



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:57 PM UTC

PDB ID : 2A0X / pdb_00002a0x
Title : Structure of human purine nucleoside phosphorylase H257F mutant
Authors : Murkin, A.S.; Shi, W.; Schramm, V.L.
Deposited on : 2005-06-17
Resolution : 2.28 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

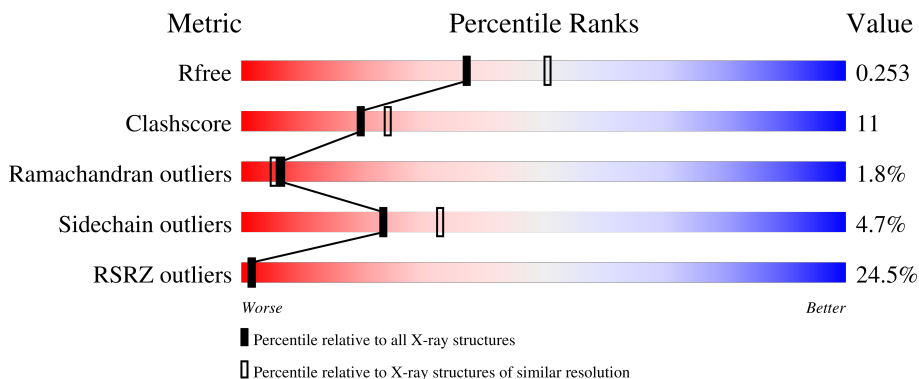
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	289	24% 71% 24% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2296 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 Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2207	1406	385	401	15	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	PHE	HIS	engineered mutation	UNP P00491

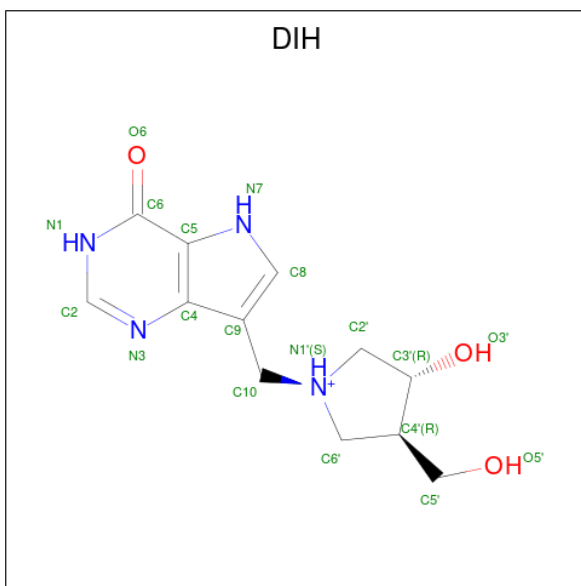
- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is 7-[[[(3R,4R)-3-(hydroxymethyl)-4-oxidanyl-pyrrolidin-1-ium-1-yl]methyl]-3,5-d

ihydropyrrolo[3,2-d]pyrimidin-4-one (CCD ID: DIH) (formula: $C_{12}H_{17}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	12	4	3		

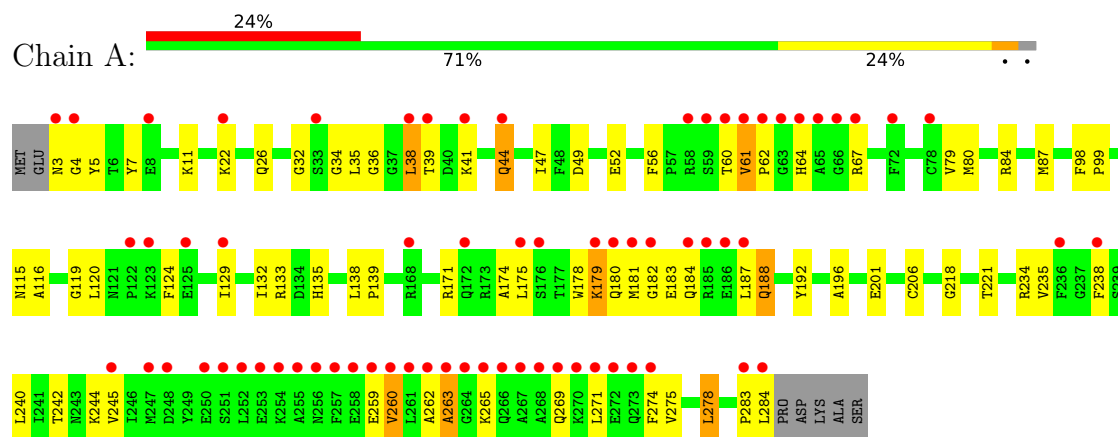
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		

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: Purine nucleoside phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	141.76Å 141.76Å 166.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.28 50.00 – 2.28	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.28) 97.5 (50.00-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.251 0.228 , 0.253	Depositor DCC
R_{free} test set	2934 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k- 2/3*l,2/3*h-2/3*k+1/3*l 0.016 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3* k+1/3*l 0.006 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3* *k+1/3*l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2296	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: SO4, DIH

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	0.42	0/2258	0.94	8/3055 (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	A	22	LYS	N-CA-C	-5.69	105.84	112.89
1	A	260	VAL	N-CA-C	5.30	115.75	110.23
1	A	26	GLN	N-CA-C	-5.27	106.91	113.55
1	A	116	ALA	N-CA-C	-5.26	101.70	110.17
1	A	263	ALA	N-CA-C	-5.16	105.74	111.36
1	A	235	VAL	N-CA-C	5.13	115.51	108.12
1	A	234	ARG	N-CA-C	-5.06	102.21	110.20
1	A	221	THR	N-CA-C	5.05	121.56	110.80

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	A	2207	0	2185	51	0
2	A	10	0	0	0	0
3	A	19	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	60	0	0	0	0
All	All	2296	0	2201	51	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 11.

All (51) 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:120:LEU:HD23	1:A:245:VAL:HG21	1.57	0.87
1:A:38:LEU:HB3	1:A:80:MET:HE1	1.63	0.81
1:A:3:ASN:ND2	1:A:5:TYR:H	1.85	0.74
1:A:3:ASN:HD22	1:A:4:GLY:N	1.88	0.71
1:A:61:VAL:N	1:A:62:PRO:HD3	2.07	0.69
1:A:188:GLN:HE21	1:A:188:GLN:HA	1.57	0.69
1:A:240:LEU:HB2	1:A:271:LEU:HD21	1.76	0.67
1:A:133:ARG:NH1	1:A:171:ARG:HH12	1.97	0.62
1:A:61:VAL:H	1:A:62:PRO:HD3	1.66	0.60
1:A:238:PHE:HE2	1:A:271:LEU:HD23	1.67	0.60
1:A:240:LEU:HD13	1:A:271:LEU:HD11	1.86	0.58
1:A:133:ARG:HD2	1:A:171:ARG:NH1	2.20	0.57
1:A:87:MET:HE3	1:A:196:ALA:HB2	1.89	0.55
1:A:262:ALA:O	1:A:265:LYS:HB3	2.08	0.54
1:A:242:THR:HB	1:A:260:VAL:HA	1.90	0.53
1:A:87:MET:HE3	1:A:196:ALA:CB	2.39	0.52
1:A:174:ALA:HA	1:A:278:LEU:HD21	1.91	0.52
1:A:38:LEU:HD22	1:A:80:MET:HE1	1.92	0.51
1:A:49:ASP:O	1:A:52:GLU:HG2	2.10	0.51
1:A:34:GLY:O	1:A:35:LEU:HD23	2.11	0.51
1:A:3:ASN:HD22	1:A:3:ASN:C	2.16	0.51
1:A:135:HIS:CD2	1:A:135:HIS:C	2.90	0.50
1:A:132:ILE:HG13	1:A:238:PHE:HA	1.94	0.49
1:A:179:LYS:HA	1:A:179:LYS:HZ1	1.77	0.49
1:A:124:PHE:O	1:A:244:LYS:HE2	2.13	0.49
1:A:271:LEU:HD12	1:A:271:LEU:H	1.78	0.49
1:A:36:GLY:O	1:A:39:THR:HG22	2.12	0.49
1:A:32:GLY:HA3	1:A:115:ASN:HA	1.94	0.48
1:A:133:ARG:CZ	1:A:171:ARG:HH12	2.25	0.48
1:A:206:CYS:SG	1:A:245:VAL:HG23	2.53	0.48
1:A:201:GLU:H	1:A:201:GLU:CD	2.22	0.48
1:A:7:TYR:CE2	1:A:11:LYS:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLY:O	1:A:245:VAL:HG22	2.14	0.47
1:A:192:TYR:OH	1:A:218:GLY:HA3	2.14	0.46
1:A:263:ALA:C	1:A:265:LYS:H	2.23	0.46
1:A:181:MET:HE2	1:A:183:GLU:OE1	2.16	0.45
1:A:175:LEU:HD23	1:A:187:LEU:HD23	1.99	0.44
1:A:138:LEU:HB2	1:A:139:PRO:HD3	1.99	0.44
1:A:61:VAL:HG12	1:A:64:HIS:NE2	2.33	0.43
1:A:274:PHE:O	1:A:278:LEU:HB2	2.19	0.43
1:A:178:TRP:CD1	1:A:187:LEU:HB2	2.53	0.43
1:A:188:GLN:HA	1:A:188:GLN:NE2	2.30	0.42
1:A:38:LEU:HD11	1:A:275:VAL:HG11	2.01	0.42
1:A:129:ILE:HD12	1:A:271:LEU:HG	2.01	0.42
1:A:41:LYS:HB3	1:A:41:LYS:NZ	2.35	0.42
1:A:98:PHE:HB3	1:A:99:PRO:HD3	2.01	0.41
1:A:79:VAL:O	1:A:79:VAL:HG13	2.19	0.41
1:A:61:VAL:N	1:A:62:PRO:CD	2.78	0.41
1:A:3:ASN:ND2	1:A:3:ASN:C	2.79	0.41
1:A:44:GLN:HE21	1:A:44:GLN:HB3	1.63	0.40
1:A:47:ILE:HD13	1:A:67:ARG:NH1	2.37	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	280/289 (97%)	262 (94%)	13 (5%)	5 (2%)	6 5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	184	GLN

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Mol	Chain	Res	Type
1	A	283	PRO
1	A	182	GLY
1	A	61	VAL

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	234/240 (98%)	223 (95%)	11 (5%)	23	33

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	44	GLN
1	A	56	PHE
1	A	84	ARG
1	A	179	LYS
1	A	180	GLN
1	A	188	GLN
1	A	259	GLU
1	A	269	GLN
1	A	278	LEU
1	A	284	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	3	ASN
1	A	44	GLN
1	A	55	ASN
1	A	172	GLN
1	A	180	GLN
1	A	188	GLN
1	A	273	GLN

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 ⓘ

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
2	SO4	A	401	-	4,4,4	1.83	2 (50%)	6,6,6	0.87	0
2	SO4	A	402	-	4,4,4	1.76	2 (50%)	6,6,6	0.84	0
3	DIH	A	300	-	21,21,21	2.11	8 (38%)	22,30,30	3.55	10 (45%)

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	DIH	A	300	-	-	0/6/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	DIH	C2-N3	4.68	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	DIH	C2-N1	4.08	1.42	1.35
3	A	300	DIH	C6'-C4'	-3.50	1.47	1.53
2	A	401	SO4	O1-S	2.97	1.62	1.44
3	A	300	DIH	C5-C4	2.70	1.41	1.38
2	A	402	SO4	O1-S	2.70	1.60	1.44
3	A	300	DIH	C2'-C3'	-2.60	1.48	1.52
3	A	300	DIH	C8-N7	-2.29	1.31	1.36
2	A	402	SO4	O3-S	-2.17	1.30	1.48
3	A	300	DIH	C10-C9	-2.16	1.49	1.51
2	A	401	SO4	O3-S	-2.10	1.30	1.48
3	A	300	DIH	C6-N1	2.04	1.43	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	DIH	C9-C10-N1'	10.60	128.23	113.38
3	A	300	DIH	O5'-C5'-C4'	7.33	127.96	111.26
3	A	300	DIH	C9-C8-N7	4.32	114.79	109.22
3	A	300	DIH	O3'-C3'-C2'	4.06	120.44	110.94
3	A	300	DIH	C2'-N1'-C6'	-3.86	98.50	104.12
3	A	300	DIH	C8-N7-C5	-3.53	105.14	109.49
3	A	300	DIH	N1-C2-N3	-3.50	121.47	125.50
3	A	300	DIH	C4-C5-N7	3.15	110.16	105.57
3	A	300	DIH	C4-C5-C6	-2.30	119.39	121.41
3	A	300	DIH	C6'-C4'-C5'	-2.29	109.56	112.71

There are no chirality outliers.

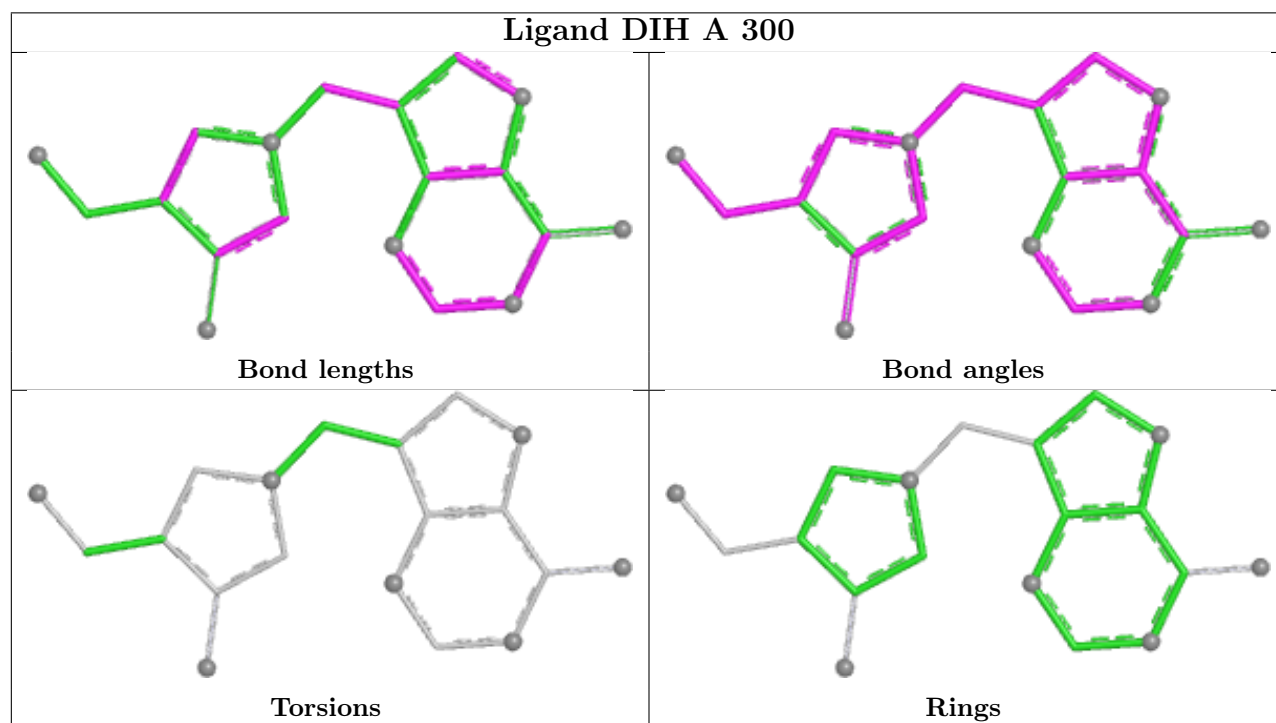
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	282/289 (97%)	1.33	69 (24%) 2 2	28, 47, 82, 86	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ALA	10.0
1	A	60	THR	9.0
1	A	63	GLY	8.6
1	A	252	LEU	8.3
1	A	59	SER	8.2
1	A	61	VAL	7.8
1	A	62	PRO	7.0
1	A	64	HIS	6.8
1	A	261	LEU	6.8
1	A	284	LEU	6.7
1	A	260	VAL	6.5
1	A	262	ALA	6.1
1	A	58	ARG	5.6
1	A	180	GLN	5.3
1	A	254	LYS	4.9
1	A	238	PHE	4.8
1	A	271	LEU	4.8
1	A	265	LYS	4.7
1	A	269	GLN	4.6
1	A	266	GLN	4.6
1	A	253	GLU	4.4
1	A	255	ALA	4.3
1	A	184	GLN	4.3
1	A	185	ARG	4.0
1	A	236	PHE	3.9
1	A	270	LYS	3.9
1	A	264	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	258	GLU	3.8
1	A	259	GLU	3.8
1	A	181	MET	3.7
1	A	66	GLY	3.7
1	A	250	GLU	3.6
1	A	187	LEU	3.6
1	A	123	LYS	3.5
1	A	182	GLY	3.4
1	A	248	ASP	3.4
1	A	257	PHE	3.3
1	A	263	ALA	3.2
1	A	129	ILE	3.2
1	A	283	PRO	3.1
1	A	251	SER	3.0
1	A	247	MET	3.0
1	A	172	GLN	3.0
1	A	33	SER	3.0
1	A	186	GLU	2.9
1	A	267	ALA	2.8
1	A	245	VAL	2.8
1	A	4	GLY	2.7
1	A	274	PHE	2.7
1	A	44	GLN	2.7
1	A	168	ARG	2.7
1	A	8	GLU	2.7
1	A	256	ASN	2.6
1	A	268	ALA	2.6
1	A	179	LYS	2.6
1	A	175	LEU	2.5
1	A	39	THR	2.4
1	A	272	GLU	2.4
1	A	72	PHE	2.4
1	A	38	LEU	2.4
1	A	125	GLU	2.4
1	A	78	CYS	2.3
1	A	273	GLN	2.3
1	A	41	LYS	2.2
1	A	67	ARG	2.2
1	A	176	SER	2.2
1	A	122	PRO	2.1
1	A	3	ASN	2.0
1	A	22	LYS	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](#)

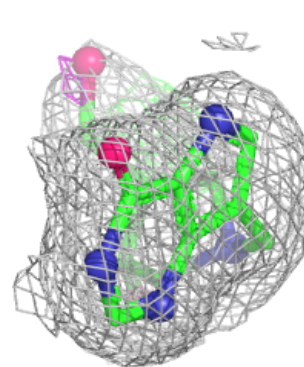
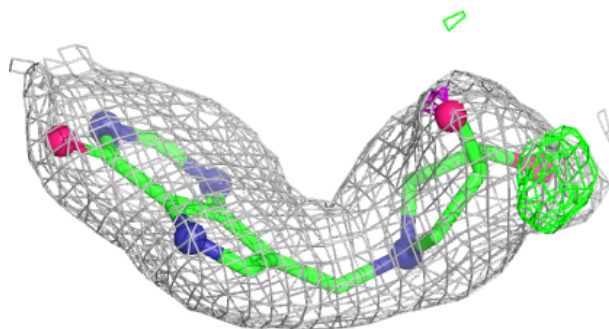
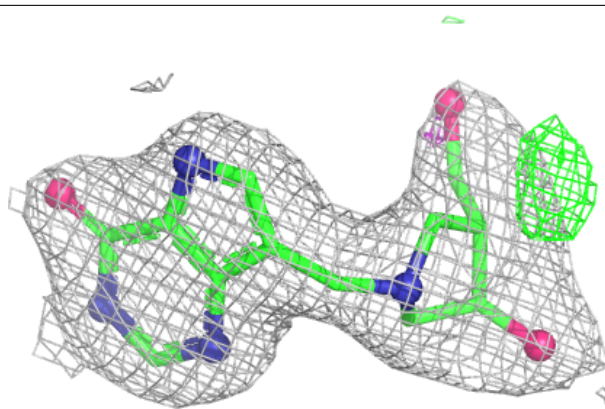
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	401	5/5	0.91	0.13	57,57,58,58	0
3	DIH	A	300	19/19	0.91	0.13	40,44,57,58	0
2	SO4	A	402	5/5	0.96	0.10	42,45,47,48	0

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

Electron density around DIH A 300:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.