



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:21 AM UTC

PDB ID : 2J3J / pdb_00002j3j
Title : Crystal structure of Arabidopsis thaliana Double Bond Reductase (AT5G16970)-Ternary Complex I
Authors : Youn, B.; Kim, S.J.; Moinuddin, S.G.; Lee, C.; Bedgar, D.L.; Harper, A.R.; Davin, L.B.; Lewis, N.G.; Kang, C.
Deposited on : 2006-08-21
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

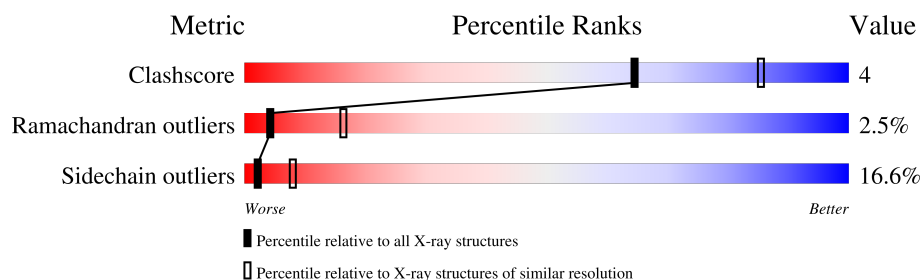
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5537 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.

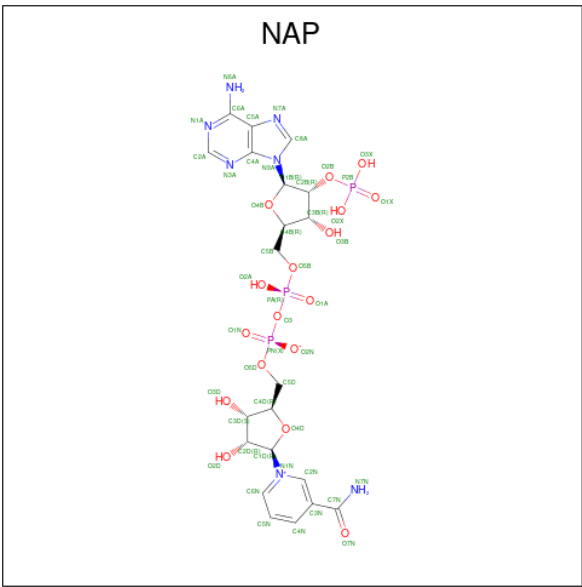
- Molecule 1 is a protein called NADPH-dependent oxidoreductase 2-alkenal reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2623	1681	432	493	17	0	0	0
1	B	345	2681	1717	441	506	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ASN	ILE	conflict	UNP Q39172
B	1279	ASN	ILE	conflict	UNP Q39172

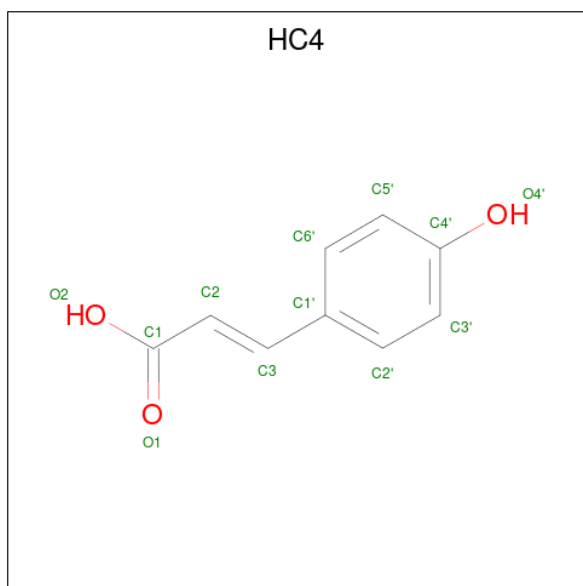
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 3 is 4'-HYDROXYCINNAMIC ACID (CCD ID: HC4) (formula: C₉H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

- Molecule 4 is water.

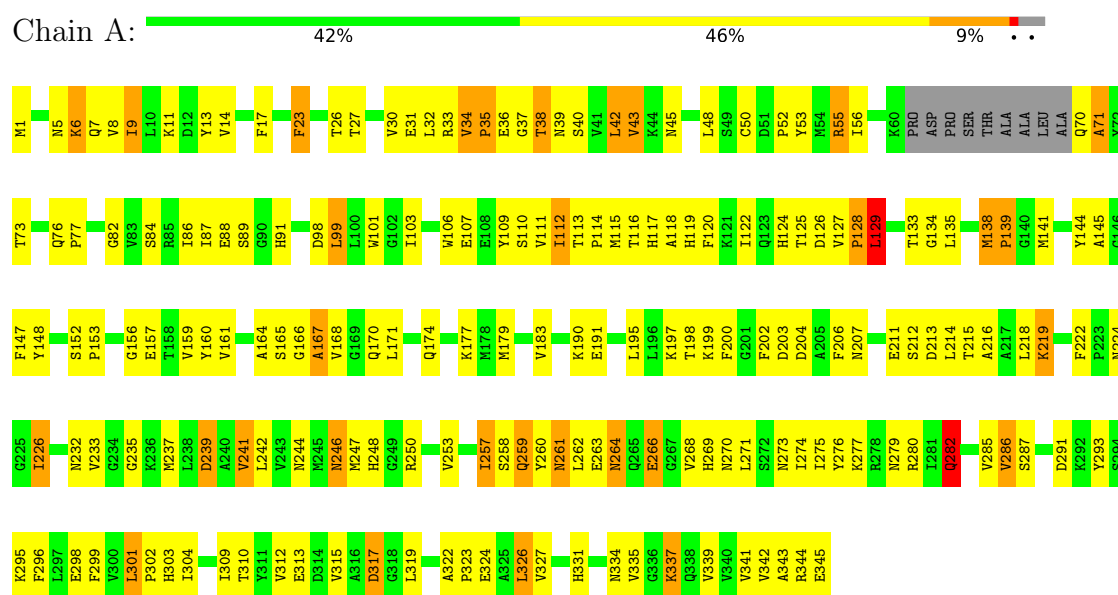
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	56	Total	O	0	0
			56	56		

3 Residue-property plots

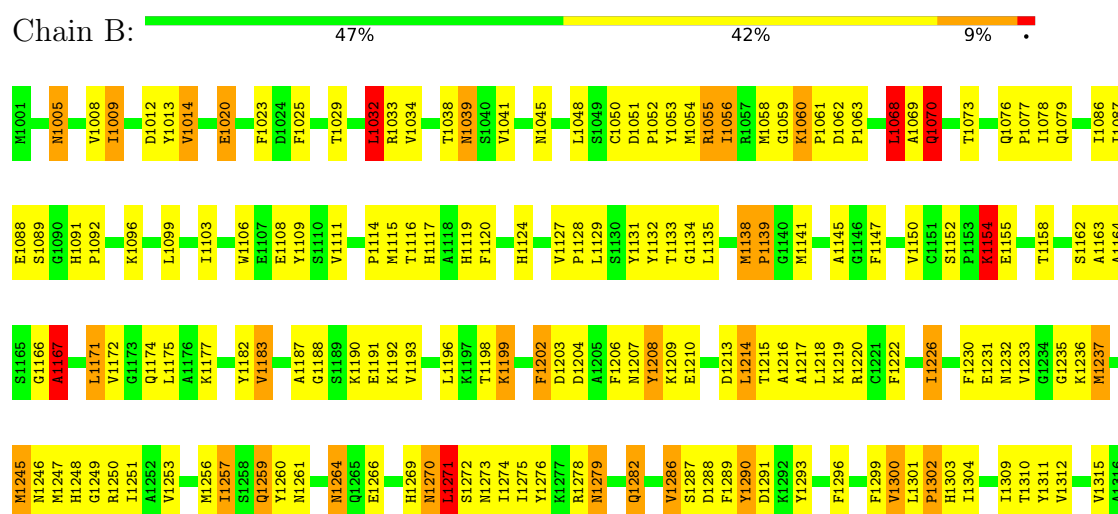
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: NADPH-dependent oxidoreductase 2-alkenal reductase



- Molecule 1: NADPH-dependent oxidoreductase 2-alkenal reductase



D1317	G1318	L1319	E1320	K1321	A1322	P1323	E1324	A1325	L1326	V1327	G1328	H1331	G1332	K1333	N1334	K1337	V1340	V1341	R1344	E1345
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.04Å 122.54Å 147.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.3 (15.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.055 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5537	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: HC4, NAP

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	1.40	20/2681 (0.7%)	2.55	211/3625 (5.8%)
1	B	1.45	28/2742 (1.0%)	2.54	231/3713 (6.2%)
All	All	1.42	48/5423 (0.9%)	2.55	442/7338 (6.0%)

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	2
1	B	0	2
All	All	0	4

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1256	MET	CA-CB	11.93	1.62	1.53
1	B	1341	VAL	CA-CB	11.33	1.66	1.53
1	B	1127	VAL	CA-CB	8.73	1.65	1.54
1	A	103	ILE	CA-CB	8.51	1.62	1.53
1	B	1290	TYR	C-N	-8.43	1.20	1.33
1	B	1119	HIS	CD2-NE2	-8.16	1.28	1.37
1	A	341	VAL	CA-CB	8.02	1.63	1.54
1	B	1253	VAL	CA-CB	7.77	1.62	1.53
1	B	1103	ILE	CA-CB	7.47	1.61	1.53
1	A	91	HIS	CD2-NE2	-7.36	1.29	1.37
1	A	119	HIS	CD2-NE2	-7.26	1.29	1.37
1	B	1056	ILE	CA-CB	7.25	1.64	1.54
1	B	1303	HIS	CD2-NE2	-7.20	1.29	1.37
1	A	248	HIS	CD2-NE2	-7.04	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	HIS	CD2-NE2	-6.99	1.30	1.37
1	B	1331	HIS	CD2-NE2	-6.96	1.30	1.37
1	B	1248	HIS	CD2-NE2	-6.86	1.30	1.37
1	B	1309	ILE	CA-CB	6.73	1.62	1.54
1	B	1117	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	124	HIS	CD2-NE2	-6.47	1.30	1.37
1	B	1124	HIS	CD2-NE2	-6.35	1.30	1.37
1	B	1340	VAL	CA-CB	6.34	1.62	1.54
1	A	56	ILE	CA-CB	6.33	1.63	1.54
1	B	1312	VAL	CA-CB	6.27	1.63	1.54
1	A	159	VAL	CA-CB	6.25	1.61	1.54
1	A	309	ILE	CA-CB	6.24	1.62	1.54
1	B	1269	HIS	CD2-NE2	-6.11	1.31	1.37
1	B	1251	ILE	CA-CB	6.08	1.62	1.54
1	B	1111	VAL	CA-CB	6.07	1.62	1.54
1	B	1041	VAL	CA-CB	6.07	1.63	1.54
1	B	1086	ILE	CA-CB	6.03	1.61	1.53
1	B	1133	THR	CA-CB	6.01	1.62	1.53
1	B	1091	HIS	CD2-NE2	-5.97	1.31	1.37
1	A	38	THR	CA-CB	5.94	1.63	1.53
1	B	1150	VAL	CA-CB	5.92	1.62	1.54
1	A	303	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	1014	VAL	CA-CB	5.79	1.61	1.54
1	A	117	HIS	CD2-NE2	-5.75	1.31	1.37
1	B	1119	HIS	CG-ND1	-5.74	1.31	1.38
1	A	269	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	1304	ILE	CA-CB	5.61	1.60	1.54
1	A	339	VAL	CA-CB	5.54	1.62	1.54
1	A	198	THR	CA-CB	5.46	1.62	1.53
1	A	268	VAL	CA-CB	5.27	1.60	1.53
1	B	1331	HIS	CG-ND1	-5.23	1.32	1.38
1	A	8	VAL	CA-CB	5.15	1.60	1.53
1	A	113	THR	CA-CB	5.04	1.60	1.53
1	A	119	HIS	CG-ND1	-5.03	1.32	1.38

All (442) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1301	LEU	CA-C-O	-13.58	105.75	118.79
1	A	23	PHE	CA-CB-CG	12.40	126.20	113.80
1	B	1290	TYR	CA-C-N	11.31	141.57	121.66
1	B	1290	TYR	C-N-CA	11.31	141.57	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ASP	CA-CB-CG	10.97	123.57	112.60
1	A	233	VAL	N-CA-C	10.85	121.68	111.48
1	B	1279	ASN	CA-CB-CG	10.69	123.29	112.60
1	A	261	ASN	CA-CB-CG	10.48	123.08	112.60
1	B	1116	THR	N-CA-C	10.24	124.85	111.75
1	B	1315	VAL	N-CA-CB	-10.17	99.63	110.72
1	B	1288	ASP	CA-CB-CG	10.09	122.69	112.60
1	A	40	SER	N-CA-C	9.32	123.64	110.50
1	B	1291	ASP	CA-CB-CG	9.31	121.91	112.60
1	A	266	GLU	N-CA-C	9.22	122.51	110.43
1	A	126	ASP	CA-CB-CG	9.12	121.72	112.60
1	A	164	ALA	CA-C-N	8.99	132.13	120.44
1	A	164	ALA	C-N-CA	8.99	132.13	120.44
1	A	319	LEU	CA-C-N	8.86	132.35	120.65
1	A	319	LEU	C-N-CA	8.86	132.35	120.65
1	A	206	PHE	CA-CB-CG	8.85	122.65	113.80
1	A	279	ASN	CA-CB-CG	8.76	121.36	112.60
1	B	1204	ASP	CA-CB-CG	8.75	121.35	112.60
1	B	1232	ASN	CA-CB-CG	8.63	121.23	112.60
1	A	214	LEU	N-CA-C	8.58	121.77	111.82
1	B	1264	ASN	CA-CB-CG	8.52	121.12	112.60
1	A	113	THR	CB-CA-C	8.48	118.56	110.17
1	A	99	LEU	N-CA-C	8.39	122.58	109.07
1	A	89	SER	N-CA-C	8.32	123.18	109.95
1	A	233	VAL	N-CA-CB	-8.18	103.47	111.57
1	A	128	PRO	N-CA-C	8.17	129.31	112.47
1	A	153	PRO	N-CA-C	8.08	125.13	111.32
1	A	299	PHE	CA-CB-CG	8.05	121.86	113.80
1	B	1275	ILE	CA-C-N	8.03	131.37	120.38
1	B	1275	ILE	C-N-CA	8.03	131.37	120.38
1	A	39	ASN	CA-CB-CG	7.99	120.59	112.60
1	B	1315	VAL	CB-CA-C	7.98	120.81	110.91
1	B	1271	LEU	CA-C-N	7.97	131.61	120.29
1	B	1271	LEU	C-N-CA	7.97	131.61	120.29
1	A	275	ILE	CA-C-N	7.94	131.43	120.63
1	A	275	ILE	C-N-CA	7.94	131.43	120.63
1	A	262	LEU	N-CA-C	7.90	122.71	109.76
1	A	116	THR	N-CA-C	7.89	121.85	111.75
1	A	279	ASN	N-CA-C	7.88	122.65	110.20
1	A	118	ALA	N-CA-C	-7.86	102.48	112.93
1	B	1167	ALA	N-CA-C	7.83	127.49	110.80
1	B	1202	PHE	CA-CB-CG	7.83	121.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1012	ASP	CA-CB-CG	7.80	120.40	112.60
1	B	1138	MET	CA-C-O	-7.77	109.52	120.16
1	B	1051	ASP	CA-CB-CG	7.76	120.36	112.60
1	A	301	LEU	CA-C-O	-7.72	109.58	120.16
1	A	43	VAL	N-CA-CB	-7.72	99.47	112.44
1	B	1199	LYS	N-CA-C	7.62	120.55	111.33
1	B	1237	MET	N-CA-C	7.60	121.81	112.23
1	A	260	TYR	CA-C-N	7.60	133.42	120.72
1	A	260	TYR	C-N-CA	7.60	133.42	120.72
1	B	1155	GLU	N-CA-C	7.57	120.95	110.35
1	B	1062	ASP	CA-C-N	7.57	127.28	119.56
1	B	1062	ASP	C-N-CA	7.57	127.28	119.56
1	B	1248	HIS	CB-CG-CD2	-7.55	121.38	131.20
1	B	1290	TYR	O-C-N	-7.54	112.56	122.59
1	B	1103	ILE	O-C-N	7.51	131.40	122.62
1	B	1275	ILE	N-CA-C	-7.51	104.47	111.45
1	B	1264	ASN	CA-C-N	7.49	131.44	120.95
1	B	1264	ASN	C-N-CA	7.49	131.44	120.95
1	A	202	PHE	CA-CB-CG	7.47	121.27	113.80
1	B	1289	PHE	CA-CB-CG	7.45	121.25	113.80
1	A	296	PHE	CA-CB-CG	7.44	121.24	113.80
1	A	138	MET	CA-C-N	7.40	127.11	119.56
1	A	138	MET	C-N-CA	7.40	127.11	119.56
1	A	37	GLY	CA-C-N	7.37	135.62	121.54
1	A	37	GLY	C-N-CA	7.37	135.62	121.54
1	A	246	ASN	CA-CB-CG	7.35	119.95	112.60
1	A	264	ASN	CA-CB-CG	7.35	119.95	112.60
1	A	101	TRP	CA-CB-CG	7.19	127.25	113.60
1	B	1164	ALA	N-CA-C	7.18	121.31	112.54
1	B	1077	PRO	N-CA-C	7.17	122.32	111.14
1	B	1323	PRO	CA-C-N	7.14	130.17	120.38
1	B	1323	PRO	C-N-CA	7.14	130.17	120.38
1	B	1053	TYR	CA-CB-CG	7.13	126.74	113.90
1	A	291	ASP	CA-CB-CG	7.08	119.68	112.60
1	B	1162	SER	CA-C-N	7.08	132.41	122.36
1	B	1162	SER	C-N-CA	7.08	132.41	122.36
1	B	1163	ALA	CA-C-O	7.06	130.03	121.84
1	B	1286	VAL	CB-CA-C	-7.03	102.65	112.14
1	B	1198	THR	CA-C-N	7.03	130.01	120.38
1	B	1198	THR	C-N-CA	7.03	130.01	120.38
1	B	1053	TYR	CA-C-N	7.00	130.61	120.38
1	B	1053	TYR	C-N-CA	7.00	130.61	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1092	PRO	N-CA-C	7.00	122.77	113.40
1	A	145	ALA	N-CA-C	6.99	118.89	111.28
1	B	1337	LYS	CB-CG-CD	6.96	127.31	111.30
1	A	241	VAL	CG1-CB-CG2	-6.96	95.49	110.80
1	A	260	TYR	O-C-N	6.96	129.49	122.12
1	B	1245	MET	CG-SD-CE	-6.95	85.60	100.90
1	B	1206	PHE	CA-CB-CG	6.94	120.74	113.80
1	A	213	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	88	GLU	CA-CB-CG	6.94	127.98	114.10
1	B	1214	LEU	CA-C-N	6.94	129.58	120.28
1	B	1214	LEU	C-N-CA	6.94	129.58	120.28
1	B	1127	VAL	CA-C-N	6.87	127.28	119.93
1	B	1127	VAL	C-N-CA	6.87	127.28	119.93
1	A	233	VAL	CA-C-O	-6.85	114.87	120.70
1	A	53	TYR	CA-CB-CG	6.85	126.23	113.90
1	A	17	PHE	CA-C-O	-6.84	113.67	119.76
1	A	246	ASN	CB-CG-ND2	6.82	126.63	116.40
1	B	1063	PRO	CA-C-N	6.82	129.71	120.44
1	B	1063	PRO	C-N-CA	6.82	129.71	120.44
1	A	33	ARG	CB-CG-CD	-6.80	95.66	111.30
1	B	1190	LYS	CA-C-N	6.78	129.67	120.38
1	B	1190	LYS	C-N-CA	6.78	129.67	120.38
1	A	257	ILE	N-CA-CB	6.77	122.40	111.23
1	A	322	ALA	CA-C-N	6.74	125.98	118.97
1	A	322	ALA	C-N-CA	6.74	125.98	118.97
1	A	239	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	246	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	B	1337	LYS	CA-CB-CG	6.72	127.54	114.10
1	B	1233	VAL	N-CA-C	6.71	123.31	109.34
1	A	30	VAL	CA-C-O	6.71	127.59	120.48
1	B	1253	VAL	CG1-CB-CG2	-6.71	96.05	110.80
1	B	1324	GLU	CA-CB-CG	6.70	127.51	114.10
1	B	1334	ASN	CA-CB-CG	6.64	119.24	112.60
1	A	204	ASP	CA-CB-CG	6.62	119.22	112.60
1	B	1191	GLU	CA-CB-CG	6.57	127.23	114.10
1	A	317	ASP	N-CA-C	6.55	119.94	107.75
1	A	331	HIS	N-CA-C	-6.55	104.22	112.93
1	A	139	PRO	CA-N-CD	-6.55	102.83	112.00
1	B	1039	ASN	CA-CB-CG	6.54	119.14	112.60
1	B	1257	ILE	N-CA-C	6.54	121.30	111.89
1	A	211	GLU	CA-C-O	6.54	127.26	120.40
1	A	9	ILE	N-CA-CB	-6.53	100.45	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASN	CA-CB-CG	6.52	119.12	112.60
1	A	77	PRO	N-CA-C	6.51	121.47	111.11
1	B	1127	VAL	N-CA-CB	-6.48	102.14	111.21
1	B	1323	PRO	CA-N-CD	-6.48	102.93	112.00
1	A	304	ILE	CA-C-N	6.46	129.59	120.28
1	A	304	ILE	C-N-CA	6.46	129.59	120.28
1	A	257	ILE	CB-CA-C	-6.45	100.71	111.29
1	A	224	ASN	CA-CB-CG	6.44	119.04	112.60
1	B	1337	LYS	CG-CD-CE	6.42	126.07	111.30
1	B	1257	ILE	CB-CA-C	-6.41	99.54	111.79
1	B	1131	TYR	CA-CB-CG	6.40	125.42	113.90
1	B	1207	ASN	CA-CB-CG	6.39	118.99	112.60
1	B	1213	ASP	CA-C-N	6.37	130.37	120.82
1	B	1213	ASP	C-N-CA	6.37	130.37	120.82
1	A	212	SER	CA-C-N	6.37	133.70	121.54
1	A	212	SER	C-N-CA	6.37	133.70	121.54
1	B	1235	GLY	CA-C-N	6.36	129.43	120.28
1	B	1235	GLY	C-N-CA	6.36	129.43	120.28
1	A	165	SER	O-C-N	6.36	128.62	122.07
1	B	1317	ASP	N-CA-C	6.36	118.97	109.25
1	B	1020	GLU	CA-C-N	6.34	131.45	120.68
1	B	1020	GLU	C-N-CA	6.34	131.45	120.68
1	B	1052	PRO	N-CA-C	6.33	125.52	112.47
1	B	1220	ARG	CA-C-N	6.33	128.67	120.44
1	B	1220	ARG	C-N-CA	6.33	128.67	120.44
1	A	110	SER	N-CA-C	6.32	119.49	109.50
1	B	1070	GLN	N-CA-C	6.31	124.25	110.80
1	B	1279	ASN	N-CA-C	6.31	118.86	110.53
1	A	216	ALA	CA-C-N	6.30	129.24	120.29
1	A	216	ALA	C-N-CA	6.30	129.24	120.29
1	A	73	THR	CB-CA-C	6.26	116.36	110.17
1	A	55	ARG	CB-CG-CD	6.25	125.67	111.30
1	A	129	LEU	N-CA-C	6.23	124.08	110.80
1	A	269	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	207	ASN	CA-CB-CG	6.22	118.83	112.60
1	A	156	GLY	CA-C-N	6.22	129.96	120.82
1	A	156	GLY	C-N-CA	6.22	129.96	120.82
1	B	1276	TYR	CA-CB-CG	6.22	125.10	113.90
1	B	1078	ILE	CB-CG1-CD1	-6.20	100.78	113.80
1	B	1045	ASN	CA-CB-CG	6.18	118.78	112.60
1	A	285	VAL	CA-C-N	6.17	130.74	120.62
1	A	285	VAL	C-N-CA	6.17	130.74	120.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ALA	N-CA-C	6.17	123.93	110.80
1	B	1304	ILE	CA-C-N	6.16	130.56	120.63
1	B	1304	ILE	C-N-CA	6.16	130.56	120.63
1	B	1129	LEU	CA-C-N	6.16	129.15	120.28
1	B	1129	LEU	C-N-CA	6.16	129.15	120.28
1	B	1260	TYR	N-CA-C	6.14	118.77	111.71
1	B	1091	HIS	CA-C-N	6.11	125.51	118.85
1	B	1091	HIS	C-N-CA	6.11	125.51	118.85
1	A	86	ILE	O-C-N	6.11	129.59	122.81
1	B	1171	LEU	CA-C-N	6.10	128.25	120.56
1	B	1171	LEU	C-N-CA	6.10	128.25	120.56
1	B	1253	VAL	CA-C-O	6.09	128.22	120.97
1	A	203	ASP	N-CA-C	6.09	117.92	111.28
1	A	237	MET	CA-C-O	-6.06	114.00	120.42
1	A	101	TRP	CG-CD2-CE3	6.06	139.96	133.90
1	B	1203	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	1114	PRO	N-CA-C	6.03	119.97	110.50
1	B	1260	TYR	O-C-N	6.03	129.27	122.22
1	B	1166	GLY	O-C-N	6.02	130.53	122.70
1	B	1246	ASN	O-C-N	6.02	129.71	122.85
1	A	282	GLN	CA-CB-CG	6.01	126.12	114.10
1	A	144	TYR	CA-C-N	6.00	128.32	120.28
1	A	144	TYR	C-N-CA	6.00	128.32	120.28
1	B	1286	VAL	CA-C-N	5.99	129.13	120.38
1	B	1286	VAL	C-N-CA	5.99	129.13	120.38
1	A	138	MET	CA-C-O	-5.99	111.95	120.16
1	A	270	ASN	N-CA-C	5.99	119.33	112.57
1	A	327	VAL	CA-CB-CG1	5.99	120.58	110.40
1	B	1154	LYS	CA-CB-CG	5.98	126.06	114.10
1	A	45	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	B	1055	ARG	CB-CG-CD	5.97	125.04	111.30
1	B	1198	THR	CA-C-O	-5.97	115.44	119.68
1	B	1187	ALA	CA-C-N	5.97	127.86	120.34
1	B	1187	ALA	C-N-CA	5.97	127.86	120.34
1	B	1303	HIS	CB-CG-CD2	-5.96	123.46	131.20
1	A	120	PHE	CA-CB-CG	5.95	119.75	113.80
1	B	1128	PRO	N-CA-C	5.95	120.95	111.26
1	A	117	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	A	42	LEU	N-CA-C	-5.94	100.02	109.76
1	B	1287	SER	N-CA-C	5.94	119.35	111.75
1	A	147	PHE	CA-C-O	-5.92	112.91	120.31
1	B	1300	VAL	CA-C-O	-5.92	114.58	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	HIS	CA-C-O	-5.89	114.71	120.19
1	A	99	LEU	CA-CB-CG	5.89	136.93	116.30
1	B	1091	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	B	1025	PHE	N-CA-C	5.88	118.99	109.40
1	B	1213	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	1009	ILE	CA-CB-CG1	-5.87	100.41	110.40
1	A	302	PRO	CA-N-CD	-5.87	103.78	112.00
1	B	1328	GLY	O-C-N	5.86	130.32	122.70
1	B	1188	GLY	N-CA-C	5.86	122.65	113.86
1	B	1302	PRO	CA-N-CD	-5.86	103.80	112.00
1	A	293	TYR	CA-C-O	-5.84	114.68	120.82
1	B	1237	MET	CG-SD-CE	-5.84	88.05	100.90
1	A	76	GLN	CA-C-N	5.83	125.83	119.89
1	A	76	GLN	C-N-CA	5.83	125.83	119.89
1	A	128	PRO	CA-N-CD	-5.83	103.84	112.00
1	B	1069	ALA	N-CA-C	-5.83	98.39	110.80
1	A	277	LYS	CA-C-N	5.83	130.68	122.46
1	A	277	LYS	C-N-CA	5.83	130.68	122.46
1	A	303	HIS	CB-CG-CD2	-5.82	123.64	131.20
1	A	32	LEU	CA-C-N	5.81	133.75	122.07
1	A	32	LEU	C-N-CA	5.81	133.75	122.07
1	A	244	ASN	N-CA-C	5.79	120.35	113.28
1	A	323	PRO	CA-C-N	5.79	128.84	120.38
1	A	323	PRO	C-N-CA	5.79	128.84	120.38
1	B	1270	ASN	CA-CB-CG	5.79	118.39	112.60
1	B	1246	ASN	CA-C-N	5.78	128.97	120.82
1	B	1246	ASN	C-N-CA	5.78	128.97	120.82
1	B	1068	LEU	CA-C-N	5.78	132.58	121.54
1	B	1068	LEU	C-N-CA	5.78	132.58	121.54
1	B	1274	ILE	CA-CB-CG1	5.76	120.19	110.40
1	B	1226	ILE	CA-CB-CG2	-5.76	100.72	110.50
1	A	148	TYR	N-CA-C	5.74	119.46	112.23
1	B	1247	MET	CA-C-N	5.73	130.51	122.08
1	B	1247	MET	C-N-CA	5.73	130.51	122.08
1	B	1059	GLY	CA-C-N	5.73	128.44	120.65
1	B	1059	GLY	C-N-CA	5.73	128.44	120.65
1	B	1208	TYR	CA-C-N	5.73	128.42	120.29
1	B	1208	TYR	C-N-CA	5.73	128.42	120.29
1	A	296	PHE	CA-C-N	5.72	127.95	120.28
1	A	296	PHE	C-N-CA	5.72	127.95	120.28
1	B	1222	PHE	CA-C-N	5.72	125.25	119.19
1	B	1222	PHE	C-N-CA	5.72	125.25	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	PRO	N-CA-C	5.72	119.48	110.50
1	B	1198	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	141	MET	CA-C-N	5.69	127.91	120.28
1	A	141	MET	C-N-CA	5.69	127.91	120.28
1	B	1232	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	B	1248	HIS	CA-C-N	5.69	127.14	120.71
1	B	1248	HIS	C-N-CA	5.69	127.14	120.71
1	A	264	ASN	CA-C-N	5.68	132.40	121.54
1	A	264	ASN	C-N-CA	5.68	132.40	121.54
1	A	167	ALA	N-CA-C	5.67	122.87	110.80
1	A	115	MET	N-CA-C	-5.66	99.29	108.52
1	B	1127	VAL	CA-C-O	-5.65	112.38	119.95
1	B	1177	LYS	CG-CD-CE	5.65	124.29	111.30
1	B	1299	PHE	CA-CB-CG	5.65	119.45	113.80
1	A	122	ILE	O-C-N	5.64	129.38	122.95
1	A	43	VAL	CB-CA-C	5.63	119.11	110.55
1	A	171	LEU	CA-C-N	5.61	128.14	120.46
1	A	171	LEU	C-N-CA	5.61	128.14	120.46
1	B	1166	GLY	CA-C-N	5.60	132.24	121.54
1	B	1166	GLY	C-N-CA	5.60	132.24	121.54
1	A	86	ILE	CG1-CB-CG2	-5.59	93.92	110.70
1	B	1331	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	296	PHE	O-C-N	5.59	128.12	122.09
1	A	327	VAL	CA-CB-CG2	-5.57	100.93	110.40
1	B	1073	THR	CA-C-O	-5.56	115.18	119.46
1	B	1193	VAL	CA-CB-CG1	5.56	119.86	110.40
1	B	1038	THR	CA-C-N	5.56	132.16	121.54
1	B	1038	THR	C-N-CA	5.56	132.16	121.54
1	A	198	THR	CA-CB-CG2	5.55	119.93	110.50
1	A	133	THR	O-C-N	5.54	129.19	122.48
1	B	1120	PHE	CA-C-N	5.54	128.58	120.71
1	B	1120	PHE	C-N-CA	5.54	128.58	120.71
1	B	1215	THR	CA-CB-OG1	-5.53	101.30	109.60
1	B	1215	THR	CA-CB-CG2	5.53	119.90	110.50
1	A	274	ILE	CA-C-O	-5.52	115.00	120.85
1	B	1296	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	27	THR	CA-CB-CG2	5.51	119.87	110.50
1	A	157	GLU	CA-C-O	-5.51	115.49	121.44
1	A	84	SER	N-CA-C	5.50	117.75	109.23
1	A	33	ARG	CA-CB-CG	5.50	125.09	114.10
1	A	7	GLN	CA-CB-CG	5.49	125.08	114.10
1	A	343	ALA	N-CA-C	5.49	118.41	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1203	ASP	N-CA-C	5.49	118.19	111.82
1	B	1099	LEU	CA-CB-CG	5.49	135.50	116.30
1	B	1032	LEU	N-CA-C	5.48	122.47	110.80
1	A	253	VAL	CG1-CB-CG2	-5.48	98.75	110.80
1	A	211	GLU	CA-CB-CG	5.48	125.05	114.10
1	B	1216	ALA	CA-C-N	5.47	127.89	120.44
1	B	1216	ALA	C-N-CA	5.47	127.89	120.44
1	B	1340	VAL	CB-CA-C	5.47	117.81	110.42
1	B	1309	ILE	N-CA-CB	5.47	118.96	111.41
1	A	344	ARG	CA-C-N	5.47	131.54	121.70
1	A	344	ARG	C-N-CA	5.47	131.54	121.70
1	B	1087	ILE	N-CA-C	-5.45	106.38	111.45
1	B	1056	ILE	CA-C-N	5.45	131.95	121.54
1	B	1056	ILE	C-N-CA	5.45	131.95	121.54
1	A	112	ILE	CA-CB-CG2	-5.44	101.25	110.50
1	A	337	LYS	CB-CG-CD	5.44	123.82	111.30
1	A	87	ILE	CA-C-O	-5.43	113.99	120.78
1	A	106	TRP	CE2-CD2-CG	-5.42	100.69	107.20
1	A	212	SER	CA-C-O	5.42	126.03	119.31
1	B	1270	ASN	N-CA-C	5.41	122.32	110.80
1	A	168	VAL	CA-C-N	5.40	126.94	120.13
1	A	168	VAL	C-N-CA	5.40	126.94	120.13
1	B	1076	GLN	CA-C-N	5.40	125.32	119.76
1	B	1076	GLN	C-N-CA	5.40	125.32	119.76
1	A	286	VAL	CA-C-N	5.40	129.23	120.60
1	A	286	VAL	C-N-CA	5.40	129.23	120.60
1	A	134	GLY	CA-C-N	5.39	127.77	120.38
1	A	134	GLY	C-N-CA	5.39	127.77	120.38
1	A	335	VAL	N-CA-CB	-5.39	106.28	111.89
1	A	103	ILE	O-C-N	5.38	128.21	122.45
1	A	287	SER	N-CA-C	5.38	118.94	112.38
1	A	303	HIS	CA-C-O	-5.38	114.27	120.24
1	B	1103	ILE	CA-C-O	5.37	127.33	121.04
1	B	1145	ALA	O-C-N	5.37	129.18	122.63
1	B	1147	PHE	CA-C-O	-5.37	114.81	120.55
1	A	70	GLN	CA-C-N	5.35	131.76	121.54
1	A	70	GLN	C-N-CA	5.35	131.76	121.54
1	A	222	PHE	CA-C-N	5.35	125.02	119.56
1	A	222	PHE	C-N-CA	5.35	125.02	119.56
1	B	1334	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	B	1183	VAL	O-C-N	5.34	128.79	123.18
1	A	342	VAL	N-CA-C	-5.33	107.22	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1106	TRP	CA-C-N	5.33	130.98	121.75
1	B	1106	TRP	C-N-CA	5.33	130.98	121.75
1	B	1089	SER	O-C-N	5.33	129.79	123.24
1	B	1231	GLU	CA-CB-CG	5.33	124.75	114.10
1	A	152	SER	CA-C-N	5.32	125.74	119.99
1	A	152	SER	C-N-CA	5.32	125.74	119.99
1	A	117	HIS	N-CA-C	5.32	119.08	112.59
1	A	107	GLU	CA-CB-CG	5.32	124.73	114.10
1	B	1132	TYR	CA-C-N	5.31	130.89	122.60
1	B	1132	TYR	C-N-CA	5.31	130.89	122.60
1	B	1198	THR	CA-CB-CG2	5.31	119.52	110.50
1	A	200	PHE	CA-CB-CG	5.30	119.10	113.80
1	B	1319	LEU	N-CA-C	5.30	118.53	111.75
1	A	35	PRO	CA-C-N	5.30	131.66	121.54
1	A	35	PRO	C-N-CA	5.30	131.66	121.54
1	B	1249	GLY	CA-C-O	-5.30	116.77	121.64
1	A	248	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	B	1172	VAL	O-C-N	5.29	127.09	121.91
1	A	9	ILE	CA-CB-CG2	5.28	119.48	110.50
1	B	1322	ALA	CA-C-N	5.28	126.44	119.84
1	B	1322	ALA	C-N-CA	5.28	126.44	119.84
1	A	50	CYS	CA-C-O	5.27	126.70	120.70
1	A	295	LYS	CA-CB-CG	5.26	124.63	114.10
1	A	261	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	A	50	CYS	O-C-N	5.25	129.84	123.01
1	B	1013	TYR	N-CA-C	5.25	117.84	110.23
1	B	1282	GLN	CB-CG-CD	5.25	121.53	112.60
1	B	1327	VAL	CA-CB-CG1	5.25	119.32	110.40
1	A	82	GLY	O-C-N	5.25	129.52	122.70
1	A	91	HIS	CA-C-N	5.24	124.85	119.56
1	A	91	HIS	C-N-CA	5.24	124.85	119.56
1	A	101	TRP	CB-CG-CD1	-5.24	119.05	126.90
1	B	1054	MET	CA-C-O	-5.23	114.34	120.20
1	B	1337	LYS	O-C-N	5.22	129.15	123.04
1	B	1218	LEU	CD1-CG-CD2	-5.22	99.32	110.80
1	B	1008	VAL	CA-C-O	5.22	125.81	120.39
1	B	1237	MET	CA-CB-CG	-5.21	103.67	114.10
1	B	1302	PRO	N-CA-C	5.21	123.21	112.47
1	B	1009	ILE	CA-CB-CG2	5.21	119.36	110.50
1	B	1192	LYS	N-CA-C	5.21	118.10	111.69
1	B	1322	ALA	CA-C-O	-5.21	113.02	120.16
1	B	1117	HIS	CB-CG-CD2	-5.20	124.44	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	GLY	CA-C-N	5.20	128.21	120.31
1	A	235	GLY	C-N-CA	5.20	128.21	120.31
1	A	35	PRO	N-CA-CB	-5.20	97.79	103.25
1	A	259	GLN	CA-C-N	5.19	127.24	120.28
1	A	259	GLN	C-N-CA	5.19	127.24	120.28
1	B	1008	VAL	CA-C-N	5.18	130.98	122.64
1	B	1008	VAL	C-N-CA	5.18	130.98	122.64
1	B	1033	ARG	CA-C-N	5.17	131.70	122.13
1	B	1033	ARG	C-N-CA	5.17	131.70	122.13
1	A	232	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	B	1050	CYS	CA-C-O	5.15	127.06	120.57
1	A	215	THR	CA-C-N	5.15	128.13	120.31
1	A	215	THR	C-N-CA	5.15	128.13	120.31
1	B	1139	PRO	CA-N-CD	-5.14	104.81	112.00
1	B	1261	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	326	LEU	CA-C-N	5.13	127.13	120.56
1	A	326	LEU	C-N-CA	5.13	127.13	120.56
1	A	219	LYS	CA-C-N	5.12	127.41	120.44
1	A	219	LYS	C-N-CA	5.12	127.41	120.44
1	A	52	PRO	N-CA-C	5.12	120.75	114.35
1	B	1259	GLN	N-CA-C	5.12	119.61	112.90
1	A	6	LYS	CA-CB-CG	5.12	124.33	114.10
1	A	263	GLU	CA-C-N	5.11	128.53	122.44
1	A	263	GLU	C-N-CA	5.11	128.53	122.44
1	B	1005	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	313	GLU	CB-CG-CD	5.10	121.27	112.60
1	B	1120	PHE	N-CA-C	5.10	117.38	108.76
1	B	1217	ALA	CA-C-N	5.09	129.23	120.72
1	B	1217	ALA	C-N-CA	5.09	129.23	120.72
1	B	1236	LYS	CA-CB-CG	5.09	124.28	114.10
1	B	1073	THR	CA-C-N	5.09	126.20	119.84
1	B	1073	THR	C-N-CA	5.09	126.20	119.84
1	A	35	PRO	N-CA-C	5.09	122.95	112.47
1	B	1226	ILE	CA-CB-CG1	5.09	119.05	110.40
1	A	327	VAL	O-C-N	5.08	127.19	121.90
1	B	1271	LEU	CA-C-O	5.08	125.78	119.12
1	A	276	TYR	CA-CB-CG	5.08	123.04	113.90
1	B	1319	LEU	CA-C-N	5.08	127.59	120.28
1	B	1319	LEU	C-N-CA	5.08	127.59	120.28
1	B	1005	ASN	N-CA-C	5.08	117.52	107.98
1	B	1023	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	1135	LEU	N-CA-C	5.07	116.49	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1230	PHE	CA-C-O	5.05	125.80	120.54
1	B	1060	LYS	CA-C-N	5.05	126.16	119.84
1	B	1060	LYS	C-N-CA	5.05	126.16	119.84
1	A	106	TRP	CG-CD2-CE3	5.05	138.95	133.90
1	A	166	GLY	O-C-N	5.04	129.25	122.70
1	A	232	ASN	CA-CB-CG	5.04	117.64	112.60
1	B	1141	MET	CA-C-N	5.04	127.44	120.29
1	B	1141	MET	C-N-CA	5.04	127.44	120.29
1	A	13	TYR	N-CA-C	5.03	117.19	110.35
1	A	113	THR	CA-CB-CG2	5.03	119.05	110.50
1	B	1135	LEU	O-C-N	5.03	127.25	122.07
1	A	273	ASN	CA-C-N	5.02	127.55	120.42
1	A	273	ASN	C-N-CA	5.02	127.55	120.42
1	B	1086	ILE	CG1-CB-CG2	-5.02	95.64	110.70
1	B	1119	HIS	CB-CG-CD2	-5.02	124.68	131.20
1	A	248	HIS	CA-C-O	5.02	127.25	121.28
1	B	1293	TYR	CA-C-N	5.01	126.96	120.44
1	B	1293	TYR	C-N-CA	5.01	126.96	120.44

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	TYR	Sidechain
1	A	34	VAL	Peptide
1	B	1152	SER	Peptide
1	B	1208	TYR	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	2623	0	2594	13	0
1	B	2681	0	2647	19	0
2	A	48	0	25	9	0
2	B	48	0	25	7	0
3	A	11	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	7	1	0
4	A	59	0	0	0	0
4	B	56	0	0	1	0
All	All	5537	0	5305	42	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 4.

All (42) 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)
2:B:2346:NAP:P2B	2:B:2346:NAP:C2B	2.11	1.38
2:A:1346:NAP:P2B	2:A:1346:NAP:C2B	2.15	1.34
2:A:1346:NAP:P2B	2:A:1346:NAP:O2B	0.86	1.26
2:B:2346:NAP:P2B	2:B:2346:NAP:O2B	0.85	1.25
2:B:2346:NAP:O2B	2:B:2346:NAP:O1X	1.78	1.00
2:A:1346:NAP:O2B	2:A:1346:NAP:O1X	1.85	0.94
2:A:1346:NAP:O2B	2:A:1346:NAP:O2X	1.87	0.91
1:B:1174:GLN:HE22	1:B:1310:THR:H	1.27	0.81
2:B:2346:NAP:P2B	2:B:2346:NAP:H2B	2.21	0.80
1:A:282:GLN:NE2	1:B:1278:ARG:HH21	1.82	0.78
2:B:2346:NAP:O2B	2:B:2346:NAP:O3X	1.99	0.75
2:B:2346:NAP:O2B	2:B:2346:NAP:O2X	2.00	0.72
1:A:259:GLN:HE22	1:A:266:GLU:H	1.44	0.65
1:B:1259:GLN:HE22	1:B:1266:GLU:H	1.42	0.65
1:B:1138:MET:HG2	1:B:1290:TYR:OH	1.99	0.63
1:A:282:GLN:HE22	1:B:1278:ARG:HH21	1.46	0.63
2:A:1346:NAP:P2B	2:A:1346:NAP:H2B	2.32	0.63
1:B:1005:ASN:HD21	1:B:1109:TYR:H	1.48	0.61
1:A:170:GLN:HE22	1:A:312:VAL:H	1.53	0.57
1:A:259:GLN:HE22	1:A:266:GLU:N	2.02	0.57
1:A:5:ASN:ND2	1:A:109:TYR:H	2.03	0.57
1:B:1068:LEU:HD11	3:B:2347:HC4:H2	1.87	0.55
1:A:174:GLN:HE22	1:A:310:THR:H	1.55	0.54
1:A:5:ASN:HD21	1:A:109:TYR:H	1.54	0.54
1:B:1014:VAL:HG21	1:B:1058:MET:HE2	1.89	0.54
1:A:286:VAL:H	2:A:1346:NAP:H72N	1.57	0.50
1:B:1167:ALA:HB2	1:B:1337:LYS:HB2	1.94	0.50
1:A:226:ILE:HD12	1:A:241:VAL:HG13	1.94	0.49
1:A:195:LEU:HD21	1:A:312:VAL:HG11	1.94	0.48
2:A:1346:NAP:H2B	2:A:1346:NAP:O3X	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1346:NAP:C2B	2:A:1346:NAP:O3X	2.60	0.47
1:B:1259:GLN:NE2	1:B:1266:GLU:H	2.09	0.46
1:B:1005:ASN:HD22	1:B:1108:GLU:HB2	1.81	0.45
1:B:1279:ASN:HB3	4:B:2042:HOH:O	2.16	0.44
1:A:138:MET:SD	2:A:1346:NAP:H5N	2.58	0.44
1:B:1322:ALA:HB2	1:B:1340:VAL:HG21	2.00	0.44
1:B:1158:THR:HG22	1:B:1182:TYR:HB3	1.99	0.43
1:B:1096:LYS:HD2	1:B:1096:LYS:H	1.84	0.43
1:B:1134:GLY:HA3	1:B:1311:TYR:OH	2.20	0.42
1:B:1167:ALA:HB3	2:B:2346:NAP:O2N	2.20	0.42
1:A:271:LEU:HD11	1:B:1271:LEU:HD11	2.02	0.42
1:B:1005:ASN:ND2	1:B:1109:TYR:H	2.15	0.41

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	332/345 (96%)	299 (90%)	24 (7%)	9 (3%)	4	15
1	B	343/345 (99%)	302 (88%)	33 (10%)	8 (2%)	5	18
All	All	675/690 (98%)	601 (89%)	57 (8%)	17 (2%)	4	16

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ALA
1	A	128	PRO
1	A	129	LEU
1	A	167	ALA
1	B	1039	ASN
1	B	1070	GLN

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Mol	Chain	Res	Type
1	B	1154	LYS
1	B	1167	ALA
1	A	38	THR
1	A	258	SER
1	B	1032	LEU
1	A	191	GLU
1	B	1068	LEU
1	A	35	PRO
1	A	36	GLU
1	B	1061	PRO
1	B	1270	ASN

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	283/289 (98%)	234 (83%)	49 (17%)	2	7
1	B	289/289 (100%)	243 (84%)	46 (16%)	2	9
All	All	572/578 (99%)	477 (83%)	95 (17%)	2	8

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	LYS
1	A	9	ILE
1	A	11	LYS
1	A	14	VAL
1	A	23	PHE
1	A	26	THR
1	A	31	GLU
1	A	34	VAL
1	A	42	LEU
1	A	43	VAL
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	55	ARG
1	A	99	LEU
1	A	111	VAL
1	A	112	ILE
1	A	125	THR
1	A	127	VAL
1	A	129	LEU
1	A	135	LEU
1	A	139	PRO
1	A	161	VAL
1	A	177	LYS
1	A	179	MET
1	A	183	VAL
1	A	190	LYS
1	A	197	LYS
1	A	199	LYS
1	A	218	LEU
1	A	219	LYS
1	A	226	ILE
1	A	239	ASP
1	A	242	LEU
1	A	246	ASN
1	A	247	MET
1	A	250	ARG
1	A	257	ILE
1	A	261	ASN
1	A	264	ASN
1	A	280	ARG
1	A	282	GLN
1	A	298	GLU
1	A	301	LEU
1	A	315	VAL
1	A	317	ASP
1	A	324	GLU
1	A	326	LEU
1	A	337	LYS
1	A	345	GLU
1	B	1009	ILE
1	B	1020	GLU
1	B	1029	THR
1	B	1032	LEU
1	B	1034	VAL

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Mol	Chain	Res	Type
1	B	1048	LEU
1	B	1055	ARG
1	B	1056	ILE
1	B	1060	LYS
1	B	1070	GLN
1	B	1079	GLN
1	B	1088	GLU
1	B	1115	MET
1	B	1139	PRO
1	B	1154	LYS
1	B	1171	LEU
1	B	1175	LEU
1	B	1183	VAL
1	B	1196	LEU
1	B	1199	LYS
1	B	1202	PHE
1	B	1209	LYS
1	B	1210	GLU
1	B	1214	LEU
1	B	1219	LYS
1	B	1226	ILE
1	B	1237	MET
1	B	1245	MET
1	B	1250	ARG
1	B	1257	ILE
1	B	1264	ASN
1	B	1271	LEU
1	B	1272	SER
1	B	1273	ASN
1	B	1282	GLN
1	B	1286	VAL
1	B	1300	VAL
1	B	1302	PRO
1	B	1317	ASP
1	B	1321	LYS
1	B	1324	GLU
1	B	1326	LEU
1	B	1333	LYS
1	B	1337	LYS
1	B	1340	VAL
1	B	1344	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	7	GLN
1	A	45	ASN
1	A	79	GLN
1	A	170	GLN
1	A	174	GLN
1	A	248	HIS
1	A	259	GLN
1	A	273	ASN
1	A	282	GLN
1	A	331	HIS
1	B	1005	ASN
1	B	1007	GLN
1	B	1123	GLN
1	B	1170	GLN
1	B	1174	GLN
1	B	1259	GLN
1	B	1261	ASN
1	B	1273	ASN
1	B	1279	ASN
1	B	1334	ASN
1	B	1338	GLN

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](#)

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	HC4	B	2347	-	11,11,12	2.99	8 (72%)	13,13,15	2.10	2 (15%)
2	NAP	A	1346	-	50,52,52	6.18	11 (22%)	71,80,80	2.25	23 (32%)
3	HC4	A	1347	-	11,11,12	3.04	8 (72%)	13,13,15	2.09	2 (15%)
2	NAP	B	2346	-	50,52,52	6.18	9 (18%)	71,80,80	2.17	24 (33%)

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	HC4	B	2347	-	-	0/4/4/5	0/1/1/1
2	NAP	A	1346	-	-	14/35/67/67	0/5/5/5
3	HC4	A	1347	-	-	0/4/4/5	0/1/1/1
2	NAP	B	2346	-	-	8/35/67/67	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2346	NAP	P2B-O2B	-42.16	0.85	1.59
2	A	1346	NAP	P2B-O2B	-41.62	0.86	1.59
3	B	2347	HC4	C2-C3	-6.80	1.21	1.34
3	A	1347	HC4	C2-C3	-6.66	1.21	1.34
2	A	1346	NAP	C2N-N1N	6.18	1.41	1.35
2	A	1346	NAP	PN-O3	5.76	1.65	1.59
2	B	2346	NAP	C2N-N1N	5.16	1.40	1.35
2	B	2346	NAP	PA-O3	4.19	1.64	1.59
2	A	1346	NAP	C5A-N7A	-3.78	1.32	1.39
2	B	2346	NAP	C5A-N7A	-3.74	1.32	1.39
2	B	2346	NAP	C6N-N1N	3.65	1.43	1.35
2	A	1346	NAP	PA-O3	3.54	1.63	1.59
2	A	1346	NAP	C6N-N1N	3.33	1.42	1.35
3	A	1347	HC4	C6'-C5'	3.17	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1347	HC4	C5'-C4'	3.12	1.44	1.39
3	A	1347	HC4	C3'-C4'	3.09	1.44	1.39
2	A	1346	NAP	O4D-C1D	3.06	1.44	1.40
3	B	2347	HC4	C3'-C4'	3.03	1.44	1.39
3	B	2347	HC4	C6'-C5'	3.03	1.43	1.38
3	B	2347	HC4	C5'-C4'	3.03	1.44	1.39
2	B	2346	NAP	PN-O3	2.94	1.62	1.59
3	A	1347	HC4	C6'-C1'	2.76	1.45	1.39
3	B	2347	HC4	C6'-C1'	2.64	1.44	1.39
2	B	2346	NAP	O4D-C1D	2.55	1.44	1.40
2	A	1346	NAP	C3N-C7N	2.50	1.54	1.50
3	A	1347	HC4	C3'-C2'	2.46	1.42	1.38
3	A	1347	HC4	C2-C1	2.37	1.51	1.44
3	B	2347	HC4	C3'-C2'	2.32	1.42	1.38
2	B	2346	NAP	C3N-C7N	2.24	1.53	1.50
3	B	2347	HC4	C2-C1	2.22	1.50	1.44
2	A	1346	NAP	PN-O5D	2.20	1.68	1.59
3	A	1347	HC4	C2'-C1'	2.15	1.43	1.39
2	A	1346	NAP	C5D-C4D	2.10	1.57	1.51
2	B	2346	NAP	C4N-C3N	2.08	1.42	1.39
2	A	1346	NAP	C1B-N9A	2.05	1.52	1.46
3	B	2347	HC4	C2'-C1'	2.00	1.43	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1346	NAP	O5D-C5D-C4D	6.93	132.59	108.99
2	A	1346	NAP	C5A-C4A-N3A	-6.60	117.63	126.72
3	A	1347	HC4	C1'-C3-C2	-6.28	116.24	127.11
2	B	2346	NAP	C5A-C4A-N3A	-6.27	118.08	126.72
2	A	1346	NAP	N3A-C4A-N9A	6.21	137.74	127.17
2	B	2346	NAP	N3A-C4A-N9A	6.02	137.41	127.17
3	B	2347	HC4	C1'-C3-C2	-6.01	116.70	127.11
2	A	1346	NAP	N3A-C2A-N1A	-4.96	121.07	128.58
2	B	2346	NAP	N3A-C2A-N1A	-4.96	121.08	128.58
2	B	2346	NAP	O5D-C5D-C4D	4.66	124.88	108.99
2	A	1346	NAP	O4D-C4D-C3D	-4.29	96.63	105.15
2	B	2346	NAP	C6N-N1N-C1D	4.05	127.67	119.73
3	B	2347	HC4	C3-C2-C1	-3.90	109.95	121.11
2	B	2346	NAP	O2B-P2B-O1X	-3.86	95.56	109.33
2	A	1346	NAP	C6A-C5A-N7A	-3.82	124.73	132.09
2	A	1346	NAP	C4D-O4D-C1D	3.78	113.39	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1346	NAP	C2A-N3A-C4A	3.77	121.04	111.83
2	B	2346	NAP	C2A-N3A-C4A	3.77	121.04	111.83
3	A	1347	HC4	C3-C2-C1	-3.60	110.82	121.11
2	B	2346	NAP	O4B-C1B-N9A	3.50	114.81	108.09
2	A	1346	NAP	O3X-P2B-O2B	3.43	119.22	105.85
2	B	2346	NAP	C2N-N1N-C1D	-3.40	111.64	119.13
2	A	1346	NAP	C6A-C5A-C4A	3.29	121.67	117.18
2	B	2346	NAP	C6A-C5A-N7A	-3.29	125.75	132.09
2	B	2346	NAP	O4B-C4B-C3B	-3.16	98.88	105.15
2	A	1346	NAP	P2B-O2B-C2B	3.11	131.74	123.43
2	A	1346	NAP	C6N-N1N-C1D	3.05	125.71	119.73
2	A	1346	NAP	O7N-C7N-C3N	3.03	123.31	119.60
2	B	2346	NAP	C6A-C5A-C4A	2.88	121.11	117.18
2	B	2346	NAP	O4B-C1B-C2B	-2.84	101.70	106.59
2	B	2346	NAP	C4D-O4D-C1D	2.82	112.50	109.92
2	B	2346	NAP	O4B-C4B-C5B	-2.78	100.42	109.33
2	A	1346	NAP	C4A-C5A-N7A	2.64	113.60	110.58
2	B	2346	NAP	O4D-C4D-C5D	2.62	117.71	109.33
2	B	2346	NAP	C5N-C4N-C3N	2.61	122.93	120.36
2	A	1346	NAP	C2B-C1B-N9A	2.60	118.03	113.75
2	A	1346	NAP	O3-PN-O1N	-2.54	103.06	110.70
2	A	1346	NAP	O3B-C3B-C2B	2.52	118.23	111.19
2	A	1346	NAP	C5N-C4N-C3N	2.49	122.82	120.36
2	A	1346	NAP	C2N-N1N-C1D	-2.45	113.72	119.13
2	B	2346	NAP	O2X-P2B-O2B	2.41	115.24	105.85
2	B	2346	NAP	C2B-C1B-N9A	2.38	117.68	113.75
2	A	1346	NAP	C3N-C7N-N7N	-2.31	114.90	117.74
2	B	2346	NAP	O3-PA-O1A	-2.28	103.83	110.70
2	A	1346	NAP	O4D-C4D-C5D	2.24	116.50	109.33
2	B	2346	NAP	C4A-C5A-N7A	2.23	113.14	110.58
2	B	2346	NAP	O3X-P2B-O2B	2.21	114.46	105.85
2	A	1346	NAP	O2B-P2B-O1X	-2.10	101.84	109.33
2	A	1346	NAP	C2A-N1A-C6A	2.07	122.12	118.73
2	B	2346	NAP	O2A-PA-O1A	2.01	121.82	112.44
2	B	2346	NAP	C5B-C4B-C3B	2.01	122.46	115.21

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1346	NAP	C5B-O5B-PA-O1A
2	A	1346	NAP	C5B-O5B-PA-O2A

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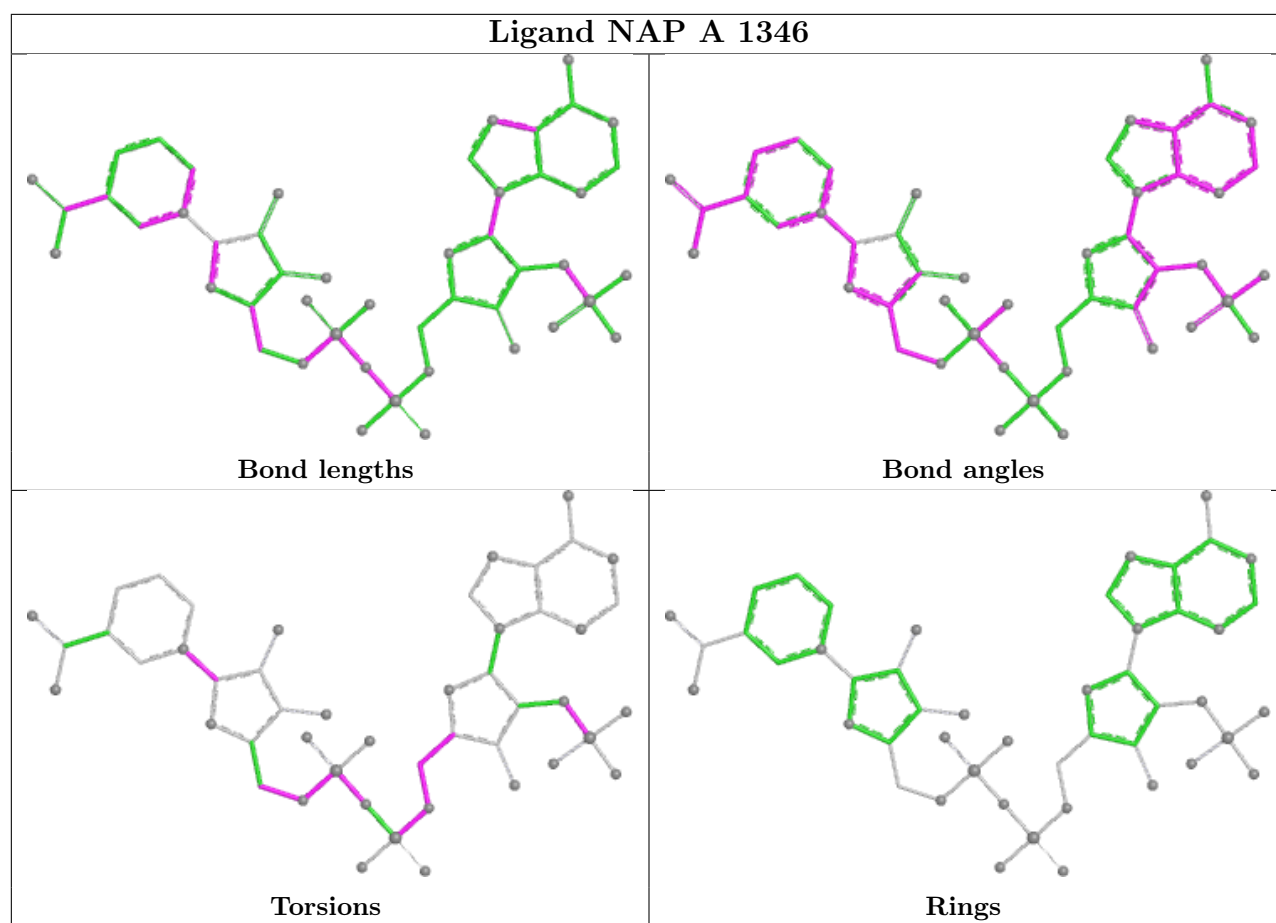
Mol	Chain	Res	Type	Atoms
2	A	1346	NAP	C5B-O5B-PA-O3
2	A	1346	NAP	C5D-O5D-PN-O3
2	A	1346	NAP	C5D-O5D-PN-O1N
2	A	1346	NAP	C4D-C5D-O5D-PN
2	A	1346	NAP	O4D-C1D-N1N-C6N
2	B	2346	NAP	O4D-C4D-C5D-O5D
2	B	2346	NAP	O4D-C1D-N1N-C6N
2	B	2346	NAP	C3D-C4D-C5D-O5D
2	A	1346	NAP	C3B-C4B-C5B-O5B
2	A	1346	NAP	O4B-C4B-C5B-O5B
2	A	1346	NAP	PA-O3-PN-O5D
2	B	2346	NAP	C4N-C3N-C7N-O7N
2	A	1346	NAP	C5D-O5D-PN-O2N
2	B	2346	NAP	C5D-O5D-PN-O1N
2	A	1346	NAP	C4B-C5B-O5B-PA
2	B	2346	NAP	C4B-C5B-O5B-PA
2	A	1346	NAP	O4D-C1D-N1N-C2N
2	B	2346	NAP	O4D-C1D-N1N-C2N
2	B	2346	NAP	O4B-C4B-C5B-O5B
2	A	1346	NAP	C2B-O2B-P2B-O1X

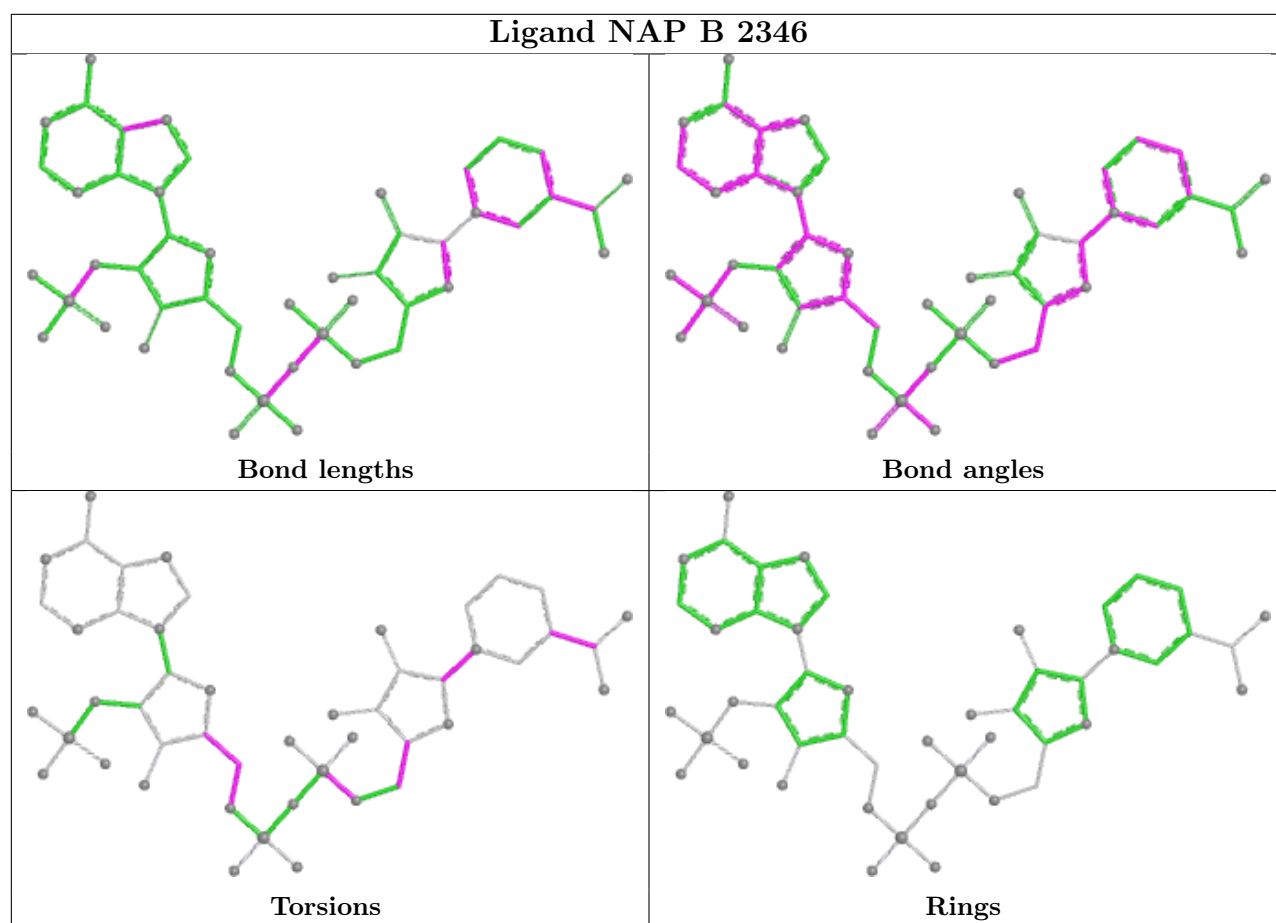
There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2347	HC4	1	0
2	A	1346	NAP	9	0
2	B	2346	NAP	7	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.