



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:01 AM UTC

PDB ID : 1DAP / pdb_00001dap
Title : C. GLUTAMICUM DAP DEHYDROGENASE IN COMPLEX WITH NADP+
Authors : Scapin, G.; Reddy, S.G.; Blanchard, J.S.
Deposited on : 1996-07-08
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

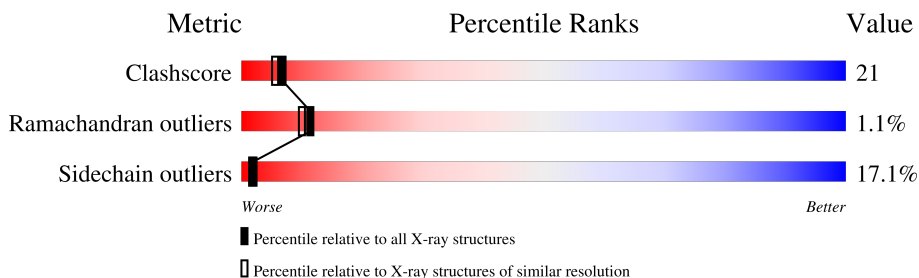
1 Overall quality at a glance

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	320	 60% 30% 10%
1	B	320	 49% 38% 11% .

2 Entry composition [i](#)

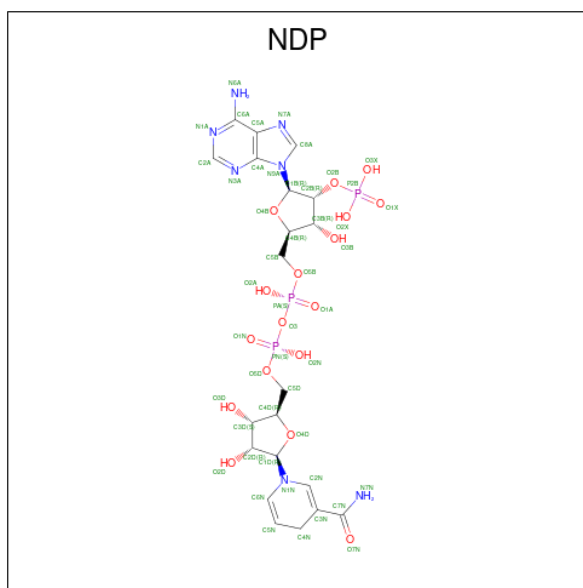
There are 4 unique types of molecules in this entry. The entry contains 5214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIAMINOPIMELIC ACID DEHYDROGENASE.

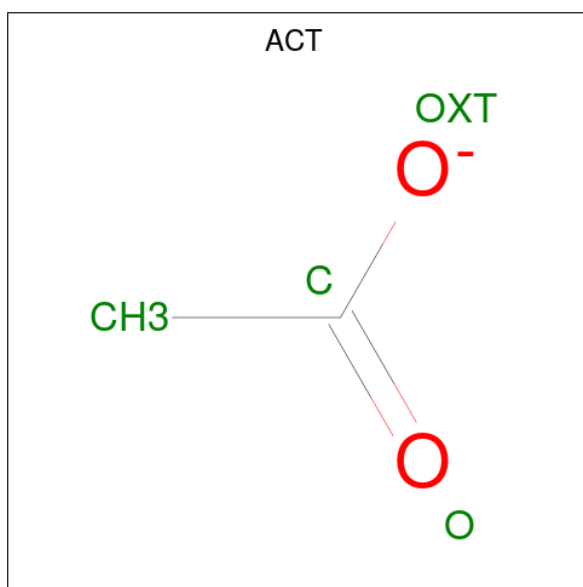
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2467	1538	441	478	10			
1	B	320	Total	C	N	O	S	0	0	0
			2460	1535	441	474	10			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is water.

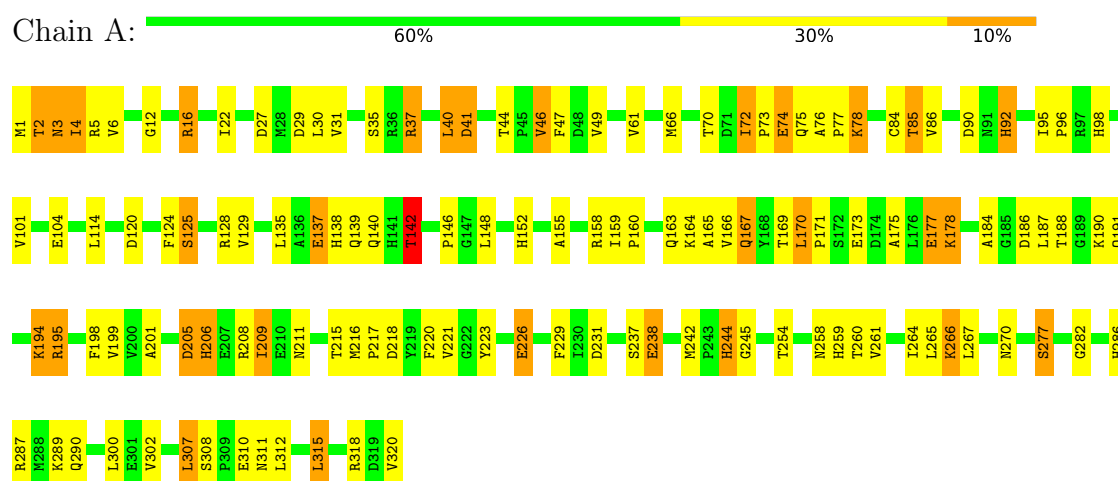
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		
4	B	91	Total	O	0	0
			91	91		

3 Residue-property plots [i](#)

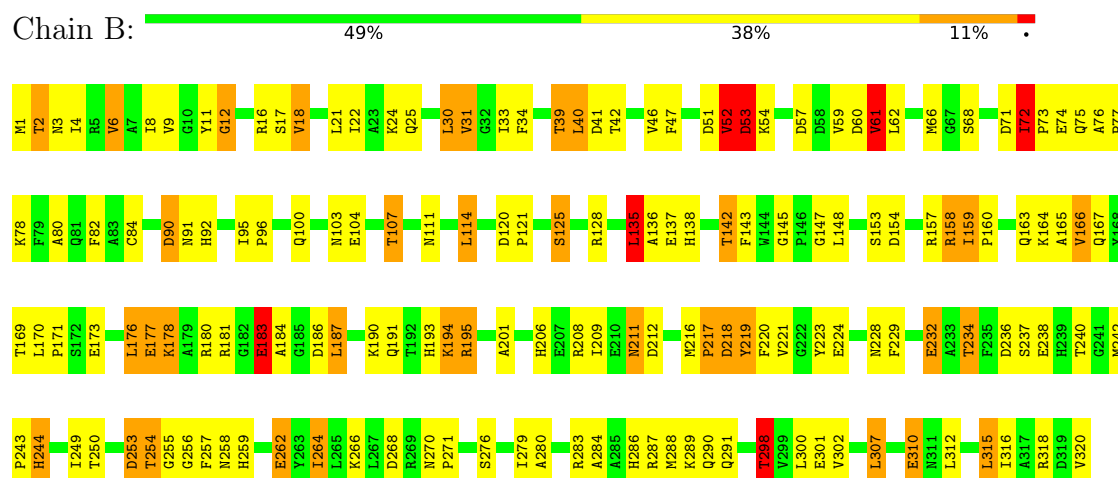
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: DIAMINOPIMELIC ACID DEHYDROGENASE



• Molecule 1: DIAMINOPIMELIC ACID DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.90Å 65.80Å 84.50Å 90.00° 106.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.0 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5214	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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: NDP, ACT

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	1.15	6/2520 (0.2%)	1.34	16/3422 (0.5%)
1	B	1.25	4/2513 (0.2%)	1.42	20/3415 (0.6%)
All	All	1.21	10/5033 (0.2%)	1.38	36/6837 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	ILE	CA-CB	16.48	1.62	1.54
1	B	61	VAL	CA-CB	6.40	1.62	1.55
1	A	264	ILE	CA-CB	-5.93	1.47	1.54
1	B	9	VAL	CA-CB	5.50	1.61	1.54
1	A	175	ALA	CA-C	5.35	1.59	1.52
1	A	261	VAL	CA-CB	-5.23	1.47	1.54
1	A	277	SER	CA-C	-5.18	1.46	1.52
1	A	142	THR	CA-CB	5.07	1.60	1.53
1	B	33	ILE	CA-CB	-5.06	1.47	1.54
1	A	46	VAL	CA-C	-5.05	1.46	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	GLY	C-N-CD	-8.35	102.23	120.60
1	A	238	GLU	N-CA-C	7.79	123.73	113.30
1	B	254	THR	N-CA-C	-7.59	98.32	109.63
1	A	206	HIS	N-CA-C	7.58	120.21	111.11
1	B	219	TYR	N-CA-C	-7.02	104.85	113.41
1	B	12	GLY	N-CA-C	-6.78	102.79	112.55
1	A	84	CYS	N-CA-C	-6.73	101.64	110.53
1	B	52	VAL	CB-CA-C	-6.64	103.38	111.88
1	B	183	GLU	N-CA-C	6.63	118.63	109.54
1	B	165	ALA	N-CA-C	6.45	118.95	108.76
1	B	135	LEU	N-CA-C	6.37	119.92	107.57
1	B	90	ASP	N-CA-C	6.29	121.72	113.30
1	B	318	ARG	N-CA-C	6.01	120.80	112.45
1	A	205	ASP	N-CA-C	5.83	120.39	113.28
1	A	137	GLU	N-CA-C	-5.83	99.69	109.07
1	A	74	GLU	N-CA-C	5.72	120.40	112.45
1	B	279	ILE	N-CA-C	5.69	115.88	110.42
1	A	92	HIS	N-CA-C	5.68	118.21	111.33
1	B	217	PRO	O-C-N	5.66	129.75	122.85
1	B	82	PHE	N-CA-C	5.58	120.24	113.38
1	B	61	VAL	O-C-N	5.42	128.40	123.19
1	A	90	ASP	N-CA-C	5.41	119.57	112.92
1	A	5	ARG	NE-CZ-NH2	5.37	124.04	119.20
1	A	142	THR	CB-CA-C	5.36	118.98	110.19
1	B	298	THR	N-CA-CB	-5.31	102.35	110.42
1	A	261	VAL	CB-CA-C	-5.29	103.26	110.77
1	A	140	GLN	N-CA-C	5.23	117.97	109.24
1	B	54	LYS	N-CA-C	5.21	119.48	113.18
1	A	124	PHE	N-CA-C	-5.15	105.84	111.82
1	B	159	ILE	CA-C-O	5.12	122.17	119.15
1	B	21	LEU	N-CA-C	5.07	118.72	112.54
1	A	165	ALA	N-CA-C	5.05	116.52	108.79
1	A	16	ARG	CA-C-N	5.04	127.44	120.29
1	A	16	ARG	C-N-CA	5.04	127.44	120.29
1	B	209	ILE	N-CA-C	-5.01	105.54	111.00
1	B	53	ASP	N-CA-CB	-5.00	102.04	110.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	SER	Mainchain
1	B	52	VAL	Mainchain

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	2467	0	2364	95	5
1	B	2460	0	2354	121	7
2	A	48	0	26	2	0
2	B	48	0	26	0	0
3	B	8	0	6	1	0
4	A	92	0	0	7	0
4	B	91	0	0	6	1
All	All	5214	0	4776	210	7

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 21.

All (210) 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:167:GLN:HE21	1:B:195:ARG:HG3	1.08	1.09
1:B:194:LYS:HE3	1:B:224:GLU:HG2	1.37	1.05
1:A:3:ASN:ND2	1:A:29:ASP:OD1	1.92	1.03
1:B:167:GLN:NE2	1:B:195:ARG:HG3	1.80	0.96
1:A:152:HIS:HB3	1:A:167:GLN:HG2	1.51	0.93
1:A:1:MET:O	1:A:3:ASN:N	2.09	0.85
1:A:265:LEU:O	1:A:266:LYS:HD3	1.76	0.85
1:A:6:VAL:HG21	1:A:22:ILE:HD13	1.60	0.82
1:A:12:GLY:O	1:A:16:ARG:HG3	1.81	0.80
1:A:128:ARG:HE	1:A:142:THR:HG21	1.47	0.79
1:B:53:ASP:HB2	4:B:472:HOH:O	1.83	0.77
1:B:169:THR:C	1:B:170:LEU:HD12	2.10	0.77
1:B:148:LEU:HD21	1:B:166:VAL:HG22	1.64	0.76
1:B:104:GLU:HG3	4:B:482:HOH:O	1.83	0.76
1:B:148:LEU:HD21	1:B:166:VAL:CG2	2.15	0.76
1:A:186:ASP:O	1:A:187:LEU:HD23	1.86	0.75
1:B:12:GLY:O	1:B:16:ARG:HG3	1.86	0.75
1:A:205:ASP:O	1:A:209:ILE:HG13	1.87	0.75
1:A:265:LEU:C	1:A:266:LYS:HD3	2.13	0.74
1:A:85:THR:HG23	4:A:405:HOH:O	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:HE3	1:B:224:GLU:CG	2.16	0.73
1:A:201:ALA:O	1:A:206:HIS:HE1	1.71	0.73
1:B:170:LEU:HD12	1:B:170:LEU:N	2.03	0.73
1:A:78:LYS:HB2	1:A:78:LYS:NZ	2.04	0.72
1:A:290:GLN:HA	1:A:290:GLN:OE1	1.89	0.72
1:A:216:MET:O	1:A:221:VAL:HG23	1.90	0.72
1:B:181:ARG:O	1:B:183:GLU:HG2	1.90	0.71
1:A:41:ASP:HB2	4:A:461:HOH:O	1.89	0.71
1:A:72:ILE:HG22	1:A:73:PRO:HD3	1.72	0.69
1:B:178:LYS:HB2	1:B:184:ALA:HB2	1.74	0.69
1:A:6:VAL:HG21	1:A:22:ILE:CD1	2.22	0.69
1:B:68:SER:CB	1:B:90:ASP:OD1	2.41	0.68
1:B:254:THR:O	1:B:256:GLY:N	2.26	0.68
1:A:155:ALA:O	1:A:158:ARG:HG2	1.92	0.68
1:A:3:ASN:HD22	1:A:29:ASP:CG	2.02	0.68
1:A:178:LYS:HG2	1:A:184:ALA:HB2	1.75	0.67
1:A:173:GLU:HG2	1:A:177:GLU:OE2	1.95	0.67
1:A:160:PRO:O	1:A:208:ARG:NH1	2.27	0.67
1:A:216:MET:C	1:A:221:VAL:HG23	2.20	0.67
1:B:298:THR:HG23	1:B:300:LEU:H	1.61	0.65
1:A:167:GLN:OE1	1:A:195:ARG:HB3	1.96	0.65
1:A:307:LEU:HD23	1:A:307:LEU:N	2.11	0.65
1:B:298:THR:HB	1:B:301:GLU:OE2	1.97	0.65
1:B:310:GLU:HB2	1:B:315:LEU:HD13	1.77	0.65
1:B:74:GLU:N	1:B:74:GLU:OE1	2.28	0.64
1:B:76:ALA:HB3	1:B:77:PRO:HD3	1.79	0.64
1:A:37:ARG:HD3	2:A:400:NDP:O1X	1.97	0.64
1:A:85:THR:CG2	4:A:405:HOH:O	2.44	0.63
1:A:159:ILE:HG23	1:A:160:PRO:HD2	1.80	0.63
1:B:310:GLU:HB2	1:B:315:LEU:CD1	2.29	0.61
1:B:6:VAL:HG11	1:B:22:ILE:HD13	1.81	0.61
1:B:75:GLN:O	1:B:78:LYS:HG2	2.01	0.61
1:B:164:LYS:NZ	1:B:232:GLU:OE2	2.25	0.61
1:B:181:ARG:NH1	1:B:183:GLU:OE2	2.30	0.60
1:B:163:GLN:NE2	1:B:201:ALA:HA	2.15	0.60
1:A:254:THR:OG1	1:A:259:HIS:HE1	1.85	0.60
1:A:37:ARG:HG3	1:A:40:LEU:HD11	1.83	0.59
1:B:208:ARG:HG2	4:B:459:HOH:O	2.03	0.59
1:B:211:ASN:OD1	1:B:212:ASP:N	2.35	0.59
1:A:152:HIS:CB	1:A:167:GLN:HG2	2.29	0.58
1:B:25:GLN:HE21	1:B:283:ARG:HH22	1.50	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:VAL:HG11	1:B:22:ILE:CD1	2.33	0.58
1:A:27:ASP:OD1	1:A:27:ASP:N	2.36	0.58
1:A:72:ILE:CD1	4:A:458:HOH:O	2.52	0.57
1:B:217:PRO:O	1:B:219:TYR:N	2.37	0.57
1:A:187:LEU:HD22	1:A:191:GLN:OE1	2.04	0.57
1:A:320:VAL:HA	1:B:125:SER:HB3	1.86	0.57
1:B:286:HIS:O	1:B:290:GLN:HG2	2.05	0.57
1:A:92:HIS:HE1	4:A:466:HOH:O	1.88	0.57
1:B:114:LEU:HD21	1:B:288:MET:CE	2.35	0.57
1:B:136:ALA:HA	4:B:486:HOH:O	2.05	0.56
1:A:270:ASN:HD22	1:A:270:ASN:C	2.13	0.56
1:B:114:LEU:HD21	1:B:288:MET:HE1	1.87	0.56
1:A:75:GLN:O	1:A:78:LYS:HG3	2.05	0.56
1:A:137:GLU:CD	1:B:24:LYS:HE2	2.31	0.56
1:B:253:ASP:HB2	1:B:258:ASN:ND2	2.21	0.56
1:B:61:VAL:HB	1:B:84:CYS:HB2	1.87	0.55
1:B:280:ALA:HB1	1:B:307:LEU:HB3	1.87	0.55
1:A:188:THR:OG1	1:A:191:GLN:NE2	2.39	0.55
1:B:148:LEU:CD2	1:B:166:VAL:HG22	2.34	0.55
1:B:307:LEU:N	1:B:307:LEU:HD23	2.22	0.55
1:A:166:VAL:HG12	1:A:198:PHE:HB2	1.89	0.55
1:A:216:MET:HB3	1:A:220:PHE:HB2	1.89	0.55
1:B:143:PHE:HA	1:B:193:HIS:CE1	2.42	0.54
1:A:310:GLU:HA	1:A:310:GLU:OE1	2.06	0.54
1:B:25:GLN:NE2	1:B:283:ARG:HH22	2.05	0.54
1:A:4:ILE:HG12	1:A:286:HIS:CD2	2.43	0.54
1:B:142:THR:HG23	4:B:488:HOH:O	2.08	0.54
1:A:190:LYS:HA	1:A:223:TYR:CE1	2.43	0.54
1:A:215:THR:O	1:A:217:PRO:HD3	2.07	0.54
1:A:217:PRO:O	1:A:218:ASP:HB2	2.08	0.54
1:B:120:ASP:CG	1:B:128:ARG:HH22	2.15	0.54
1:B:211:ASN:OD1	1:B:212:ASP:OD1	2.26	0.54
1:A:169:THR:C	1:A:170:LEU:HD23	2.33	0.53
1:B:164:LYS:HE2	1:B:236:ASP:OD1	2.08	0.53
1:A:125:SER:HB3	1:B:320:VAL:HA	1.90	0.53
1:A:78:LYS:HB2	1:A:78:LYS:HZ2	1.71	0.53
1:B:194:LYS:HD2	1:B:224:GLU:HB3	1.90	0.53
1:B:92:HIS:HA	1:B:95:ILE:HD12	1.91	0.53
1:B:217:PRO:C	1:B:219:TYR:H	2.17	0.52
1:B:135:LEU:HD13	1:B:138:HIS:HB3	1.90	0.52
1:B:194:LYS:CE	1:B:224:GLU:HG2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:HD2	1:B:320:VAL:O	1.91	0.52
1:A:287:ARG:NH2	1:A:308:SER:O	2.41	0.52
1:B:181:ARG:HH12	1:B:183:GLU:CD	2.18	0.52
1:B:216:MET:HG2	1:B:217:PRO:HD2	1.91	0.52
1:A:104:GLU:HG3	4:A:454:HOH:O	2.10	0.52
1:A:72:ILE:N	1:A:73:PRO:HD2	2.25	0.51
1:B:167:GLN:HE21	1:B:195:ARG:CG	2.00	0.51
1:B:254:THR:OG1	1:B:259:HIS:HE1	1.93	0.51
1:A:1:MET:O	1:A:2:THR:C	2.52	0.51
1:B:1:MET:N	1:B:2:THR:CB	2.73	0.51
1:B:180:ARG:HH11	1:B:180:ARG:HG3	1.75	0.51
1:B:184:ALA:O	1:B:187:LEU:HB2	2.11	0.51
1:B:17:SER:OG	1:B:271:PRO:HB2	2.11	0.51
1:B:6:VAL:HG12	1:B:30:LEU:HA	1.92	0.51
1:B:186:ASP:O	1:B:187:LEU:HD12	2.10	0.51
1:B:128:ARG:HE	1:B:142:THR:HG21	1.76	0.51
1:B:4:ILE:HG12	1:B:286:HIS:CD2	2.46	0.50
1:B:201:ALA:O	1:B:206:HIS:HE1	1.94	0.50
1:B:287:ARG:O	1:B:291:GLN:HB2	2.10	0.50
1:B:237:SER:OG	1:B:238:GLU:N	2.45	0.50
1:A:152:HIS:HB3	1:A:167:GLN:CG	2.34	0.50
1:B:167:GLN:HE22	1:B:195:ARG:HE	1.60	0.50
1:A:159:ILE:HD11	1:A:216:MET:CE	2.42	0.49
1:B:8:ILE:CD1	1:B:18:VAL:HG22	2.42	0.49
1:B:253:ASP:HA	1:B:257:PHE:O	2.13	0.49
1:A:78:LYS:HB2	1:A:78:LYS:HZ3	1.75	0.49
1:A:188:THR:HG23	1:A:191:GLN:HE22	1.78	0.49
1:B:72:ILE:HB	1:B:73:PRO:HD3	1.94	0.49
1:B:170:LEU:N	1:B:170:LEU:CD1	2.74	0.49
1:B:71:ASP:OD2	1:B:158:ARG:NH2	2.46	0.49
1:B:153:SER:HB3	1:B:157:ARG:NH2	2.28	0.49
1:B:218:ASP:N	1:B:221:VAL:HG22	2.27	0.49
1:B:178:LYS:HB3	1:B:183:GLU:O	2.11	0.48
1:B:31:VAL:HG21	1:B:59:VAL:HG12	1.95	0.48
1:B:148:LEU:HD21	1:B:166:VAL:HG21	1.94	0.48
1:B:298:THR:CG2	1:B:300:LEU:H	2.25	0.48
1:A:199:VAL:O	1:A:229:PHE:HA	2.14	0.48
1:A:311:ASN:OD1	1:A:312:LEU:N	2.47	0.47
1:B:170:LEU:HA	1:B:171:PRO:HD3	1.68	0.47
1:A:72:ILE:HG22	1:A:73:PRO:CD	2.43	0.47
1:B:180:ARG:HG3	1:B:180:ARG:NH1	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:N	1:B:271:PRO:HD2	2.29	0.47
1:B:135:LEU:O	1:B:138:HIS:HD2	1.97	0.47
1:B:84:CYS:SG	1:B:289:LYS:HD2	2.54	0.47
1:B:147:GLY:HA3	1:B:244:HIS:HA	1.96	0.47
1:B:135:LEU:O	1:B:138:HIS:CD2	2.69	0.46
1:B:181:ARG:NH1	1:B:183:GLU:CD	2.74	0.46
1:A:266:LYS:C	1:A:267:LEU:HD23	2.41	0.46
1:B:173:GLU:O	1:B:177:GLU:HG2	2.16	0.46
1:A:46:VAL:HG12	1:A:47:PHE:N	2.30	0.46
1:A:78:LYS:NZ	1:A:78:LYS:CB	2.73	0.46
1:B:1:MET:CA	1:B:2:THR:CB	2.94	0.46
1:B:103:ASN:O	1:B:107:THR:OG1	2.28	0.46
1:B:68:SER:OG	1:B:90:ASP:OD1	2.33	0.45
1:A:95:ILE:HB	1:A:96:PRO:HD3	1.99	0.45
1:A:86:VAL:HG21	1:A:282:GLY:HA2	1.98	0.45
1:B:253:ASP:HB2	1:B:258:ASN:HD21	1.81	0.45
1:A:148:LEU:HD11	1:A:166:VAL:CG2	2.46	0.45
1:A:98:HIS:O	1:A:101:VAL:HG12	2.16	0.45
1:A:129:VAL:HG21	1:A:300:LEU:CD2	2.46	0.45
1:B:154:ASP:O	1:B:158:ARG:HG2	2.17	0.45
1:A:308:SER:CB	1:A:315:LEU:HD21	2.47	0.45
1:A:35:SER:C	1:A:49:VAL:HG13	2.42	0.45
1:A:2:THR:HG22	4:A:447:HOH:O	2.16	0.44
1:A:2:THR:OG1	1:A:3:ASN:N	2.51	0.44
1:A:128:ARG:NE	1:A:142:THR:HG21	2.23	0.44
1:A:170:LEU:HD23	1:A:170:LEU:N	2.32	0.44
1:A:160:PRO:HB2	1:A:208:ARG:NH1	2.32	0.44
1:B:195:ARG:NH2	3:B:402:ACT:OXT	2.50	0.44
1:A:135:LEU:O	1:A:138:HIS:HD2	2.00	0.44
1:A:201:ALA:O	1:A:206:HIS:CE1	2.60	0.44
1:B:135:LEU:HD11	1:B:250:THR:CG2	2.47	0.44
1:A:146:PRO:HD2	1:A:266:LYS:NZ	2.33	0.44
1:B:135:LEU:CD1	1:B:138:HIS:HB3	2.48	0.44
1:B:284:ALA:O	1:B:288:MET:HG3	2.17	0.44
1:B:216:MET:HB3	1:B:220:PHE:HB2	2.00	0.43
1:B:176:LEU:HD21	1:B:249:ILE:HD11	2.01	0.43
1:B:195:ARG:NH1	1:B:223:TYR:CZ	2.86	0.43
1:B:135:LEU:HD11	1:B:250:THR:HG21	1.99	0.43
1:B:163:GLN:HE21	1:B:201:ALA:HA	1.81	0.43
1:A:92:HIS:CD2	1:B:320:VAL:O	2.72	0.43
1:A:3:ASN:O	1:A:4:ILE:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:N	1:A:307:LEU:CD2	2.82	0.43
1:B:262:GLU:HG3	4:B:451:HOH:O	2.18	0.43
1:B:262:GLU:OE1	1:B:264:ILE:HG12	2.19	0.42
1:A:120:ASP:CG	1:A:128:ARG:HH22	2.26	0.42
1:A:270:ASN:HD21	2:A:400:NDP:H5N	1.83	0.42
1:B:312:LEU:HG	1:B:316:ILE:HD12	2.01	0.42
1:A:258:ASN:O	1:B:268:ASP:HB2	2.19	0.42
1:B:91:ASN:HD22	1:B:91:ASN:C	2.26	0.42
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.79	0.42
1:A:135:LEU:O	1:A:138:HIS:CD2	2.73	0.42
1:B:76:ALA:N	1:B:77:PRO:CD	2.82	0.42
1:A:152:HIS:CB	1:A:167:GLN:CG	2.94	0.41
1:A:244:HIS:CD2	1:A:245:GLY:H	2.38	0.41
1:B:1:MET:CB	1:B:2:THR:CA	2.98	0.41
1:B:11:TYR:CD2	1:B:40:LEU:HG	2.54	0.41
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.87	0.41
1:B:34:PHE:CD1	1:B:47:PHE:HB2	2.56	0.41
1:B:242:MET:N	1:B:243:PRO:CD	2.83	0.41
1:A:76:ALA:HB3	1:A:77:PRO:HD3	2.01	0.41
1:B:60:ASP:C	1:B:61:VAL:HG12	2.46	0.41
1:B:159:ILE:HA	1:B:160:PRO:HD2	1.82	0.41
1:A:159:ILE:HG23	1:A:160:PRO:CD	2.47	0.41
1:A:194:LYS:HB2	1:A:194:LYS:HE2	1.91	0.40
1:B:92:HIS:CE1	1:B:121:PRO:HD3	2.57	0.40
1:B:80:ALA:O	1:B:111:ASN:ND2	2.46	0.40
1:B:95:ILE:N	1:B:96:PRO:CD	2.85	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:OD2	1:B:190:LYS:NZ[2_646]	1.97	0.23
1:A:226:GLU:OE2	1:B:234:THR:OG1[2_556]	2.04	0.16
1:A:229:PHE:N	1:B:229:PHE:O[2_556]	2.11	0.09
1:B:39:THR:N	4:B:416:HOH:O[2_646]	2.11	0.09
1:A:206:HIS:CD2	1:B:206:HIS:CD2[2_556]	2.12	0.08
1:A:231:ASP:N	1:B:228:ASN:OD1[2_556]	2.14	0.06
1:A:229:PHE:O	1:B:229:PHE:N[2_556]	2.17	0.03

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	318/320 (99%)	295 (93%)	20 (6%)	3 (1%)	14	14
1	B	318/320 (99%)	301 (95%)	13 (4%)	4 (1%)	9	8
All	All	636/640 (99%)	596 (94%)	33 (5%)	7 (1%)	11	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	B	53	ASP
1	B	218	ASP
1	B	255	GLY
1	A	4	ILE
1	B	2	THR
1	A	41	ASP

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	258/261 (99%)	218 (84%)	40 (16%)	2	2
1	B	256/261 (98%)	208 (81%)	48 (19%)	1	1
All	All	514/522 (98%)	426 (83%)	88 (17%)	2	2

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	30	LEU
1	A	31	VAL
1	A	37	ARG
1	A	40	LEU
1	A	44	THR
1	A	61	VAL
1	A	66	MET
1	A	70	THR
1	A	72	ILE
1	A	74	GLU
1	A	78	LYS
1	A	85	THR
1	A	114	LEU
1	A	125	SER
1	A	139	GLN
1	A	142	THR
1	A	163	GLN
1	A	164	LYS
1	A	167	GLN
1	A	170	LEU
1	A	171	PRO
1	A	177	GLU
1	A	178	LYS
1	A	194	LYS
1	A	195	ARG
1	A	209	ILE
1	A	211	ASN
1	A	226	GLU
1	A	237	SER
1	A	238	GLU
1	A	242	MET
1	A	244	HIS
1	A	260	THR
1	A	266	LYS
1	A	289	LYS
1	A	302	VAL
1	A	307	LEU
1	A	315	LEU
1	A	318	ARG
1	B	3	ASN
1	B	6	VAL
1	B	18	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	30	LEU
1	B	31	VAL
1	B	39	THR
1	B	40	LEU
1	B	41	ASP
1	B	42	THR
1	B	46	VAL
1	B	52	VAL
1	B	57	ASP
1	B	61	VAL
1	B	62	LEU
1	B	66	MET
1	B	72	ILE
1	B	100	GLN
1	B	107	THR
1	B	114	LEU
1	B	125	SER
1	B	135	LEU
1	B	137	GLU
1	B	142	THR
1	B	158	ARG
1	B	166	VAL
1	B	176	LEU
1	B	177	GLU
1	B	178	LYS
1	B	183	GLU
1	B	187	LEU
1	B	191	GLN
1	B	194	LYS
1	B	195	ARG
1	B	211	ASN
1	B	232	GLU
1	B	234	THR
1	B	240	THR
1	B	244	HIS
1	B	253	ASP
1	B	262	GLU
1	B	264	ILE
1	B	266	LYS
1	B	276	SER
1	B	298	THR
1	B	302	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	307	LEU
1	B	310	GLU
1	B	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	92	HIS
1	A	100	GLN
1	A	138	HIS
1	A	141	HIS
1	A	191	GLN
1	A	196	GLN
1	A	206	HIS
1	A	244	HIS
1	A	258	ASN
1	A	259	HIS
1	A	270	ASN
1	A	286	HIS
1	B	25	GLN
1	B	81	GLN
1	B	91	ASN
1	B	127	ASN
1	B	138	HIS
1	B	141	HIS
1	B	152	HIS
1	B	163	GLN
1	B	167	GLN
1	B	206	HIS
1	B	258	ASN
1	B	259	HIS
1	B	278	GLN
1	B	286	HIS

5.3.3 RNA ⓘ

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](#)

4 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	ACT	B	401	-	3,3,3	1.30	0	3,3,3	0.74	0
2	NDP	A	400	-	51,52,52	2.33	8 (15%)	71,80,80	1.60	15 (21%)
3	ACT	B	402	-	3,3,3	1.33	0	3,3,3	0.38	0
2	NDP	B	400	-	51,52,52	2.02	11 (21%)	71,80,80	1.72	14 (19%)

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	NDP	A	400	-	-	2/34/77/77	0/5/5/5
2	NDP	B	400	-	-	1/34/77/77	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NDP	PN-O3	-9.26	1.49	1.59
2	B	400	NDP	PN-O3	-7.51	1.51	1.59
2	A	400	NDP	O7N-C7N	7.14	1.41	1.24
2	A	400	NDP	PA-O3	-6.86	1.52	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	NDP	C4N-C3N	-5.13	1.40	1.50
2	B	400	NDP	C2A-N3A	5.00	1.42	1.33
2	B	400	NDP	O7N-C7N	4.67	1.35	1.24
2	B	400	NDP	PA-O3	-4.45	1.54	1.59
2	B	400	NDP	C4N-C5N	-3.89	1.38	1.49
2	A	400	NDP	C2A-N3A	3.87	1.40	1.33
2	A	400	NDP	C4N-C5N	-3.79	1.39	1.49
2	A	400	NDP	C6N-C5N	3.04	1.42	1.33
2	B	400	NDP	C6N-C5N	2.78	1.41	1.33
2	B	400	NDP	C4N-C3N	-2.68	1.44	1.50
2	B	400	NDP	C7N-C3N	-2.66	1.43	1.48
2	A	400	NDP	C7N-C3N	-2.47	1.43	1.48
2	B	400	NDP	O3B-C3B	-2.18	1.37	1.43
2	B	400	NDP	P2B-O2B	2.11	1.63	1.59
2	B	400	NDP	P2B-O3X	-2.05	1.47	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NDP	N3A-C2A-N1A	-4.95	121.09	128.58
2	A	400	NDP	C3D-C2D-C1D	4.84	110.61	101.46
2	B	400	NDP	O2D-C2D-C1D	-3.92	96.59	110.10
2	B	400	NDP	C2D-C1D-N1N	-3.89	103.73	113.31
2	A	400	NDP	N3A-C2A-N1A	-3.87	122.72	128.58
2	B	400	NDP	C1D-N1N-C2N	-3.73	115.00	121.14
2	B	400	NDP	C2A-N1A-C6A	3.72	124.85	118.73
2	A	400	NDP	O3-PA-O1A	-3.68	99.64	110.70
2	B	400	NDP	O5D-PN-O1N	-3.27	95.99	108.94
2	A	400	NDP	C2A-N1A-C6A	3.08	123.78	118.73
2	B	400	NDP	O4B-C1B-N9A	-3.00	102.33	108.09
2	A	400	NDP	O4D-C1D-C2D	-2.99	100.22	106.62
2	A	400	NDP	O3D-C3D-C4D	2.98	119.65	111.08
2	A	400	NDP	C2D-C3D-C4D	-2.82	97.17	102.61
2	B	400	NDP	O2N-PN-O3	2.77	114.77	107.27
2	B	400	NDP	O7N-C7N-C3N	-2.70	115.82	120.90
2	A	400	NDP	O4D-C4D-C3D	2.66	110.43	105.15
2	B	400	NDP	C6N-N1N-C2N	2.64	122.14	119.32
2	B	400	NDP	O3X-P2B-O1X	2.60	120.96	110.83
2	B	400	NDP	C5D-C4D-C3D	2.60	124.56	115.21
2	A	400	NDP	C1B-N9A-C8A	-2.59	121.34	127.09
2	A	400	NDP	O2A-PA-O3	2.57	114.21	107.27
2	A	400	NDP	O3X-P2B-O1X	2.48	120.48	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	NDP	C2B-C1B-N9A	-2.42	109.78	113.75
2	A	400	NDP	N6A-C6A-N1A	2.34	123.59	118.38
2	A	400	NDP	O2N-PN-O3	2.30	113.48	107.27
2	B	400	NDP	C3N-C7N-N7N	2.29	121.73	117.67
2	A	400	NDP	C4A-N9A-C1B	2.19	131.74	126.63
2	A	400	NDP	C4D-O4D-C1D	-2.13	104.77	109.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

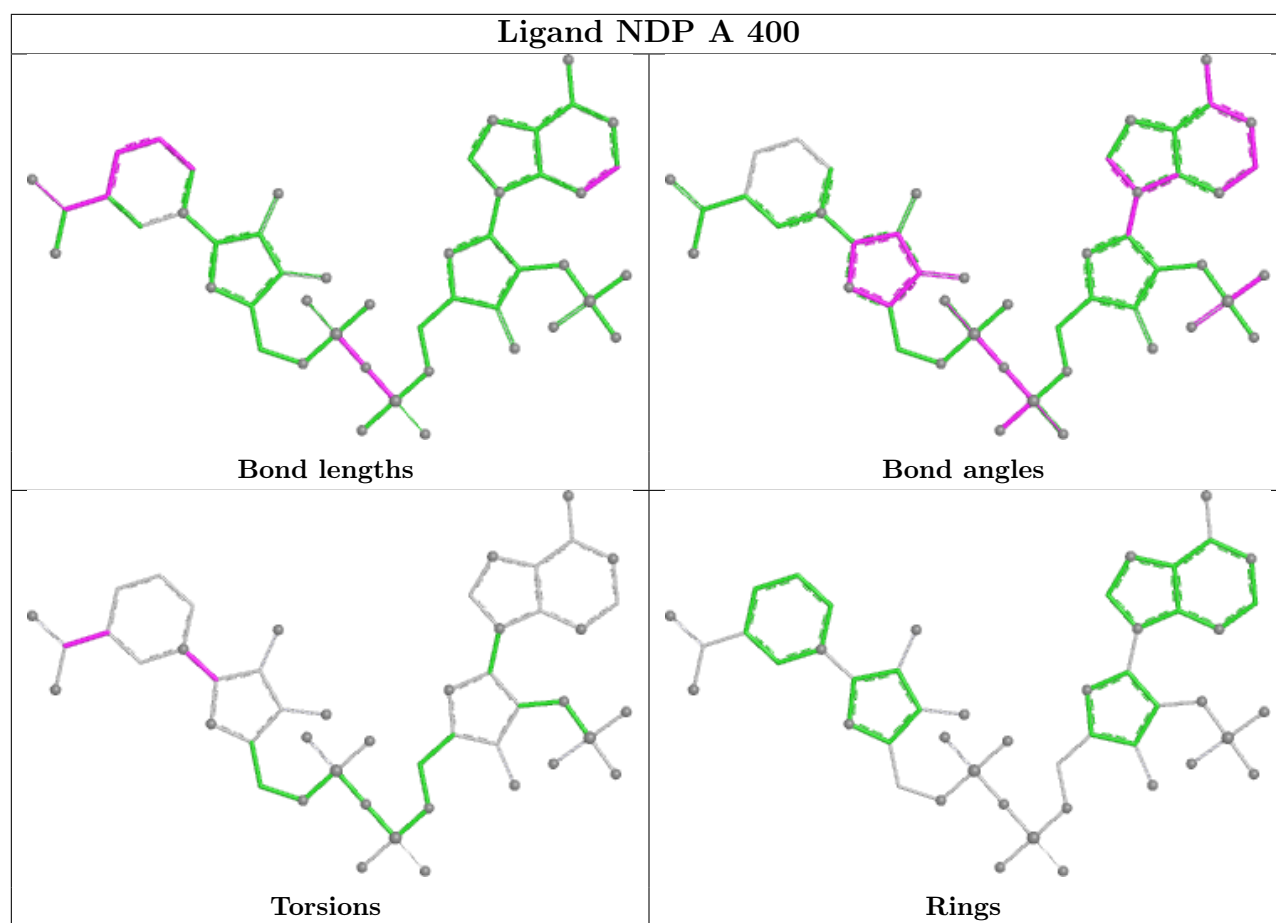
Mol	Chain	Res	Type	Atoms
2	A	400	NDP	O4D-C1D-N1N-C2N
2	B	400	NDP	O4D-C1D-N1N-C2N
2	A	400	NDP	C2N-C3N-C7N-N7N

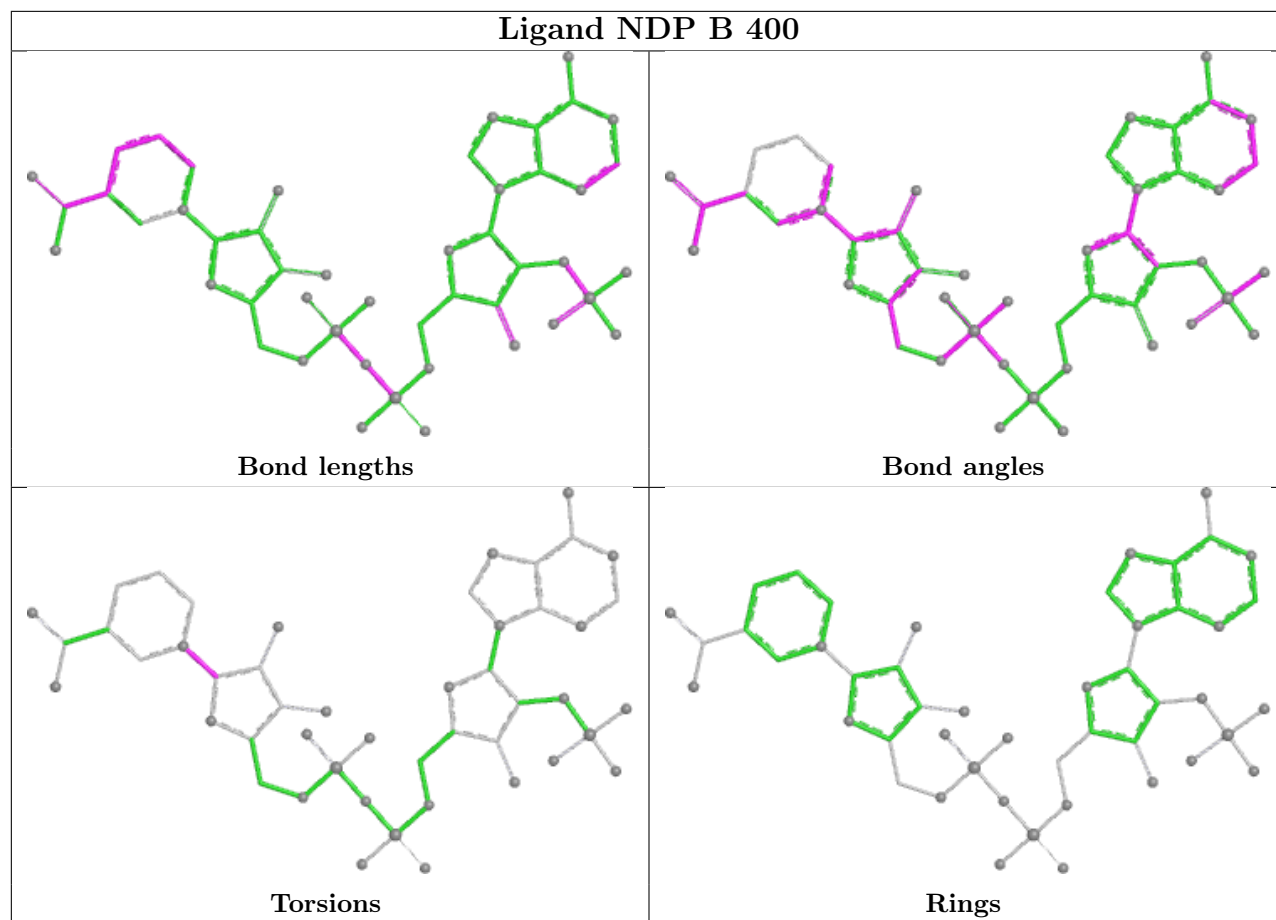
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	NDP	2	0
3	B	402	ACT	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.