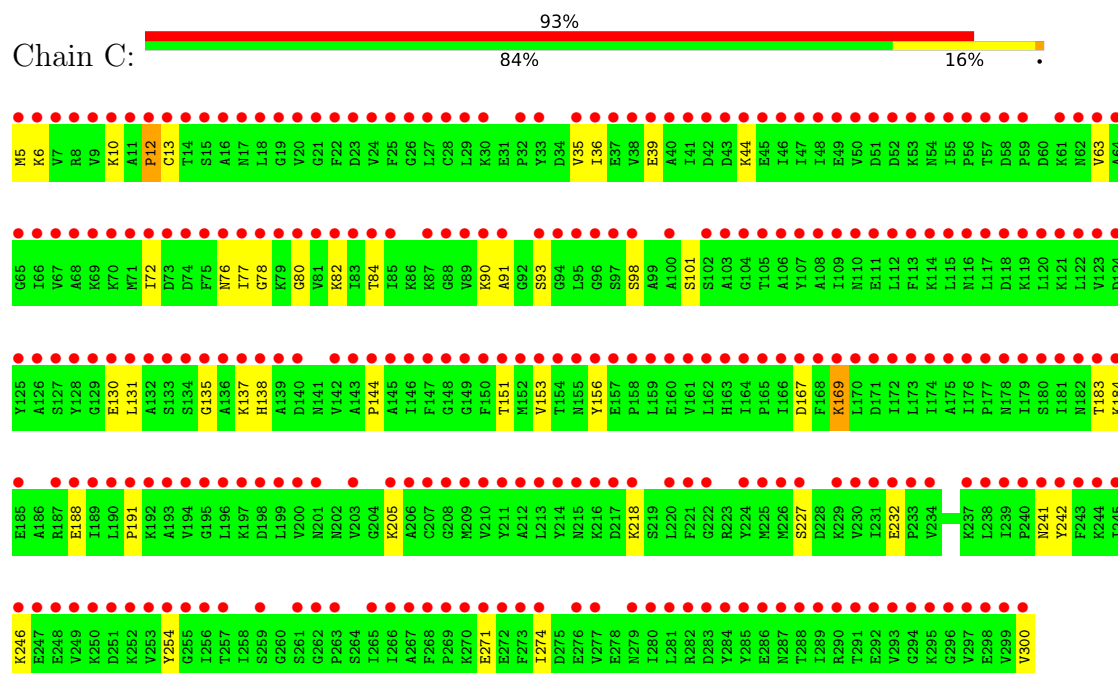
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	308	Total 308	O 308	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: HOMOSERINE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.99Å 87.99Å 99.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.80) 98.7 (50.00-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 1.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.177 , 0.207 0.387 , 0.408	Depositor DCC
R_{free} test set	1709 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2669	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	C	0.78	0/2350	1.09	8/3169 (0.3%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	PRO	N-CA-C	6.00	121.70	111.68
1	C	80	GLY	N-CA-C	-5.84	103.35	112.58
1	C	274	ILE	N-CA-C	5.83	116.48	110.36
1	C	232	GLU	CA-C-N	-5.38	114.13	119.56
1	C	232	GLU	C-N-CA	-5.38	114.13	119.56
1	C	13	CYS	N-CA-C	-5.32	103.51	110.53
1	C	254	TYR	N-CA-C	-5.17	105.82	111.82
1	C	35	VAL	N-CA-C	-5.14	100.35	107.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2314	0	2374	34	1
2	C	8	0	3	0	0
3	C	31	0	13	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	8	0	12	1	1
5	C	308	0	0	15	1
All	All	2669	0	2402	35	2

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 7.

All (35) 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:C:183:THR:OG1	3:C:1301:ANP:O1B	2.02	0.78
1:C:91:ALA:HB1	3:C:1301:ANP:H5'2	1.68	0.75
1:C:5:MET:N	5:C:2001:HOH:O	2.23	0.72
1:C:184:LYS:O	1:C:188:GLU:HG3	1.92	0.69
1:C:5:MET:HB3	5:C:2002:HOH:O	1.92	0.69
1:C:137:LYS:O	1:C:137:LYS:HG2	1.98	0.64
1:C:242:TYR:CZ	1:C:246:LYS:HD2	2.34	0.62
1:C:138:HIS:HB2	5:C:2167:HOH:O	2.02	0.59
1:C:169:LYS:HA	5:C:2187:HOH:O	2.01	0.59
1:C:98[B]:SER:HB2	3:C:1301:ANP:O5'	2.03	0.58
1:C:169:LYS:O	1:C:218:LYS:HE2	2.06	0.55
4:C:1302:TRS:H31	5:C:2122:HOH:O	2.05	0.55
1:C:271:GLU:HG3	5:C:2188:HOH:O	2.08	0.53
1:C:167:ASP:HB3	5:C:2183:HOH:O	2.09	0.52
1:C:72:ILE:HA	1:C:77:ILE:HD12	1.92	0.52
1:C:169:LYS:NZ	5:C:2185:HOH:O	2.45	0.50
1:C:63:VAL:HG11	1:C:98[B]:SER:OG	2.11	0.50
1:C:130:GLU:OE1	5:C:2163:HOH:O	2.20	0.48
1:C:6:LYS:HG2	1:C:39:GLU:HB2	1.96	0.47
1:C:191:PRO:HG3	5:C:2121:HOH:O	2.15	0.47
1:C:98[A]:SER:HB3	3:C:1301:ANP:O5'	2.14	0.47
1:C:36:ILE:HD11	1:C:101:SER:HA	1.96	0.47
1:C:184:LYS:HG3	5:C:2198:HOH:O	2.15	0.47
1:C:205:LYS:HG3	1:C:227[A]:SER:OG	2.15	0.47
1:C:10:LYS:HG2	1:C:300[B]:VAL:HG13	1.96	0.46
1:C:82:LYS:NZ	5:C:2111:HOH:O	2.49	0.45
1:C:84[B]:THR:HG23	5:C:2112:HOH:O	2.18	0.44
1:C:153:VAL:HG11	1:C:156:TYR:CZ	2.53	0.43
1:C:44:LYS:HE2	1:C:78:GLY:O	2.18	0.42
1:C:241:ASN:ND2	5:C:2245:HOH:O	2.28	0.42
1:C:91:ALA:HA	3:C:1301:ANP:O2A	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:HIS:CB	5:C:2167:HOH:O	2.65	0.42
1:C:90:LYS:HG3	1:C:93[B]:SER:OG	2.19	0.41
1:C:131:LEU:O	1:C:135:GLY:N	2.50	0.41
1:C:144:PRO:HD3	1:C:151:THR:OG1	2.21	0.40

All (2) 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)
5:C:2197:HOH:O	5:C:2197:HOH:O[8_665]	2.04	0.16
1:C:76:ASN:OD1	4:C:1302:TRS:O3[3_644]	2.18	0.02

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	C	300/296 (101%)	296 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	255/248 (103%)	253 (99%)	2 (1%)	73	70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	12	PRO
1	C	169	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	141	ASN

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](#)

3 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	C	1301	-	33,33,33	2.05	9 (27%)	45,52,52	2.62	20 (44%)
2	HSE	C	1300	-	6,7,7	2.06	1 (16%)	5,8,8	1.89	1 (20%)
4	TRS	C	1302	-	7,7,7	1.47	1 (14%)	9,9,9	2.18	4 (44%)

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	C	1301	-	-	5/18/38/38	0/3/3/3
2	HSE	C	1300	-	-	3/7/7/7	-
4	TRS	C	1302	-	-	3/9/9/9	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1301	ANP	PA-O3A	-5.76	1.53	1.59
3	C	1301	ANP	PG-N3B	5.39	1.77	1.63
2	C	1300	HSE	OXT-C	4.87	1.46	1.30
3	C	1301	ANP	PB-O2B	-3.53	1.47	1.56
3	C	1301	ANP	PG-O1G	3.52	1.51	1.46
4	C	1302	TRS	C1-C	2.99	1.61	1.53
3	C	1301	ANP	C2-N1	2.31	1.38	1.33
3	C	1301	ANP	C5'-C4'	2.08	1.57	1.51
3	C	1301	ANP	PA-O5'	2.03	1.67	1.59
3	C	1301	ANP	PB-O1B	2.02	1.49	1.46
3	C	1301	ANP	C2'-C1'	-2.02	1.47	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1301	ANP	C5-C4-N3	-6.62	117.61	126.72
3	C	1301	ANP	N3-C4-N9	5.98	137.33	127.17
3	C	1301	ANP	O1B-PB-N3B	-5.95	103.00	111.77
3	C	1301	ANP	O4'-C1'-N9	5.77	119.18	108.09
3	C	1301	ANP	C2-N3-C4	4.09	121.81	111.83
3	C	1301	ANP	C4'-O4'-C1'	3.71	117.66	109.47
3	C	1301	ANP	N3-C2-N1	-3.53	123.23	128.58
2	C	1300	HSE	C4-C3-CA	3.50	119.40	113.27
4	C	1302	TRS	C2-C-C1	-3.40	101.60	110.66
3	C	1301	ANP	O1G-PG-N3B	-3.38	106.79	111.77
3	C	1301	ANP	O4'-C4'-C3'	-3.37	98.47	105.15
3	C	1301	ANP	O4'-C1'-C2'	-3.09	100.00	106.62
4	C	1302	TRS	O1-C1-C	-2.88	102.84	110.88
4	C	1302	TRS	C2-C-N	2.80	115.30	108.17
3	C	1301	ANP	O3'-C3'-C4'	-2.75	103.18	111.08
3	C	1301	ANP	O3A-PB-N3B	2.67	113.98	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1301	ANP	O4'-C4'-C5'	2.57	117.56	109.33
3	C	1301	ANP	O3A-PA-O1A	-2.56	103.01	110.70
3	C	1301	ANP	O2'-C2'-C3'	2.53	119.91	111.82
4	C	1302	TRS	C3-C-N	2.35	114.16	108.17
3	C	1301	ANP	C4-N9-C8	2.31	108.17	105.74
3	C	1301	ANP	C3'-C2'-C1'	2.24	105.70	101.46
3	C	1301	ANP	C6-C5-C4	2.20	120.18	117.18
3	C	1301	ANP	O5'-C5'-C4'	2.16	116.35	108.99
3	C	1301	ANP	O2A-PA-O3A	2.02	112.73	107.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1301	ANP	PB-N3B-PG-O1G
3	C	1301	ANP	PG-N3B-PB-O1B
3	C	1301	ANP	O4'-C4'-C5'-O5'
4	C	1302	TRS	N-C-C2-O2
3	C	1301	ANP	C3'-C4'-C5'-O5'
2	C	1300	HSE	OXT-C-CA-N
2	C	1300	HSE	O-C-CA-N
3	C	1301	ANP	PB-O3A-PA-O2A
4	C	1302	TRS	C3-C-C2-O2
4	C	1302	TRS	N-C-C1-O1
2	C	1300	HSE	O-C-CA-C3

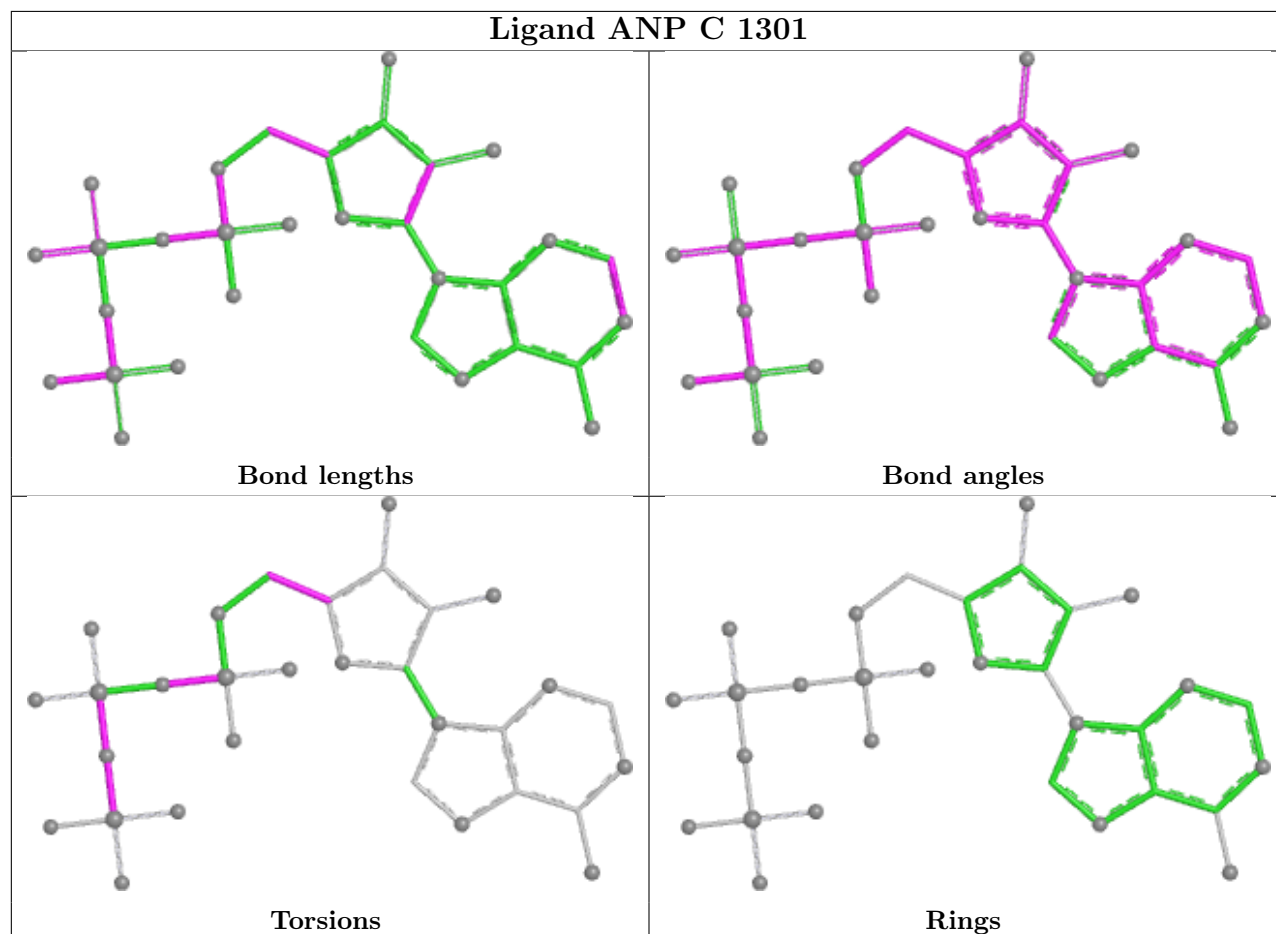
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	ANP	5	0
4	C	1302	TRS	1	1

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	C	296/296 (100%)	3.44	275 (92%) 0 0	8, 22, 42, 55	7 (2%)

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	GLY	9.5
1	C	136	ALA	7.4
1	C	7	VAL	7.3
1	C	179	ILE	6.9
1	C	134	SER	6.6
1	C	131	LEU	6.2
1	C	168	PHE	6.1
1	C	148	GLY	6.0
1	C	158	PRO	6.0
1	C	5	MET	5.9
1	C	41	ILE	5.8
1	C	189	ILE	5.8
1	C	300[A]	VAL	5.7
1	C	135	GLY	5.6
1	C	46	ILE	5.5
1	C	231	ILE	5.5
1	C	77	ILE	5.4
1	C	109	ILE	5.2
1	C	273	PHE	5.2
1	C	191	PRO	5.1
1	C	165	PRO	5.1
1	C	162	LEU	5.0
1	C	170	LEU	5.0
1	C	299	VAL	5.0
1	C	156	TYR	5.0
1	C	25	PHE	5.0
1	C	35	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	249	VAL	4.9
1	C	274	ILE	4.9
1	C	211	TYR	4.8
1	C	44	LYS	4.8
1	C	79	LYS	4.8
1	C	117	LEU	4.8
1	C	115	LEU	4.8
1	C	182	ASN	4.7
1	C	245	ILE	4.7
1	C	190	LEU	4.7
1	C	93[A]	SER	4.7
1	C	221	PHE	4.7
1	C	166	ILE	4.7
1	C	84[A]	THR	4.6
1	C	28	CYS	4.6
1	C	47	ILE	4.6
1	C	132	ALA	4.6
1	C	194	VAL	4.6
1	C	234	VAL	4.6
1	C	133	SER	4.5
1	C	125	TYR	4.5
1	C	164	ILE	4.5
1	C	128	TYR	4.5
1	C	75	PHE	4.5
1	C	16	ALA	4.5
1	C	147	PHE	4.4
1	C	21	GLY	4.4
1	C	29	LEU	4.4
1	C	280	ILE	4.4
1	C	183	THR	4.4
1	C	6	LYS	4.3
1	C	214	TYR	4.3
1	C	137	LYS	4.3
1	C	268	PHE	4.3
1	C	50	VAL	4.3
1	C	174	ILE	4.3
1	C	192	LYS	4.3
1	C	110	ASN	4.3
1	C	277	VAL	4.2
1	C	129	GLY	4.2
1	C	196	LEU	4.2
1	C	66	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	296	GLY	4.1
1	C	91	ALA	4.1
1	C	172	ILE	4.1
1	C	224	TYR	4.1
1	C	113	PHE	4.1
1	C	33	TYR	4.1
1	C	169	LYS	4.1
1	C	83	ILE	4.0
1	C	185	GLU	4.0
1	C	120	LEU	4.0
1	C	272	GLU	4.0
1	C	199	LEU	4.0
1	C	126	ALA	4.0
1	C	78	GLY	3.9
1	C	53	LYS	3.9
1	C	197	LYS	3.9
1	C	178	ASN	3.9
1	C	98[A]	SER	3.9
1	C	289	ILE	3.9
1	C	292	GLU	3.9
1	C	270	LYS	3.9
1	C	163	HIS	3.9
1	C	213	LEU	3.9
1	C	97	SER	3.9
1	C	20	VAL	3.9
1	C	27	LEU	3.9
1	C	112	LEU	3.9
1	C	74	ASP	3.9
1	C	139	ALA	3.8
1	C	149	GLY	3.8
1	C	81	VAL	3.8
1	C	216	LYS	3.8
1	C	281	LEU	3.8
1	C	94	GLY	3.8
1	C	96	GLY	3.8
1	C	130	GLU	3.8
1	C	72	ILE	3.8
1	C	253	VAL	3.8
1	C	22	PHE	3.8
1	C	138	HIS	3.7
1	C	181	ILE	3.7
1	C	142	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	247	GLU	3.7
1	C	64	ALA	3.7
1	C	188	GLU	3.7
1	C	65	GLY	3.7
1	C	263	PRO	3.7
1	C	201	ASN	3.7
1	C	30	LYS	3.7
1	C	38	VAL	3.6
1	C	89	VAL	3.6
1	C	161	VAL	3.6
1	C	200	VAL	3.6
1	C	210	VAL	3.6
1	C	173	LEU	3.6
1	C	220	LEU	3.6
1	C	251	ASP	3.6
1	C	206	ALA	3.6
1	C	32	PRO	3.6
1	C	123	VAL	3.6
1	C	238	LEU	3.6
1	C	36	ILE	3.5
1	C	42	ASP	3.5
1	C	159	LEU	3.5
1	C	284	TYR	3.5
1	C	48	ILE	3.5
1	C	10	LYS	3.5
1	C	59	PRO	3.4
1	C	243	PHE	3.4
1	C	269	PRO	3.4
1	C	180	SER	3.4
1	C	177	PRO	3.4
1	C	63	VAL	3.4
1	C	155	ASN	3.4
1	C	118	ASP	3.3
1	C	160	GLU	3.3
1	C	80	GLY	3.3
1	C	250	LYS	3.3
1	C	150	PHE	3.3
1	C	62	ASN	3.3
1	C	271	GLU	3.2
1	C	237	LYS	3.2
1	C	107	TYR	3.2
1	C	285	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	283	ASP	3.2
1	C	105	THR	3.2
1	C	54	ASN	3.2
1	C	215	ASN	3.2
1	C	88	GLY	3.2
1	C	167	ASP	3.2
1	C	230	VAL	3.2
1	C	95	LEU	3.2
1	C	68	ALA	3.2
1	C	254	TYR	3.2
1	C	18	LEU	3.2
1	C	140	ASP	3.2
1	C	256	ILE	3.1
1	C	9	VAL	3.1
1	C	40	ALA	3.1
1	C	114	LYS	3.1
1	C	152	MET	3.1
1	C	184	LYS	3.1
1	C	154	THR	3.1
1	C	252	LYS	3.0
1	C	76	ASN	3.0
1	C	52	ASP	3.0
1	C	85	ILE	3.0
1	C	171	ASP	3.0
1	C	175	ALA	3.0
1	C	157	GLU	3.0
1	C	58	ASP	2.9
1	C	262	GLY	2.9
1	C	56	PRO	2.9
1	C	71	MET	2.9
1	C	116	ASN	2.9
1	C	11	ALA	2.9
1	C	119	LYS	2.9
1	C	55	ILE	2.9
1	C	24	VAL	2.9
1	C	242	TYR	2.9
1	C	291	THR	2.9
1	C	233	PRO	2.9
1	C	212	ALA	2.9
1	C	13	CYS	2.9
1	C	61	LYS	2.8
1	C	282	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	100	ALA	2.8
1	C	23	ASP	2.8
1	C	146	ILE	2.8
1	C	287	ASN	2.8
1	C	276	GLU	2.8
1	C	103	ALA	2.8
1	C	226	MET	2.8
1	C	290	ARG	2.8
1	C	293	VAL	2.8
1	C	127	SER	2.8
1	C	145	ALA	2.8
1	C	90	LYS	2.7
1	C	122	LEU	2.7
1	C	51	ASP	2.7
1	C	266	ILE	2.7
1	C	15[A]	SER	2.7
1	C	14	THR	2.7
1	C	57	THR	2.7
1	C	17	ASN	2.7
1	C	121	LYS	2.7
1	C	297	VAL	2.7
1	C	106	ALA	2.6
1	C	279	ASN	2.6
1	C	67	VAL	2.6
1	C	8	ARG	2.6
1	C	39	GLU	2.6
1	C	246	LYS	2.6
1	C	295	LYS	2.6
1	C	104	GLY	2.6
1	C	195	GLY	2.6
1	C	203	VAL	2.6
1	C	227[A]	SER	2.6
1	C	257	THR	2.6
1	C	207	CYS	2.6
1	C	143	ALA	2.5
1	C	144	PRO	2.5
1	C	248	GLU	2.5
1	C	267	ALA	2.5
1	C	45	GLU	2.5
1	C	298	GLU	2.5
1	C	43	ASP	2.5
1	C	87	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	244	LYS	2.5
1	C	208	GLY	2.4
1	C	124	ASP	2.4
1	C	265	ILE	2.4
1	C	153	VAL	2.4
1	C	19	GLY	2.4
1	C	239	ILE	2.4
1	C	261	SER	2.4
1	C	205	LYS	2.4
1	C	198	ASP	2.3
1	C	82	LYS	2.3
1	C	232	GLU	2.3
1	C	241	ASN	2.3
1	C	222	GLY	2.3
1	C	73	ASP	2.3
1	C	49	GLU	2.3
1	C	229	LYS	2.3
1	C	108	ALA	2.3
1	C	187	ARG	2.3
1	C	259	SER	2.3
1	C	286	GLU	2.3
1	C	111	GLU	2.2
1	C	217	ASP	2.2
1	C	240	PRO	2.2
1	C	69	LYS	2.2
1	C	151	THR	2.2
1	C	193	ALA	2.2
1	C	26	GLY	2.2
1	C	12	PRO	2.2
1	C	209	MET	2.1
1	C	70	LYS	2.1
1	C	218	LYS	2.1
1	C	255	GLY	2.1
1	C	288	THR	2.1
1	C	37	GLU	2.0
1	C	176	ILE	2.0
1	C	225	MET	2.0
1	C	102	SER	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](#)

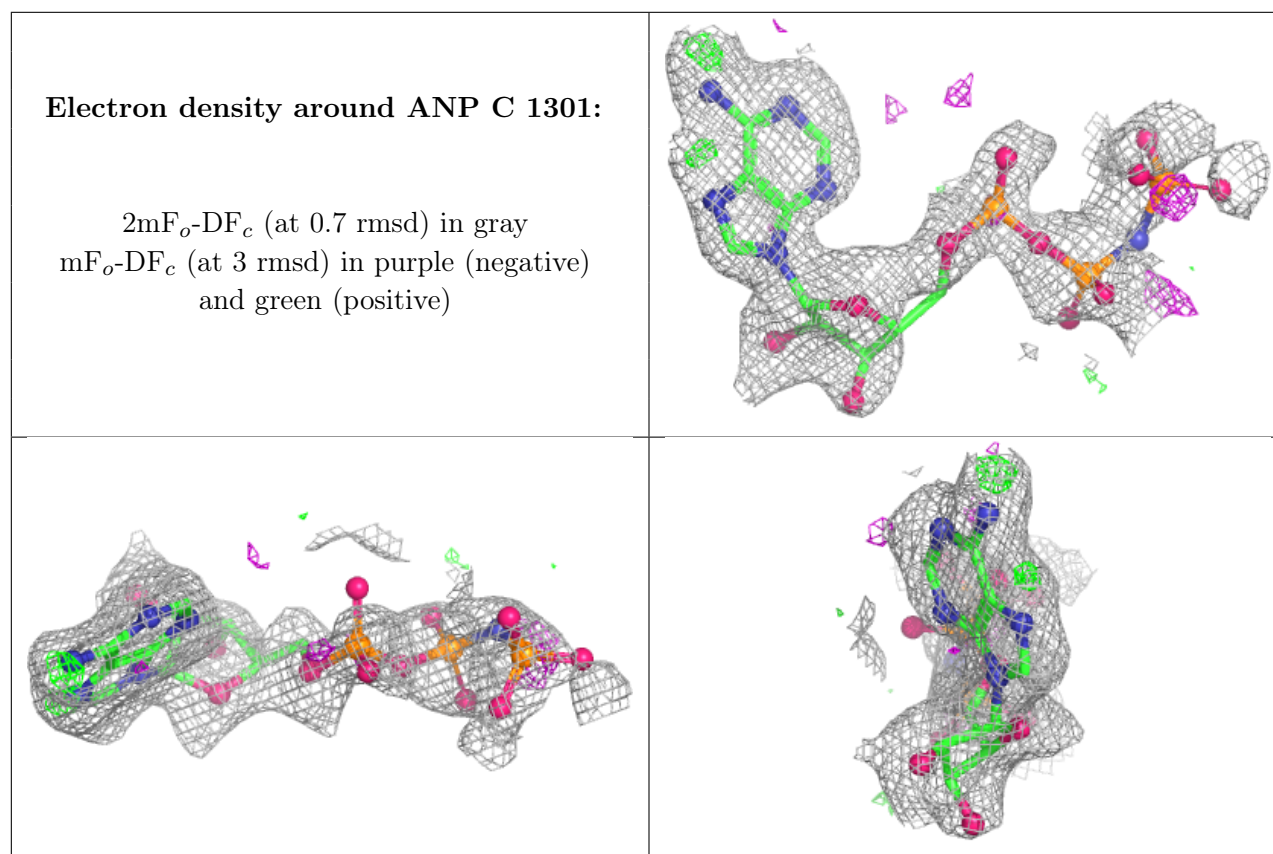
There are no oligosaccharides in this entry.

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
4	TRS	C	1302	8/8	0.62	0.21	20,33,36,36	0
3	ANP	C	1301	31/31	0.69	0.25	18,41,73,73	0
2	HSE	C	1300	8/8	0.71	0.17	26,28,32,32	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.