



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:55 AM UTC

PDB ID : 2NTV / pdb_00002ntv
Title : Mycobacterium leprae InhA bound with PTH-NAD adduct
Authors : Wang, F.; Sacchettini, J.C.
Deposited on : 2006-11-08
Resolution : 2.10 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

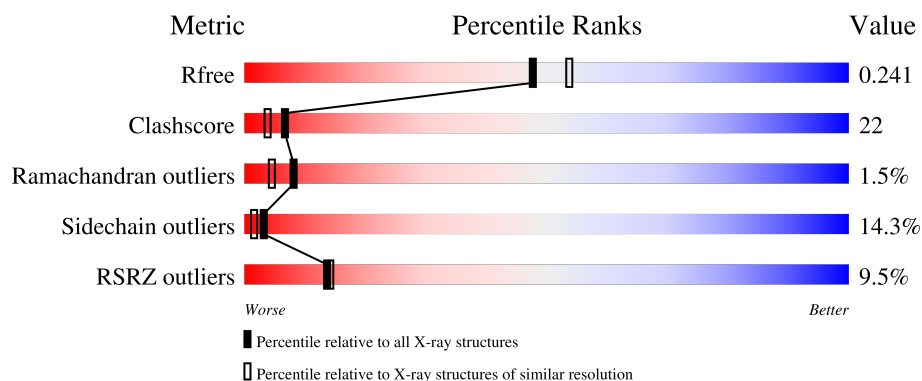
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	268	5% 73% 22% .
1	B	268	14% 65% 24% 8% .

2 Entry composition [i](#)

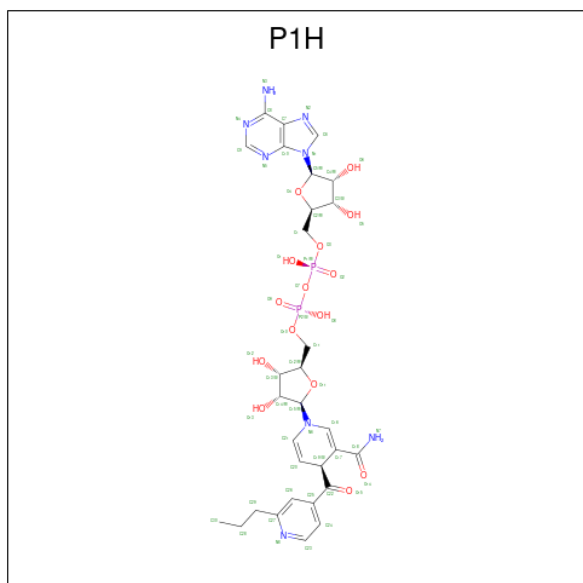
There are 3 unique types of molecules in this entry. The entry contains 4329 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Enoyl-[ACP] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2008	1271	344	383	10			
1	B	268	Total	C	N	O	S	0	0	0
			2008	1271	344	383	10			

- Molecule 2 is {(2R,3S,4R,5R)-5-[(4S)-3-(AMINOCARBONYL)-4-(2-PROPYLISONIC OTINOYL)PYRIDIN-1(4H)-YL]-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL}M ETHYL [(2R,3S,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL DIHYDROGEN DIPHOSPHATE (CCD ID: P1H) (formula: C₃₀H₃₈N₈O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			55	30	8	15	2		
2	B	1	Total	C	N	O	P	0	0
			55	30	8	15	2		

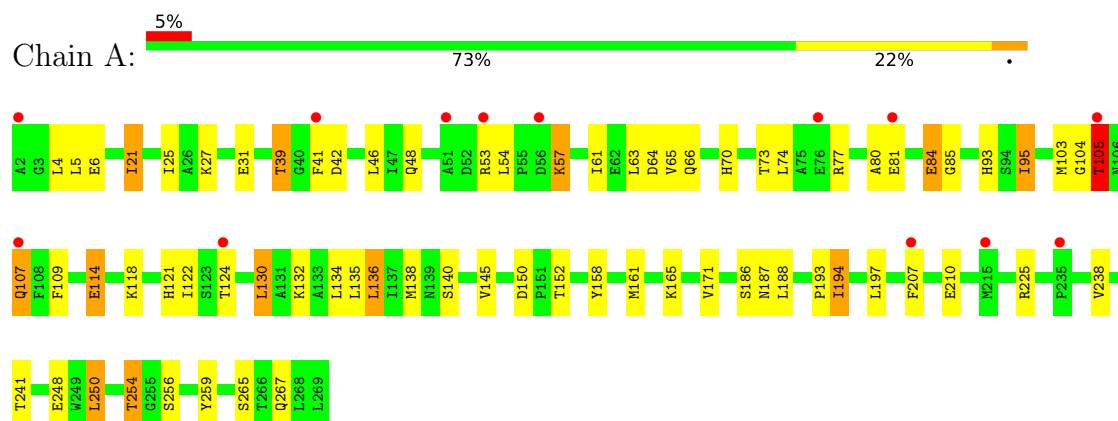
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total 124	O 124	0	0
3	B	79	Total 79	O 79	0	0

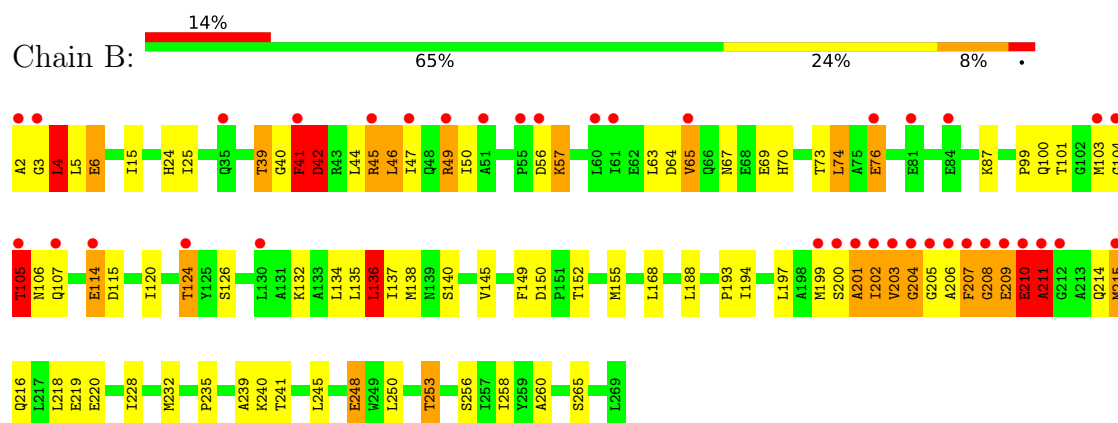
3 Residue-property plots

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: Enoyl-[ACP] reductase



• Molecule 1: Enoyl-[ACP] reductase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.23Å 100.02Å 186.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.10 19.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.89-2.10) 99.2 (19.89-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.244 0.215 , 0.241	Depositor DCC
R_{free} test set	2528 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.5	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	0.95	EDS
Total number of atoms	4329	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: P1H

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	0.78	0/2044	1.05	5/2771 (0.2%)
1	B	1.09	5/2044 (0.2%)	1.15	12/2771 (0.4%)
All	All	0.95	5/4088 (0.1%)	1.10	17/5542 (0.3%)

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	B	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	PHE	CB-CG	20.31	1.97	1.50
1	B	41	PHE	CA-CB	-19.71	1.20	1.53
1	B	41	PHE	CA-C	-14.95	1.32	1.52
1	B	41	PHE	CD1-CE1	11.57	1.73	1.38
1	B	41	PHE	N-CA	6.38	1.54	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	PHE	CA-CB-CG	-14.41	99.39	113.80
1	B	41	PHE	CB-CG-CD1	-12.40	99.61	120.70
1	B	41	PHE	CB-CG-CD2	11.28	139.87	120.70
1	B	41	PHE	CB-CA-C	9.82	129.96	110.42
1	B	41	PHE	N-CA-CB	-8.04	96.91	110.49
1	A	105	THR	CB-CA-C	-7.50	99.10	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLY	CA-C-N	6.34	128.68	120.44
1	A	104	GLY	C-N-CA	6.34	128.68	120.44
1	B	211	ALA	N-CA-C	5.98	119.23	109.06
1	B	41	PHE	CA-C-N	-5.76	111.95	121.92
1	B	41	PHE	C-N-CA	-5.76	111.95	121.92
1	B	40	GLY	CA-C-N	5.72	132.46	121.54
1	B	40	GLY	C-N-CA	5.72	132.46	121.54
1	B	42	ASP	CB-CA-C	5.32	118.96	109.29
1	B	136	LEU	CA-CB-CG	-5.16	98.23	116.30
1	A	54	LEU	CA-C-N	5.07	125.35	119.47
1	A	54	LEU	C-N-CA	5.07	125.35	119.47

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	208	GLY	Peptide
1	B	210	GLU	Peptide
1	B	211	ALA	Peptide
1	B	41	PHE	Sidechain

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	2008	0	2018	55	0
1	B	2008	0	2018	124	0
2	A	55	0	36	3	0
2	B	55	0	36	9	0
3	A	124	0	0	12	0
3	B	79	0	0	9	0
All	All	4329	0	4108	177	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 22.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:PHE:CB	1:B:41:PHE:CG	1.97	1.48
1:A:136:LEU:H	1:A:136:LEU:CD1	1.42	1.30
1:A:136:LEU:HD12	1:A:136:LEU:N	1.53	1.20
1:B:202:ILE:CG2	1:B:203:VAL:HG12	1.75	1.16
1:B:45:ARG:HA	1:B:45:ARG:HE	1.07	1.12
1:B:202:ILE:HG22	1:B:203:VAL:HG12	1.08	1.07
1:B:203:VAL:HA	1:B:204:GLY:C	1.74	1.06
1:B:41:PHE:HA	1:B:41:PHE:CD1	1.94	1.02
1:B:64:ASP:H	1:B:70:HIS:CD2	1.80	0.99
1:B:203:VAL:HG23	1:B:207:PHE:O	1.63	0.98
1:B:202:ILE:HG22	1:B:203:VAL:CG1	1.95	0.97
1:B:45:ARG:HA	1:B:45:ARG:NE	1.79	0.96
1:A:64:ASP:H	1:A:70:HIS:HD2	0.99	0.96
1:B:203:VAL:O	1:B:215:MET:HE1	1.66	0.96
1:B:41:PHE:CG	1:B:41:PHE:CA	2.47	0.96
1:B:41:PHE:HA	1:B:41:PHE:HD1	1.30	0.95
1:A:77:ARG:O	1:A:81:GLU:HG2	1.69	0.93
1:B:203:VAL:HA	1:B:204:GLY:O	1.70	0.92
1:B:211:ALA:HB1	1:B:214:GLN:H	1.36	0.90
1:A:136:LEU:H	1:A:136:LEU:HD12	0.75	0.90
1:B:207:PHE:HB2	1:B:208:GLY:HA2	1.51	0.90
1:B:41:PHE:CG	1:B:42:ASP:N	2.40	0.89
1:B:64:ASP:H	1:B:70:HIS:HD2	0.89	0.87
1:A:64:ASP:H	1:A:70:HIS:CD2	1.92	0.84
1:B:49:ARG:HH11	1:B:49:ARG:HB3	1.42	0.84
1:A:254:THR:HG21	3:A:316:HOH:O	1.76	0.84
1:B:41:PHE:CD1	1:B:41:PHE:CA	2.60	0.84
1:B:41:PHE:CB	1:B:41:PHE:CD1	2.61	0.84
1:B:204:GLY:O	1:B:206:ALA:HA	1.78	0.83
1:B:2:ALA:HA	1:B:6:GLU:OE2	1.77	0.83
1:B:41:PHE:CZ	2:B:400:P1H:N3	2.47	0.83
1:B:64:ASP:N	1:B:70:HIS:HD2	1.73	0.83
1:B:215:MET:HE3	1:B:215:MET:HA	1.62	0.81
1:B:206:ALA:HB1	1:B:208:GLY:O	1.81	0.80
1:B:105:THR:OG1	1:B:106:ASN:N	2.12	0.80
1:B:101:THR:HG21	1:B:115:ASP:OD2	1.81	0.79
1:B:2:ALA:N	1:B:6:GLU:HB2	1.97	0.78
1:B:204:GLY:O	1:B:207:PHE:O	1.99	0.78
1:B:219:GLU:HA	1:B:232:MET:HE3	1.63	0.78
1:B:41:PHE:CE1	2:B:400:P1H:N4	2.53	0.77
1:A:265:SER:OG	3:A:413:HOH:O	2.03	0.75
1:B:206:ALA:HB1	1:B:207:PHE:HA	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ILE:H	2:B:400:P1H:HN72	1.34	0.74
1:B:103:MET:O	1:B:105:THR:N	2.21	0.72
1:B:211:ALA:HB3	1:B:214:GLN:HG2	1.71	0.72
1:B:114:GLU:H	1:B:114:GLU:CD	1.96	0.71
1:B:136:LEU:HD12	1:B:136:LEU:H	1.55	0.71
1:A:39:THR:CG2	3:A:319:HOH:O	2.37	0.71
1:A:95:ILE:CD1	1:A:122:ILE:HG23	2.21	0.70
1:A:61:ILE:HG23	1:A:77:ARG:NH1	2.07	0.69
1:A:186:SER:H	1:A:254:THR:HG23	1.58	0.68
1:B:218:LEU:HG	1:B:232:MET:HE1	1.76	0.68
1:B:73:THR:HA	1:B:76:GLU:HG3	1.76	0.67
1:B:201:ALA:O	1:B:205:GLY:O	2.14	0.65
1:A:150:ASP:OD1	1:A:152:THR:HG23	1.97	0.65
1:A:136:LEU:CD1	1:A:136:LEU:N	2.24	0.65
1:B:193:PRO:HG2	1:B:232:MET:HE2	1.78	0.65
1:B:3:GLY:O	1:B:4:LEU:HB2	1.95	0.64
1:B:207:PHE:CB	1:B:208:GLY:HA2	2.17	0.63
3:A:301:HOH:O	1:B:253:THR:HG22	1.98	0.63
1:B:132:LYS:O	1:B:136:LEU:HD11	1.99	0.63
1:A:186:SER:H	1:A:254:THR:CG2	2.12	0.62
1:A:21:ILE:HD11	1:A:25:ILE:HD11	1.82	0.62
1:B:45:ARG:HE	1:B:45:ARG:CA	1.98	0.62
1:A:80:ALA:HB1	3:A:407:HOH:O	1.99	0.62
1:B:45:ARG:NE	1:B:45:ARG:CA	2.58	0.62
1:B:41:PHE:CD1	2:B:400:P1H:N4	2.67	0.61
1:A:194:ILE:H	2:A:300:P1H:HN72	1.44	0.61
1:B:63:LEU:O	2:B:400:P1H:H9	2.01	0.61
1:A:39:THR:HG23	1:A:63:LEU:HB3	1.83	0.61
1:A:105:THR:HG23	3:A:359:HOH:O	2.00	0.60
1:A:132:LYS:O	1:A:136:LEU:HD11	2.00	0.60
1:B:41:PHE:CG	1:B:41:PHE:C	2.79	0.60
1:B:200:SER:O	1:B:201:ALA:CB	2.48	0.60
1:A:95:ILE:HD11	1:A:122:ILE:HG23	1.84	0.59
1:B:149:PHE:HB3	2:B:400:P1H:H20	1.83	0.59
1:A:114:GLU:CD	1:A:114:GLU:H	2.09	0.59
1:B:41:PHE:CD1	1:B:41:PHE:C	2.80	0.59
1:A:27:LYS:O	1:A:31:GLU:HG3	2.03	0.58
1:B:201:ALA:O	1:B:205:GLY:C	2.46	0.58
1:B:205:GLY:HA2	1:B:206:ALA:HB2	1.86	0.58
1:B:211:ALA:CB	1:B:214:GLN:H	2.15	0.57
1:B:49:ARG:HH11	1:B:49:ARG:CB	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:HG13	3:B:441:HOH:O	2.04	0.57
1:A:225:ARG:HD2	1:A:267:GLN:O	2.05	0.56
1:B:39:THR:HG23	1:B:63:LEU:HB3	1.88	0.56
1:B:200:SER:O	1:B:201:ALA:HB2	2.05	0.56
1:A:152:THR:HG22	3:A:313:HOH:O	2.05	0.55
1:A:39:THR:HG22	3:A:319:HOH:O	2.03	0.55
1:A:73:THR:HG23	3:A:420:HOH:O	2.05	0.55
2:A:300:P1H:H161	2:A:300:P1H:O8	2.07	0.55
1:A:107:GLN:NE2	1:A:109:PHE:H	2.05	0.55
1:A:134:LEU:O	1:A:138:MET:HG3	2.06	0.55
1:A:57:LYS:HE2	1:A:57:LYS:H	1.71	0.54
1:A:41:PHE:C	1:A:41:PHE:CD1	2.86	0.53
1:B:46:LEU:HD23	1:B:49:ARG:HH12	1.74	0.53
1:B:87:LYS:HD2	1:B:137:ILE:HA	1.90	0.53
1:B:206:ALA:HB1	1:B:208:GLY:C	2.33	0.53
1:B:211:ALA:HB1	1:B:214:GLN:N	2.17	0.53
1:B:136:LEU:H	1:B:136:LEU:CD1	2.17	0.53
1:A:105:THR:OG1	1:A:207:PHE:O	2.24	0.53
1:B:208:GLY:O	1:B:209:GLU:HB2	2.09	0.53
1:B:215:MET:HA	1:B:215:MET:CE	2.37	0.52
1:B:49:ARG:HB3	1:B:49:ARG:NH1	2.20	0.52
1:B:201:ALA:O	1:B:202:ILE:C	2.51	0.52
1:B:74:LEU:HD13	1:B:134:LEU:HD21	1.92	0.52
1:B:41:PHE:CZ	2:B:400:P1H:C8	2.93	0.52
1:B:99:PRO:HB2	1:B:101:THR:HG22	1.92	0.52
1:B:203:VAL:CA	1:B:204:GLY:C	2.66	0.51
1:A:95:ILE:CD1	1:A:122:ILE:CG2	2.87	0.51
1:A:121:HIS:HD2	3:A:403:HOH:O	1.93	0.51
1:B:56:ASP:OD1	1:B:57:LYS:HD2	2.10	0.50
1:B:46:LEU:O	1:B:50:ILE:HG12	2.10	0.50
1:B:197:LEU:O	1:B:200:SER:O	2.28	0.50
1:B:105:THR:HA	3:B:416:HOH:O	2.12	0.50
1:B:120:ILE:O	1:B:124:THR:HG23	2.12	0.50
1:B:193:PRO:O	1:B:232:MET:HG3	2.12	0.49
1:B:248:GLU:HB2	3:B:428:HOH:O	2.12	0.49
1:A:42:ASP:N	3:A:417:HOH:O	2.05	0.49
1:B:215:MET:HE3	1:B:215:MET:CA	2.39	0.49
1:B:202:ILE:HG23	1:B:203:VAL:HG12	1.84	0.48
1:B:211:ALA:CB	1:B:214:GLN:HG2	2.43	0.48
1:A:124:THR:CG2	1:A:171:VAL:HG21	2.43	0.48
1:A:161:MET:HE3	1:A:165:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:MET:CE	1:A:165:LYS:HE2	2.44	0.48
1:B:64:ASP:HB3	1:B:67:ASN:HB2	1.96	0.48
1:A:259:TYR:O	1:B:253:THR:HB	2.14	0.48
1:A:210:GLU:H	1:A:210:GLU:CD	2.22	0.48
1:B:258:ILE:HD12	1:B:258:ILE:N	2.28	0.48
1:B:149:PHE:HB3	2:B:400:P1H:C20	2.44	0.47
1:B:49:ARG:CB	1:B:49:ARG:NH1	2.77	0.47
1:B:67:ASN:OD1	1:B:69:GLU:HB2	2.14	0.47
1:B:202:ILE:HG22	1:B:203:VAL:N	2.30	0.47
1:A:193:PRO:HA	2:A:300:P1H:HN71	1.80	0.47
1:A:241:THR:HG23	1:B:250:LEU:HD23	1.96	0.47
1:B:206:ALA:CB	1:B:208:GLY:O	2.59	0.47
1:B:219:GLU:HA	1:B:232:MET:CE	2.41	0.47
1:A:39:THR:HG21	1:A:63:LEU:HD23	1.97	0.46
1:A:225:ARG:HH11	1:A:225:ARG:HG3	1.80	0.46
1:B:265:SER:OG	3:B:476:HOH:O	2.21	0.46
1:B:193:PRO:HA	2:B:400:P1H:HN71	1.79	0.46
1:A:93:HIS:HD2	1:A:130:LEU:HD13	1.81	0.46
1:B:73:THR:HG22	1:B:76:GLU:OE1	2.15	0.46
1:B:100:GLN:O	1:B:105:THR:HG23	2.15	0.46
1:A:250:LEU:HD12	1:B:241:THR:HG23	1.96	0.46
1:B:209:GLU:HB3	3:B:444:HOH:O	2.16	0.45
1:B:65:VAL:HG11	1:B:126:SER:CB	2.47	0.45
1:B:209:GLU:O	1:B:210:GLU:C	2.60	0.45
1:A:27:LYS:HB3	1:A:27:LYS:HE3	1.78	0.44
1:B:41:PHE:O	1:B:44:LEU:CD2	2.65	0.44
1:B:107:GLN:HB3	3:B:419:HOH:O	2.17	0.44
3:A:301:HOH:O	1:B:253:THR:CG2	2.60	0.44
1:B:150:ASP:OD1	1:B:152:THR:HG23	2.18	0.44
1:A:84:GLU:OE1	1:A:85:GLY:N	2.47	0.43
1:B:218:LEU:HG	1:B:232:MET:CE	2.47	0.43
1:B:25:ILE:CD1	1:B:239:ALA:HA	2.48	0.43
1:B:211:ALA:HB3	1:B:214:GLN:CG	2.44	0.43
1:B:199:MET:HA	1:B:199:MET:HE2	2.01	0.43
1:B:219:GLU:CA	1:B:232:MET:HE3	2.41	0.43
1:A:103:MET:HE3	1:A:158:TYR:HA	2.02	0.42
1:B:152:THR:HG22	3:B:421:HOH:O	2.19	0.42
1:B:207:PHE:HB3	3:B:416:HOH:O	2.20	0.42
1:B:41:PHE:O	1:B:44:LEU:HD21	2.20	0.42
1:B:65:VAL:CG1	1:B:126:SER:CB	2.97	0.42
1:B:45:ARG:HG3	3:B:451:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:THR:HG21	1:B:260:ALA:HB2	2.01	0.41
1:B:134:LEU:O	1:B:138:MET:HG3	2.21	0.41
1:A:145:VAL:HA	1:A:187:ASN:O	2.21	0.41
1:B:101:THR:HG21	1:B:115:ASP:CG	2.44	0.41
1:A:194:ILE:HD11	1:A:238:VAL:HG21	2.03	0.41
1:A:61:ILE:CG2	1:A:77:ARG:NH1	2.78	0.41
1:A:95:ILE:HD12	1:A:122:ILE:CG2	2.51	0.41
1:B:24:HIS:CD2	1:B:235:PRO:HG3	2.55	0.41
1:B:216:GLN:O	1:B:220:GLU:HG2	2.20	0.41
1:B:46:LEU:O	1:B:46:LEU:HD22	2.21	0.40
1:A:66:GLN:HE22	1:A:118:LYS:HE3	1.85	0.40
1:B:245:LEU:HD11	1:B:258:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	266/268 (99%)	258 (97%)	8 (3%)	0	100	100
1	B	266/268 (99%)	242 (91%)	16 (6%)	8 (3%)	3	1
All	All	532/536 (99%)	500 (94%)	24 (4%)	8 (2%)	8	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	GLY
1	B	105	THR
1	B	201	ALA
1	B	203	VAL
1	B	4	LEU
1	B	41	PHE

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Mol	Chain	Res	Type
1	B	204	GLY
1	B	209	GLU

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	207/207 (100%)	180 (87%)	27 (13%)	4	2
1	B	207/207 (100%)	175 (84%)	32 (16%)	2	1
All	All	414/414 (100%)	355 (86%)	59 (14%)	3	1

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	LEU
1	A	6	GLU
1	A	21	ILE
1	A	39	THR
1	A	46	LEU
1	A	48	GLN
1	A	53	ARG
1	A	57	LYS
1	A	65	VAL
1	A	74	LEU
1	A	84	GLU
1	A	95	ILE
1	A	105	THR
1	A	107	GLN
1	A	114	GLU
1	A	130	LEU
1	A	135	LEU
1	A	136	LEU
1	A	140	SER
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	194	ILE
1	A	197	LEU
1	A	248	GLU
1	A	250	LEU
1	A	254	THR
1	A	256	SER
1	B	4	LEU
1	B	5	LEU
1	B	6	GLU
1	B	39	THR
1	B	42	ASP
1	B	45	ARG
1	B	46	LEU
1	B	47	ILE
1	B	49	ARG
1	B	57	LYS
1	B	65	VAL
1	B	74	LEU
1	B	76	GLU
1	B	105	THR
1	B	114	GLU
1	B	124	THR
1	B	135	LEU
1	B	136	LEU
1	B	140	SER
1	B	145	VAL
1	B	155	MET
1	B	168	LEU
1	B	188	LEU
1	B	202	ILE
1	B	207	PHE
1	B	210	GLU
1	B	215	MET
1	B	228	ILE
1	B	240	LYS
1	B	248	GLU
1	B	253	THR
1	B	256	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	70	HIS
1	A	100	GLN
1	A	107	GLN
1	A	121	HIS
1	A	216	GLN
1	B	24	HIS
1	B	66	GLN
1	B	70	HIS
1	B	121	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	P1H	B	400	-	57,60,60	4.91	23 (40%)	76,90,90	3.70	30 (39%)
2	P1H	A	300	-	57,60,60	4.50	25 (43%)	76,90,90	3.09	21 (27%)

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	P1H	B	400	-	-	7/40/86/86	0/6/6/6
2	P1H	A	300	-	-	5/40/86/86	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	P1H	O15-C22	15.57	1.42	1.22
2	A	300	P1H	O15-C22	15.04	1.42	1.22
2	B	400	P1H	C7-C10	12.75	1.61	1.39
2	A	300	P1H	C16-C17	12.64	1.53	1.35
2	B	400	P1H	C16-C17	12.04	1.52	1.35
2	B	400	P1H	C24-C25	8.78	1.52	1.39
2	B	400	P1H	C21-C20	8.68	1.51	1.33
2	A	300	P1H	C21-C20	8.58	1.51	1.33
2	A	300	P1H	C24-C25	8.58	1.52	1.39
2	B	400	P1H	C26-C25	8.58	1.52	1.39
2	B	400	P1H	C26-C27	8.50	1.53	1.38
2	B	400	P1H	C8-N4	8.42	1.59	1.35
2	A	300	P1H	O14-C18	8.21	1.43	1.24
2	A	300	P1H	C26-C25	7.84	1.51	1.39
2	B	400	P1H	C9-N4	7.79	1.47	1.33
2	A	300	P1H	C26-C27	7.75	1.51	1.38
2	B	400	P1H	C6-N2	7.58	1.46	1.31
2	A	300	P1H	C6-N2	7.54	1.46	1.31
2	A	300	P1H	C9-N4	7.31	1.46	1.33
2	B	400	P1H	O14-C18	7.22	1.41	1.24
2	A	300	P1H	C9-N5	6.94	1.46	1.33
2	B	400	P1H	C6-N1	6.91	1.49	1.37
2	B	400	P1H	C24-C23	6.34	1.50	1.38
2	A	300	P1H	C6-N1	6.27	1.48	1.37
2	A	300	P1H	C24-C23	5.91	1.50	1.38
2	B	400	P1H	C10-N1	5.68	1.49	1.37
2	B	400	P1H	C27-N8	5.68	1.46	1.34
2	B	400	P1H	C23-N8	5.33	1.45	1.34
2	B	400	P1H	C8-N3	5.28	1.47	1.34
2	A	300	P1H	C27-N8	5.27	1.45	1.34
2	A	300	P1H	C7-C10	5.19	1.48	1.39
2	A	300	P1H	C10-N5	4.54	1.42	1.34
2	A	300	P1H	C18-N7	4.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	P1H	C23-N8	4.06	1.43	1.34
2	B	400	P1H	C10-N5	3.95	1.41	1.34
2	A	300	P1H	C8-N3	3.69	1.43	1.34
2	B	400	P1H	C21-N6	3.58	1.46	1.37
2	A	300	P1H	C21-N6	3.55	1.45	1.37
2	A	300	P1H	C7-N2	3.50	1.45	1.39
2	A	300	P1H	C8-N4	3.25	1.44	1.35
2	A	300	P1H	C7-C8	3.25	1.50	1.41
2	B	400	P1H	P2-O7	3.04	1.62	1.59
2	B	400	P1H	C18-N7	3.00	1.42	1.33
2	A	300	P1H	P1-O7	2.96	1.62	1.59
2	B	400	P1H	P1-O7	2.81	1.62	1.59
2	B	400	P1H	C25-C22	2.79	1.53	1.49
2	A	300	P1H	C10-N1	2.57	1.43	1.37
2	A	300	P1H	P2-O7	2.28	1.62	1.59

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	P1H	N4-C9-N5	-16.05	104.28	128.58
2	A	300	P1H	C21-N6-C16	11.13	131.24	119.32
2	A	300	P1H	C17-C16-N6	-11.00	110.69	122.84
2	B	400	P1H	C21-N6-C16	10.17	130.20	119.32
2	B	400	P1H	C17-C16-N6	-9.67	112.16	122.84
2	A	300	P1H	N4-C9-N5	-9.11	114.80	128.58
2	A	300	P1H	C25-C26-C27	-8.65	111.32	119.93
2	B	400	P1H	O4-C5-N1	8.10	123.64	108.09
2	B	400	P1H	C4-C5-N1	-7.77	94.00	113.30
2	B	400	P1H	C23-N8-C27	7.52	127.96	117.41
2	A	300	P1H	N1-C6-N2	-6.24	105.09	113.94
2	A	300	P1H	C24-C23-N8	-6.23	116.33	123.97
2	B	400	P1H	C9-N5-C10	6.22	127.02	111.83
2	A	300	P1H	C23-N8-C27	6.19	126.09	117.41
2	B	400	P1H	C8-C7-C10	-5.91	109.11	117.18
2	B	400	P1H	N1-C6-N2	-5.80	105.71	113.94
2	A	300	P1H	C10-N1-C6	5.51	111.52	105.74
2	B	400	P1H	C15-N6-C21	-4.84	110.54	120.77
2	B	400	P1H	C24-C23-N8	-4.83	118.05	123.97
2	A	300	P1H	C24-C25-C26	4.59	124.56	119.25
2	B	400	P1H	C7-N2-C6	4.58	110.66	103.45
2	B	400	P1H	C29-C27-C26	-4.45	115.21	121.65
2	A	300	P1H	C9-N4-C8	4.43	126.01	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	P1H	C10-N1-C6	4.29	110.24	105.74
2	A	300	P1H	C15-N6-C21	-4.25	111.78	120.77
2	B	400	P1H	C7-C10-N1	-4.18	101.25	105.81
2	B	400	P1H	C24-C25-C26	4.00	123.87	119.25
2	B	400	P1H	C26-C27-N8	-3.95	116.19	122.01
2	B	400	P1H	O15-C22-C25	-3.79	115.99	120.70
2	B	400	P1H	C7-C8-N4	-3.72	108.06	117.51
2	B	400	P1H	C7-C8-N3	-3.53	114.55	123.29
2	A	300	P1H	C8-C7-C10	-3.34	112.62	117.18
2	B	400	P1H	C25-C26-C27	-3.14	116.80	119.93
2	A	300	P1H	O15-C22-C25	-3.08	116.87	120.70
2	A	300	P1H	O4-C5-N1	2.99	113.83	108.09
2	A	300	P1H	C9-N5-C10	2.95	119.04	111.83
2	A	300	P1H	C29-C27-C26	-2.95	117.38	121.65
2	B	400	P1H	C23-C24-C25	-2.93	115.84	119.05
2	B	400	P1H	O11-C15-N6	2.78	113.38	108.08
2	B	400	P1H	C5-N1-C6	-2.61	121.31	127.09
2	A	300	P1H	O11-C15-C14	-2.57	101.12	106.62
2	A	300	P1H	C15-N6-C16	-2.56	116.93	121.14
2	A	300	P1H	C7-N2-C6	2.54	107.45	103.45
2	B	400	P1H	C25-C22-C19	2.44	121.83	118.83
2	B	400	P1H	O13-C14-C15	2.40	118.37	110.10
2	B	400	P1H	C19-C17-C16	2.25	124.65	121.86
2	B	400	P1H	C9-N4-C8	2.16	122.29	118.73
2	A	300	P1H	C2-O4-C5	-2.12	104.78	109.47
2	B	400	P1H	C10-C7-N2	-2.11	108.17	110.58
2	A	300	P1H	C7-C8-N3	-2.05	118.20	123.29
2	B	400	P1H	C7-C10-N5	-2.03	123.92	126.72

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	P1H	C11-O10-P2-O8
2	A	300	P1H	C11-O10-P2-O7
2	B	400	P1H	C11-O10-P2-O9
2	B	400	P1H	C11-O10-P2-O7
2	B	400	P1H	C30-C28-C29-C27
2	A	300	P1H	C30-C28-C29-C27
2	A	300	P1H	O11-C15-N6-C21
2	B	400	P1H	O11-C15-N6-C21
2	B	400	P1H	C11-O10-P2-O8

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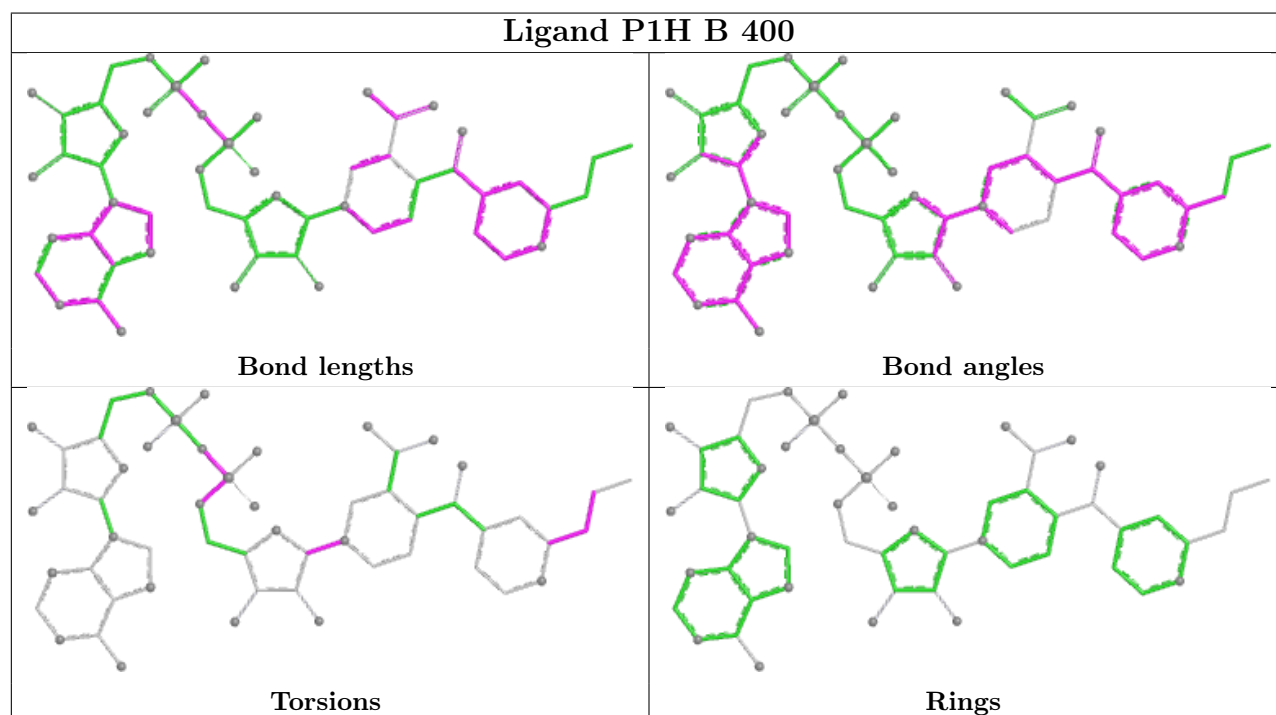
Mol	Chain	Res	Type	Atoms
2	A	300	P1H	C26-C27-C29-C28
2	B	400	P1H	N8-C27-C29-C28
2	B	400	P1H	P1-O7-P2-O8

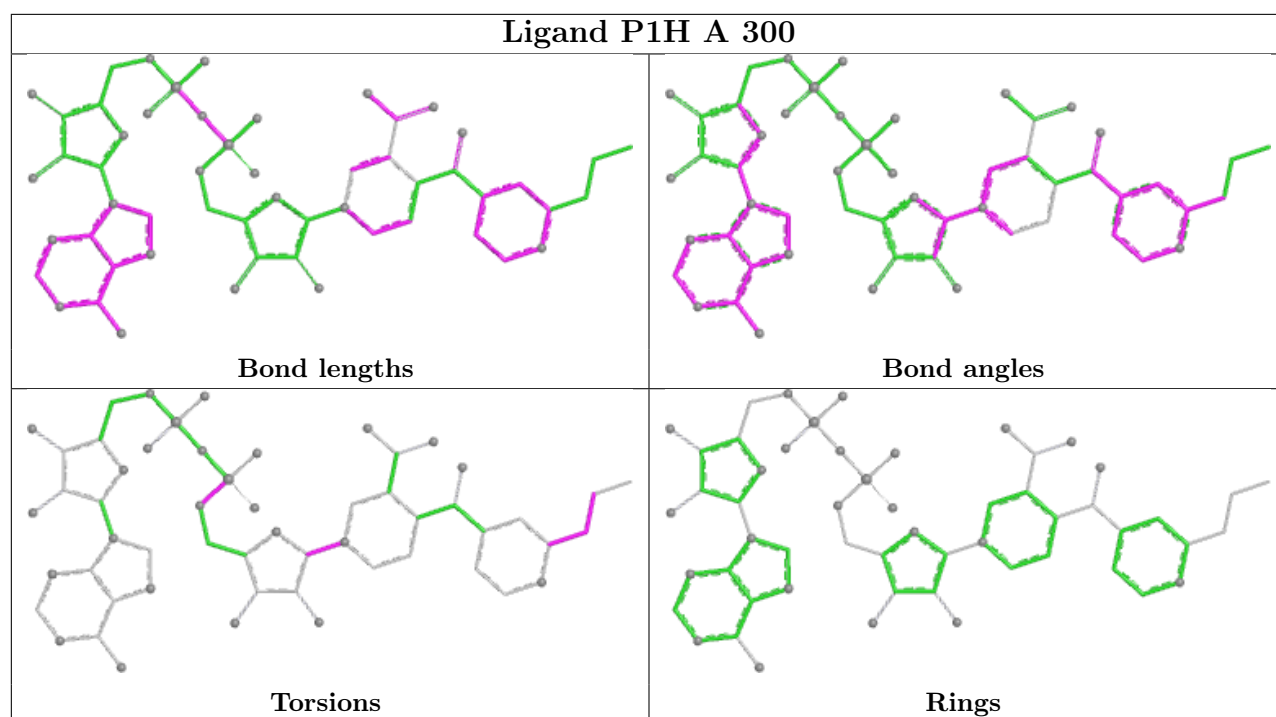
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	P1H	9	0
2	A	300	P1H	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	268/268 (100%)	0.07	13 (4%) 35 37	25, 35, 48, 57	0
1	B	268/268 (100%)	0.71	38 (14%) 6 6	27, 42, 66, 78	0
All	All	536/536 (100%)	0.39	51 (9%) 14 14	25, 37, 63, 78	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	203	VAL	8.1
1	B	207	PHE	6.8
1	B	41	PHE	6.2
1	B	201	ALA	5.7
1	B	105	THR	4.9
1	B	49	ARG	4.7
1	B	124	THR	4.2
1	B	3	GLY	4.2
1	A	105	THR	3.9
1	B	56	ASP	3.8
1	A	2	ALA	3.7
1	A	215	MET	3.7
1	B	47	ILE	3.7
1	B	205	GLY	3.6
1	B	211	ALA	3.5
1	B	208	GLY	3.5
1	A	81	GLU	3.4
1	A	107	GLN	3.4
1	A	76	GLU	3.4
1	B	51	ALA	3.4
1	B	204	GLY	3.3
1	B	76	GLU	3.3
1	A	56	ASP	3.3
1	B	202	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	45	ARG	3.2
1	B	81	GLU	3.1
1	A	207	PHE	3.0
1	B	206	ALA	3.0
1	B	212	GLY	2.9
1	A	53	ARG	2.9
1	B	215	MET	2.8
1	A	124	THR	2.8
1	B	200	SER	2.8
1	B	60	LEU	2.8
1	B	2	ALA	2.7
1	B	35	GLN	2.7
1	B	61	ILE	2.7
1	B	130	LEU	2.6
1	B	84	GLU	2.5
1	B	210	GLU	2.5
1	A	235	PRO	2.5
1	B	103	MET	2.4
1	A	41	PHE	2.3
1	B	114	GLU	2.2
1	B	107	GLN	2.2
1	B	55	PRO	2.2
1	B	209	GLU	2.2
1	A	51	ALA	2.1
1	B	199	MET	2.1
1	B	65	VAL	2.1
1	B	104	GLY	2.1

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,

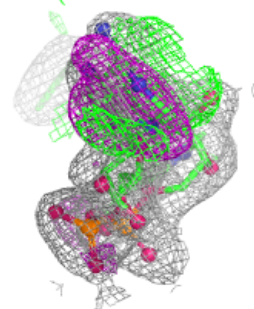
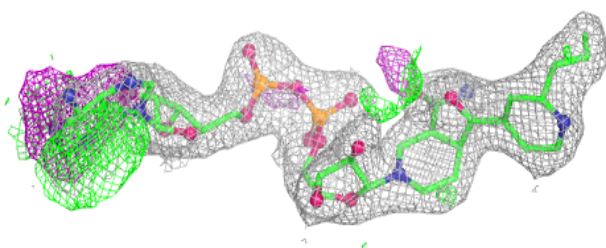
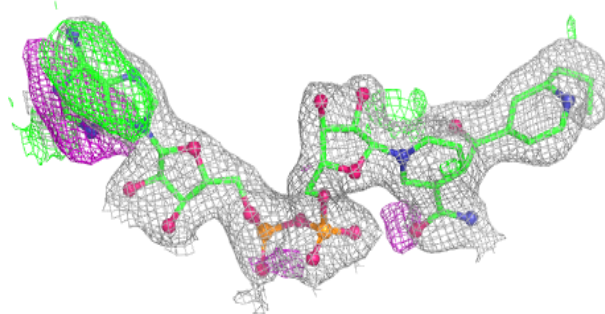
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

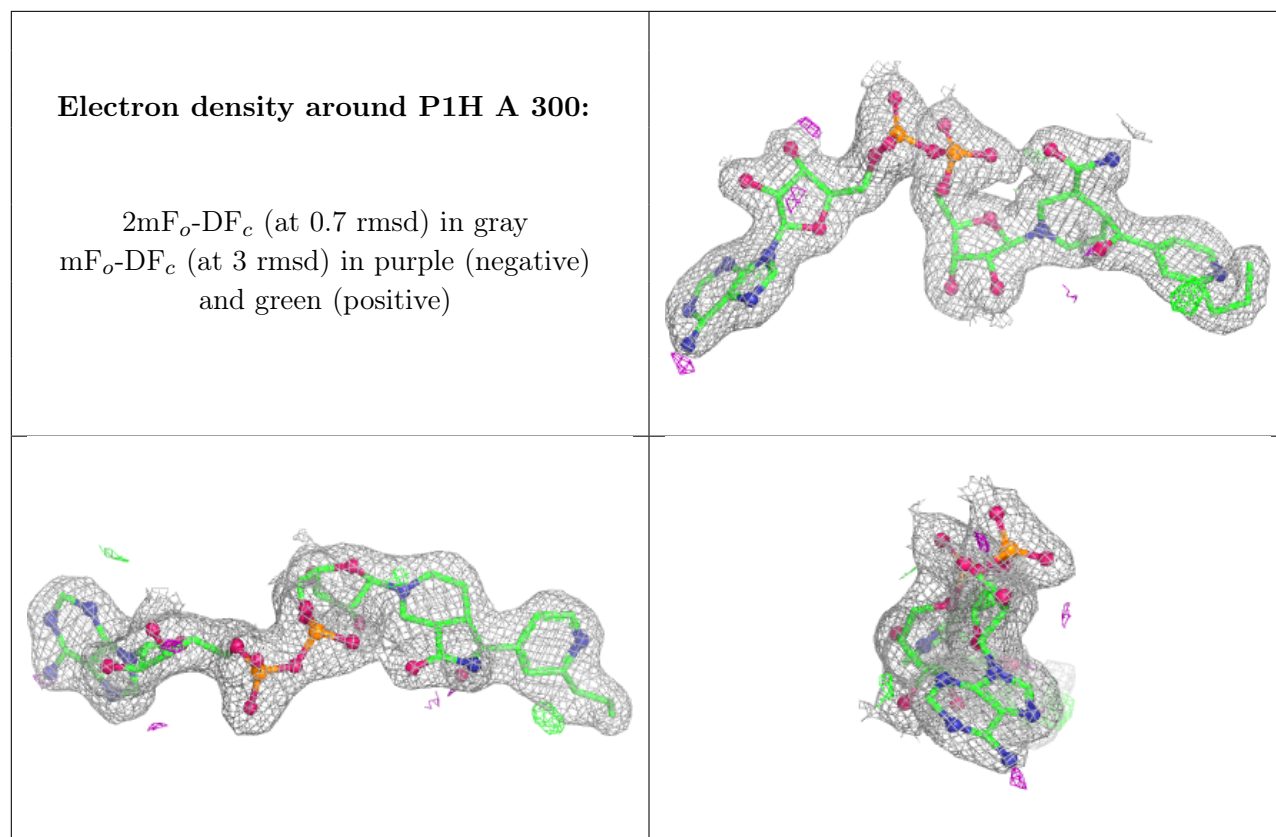
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	P1H	B	400	55/55	0.82	0.13	31,37,44,46	0
2	P1H	A	300	55/55	0.96	0.06	26,30,34,35	0

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 P1H B 400:

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.