



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:47 PM UTC

PDB ID : 1DRW / pdb_00001drw
Title : ESCHERICHIA COLI DHPR/NHDH COMPLEX
Authors : Reddy, S.G.; Scapin, G.; Blanchard, J.S.
Deposited on : 1996-06-28
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

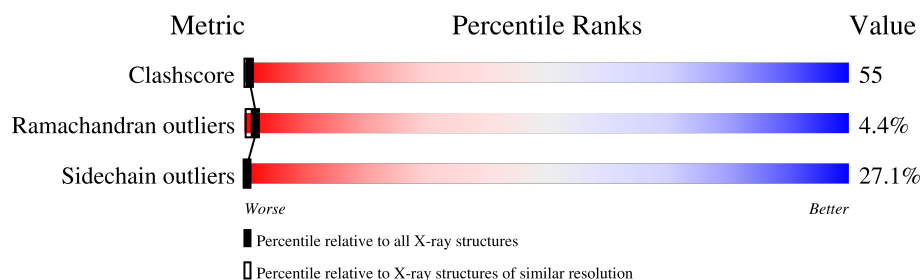
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	273	

2 Entry composition [i](#)

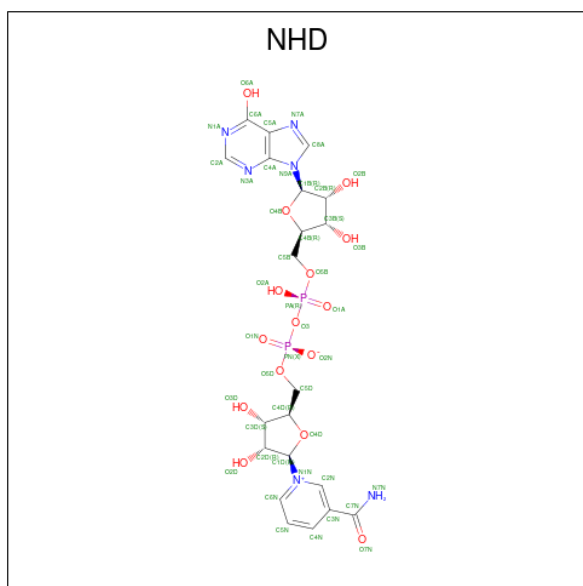
There are 3 unique types of molecules in this entry. The entry contains 2105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDRODIPICOLINATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	1980	1232	354	384	10	0	0	0

- Molecule 2 is NICOTINAMIDE PURIN-6-OL-DINUCLEOTIDE (CCD ID: NHD) (formula: $C_{21}H_{26}N_6O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	44	21	6	15	2	0	0

- Molecule 3 is water.

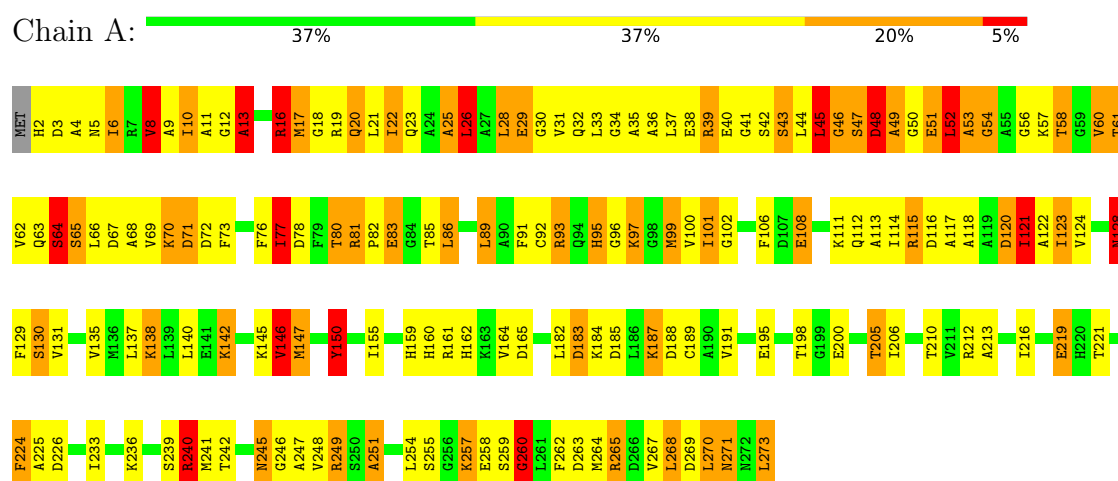
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	81	Total 81 O 81	0	0

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. 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. 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.

Note EDS was not executed.

• Molecule 1: DIHYDRODIPICOLINATE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	75.60 Å 81.70 Å 93.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	82.0 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2105	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	2.20	18/2006 (0.9%)	1.48	21/2705 (0.8%)

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	1	17

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	LEU	C-OXT	70.38	2.64	1.23
1	A	99	MET	SD-CE	-7.43	1.60	1.79
1	A	128	ASN	CA-C	-6.08	1.46	1.52
1	A	123	ILE	CA-CB	5.96	1.62	1.54
1	A	205	THR	CA-CB	-5.96	1.43	1.53
1	A	270	LEU	CA-C	-5.85	1.44	1.52
1	A	135	VAL	CA-CB	5.68	1.61	1.54
1	A	86	LEU	CA-C	5.55	1.60	1.52
1	A	121	ILE	CA-CB	5.50	1.62	1.54
1	A	101	ILE	CA-CB	-5.41	1.47	1.54
1	A	77	ILE	CA-CB	-5.39	1.47	1.54
1	A	124	VAL	CA-CB	-5.25	1.48	1.54
1	A	131	VAL	CA-CB	-5.18	1.47	1.54
1	A	65	SER	CA-C	-5.17	1.46	1.52
1	A	130	SER	C-O	-5.17	1.17	1.23
1	A	131	VAL	CA-C	5.08	1.59	1.52
1	A	270	LEU	N-CA	-5.05	1.39	1.46
1	A	206	ILE	C-O	-5.03	1.18	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	VAL	N-CA-C	14.04	124.44	110.82
1	A	48	ASP	N-CA-C	10.38	132.90	110.80
1	A	52	LEU	N-CA-C	-9.56	102.13	113.88
1	A	198	THR	N-CA-C	-7.71	104.77	114.56
1	A	13	ALA	N-CA-C	7.57	126.93	110.80
1	A	25	ALA	N-CA-C	-7.22	103.35	111.07
1	A	270	LEU	N-CA-C	-6.72	104.18	112.38
1	A	17	MET	N-CA-C	6.58	118.11	111.07
1	A	45	LEU	N-CA-C	6.41	118.57	110.24
1	A	28	LEU	N-CA-C	6.10	118.55	109.59
1	A	43	SER	N-CA-C	-5.95	106.18	113.50
1	A	16	ARG	N-CA-C	-5.89	104.86	111.28
1	A	150	TYR	N-CA-C	-5.88	105.19	112.90
1	A	101	ILE	N-CA-C	5.62	116.20	107.99
1	A	123	ILE	N-CA-C	5.54	116.10	108.12
1	A	113	ALA	N-CA-C	-5.43	105.37	111.28
1	A	240	ARG	N-CA-C	-5.24	106.89	113.28
1	A	53	ALA	N-CA-C	-5.22	107.44	112.97
1	A	268	LEU	N-CA-C	-5.17	107.15	113.50
1	A	251	ALA	N-CA-C	-5.05	105.05	111.11
1	A	146	VAL	N-CA-CB	5.02	117.75	110.52

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	146	VAL	CA

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ASP	Sidechain
1	A	150	TYR	Sidechain
1	A	155	ILE	Mainchain
1	A	16	ARG	Mainchain
1	A	183	ASP	Mainchain
1	A	219	GLU	Mainchain
1	A	224	PHE	Sidechain
1	A	225	ALA	Mainchain
1	A	226	ASP	Mainchain
1	A	26	LEU	Mainchain
1	A	260	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	262	PHE	Sidechain
1	A	48	ASP	Mainchain
1	A	54	GLY	Mainchain
1	A	6	ILE	Mainchain
1	A	77	ILE	Mainchain
1	A	8	VAL	Mainchain

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	1980	0	1940	218	0
2	A	44	0	25	2	0
3	A	81	0	0	9	0
All	All	2105	0	1965	218	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 55.

All (218) 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:3:ASP:HA	1:A:32:GLN:HG3	1.33	1.10
1:A:69:VAL:HG22	1:A:72:ASP:HB2	1.26	1.09
1:A:45:LEU:HD12	1:A:46:GLY:H	1.15	1.09
1:A:80:THR:HG22	1:A:81:ARG:H	1.18	1.08
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.19	1.02
1:A:23:GLN:HG2	1:A:53:ALA:CB	1.97	0.94
1:A:122:ALA:HB2	1:A:258:GLU:HA	1.49	0.91
1:A:45:LEU:HD12	1:A:46:GLY:N	1.84	0.91
1:A:23:GLN:HG2	1:A:53:ALA:HB1	1.53	0.91
1:A:69:VAL:CG2	1:A:72:ASP:HB2	2.02	0.89
1:A:28:LEU:HD12	1:A:29:GLU:N	1.86	0.89
1:A:128:ASN:ND2	1:A:130:SER:H	1.71	0.88
1:A:80:THR:CG2	1:A:81:ARG:H	1.87	0.87
1:A:128:ASN:HD22	1:A:130:SER:H	1.24	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:HA	1:A:60:VAL:O	1.76	0.85
1:A:50:GLY:H	1:A:58:THR:HG23	1.41	0.85
1:A:28:LEU:HD22	1:A:249:ARG:HD2	1.57	0.85
1:A:39:ARG:HG2	1:A:39:ARG:NH1	1.86	0.84
1:A:20:GLN:NE2	1:A:241:MET:HG2	1.93	0.82
1:A:51:GLU:HA	1:A:54:GLY:O	1.80	0.80
1:A:50:GLY:H	1:A:58:THR:CG2	1.96	0.79
1:A:80:THR:HG22	1:A:81:ARG:N	1.99	0.77
1:A:76:PHE:HB3	1:A:99:MET:HG2	1.67	0.76
1:A:70:LYS:NZ	1:A:71:ASP:HB3	2.00	0.75
1:A:19:ARG:CB	1:A:52:LEU:HD13	2.16	0.75
1:A:160:HIS:HD2	1:A:162:HIS:H	1.34	0.75
1:A:245:ASN:H	1:A:245:ASN:ND2	1.83	0.75
1:A:116:ASP:HB2	3:A:413:HOH:O	1.85	0.74
1:A:86:LEU:CD2	1:A:89:LEU:HD12	2.17	0.74
1:A:241:MET:O	1:A:245:ASN:ND2	2.20	0.73
1:A:51:GLU:HG2	1:A:56:GLY:O	1.87	0.73
1:A:16:ARG:HD2	1:A:240:ARG:NH2	2.03	0.72
1:A:45:LEU:HD11	1:A:63:GLN:O	1.90	0.72
1:A:93:ARG:NH1	1:A:120:ASP:OD2	2.23	0.72
1:A:70:LYS:HZ3	1:A:71:ASP:HB3	1.53	0.71
1:A:257:LYS:O	1:A:258:GLU:HG3	1.91	0.71
1:A:70:LYS:HB2	1:A:91:PHE:HZ	1.56	0.70
1:A:49:ALA:HB1	1:A:58:THR:HG23	1.72	0.70
1:A:8:VAL:HG21	1:A:77:ILE:HD11	1.74	0.70
1:A:93:ARG:NH2	1:A:116:ASP:OD2	2.24	0.69
1:A:8:VAL:HG21	1:A:77:ILE:CD1	2.22	0.69
1:A:112:GLN:HG3	3:A:482:HOH:O	1.92	0.69
1:A:3:ASP:HA	1:A:32:GLN:CG	2.17	0.69
1:A:62:VAL:C	1:A:63:GLN:HG2	2.18	0.69
1:A:44:LEU:O	1:A:62:VAL:HG11	1.93	0.69
1:A:86:LEU:HD22	1:A:89:LEU:HD12	1.75	0.68
1:A:187:LYS:HA	3:A:474:HOH:O	1.94	0.68
1:A:122:ALA:HA	1:A:259:SER:O	1.94	0.68
1:A:16:ARG:CB	1:A:240:ARG:HH22	2.07	0.68
1:A:96:GLY:HA2	1:A:121:ILE:CD1	2.24	0.68
1:A:150:TYR:N	1:A:150:TYR:CD1	2.59	0.66
1:A:80:THR:CG2	1:A:81:ARG:N	2.51	0.66
1:A:184:LYS:HG2	1:A:185:ASP:H	1.61	0.66
1:A:37:LEU:HD21	1:A:66:LEU:HD23	1.78	0.64
1:A:16:ARG:HD2	1:A:240:ARG:HH22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:C	1:A:47:SER:H	2.04	0.62
1:A:96:GLY:C	1:A:121:ILE:HD11	2.24	0.62
1:A:42:SER:CB	1:A:45:LEU:HD22	2.30	0.62
1:A:45:LEU:CD1	1:A:62:VAL:HG22	2.30	0.62
1:A:160:HIS:CD2	1:A:162:HIS:H	2.17	0.62
1:A:185:ASP:OD2	1:A:187:LYS:HD3	1.99	0.62
1:A:118:ALA:HA	1:A:121:ILE:O	2.00	0.62
1:A:23:GLN:HG2	1:A:53:ALA:HB2	1.82	0.61
1:A:189:CYS:HB2	1:A:205:THR:HA	1.82	0.61
1:A:4:ALA:HB1	1:A:30:GLY:HA2	1.82	0.61
1:A:219:GLU:HG2	1:A:236:LYS:HG2	1.83	0.60
1:A:70:LYS:HB2	1:A:91:PHE:CZ	2.35	0.60
1:A:36:ALA:O	1:A:62:VAL:HA	2.01	0.60
1:A:28:LEU:HD23	1:A:248:VAL:HG12	1.82	0.60
1:A:239:SER:OG	1:A:241:MET:HB2	2.02	0.59
1:A:4:ALA:H	1:A:32:GLN:HB2	1.66	0.59
1:A:22:ILE:HG22	1:A:53:ALA:CB	2.33	0.59
1:A:69:VAL:HG13	1:A:73:PHE:HE2	1.67	0.59
1:A:18:GLY:O	1:A:22:ILE:HD12	2.04	0.58
1:A:240:ARG:NH1	1:A:240:ARG:HG2	2.17	0.58
1:A:108:GLU:HA	1:A:111:LYS:HD2	1.84	0.58
1:A:264:MET:O	1:A:268:LEU:HB2	2.03	0.57
1:A:121:ILE:HG23	1:A:123:ILE:HG13	1.86	0.57
1:A:128:ASN:HD22	1:A:128:ASN:C	2.11	0.57
1:A:263:ASP:O	1:A:267:VAL:HG23	2.05	0.57
1:A:45:LEU:O	1:A:47:SER:N	2.26	0.56
1:A:118:ALA:O	1:A:260:GLY:HA2	2.04	0.56
1:A:147:MET:HE2	1:A:224:PHE:HB3	1.86	0.56
1:A:28:LEU:O	1:A:31:VAL:HG22	2.06	0.56
1:A:20:GLN:HE22	1:A:241:MET:HG2	1.68	0.56
1:A:28:LEU:HD12	1:A:28:LEU:C	2.30	0.56
1:A:245:ASN:ND2	1:A:245:ASN:N	2.53	0.55
1:A:16:ARG:HB3	1:A:240:ARG:NH2	2.21	0.55
1:A:9:ALA:HA	1:A:35:ALA:O	2.07	0.55
1:A:28:LEU:CD2	1:A:249:ARG:HD2	2.32	0.55
1:A:150:TYR:HD2	3:A:465:HOH:O	1.89	0.54
1:A:91:PHE:CE1	1:A:95:HIS:CD2	2.96	0.54
1:A:8:VAL:O	1:A:34:GLY:N	2.39	0.54
1:A:47:SER:O	1:A:61:THR:OG1	2.23	0.54
1:A:91:PHE:CZ	1:A:95:HIS:CD2	2.96	0.54
1:A:39:ARG:HH11	1:A:39:ARG:CG	2.04	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:O	1:A:138:LYS:HD2	2.09	0.53
1:A:240:ARG:HG2	1:A:240:ARG:HH11	1.72	0.53
1:A:3:ASP:O	1:A:4:ALA:HB2	2.08	0.52
1:A:21:LEU:HD22	1:A:77:ILE:HG21	1.89	0.52
1:A:66:LEU:HB3	1:A:91:PHE:CZ	2.43	0.52
1:A:117:ALA:O	1:A:121:ILE:HG22	2.09	0.52
1:A:8:VAL:HG13	1:A:10:ILE:CD1	2.39	0.52
1:A:48:ASP:N	1:A:48:ASP:OD1	2.40	0.52
1:A:86:LEU:HD23	1:A:89:LEU:HD12	1.88	0.52
1:A:249:ARG:HD3	1:A:249:ARG:N	2.25	0.52
1:A:85:THR:HG21	1:A:106:PHE:HZ	1.74	0.52
1:A:12:GLY:O	2:A:301:NHD:O3B	2.27	0.52
1:A:108:GLU:HB3	3:A:485:HOH:O	2.10	0.51
1:A:28:LEU:HD12	1:A:29:GLU:H	1.73	0.51
1:A:3:ASP:CA	1:A:32:GLN:HG3	2.23	0.51
1:A:4:ALA:CB	1:A:30:GLY:HA2	2.40	0.51
1:A:4:ALA:HB3	1:A:30:GLY:C	2.35	0.51
1:A:96:GLY:HA2	1:A:121:ILE:HD13	1.93	0.51
1:A:8:VAL:HG13	1:A:10:ILE:HD13	1.93	0.51
1:A:269:ASP:C	1:A:271:ASN:N	2.67	0.51
1:A:25:ALA:O	1:A:26:LEU:O	2.29	0.50
1:A:184:LYS:HG2	1:A:185:ASP:N	2.25	0.50
1:A:81:ARG:HD3	1:A:82:PRO:CD	2.41	0.50
1:A:69:VAL:C	1:A:71:ASP:H	2.19	0.50
1:A:69:VAL:O	1:A:71:ASP:N	2.45	0.50
1:A:118:ALA:HB1	1:A:260:GLY:CA	2.41	0.50
1:A:61:THR:O	1:A:63:GLN:HG2	2.12	0.50
1:A:69:VAL:HG13	1:A:73:PHE:CE2	2.46	0.50
1:A:76:PHE:HB3	1:A:99:MET:CG	2.40	0.50
1:A:66:LEU:HB3	1:A:91:PHE:CE2	2.47	0.49
1:A:37:LEU:CD2	1:A:66:LEU:HD23	2.41	0.49
1:A:45:LEU:HD13	1:A:62:VAL:HG22	1.94	0.49
1:A:269:ASP:HA	3:A:450:HOH:O	2.12	0.49
1:A:28:LEU:HD22	1:A:249:ARG:CD	2.38	0.49
1:A:242:THR:HA	1:A:245:ASN:HD21	1.77	0.49
1:A:2:HIS:CA	1:A:26:LEU:O	2.61	0.49
1:A:49:ALA:CB	1:A:58:THR:HG23	2.41	0.48
1:A:81:ARG:HD3	1:A:82:PRO:HD3	1.95	0.48
1:A:16:ARG:HB2	1:A:240:ARG:HH22	1.77	0.48
1:A:22:ILE:CG2	1:A:53:ALA:CB	2.91	0.48
1:A:38:GLU:HG3	1:A:39:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:CB	1:A:91:PHE:CE2	2.97	0.48
1:A:40:GLU:HA	1:A:64:SER:OG	2.13	0.48
1:A:129:PHE:O	1:A:246:GLY:HA3	2.13	0.48
1:A:69:VAL:C	1:A:71:ASP:N	2.69	0.47
1:A:97:LYS:N	1:A:121:ILE:HD11	2.29	0.47
1:A:83:GLU:OE2	3:A:469:HOH:O	2.20	0.47
1:A:13:ALA:HB3	1:A:37:LEU:O	2.15	0.47
1:A:44:LEU:O	1:A:62:VAL:CG1	2.61	0.46
1:A:102:GLY:O	2:A:301:NHD:H2N	2.15	0.46
1:A:142:LYS:N	1:A:142:LYS:CD	2.77	0.46
1:A:83:GLU:CD	1:A:83:GLU:H	2.23	0.46
1:A:128:ASN:ND2	1:A:128:ASN:C	2.74	0.46
1:A:50:GLY:N	1:A:58:THR:CG2	2.73	0.46
1:A:22:ILE:CG2	1:A:53:ALA:HB2	2.45	0.46
1:A:45:LEU:C	1:A:47:SER:N	2.70	0.46
1:A:111:LYS:O	1:A:114:ILE:HB	2.16	0.46
1:A:147:MET:HA	1:A:150:TYR:CE2	2.50	0.46
1:A:2:HIS:N	1:A:25:ALA:O	2.50	0.45
1:A:254:LEU:O	1:A:257:LYS:HG2	2.16	0.45
1:A:115:ARG:HE	1:A:115:ARG:HB2	1.56	0.45
1:A:138:LYS:HD3	1:A:138:LYS:HA	1.54	0.45
1:A:69:VAL:O	1:A:72:ASP:N	2.34	0.45
1:A:160:HIS:HD2	1:A:162:HIS:N	2.08	0.45
1:A:17:MET:O	1:A:21:LEU:HD12	2.16	0.45
1:A:52:LEU:C	1:A:54:GLY:H	2.25	0.45
1:A:93:ARG:NH1	3:A:455:HOH:O	2.42	0.45
1:A:38:GLU:CG	1:A:39:ARG:N	2.81	0.44
1:A:118:ALA:HB1	1:A:260:GLY:HA2	1.99	0.44
1:A:85:THR:O	1:A:89:LEU:HB2	2.18	0.44
1:A:248:VAL:O	1:A:251:ALA:HB3	2.17	0.44
1:A:22:ILE:HG22	1:A:53:ALA:HB2	1.99	0.44
1:A:81:ARG:HB3	1:A:83:GLU:HG2	2.00	0.44
1:A:101:ILE:HD12	1:A:123:ILE:HG23	2.00	0.44
1:A:142:LYS:N	1:A:142:LYS:HD3	2.33	0.43
1:A:37:LEU:N	1:A:37:LEU:HD12	2.32	0.43
1:A:4:ALA:N	1:A:32:GLN:HB2	2.33	0.43
1:A:140:LEU:HD23	1:A:233:ILE:HD12	2.00	0.43
1:A:45:LEU:HD11	1:A:62:VAL:HG22	1.98	0.43
1:A:78:ASP:OD1	1:A:80:THR:HB	2.18	0.43
1:A:142:LYS:HD2	1:A:142:LYS:HA	1.58	0.43
1:A:100:VAL:HG11	1:A:247:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ALA:CB	1:A:30:GLY:CA	2.96	0.43
1:A:66:LEU:O	1:A:70:LYS:N	2.51	0.43
1:A:70:LYS:NZ	1:A:71:ASP:CB	2.79	0.43
1:A:81:ARG:HG3	1:A:83:GLU:OE2	2.18	0.43
1:A:121:ILE:CG2	1:A:123:ILE:HD11	2.49	0.43
1:A:159:HIS:O	1:A:212:ARG:HA	2.18	0.43
1:A:69:VAL:HG22	1:A:69:VAL:O	2.18	0.43
1:A:65:SER:HB3	1:A:68:ALA:HB2	2.00	0.42
1:A:210:THR:HG23	1:A:212:ARG:NH1	2.35	0.42
1:A:45:LEU:HD13	1:A:45:LEU:HA	1.10	0.42
1:A:38:GLU:CD	1:A:39:ARG:H	2.27	0.42
1:A:86:LEU:HA	1:A:89:LEU:HB2	2.02	0.42
1:A:146:VAL:HG23	1:A:146:VAL:O	2.18	0.42
1:A:40:GLU:C	1:A:42:SER:H	2.27	0.42
1:A:121:ILE:HG23	1:A:123:ILE:CG1	2.49	0.42
1:A:3:ASP:H	1:A:32:GLN:HA	1.84	0.42
1:A:9:ALA:HB2	1:A:73:PHE:CG	2.54	0.42
1:A:48:ASP:HB3	1:A:49:ALA:H	1.39	0.42
1:A:61:THR:CG2	1:A:63:GLN:OE1	2.68	0.42
1:A:129:PHE:C	1:A:264:MET:HE2	2.44	0.41
1:A:17:MET:C	1:A:21:LEU:HD12	2.45	0.41
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.85	0.41
1:A:185:ASP:O	1:A:188:ASP:N	2.43	0.41
1:A:91:PHE:CD1	1:A:91:PHE:C	2.97	0.41
1:A:213:ALA:O	1:A:216:ILE:HD12	2.21	0.41
1:A:85:THR:O	1:A:89:LEU:N	2.38	0.41
1:A:50:GLY:N	1:A:58:THR:HG21	2.36	0.41
1:A:99:MET:HE3	1:A:99:MET:HB2	1.71	0.41
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.89	0.41
1:A:147:MET:HE3	1:A:147:MET:HB3	1.97	0.41
1:A:66:LEU:HB2	1:A:91:PHE:CE2	2.56	0.41
1:A:70:LYS:HG3	1:A:95:HIS:CD2	2.57	0.41
1:A:263:ASP:HB2	3:A:415:HOH:O	2.21	0.41
1:A:182:LEU:O	1:A:183:ASP:HB2	2.21	0.40
1:A:138:LYS:HE2	1:A:270:LEU:O	2.21	0.40
1:A:37:LEU:HD12	1:A:37:LEU:H	1.86	0.40
1:A:146:VAL:O	1:A:150:TYR:CZ	2.75	0.40
1:A:265:ARG:HE	1:A:265:ARG:HB2	1.58	0.40
1:A:92:CYS:CB	1:A:97:LYS:HB2	2.51	0.40
1:A:273:LEU:OXT	1:A:273:LEU:C	2.64	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	270/273 (99%)	230 (85%)	28 (10%)	12 (4%)	2 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	11	ALA
1	A	47	SER
1	A	48	ASP
1	A	13	ALA
1	A	49	ALA
1	A	5	ASN
1	A	26	LEU
1	A	46	GLY
1	A	64	SER
1	A	41	GLY
1	A	260	GLY

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	192/201 (96%)	140 (73%)	52 (27%)	0 0

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

Mol	Chain	Res	Type
1	A	8	VAL
1	A	10	ILE
1	A	20	GLN
1	A	22	ILE
1	A	26	LEU
1	A	29	GLU
1	A	33	LEU
1	A	39	ARG
1	A	43	SER
1	A	45	LEU
1	A	51	GLU
1	A	52	LEU
1	A	57	LYS
1	A	58	THR
1	A	60	VAL
1	A	61	THR
1	A	64	SER
1	A	67	ASP
1	A	70	LYS
1	A	71	ASP
1	A	80	THR
1	A	81	ARG
1	A	83	GLU
1	A	89	LEU
1	A	93	ARG
1	A	95	HIS
1	A	97	LYS
1	A	108	GLU
1	A	115	ARG
1	A	121	ILE
1	A	128	ASN
1	A	138	LYS
1	A	142	LYS
1	A	145	LYS
1	A	146	VAL
1	A	147	MET
1	A	150	TYR
1	A	161	ARG
1	A	164	VAL
1	A	165	ASP
1	A	187	LYS
1	A	191	VAL
1	A	195	GLU

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Mol	Chain	Res	Type
1	A	200	GLU
1	A	221	THR
1	A	240	ARG
1	A	245	ASN
1	A	249	ARG
1	A	255	SER
1	A	257	LYS
1	A	265	ARG
1	A	271	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	88	HIS
1	A	128	ASN
1	A	160	HIS
1	A	245	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](#)

1 ligand is 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	NHD	A	301	-	46,48,48	2.49	6 (13%)	62,73,73	2.05	18 (29%)

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	NHD	A	301	-	-	3/30/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NHD	O7N-C7N	9.71	1.42	1.24
2	A	301	NHD	PN-O3	-8.83	1.50	1.59
2	A	301	NHD	PA-O3	-7.18	1.51	1.59
2	A	301	NHD	C3N-C7N	-4.40	1.44	1.50
2	A	301	NHD	O3D-C3D	3.53	1.51	1.43
2	A	301	NHD	C6N-C5N	2.11	1.43	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NHD	C2N-C3N-C4N	-7.49	109.55	118.26
2	A	301	NHD	C5N-C4N-C3N	5.83	126.10	120.36
2	A	301	NHD	C4A-N9A-C1B	-3.85	117.64	126.63
2	A	301	NHD	O3-PN-O1N	-3.47	100.27	110.70
2	A	301	NHD	O2N-PN-O3	3.44	116.56	107.27
2	A	301	NHD	C5N-C6N-N1N	-3.39	115.76	120.38
2	A	301	NHD	C6N-N1N-C2N	-2.98	119.34	121.88
2	A	301	NHD	O3B-C3B-C4B	-2.96	102.59	111.08
2	A	301	NHD	O2N-PN-O1N	2.94	126.11	112.44
2	A	301	NHD	C1B-N9A-C8A	2.84	133.39	127.09
2	A	301	NHD	O2B-C2B-C3B	2.70	120.47	111.82
2	A	301	NHD	C2B-C3B-C4B	-2.47	97.83	102.61
2	A	301	NHD	O5D-PN-O1N	-2.47	99.14	108.94
2	A	301	NHD	C5A-C4A-N9A	-2.42	103.17	105.81
2	A	301	NHD	O5B-PA-O1A	-2.41	99.39	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	NHD	O2A-PA-O1A	2.35	123.40	112.44
2	A	301	NHD	C4A-N9A-C8A	2.22	108.06	105.74
2	A	301	NHD	C3N-C7N-N7N	-2.13	115.12	117.74

There are no chirality outliers.

All (3) torsion outliers are listed below:

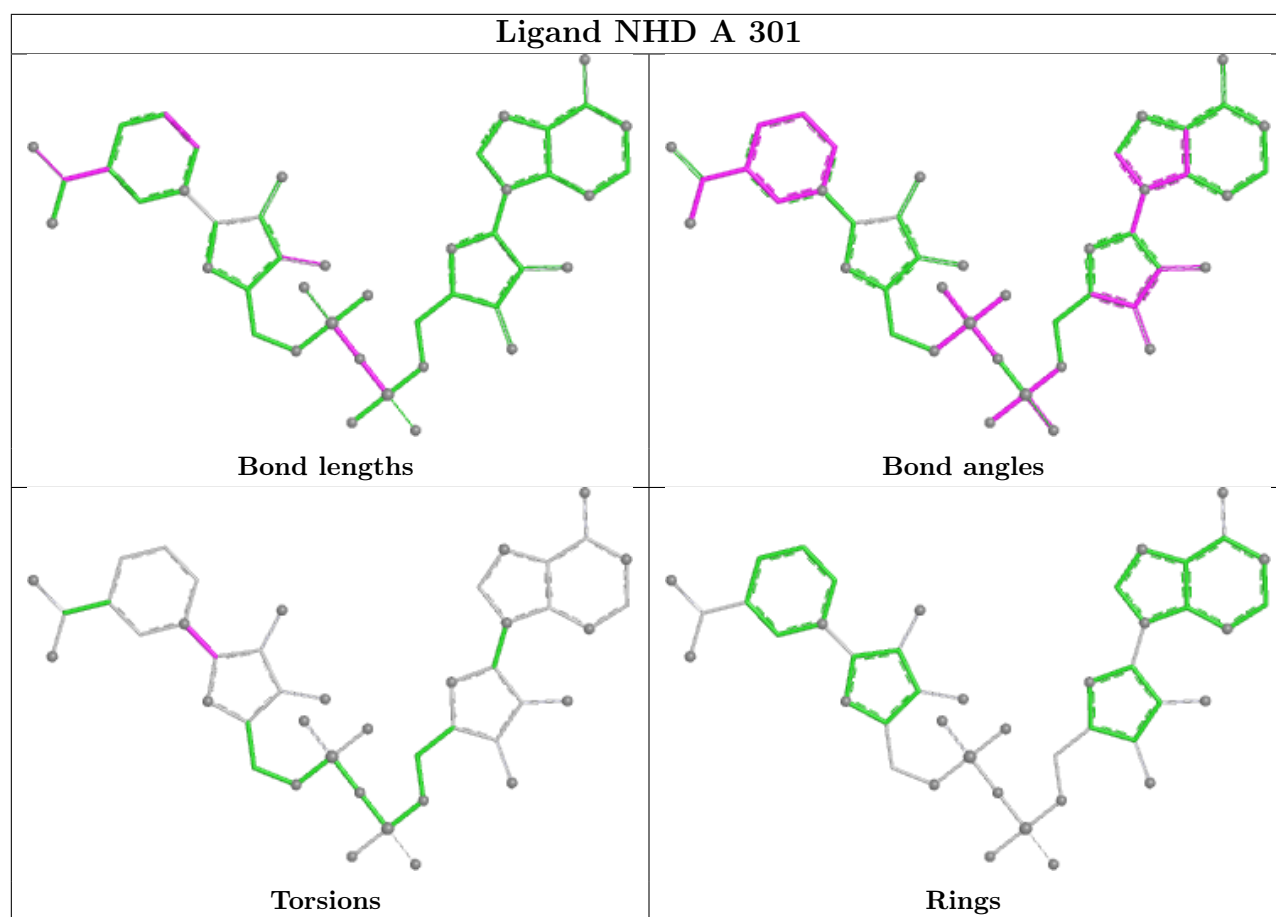
Mol	Chain	Res	Type	Atoms
2	A	301	NHD	O4D-C1D-N1N-C6N
2	A	301	NHD	C2D-C1D-N1N-C2N
2	A	301	NHD	O4D-C1D-N1N-C2N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NHD	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.