



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:22 PM UTC

PDB ID : 2J3K / pdb_00002j3k
Title : Crystal structure of Arabidopsis thaliana Double Bond Reductase (AT5G16970)-Ternary Complex II
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 : 2006-08-22
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

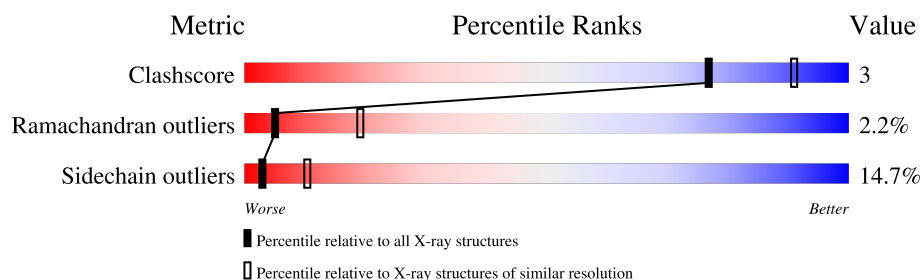
1 Overall quality at a glance

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	 44% 43% 10% . .
1	B	345	 44% 42% 13% .

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.

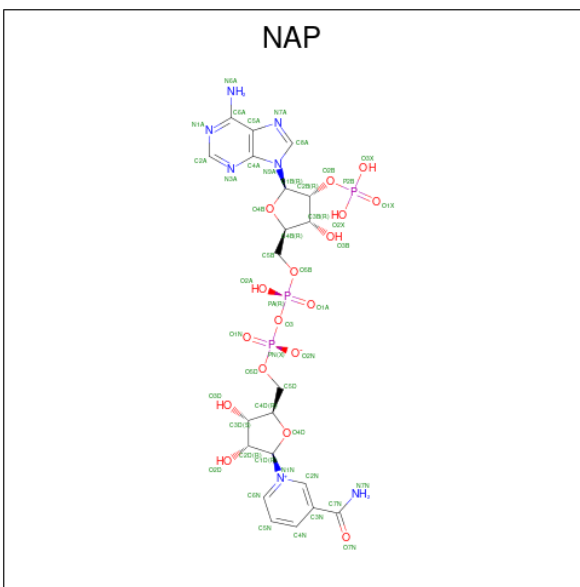
- Molecule 1 is a protein called NADPH-dependent oxidoreductase 2-alkenal reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total 2623	C 1681	N 432	O 493	S 17	0	0	0
1	B	345	Total 2681	C 1717	N 441	O 506	S 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: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



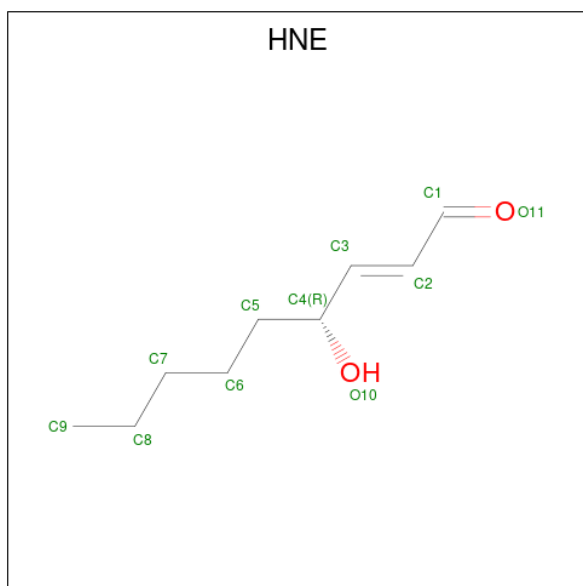
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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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 (2E,4R)-4-HYDROXYNON-2-ENAL (CCD ID: HNE) (formula: C₉H₁₆O₂).



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.

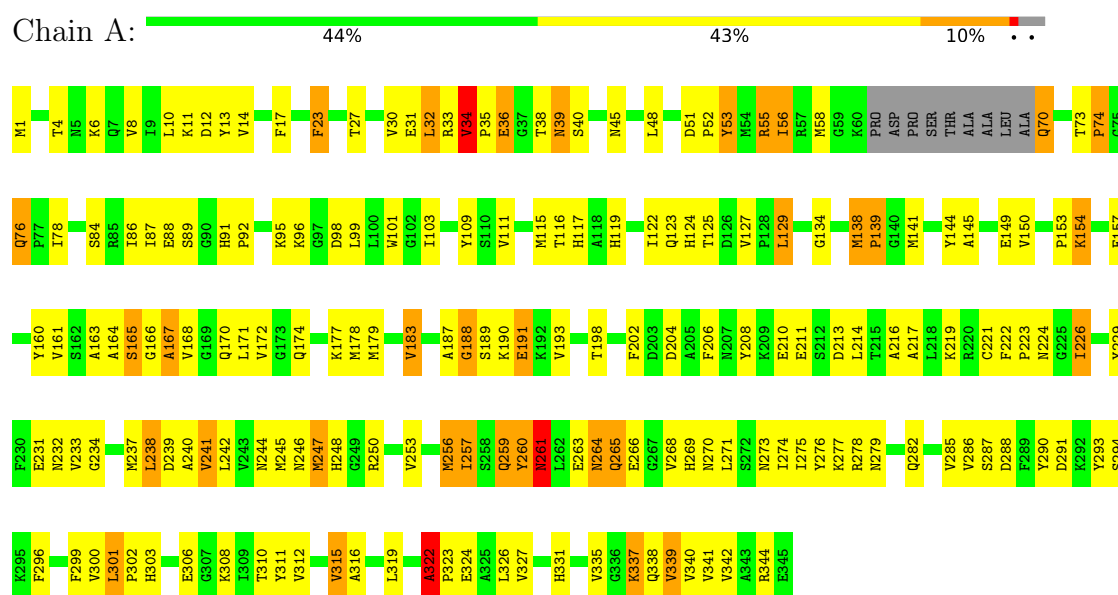
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	72	Total	O	0	0
			72	72		

3 Residue-property plots

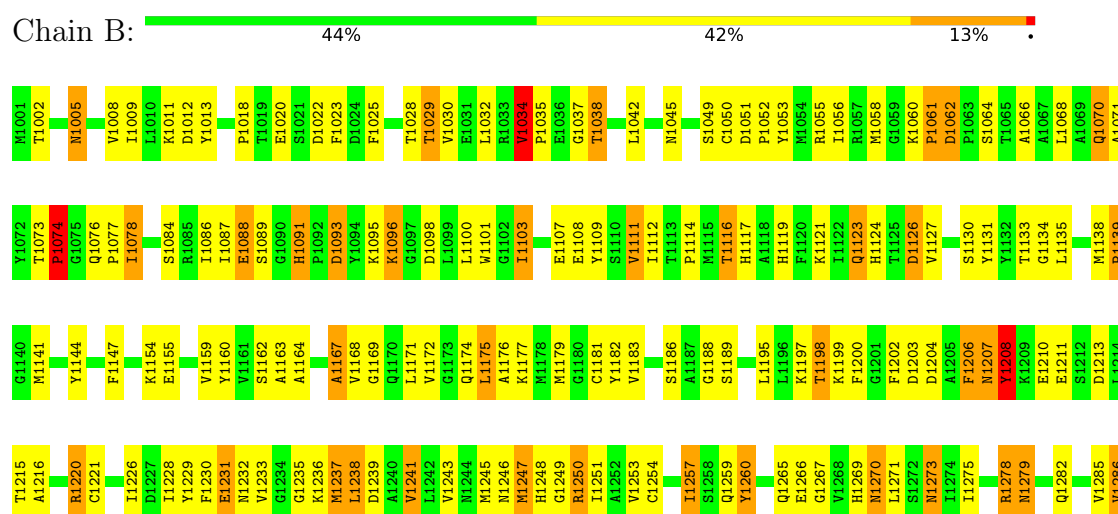
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



S1287	D1288	F1289	Y1290	D1291	K1292	Y1293
F1296	L1297	E1298	F1299	V1300	L1301	P1302
H1303	I1304	R1305	E1306	I1309	T1310	Y1311
V1312	E1313	D1314	D1317	G1318	L1319	A1322
P1323	E1324	H1331	H1334	K1337	Q1338	V1339
V1340	V1341	V1342	A1343	R1344	E1345	

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	49.08 Å 122.45 Å 147.84 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	82.6 (15.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5556	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: HNE, 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	1.42	26/2681 (1.0%)	2.59	235/3625 (6.5%)
1	B	1.45	25/2742 (0.9%)	2.62	241/3713 (6.5%)
All	All	1.44	51/5423 (0.9%)	2.61	476/7338 (6.5%)

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	4
1	B	0	6
All	All	0	10

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1086	ILE	CA-CB	9.10	1.64	1.53
1	B	1119	HIS	CD2-NE2	-8.12	1.28	1.37
1	A	256	MET	CA-CB	8.10	1.59	1.53
1	A	111	VAL	CA-CB	7.52	1.62	1.54
1	A	91	HIS	CD2-NE2	-7.42	1.29	1.37
1	B	1269	HIS	CD2-NE2	-7.31	1.29	1.37
1	B	1103	ILE	CA-CB	7.18	1.62	1.53
1	B	1309	ILE	CA-CB	7.12	1.63	1.54
1	B	1091	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	119	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	274	ILE	CA-CB	6.92	1.63	1.54
1	A	303	HIS	CD2-NE2	-6.89	1.30	1.37
1	B	1248	HIS	CD2-NE2	-6.89	1.30	1.37
1	B	1111	VAL	CA-CB	6.77	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1303	HIS	CD2-NE2	-6.75	1.30	1.37
1	B	1251	ILE	CA-CB	6.70	1.63	1.54
1	B	1078	ILE	CA-CB	6.52	1.63	1.53
1	B	1159	VAL	CA-CB	6.49	1.62	1.54
1	A	127	VAL	CA-CB	6.46	1.62	1.54
1	A	331	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	87	ILE	CA-CB	6.33	1.62	1.54
1	A	269	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	248	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	1253	VAL	CA-CB	6.17	1.60	1.53
1	B	1119	HIS	CG-ND1	-6.15	1.31	1.38
1	B	1117	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	1331	HIS	CD2-NE2	-6.07	1.31	1.37
1	A	124	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	103	ILE	CA-CB	5.94	1.60	1.53
1	A	117	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	78	ILE	CA-CB	5.88	1.61	1.54
1	B	1228	ILE	CA-CB	5.83	1.61	1.54
1	B	1124	HIS	CD2-NE2	-5.82	1.31	1.37
1	B	1243	VAL	CA-CB	5.79	1.61	1.54
1	A	8	VAL	CA-CB	5.66	1.60	1.53
1	A	56	ILE	CA-CB	5.66	1.62	1.54
1	A	86	ILE	CA-CB	5.65	1.61	1.54
1	A	303	HIS	CG-ND1	-5.64	1.32	1.38
1	B	1300	VAL	CA-CB	5.55	1.61	1.54
1	A	125	THR	CA-CB	5.42	1.62	1.53
1	B	1304	ILE	CA-CB	5.37	1.60	1.54
1	B	1341	VAL	CA-CB	5.37	1.60	1.53
1	B	1034	VAL	CA-CB	5.32	1.61	1.54
1	A	34	VAL	CA-CB	5.25	1.60	1.54
1	A	341	VAL	CA-CB	5.18	1.60	1.54
1	B	1182	TYR	CA-CB	5.16	1.59	1.53
1	A	119	HIS	CG-ND1	-5.14	1.32	1.38
1	A	91	HIS	CG-ND1	-5.10	1.32	1.38
1	A	248	HIS	CG-ND1	-5.09	1.32	1.38
1	B	1248	HIS	CG-ND1	-5.06	1.32	1.38
1	A	256	MET	C-N	5.02	1.39	1.34

All (476) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1181	CYS	N-CA-C	11.82	126.43	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ASN	CA-CB-CG	11.35	123.95	112.60
1	A	23	PHE	CA-CB-CG	11.10	124.89	113.80
1	A	164	ALA	CA-C-N	10.69	134.33	120.44
1	A	164	ALA	C-N-CA	10.69	134.33	120.44
1	A	315	VAL	N-CA-C	10.19	126.66	112.50
1	B	1138	MET	CA-C-O	-9.97	106.50	120.16
1	A	279	ASN	CA-CB-CG	9.85	122.45	112.60
1	B	1301	LEU	CA-C-O	-9.67	106.91	120.16
1	A	214	LEU	N-CA-C	9.59	122.74	111.71
1	A	335	VAL	CA-C-N	9.52	129.96	121.86
1	A	335	VAL	C-N-CA	9.52	129.96	121.86
1	B	1103	ILE	N-CA-CB	-9.47	102.87	112.06
1	A	98	ASP	CA-CB-CG	9.43	122.03	112.60
1	A	296	PHE	CA-CB-CG	9.34	123.14	113.80
1	B	1279	ASN	CA-CB-CG	9.25	121.85	112.60
1	A	206	PHE	CA-CB-CG	9.21	123.00	113.80
1	A	291	ASP	CA-CB-CG	9.20	121.80	112.60
1	A	89	SER	N-CA-C	9.15	124.62	109.06
1	B	1052	PRO	N-CA-C	9.15	125.18	114.20
1	B	1232	ASN	CA-CB-CG	9.12	121.72	112.60
1	B	1334	ASN	CA-CB-CG	9.05	121.65	112.60
1	B	1291	ASP	CA-CB-CG	8.91	121.51	112.60
1	A	52	PRO	N-CA-C	8.80	124.86	114.03
1	B	1093	ASP	CA-CB-CG	8.75	121.35	112.60
1	B	1288	ASP	CA-CB-CG	8.71	121.31	112.60
1	B	1116	THR	N-CA-C	8.62	121.76	111.33
1	B	1267	GLY	O-C-N	8.53	129.66	123.35
1	B	1199	LYS	N-CA-C	8.53	120.57	111.28
1	B	1013	TYR	N-CA-C	8.52	122.26	110.24
1	B	1029	THR	CA-CB-OG1	-8.51	96.83	109.60
1	A	39	ASN	CA-CB-CG	8.49	121.09	112.60
1	B	1342	VAL	N-CA-C	-8.43	104.56	111.81
1	A	204	ASP	CA-CB-CG	8.41	121.01	112.60
1	A	273	ASN	CA-CB-CG	8.33	120.93	112.60
1	B	1126	ASP	CA-CB-CG	8.29	120.89	112.60
1	A	92	PRO	N-CA-C	8.28	124.49	113.40
1	B	1029	THR	CA-CB-CG2	8.17	124.40	110.50
1	B	1045	ASN	CA-CB-CG	8.13	120.73	112.60
1	A	198	THR	CA-CB-OG1	-8.11	97.44	109.60
1	B	1076	GLN	CA-C-N	8.04	129.89	119.84
1	B	1076	GLN	C-N-CA	8.04	129.89	119.84
1	B	1167	ALA	N-CA-C	8.03	127.90	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1231	GLU	CA-CB-CG	8.02	130.14	114.10
1	B	1289	PHE	CA-CB-CG	8.01	121.81	113.80
1	A	312	VAL	CG1-CB-CG2	-8.00	93.20	110.80
1	A	139	PRO	N-CA-C	7.99	124.44	113.65
1	B	1253	VAL	CA-C-O	7.93	130.41	120.97
1	A	40	SER	N-CA-C	7.92	121.79	110.14
1	A	275	ILE	CA-C-N	7.88	131.05	120.65
1	A	275	ILE	C-N-CA	7.88	131.05	120.65
1	A	198	THR	CA-CB-CG2	7.87	123.88	110.50
1	B	1270	ASN	N-CA-C	7.83	122.83	110.70
1	B	1114	PRO	O-C-N	7.72	131.75	123.10
1	A	99	LEU	N-CA-C	7.71	122.00	109.59
1	B	1299	PHE	CA-CB-CG	7.66	121.46	113.80
1	B	1208	TYR	CA-C-N	7.64	130.83	120.44
1	B	1208	TYR	C-N-CA	7.64	130.83	120.44
1	A	187	ALA	CA-C-N	7.61	128.23	119.94
1	A	187	ALA	C-N-CA	7.61	128.23	119.94
1	B	1023	PHE	CA-CB-CG	7.56	121.36	113.80
1	B	1232	ASN	OD1-CG-ND2	-7.55	115.05	122.60
1	B	1253	VAL	CG1-CB-CG2	-7.55	94.20	110.80
1	B	1290	TYR	N-CA-C	7.50	122.12	113.19
1	A	163	ALA	CA-C-N	7.46	131.65	120.31
1	A	163	ALA	C-N-CA	7.46	131.65	120.31
1	A	216	ALA	CA-C-N	7.44	130.85	120.29
1	A	216	ALA	C-N-CA	7.44	130.85	120.29
1	B	1103	ILE	CA-C-O	7.42	129.56	121.70
1	B	1265	GLN	CA-CB-CG	-7.38	99.33	114.10
1	A	259	GLN	N-CA-C	7.33	122.90	113.88
1	B	1139	PRO	CA-N-CD	-7.32	101.75	112.00
1	A	301	LEU	CA-C-O	-7.32	110.14	120.16
1	B	1032	LEU	CA-C-N	7.30	131.08	120.71
1	B	1032	LEU	C-N-CA	7.30	131.08	120.71
1	B	1073	THR	CA-C-N	7.29	128.96	119.84
1	B	1073	THR	C-N-CA	7.29	128.96	119.84
1	B	1207	ASN	CA-CB-CG	7.28	119.88	112.60
1	A	116	THR	N-CA-C	7.27	123.36	111.37
1	B	1331	HIS	N-CA-C	-7.27	103.42	112.72
1	B	1319	LEU	CA-C-N	7.26	130.33	120.38
1	B	1319	LEU	C-N-CA	7.26	130.33	120.38
1	B	1163	ALA	CA-C-O	7.25	130.51	122.03
1	A	239	ASP	CA-CB-CG	7.24	119.84	112.60
1	A	145	ALA	N-CA-C	7.23	119.16	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1028	THR	CA-CB-OG1	-7.23	98.75	109.60
1	A	202	PHE	CA-CB-CG	7.21	121.01	113.80
1	A	231	GLU	CA-CB-CG	7.20	128.49	114.10
1	A	213	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	269	HIS	N-CA-C	7.18	122.18	113.41
1	B	1206	PHE	CA-CB-CG	7.18	120.98	113.80
1	A	219	LYS	CA-CB-CG	7.17	128.43	114.10
1	B	1028	THR	CA-CB-CG2	7.15	122.66	110.50
1	A	342	VAL	N-CA-C	-7.14	105.67	111.81
1	A	265	GLN	N-CA-C	7.12	121.45	110.20
1	A	73	THR	CA-C-N	7.12	128.74	119.84
1	A	73	THR	C-N-CA	7.12	128.74	119.84
1	A	319	LEU	CA-C-N	7.02	129.99	120.44
1	A	319	LEU	C-N-CA	7.02	129.99	120.44
1	B	1236	LYS	CA-CB-CG	7.01	128.13	114.10
1	B	1230	PHE	CA-C-O	6.99	127.81	120.54
1	B	1257	ILE	CB-CA-C	-6.97	98.47	111.79
1	A	323	PRO	CA-C-N	6.97	129.93	120.38
1	A	323	PRO	C-N-CA	6.97	129.93	120.38
1	B	1278	ARG	N-CA-C	6.95	121.08	111.90
1	A	165	SER	O-C-N	6.95	129.23	122.07
1	A	274	ILE	CG1-CB-CG2	-6.93	89.91	110.70
1	A	239	ASP	CA-C-N	6.93	130.13	120.29
1	A	239	ASP	C-N-CA	6.93	130.13	120.29
1	A	246	ASN	CA-CB-CG	6.92	119.52	112.60
1	B	1248	HIS	CB-CG-CD2	-6.92	122.20	131.20
1	A	103	ILE	O-C-N	6.92	130.22	122.68
1	A	238	LEU	CA-C-O	-6.92	113.22	120.55
1	A	279	ASN	N-CA-C	6.91	121.56	109.96
1	B	1286	VAL	CB-CA-C	-6.86	101.14	112.26
1	B	1037	GLY	CA-C-N	6.86	134.65	121.54
1	B	1037	GLY	C-N-CA	6.86	134.65	121.54
1	A	269	HIS	CB-CG-CD2	-6.81	122.34	131.20
1	B	1233	VAL	N-CA-C	6.81	123.51	109.34
1	A	288	ASP	CA-CB-CG	6.80	119.41	112.60
1	B	1141	MET	CA-C-N	6.78	129.37	120.28
1	B	1141	MET	C-N-CA	6.78	129.37	120.28
1	A	303	HIS	CB-CG-CD2	-6.78	122.39	131.20
1	B	1135	LEU	N-CA-C	6.78	119.25	111.11
1	A	300	VAL	CA-C-O	-6.76	112.95	120.25
1	B	1005	ASN	CA-CB-CG	6.73	119.33	112.60
1	B	1172	VAL	O-C-N	6.70	128.37	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	LYS	CA-C-N	6.68	131.88	122.46
1	A	277	LYS	C-N-CA	6.68	131.88	122.46
1	B	1062	ASP	CA-C-N	6.68	126.31	119.56
1	B	1062	ASP	C-N-CA	6.68	126.31	119.56
1	A	232	ASN	OD1-CG-ND2	-6.68	115.92	122.60
1	B	1266	GLU	CA-CB-CG	6.66	127.42	114.10
1	A	338	GLN	N-CA-C	6.65	119.69	107.99
1	A	178	MET	N-CA-C	-6.64	107.05	114.62
1	B	1035	PRO	N-CA-C	6.62	121.35	110.55
1	B	1313	GLU	CA-CB-CG	6.62	127.33	114.10
1	A	224	ASN	CA-CB-CG	6.59	119.19	112.60
1	A	245	MET	N-CA-C	6.57	118.49	110.41
1	B	1162	SER	CA-C-N	6.56	131.71	122.46
1	B	1162	SER	C-N-CA	6.56	131.71	122.46
1	B	1168	VAL	N-CA-C	-6.53	105.38	111.45
1	B	1096	LYS	N-CA-C	6.51	124.66	110.80
1	A	211	GLU	CA-C-O	6.50	127.41	120.46
1	B	1164	ALA	N-CA-C	6.49	120.46	112.54
1	A	6	LYS	CA-CB-CG	6.48	127.07	114.10
1	A	172	VAL	O-C-N	6.48	128.16	121.87
1	A	141	MET	CA-C-N	6.48	129.61	120.28
1	A	141	MET	C-N-CA	6.48	129.61	120.28
1	B	1304	ILE	N-CA-C	-6.47	104.85	110.74
1	B	1005	ASN	N-CA-C	6.47	119.78	107.75
1	A	188	GLY	N-CA-C	6.46	120.31	112.49
1	B	1239	ASP	N-CA-C	6.46	119.14	111.71
1	B	1053	TYR	CA-C-O	6.46	127.40	119.97
1	B	1103	ILE	N-CA-C	6.46	115.92	106.55
1	B	1278	ARG	CA-C-N	6.46	130.04	120.87
1	B	1278	ARG	C-N-CA	6.46	130.04	120.87
1	B	1236	LYS	CA-C-N	6.45	129.21	120.44
1	B	1236	LYS	C-N-CA	6.45	129.21	120.44
1	A	74	PRO	CA-N-CD	-6.40	103.04	112.00
1	A	276	TYR	CA-CB-CG	6.39	125.41	113.90
1	B	1111	VAL	N-CA-CB	6.37	119.24	111.60
1	B	1344	ARG	CA-C-N	6.37	133.16	121.70
1	B	1344	ARG	C-N-CA	6.37	133.16	121.70
1	B	1215	THR	CA-CB-OG1	-6.36	100.06	109.60
1	A	286	VAL	CA-C-N	6.35	129.66	120.38
1	A	286	VAL	C-N-CA	6.35	129.66	120.38
1	A	101	TRP	CA-CB-CG	6.33	125.63	113.60
1	A	153	PRO	N-CA-C	6.30	124.11	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1123	GLN	CB-CG-CD	6.29	123.30	112.60
1	A	287	SER	N-CA-C	6.29	119.80	111.75
1	B	1175	LEU	CA-C-N	6.29	128.99	120.44
1	B	1175	LEU	C-N-CA	6.29	128.99	120.44
1	B	1302	PRO	N-CA-C	6.29	122.93	113.81
1	B	1286	VAL	CA-CB-CG1	-6.28	99.72	110.40
1	B	1200	PHE	CA-CB-CG	6.27	120.07	113.80
1	B	1070	GLN	CA-C-N	6.27	133.51	121.54
1	B	1070	GLN	C-N-CA	6.27	133.51	121.54
1	B	1345	GLU	CA-CB-CG	6.27	126.64	114.10
1	B	1087	ILE	CA-C-N	6.26	133.50	121.54
1	B	1087	ILE	C-N-CA	6.26	133.50	121.54
1	A	84	SER	N-CA-C	6.25	119.44	108.75
1	B	1098	ASP	CA-CB-CG	6.25	118.85	112.60
1	A	312	VAL	CA-CB-CG1	6.23	121.00	110.40
1	B	1285	VAL	CG1-CB-CG2	-6.23	97.10	110.80
1	B	1064	SER	CA-C-N	6.22	129.13	120.29
1	B	1064	SER	C-N-CA	6.22	129.13	120.29
1	B	1305	ARG	CB-CG-CD	-6.22	97.00	111.30
1	A	322	ALA	CA-C-N	6.21	125.43	118.97
1	A	322	ALA	C-N-CA	6.21	125.43	118.97
1	A	264	ASN	O-C-N	6.21	130.29	122.84
1	B	1271	LEU	CA-C-N	6.21	131.23	120.68
1	B	1271	LEU	C-N-CA	6.21	131.23	120.68
1	A	257	ILE	CB-CG1-CD1	6.20	126.82	113.80
1	A	144	TYR	CA-C-N	6.19	128.57	120.28
1	A	144	TYR	C-N-CA	6.19	128.57	120.28
1	B	1077	PRO	N-CA-C	6.19	125.21	112.47
1	A	226	ILE	CA-CB-CG2	-6.18	99.99	110.50
1	B	1237	MET	CG-SD-CE	-6.18	87.30	100.90
1	B	1220	ARG	CA-CB-CG	6.18	126.46	114.10
1	B	1012	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	36	GLU	CA-CB-CG	6.16	126.42	114.10
1	A	74	PRO	N-CA-C	6.15	125.15	112.47
1	B	1317	ASP	N-CA-C	6.15	118.74	108.96
1	B	1202	PHE	CA-CB-CG	6.14	119.94	113.80
1	A	234	GLY	O-C-N	6.12	129.72	122.68
1	A	226	ILE	CA-CB-CG1	6.11	120.79	110.40
1	B	1070	GLN	N-CA-C	-6.11	106.44	114.31
1	B	1313	GLU	N-CA-CB	-6.09	101.48	111.66
1	A	70	GLN	CA-CB-CG	6.09	126.27	114.10
1	A	326	LEU	CA-C-N	6.08	128.45	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	LEU	C-N-CA	6.08	128.45	120.60
1	B	1051	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	91	HIS	CA-CB-CG	6.08	119.88	113.80
1	B	1238	LEU	CA-C-O	-6.08	113.97	120.42
1	A	154	LYS	CG-CD-CE	6.08	125.28	111.30
1	A	134	GLY	CA-C-N	6.08	128.74	120.54
1	A	134	GLY	C-N-CA	6.08	128.74	120.54
1	A	290	TYR	N-CA-C	6.07	120.16	112.87
1	A	55	ARG	CB-CG-CD	6.07	125.26	111.30
1	B	1131	TYR	CA-CB-CG	6.06	124.81	113.90
1	A	327	VAL	CA-CB-CG2	-6.05	100.11	110.40
1	B	1078	ILE	CB-CG1-CD1	-6.04	101.12	113.80
1	B	1127	VAL	CA-C-N	6.04	125.98	119.76
1	B	1127	VAL	C-N-CA	6.04	125.98	119.76
1	B	1337	LYS	CB-CG-CD	6.04	125.18	111.30
1	A	327	VAL	CA-CB-CG1	6.03	120.66	110.40
1	B	1076	GLN	CA-C-O	-6.03	113.77	119.80
1	B	1314	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	1123	GLN	CA-CB-CG	6.02	126.14	114.10
1	B	1247	MET	CA-C-N	6.01	131.12	122.40
1	B	1247	MET	C-N-CA	6.01	131.12	122.40
1	B	1296	PHE	CA-C-O	-6.01	114.49	120.80
1	A	168	VAL	CA-C-N	6.01	126.76	120.03
1	A	168	VAL	C-N-CA	6.01	126.76	120.03
1	A	263	GLU	CA-CB-CG	6.00	126.11	114.10
1	A	167	ALA	N-CA-C	6.00	123.58	110.80
1	A	12	ASP	CA-C-N	5.99	129.34	120.90
1	A	12	ASP	C-N-CA	5.99	129.34	120.90
1	A	221	CYS	N-CA-C	5.98	119.67	112.38
1	A	127	VAL	N-CA-CB	-5.97	102.85	111.21
1	B	1297	LEU	N-CA-C	5.97	118.58	111.71
1	B	1198	THR	CA-C-N	5.96	128.26	120.28
1	B	1198	THR	C-N-CA	5.96	128.26	120.28
1	B	1117	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	B	1076	GLN	N-CA-C	5.95	118.25	109.50
1	B	1216	ALA	CA-C-N	5.93	128.72	120.29
1	B	1216	ALA	C-N-CA	5.93	128.72	120.29
1	B	1074	PRO	N-CA-C	5.93	124.68	112.47
1	B	1237	MET	N-CA-C	5.92	117.53	111.14
1	B	1271	LEU	CA-C-O	5.91	126.58	119.43
1	A	17	PHE	CA-CB-CG	5.91	119.71	113.80
1	B	1174	GLN	CA-C-N	5.91	128.79	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1174	GLN	C-N-CA	5.91	128.79	120.28
1	A	335	VAL	O-C-N	5.91	129.76	122.32
1	A	17	PHE	CA-C-N	5.88	125.64	119.76
1	A	17	PHE	C-N-CA	5.88	125.64	119.76
1	B	1311	TYR	CA-CB-CG	5.88	124.48	113.90
1	B	1168	VAL	CG1-CB-CG2	-5.87	97.89	110.80
1	A	282	GLN	CA-CB-CG	5.86	125.81	114.10
1	A	27	THR	CA-CB-CG2	5.85	120.45	110.50
1	A	191	GLU	CA-CB-CG	5.84	125.78	114.10
1	B	1147	PHE	CA-C-O	-5.84	113.01	120.31
1	B	1089	SER	N-CA-C	5.83	119.07	109.85
1	B	1127	VAL	CA-C-O	-5.82	112.15	119.95
1	B	1155	GLU	N-CA-C	5.82	118.45	110.24
1	B	1331	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	B	1053	TYR	CA-CB-CG	5.80	124.35	113.90
1	B	1008	VAL	CA-C-O	5.80	126.42	120.39
1	A	285	VAL	CA-C-N	5.80	128.41	120.46
1	A	285	VAL	C-N-CA	5.80	128.41	120.46
1	B	1073	THR	CA-C-O	-5.80	115.00	119.46
1	A	260	TYR	O-C-N	5.79	128.25	122.12
1	A	259	GLN	CA-C-N	5.78	128.02	120.28
1	A	259	GLN	C-N-CA	5.78	128.02	120.28
1	A	237	MET	CA-CB-CG	-5.78	102.55	114.10
1	A	150	VAL	N-CA-C	5.77	118.30	111.09
1	B	1260	TYR	N-CA-C	5.76	119.13	111.75
1	B	1273	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	163	ALA	O-C-N	5.75	129.76	122.57
1	B	1018	PRO	O-C-N	5.75	130.37	123.13
1	B	1002	THR	CA-CB-OG1	-5.74	100.99	109.60
1	B	1235	GLY	CA-C-N	5.74	129.43	120.82
1	B	1235	GLY	C-N-CA	5.74	129.43	120.82
1	B	1293	TYR	CA-C-N	5.74	128.24	120.44
1	B	1293	TYR	C-N-CA	5.74	128.24	120.44
1	B	1095	LYS	CA-C-N	5.73	132.49	121.54
1	B	1095	LYS	C-N-CA	5.73	132.49	121.54
1	A	129	LEU	CA-CB-CG	5.73	136.35	116.30
1	B	1259	GLN	CA-C-N	5.72	128.74	120.38
1	B	1259	GLN	C-N-CA	5.72	128.74	120.38
1	A	149	GLU	CA-C-N	5.72	129.68	120.30
1	A	149	GLU	C-N-CA	5.72	129.68	120.30
1	A	35	PRO	N-CA-C	5.72	124.25	112.47
1	B	1279	ASN	N-CA-C	5.72	118.74	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	TRP	CG-CD2-CE3	5.70	139.60	133.90
1	B	1309	ILE	O-C-N	5.70	129.36	123.20
1	A	217	ALA	O-C-N	5.70	128.65	122.15
1	B	1134	GLY	CA-C-N	5.70	128.23	120.54
1	B	1134	GLY	C-N-CA	5.70	128.23	120.54
1	B	1323	PRO	CA-C-N	5.68	128.46	120.28
1	B	1323	PRO	C-N-CA	5.68	128.46	120.28
1	A	238	LEU	CA-C-N	5.68	127.89	120.28
1	A	238	LEU	C-N-CA	5.68	127.89	120.28
1	A	278	ARG	N-CA-C	5.67	119.01	111.30
1	B	1275	ILE	N-CA-C	-5.67	105.58	110.74
1	A	38	THR	CA-C-N	5.66	132.35	121.54
1	A	38	THR	C-N-CA	5.66	132.35	121.54
1	B	1002	THR	CA-CB-CG2	5.66	120.12	110.50
1	B	1303	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	A	117	HIS	CA-C-O	5.66	128.60	120.51
1	A	183	VAL	CB-CA-C	-5.64	102.28	110.63
1	A	247	MET	CA-C-N	5.63	131.43	122.93
1	A	247	MET	C-N-CA	5.63	131.43	122.93
1	A	101	TRP	CB-CG-CD1	-5.62	118.47	126.90
1	B	1260	TYR	CA-CB-CG	5.62	124.01	113.90
1	B	1259	GLN	N-CA-C	5.61	120.24	112.90
1	A	30	VAL	CG1-CB-CG2	-5.60	98.47	110.80
1	B	1270	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	11	LYS	O-C-N	5.59	128.13	122.09
1	A	237	MET	CA-C-O	-5.59	114.04	120.24
1	A	35	PRO	CA-C-N	5.58	132.19	121.54
1	A	35	PRO	C-N-CA	5.58	132.19	121.54
1	B	1215	THR	CA-CB-CG2	5.57	119.97	110.50
1	A	270	ASN	N-CA-C	5.57	118.86	112.57
1	B	1203	ASP	N-CA-C	5.56	117.34	111.28
1	B	1177	LYS	CG-CD-CE	5.55	124.06	111.30
1	A	139	PRO	CA-N-CD	-5.54	104.25	112.00
1	B	1204	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	87	ILE	N-CA-C	-5.54	107.05	111.81
1	A	265	GLN	CA-C-N	5.54	128.71	120.90
1	A	265	GLN	C-N-CA	5.54	128.71	120.90
1	B	1086	ILE	CG1-CB-CG2	-5.52	94.15	110.70
1	A	32	LEU	N-CA-C	5.51	117.89	109.62
1	A	119	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	B	1038	THR	CA-CB-OG1	-5.50	101.34	109.60
1	B	1061	PRO	N-CA-C	5.50	123.79	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	PHE	CA-C-N	5.50	126.22	120.12
1	A	222	PHE	C-N-CA	5.50	126.22	120.12
1	B	1101	TRP	CA-CB-CG	5.49	124.03	113.60
1	A	10	LEU	N-CA-C	-5.49	99.58	108.52
1	B	1248	HIS	CA-C-N	5.48	126.90	120.71
1	B	1248	HIS	C-N-CA	5.48	126.90	120.71
1	A	324	GLU	O-C-N	5.47	127.92	122.12
1	A	76	GLN	CA-C-O	-5.47	113.90	120.41
1	B	1339	VAL	CG1-CB-CG2	-5.46	98.78	110.80
1	A	268	VAL	CG1-CB-CG2	-5.46	98.79	110.80
1	A	294	SER	CA-C-N	5.45	128.03	120.29
1	A	294	SER	C-N-CA	5.45	128.03	120.29
1	B	1133	THR	N-CA-C	-5.45	106.31	113.12
1	A	171	LEU	CA-C-N	5.44	127.91	120.46
1	A	171	LEU	C-N-CA	5.44	127.91	120.46
1	A	87	ILE	CA-C-O	-5.43	114.35	120.32
1	B	1300	VAL	O-C-N	5.43	127.42	121.83
1	B	1278	ARG	CG-CD-NE	5.42	123.92	112.00
1	A	293	TYR	CA-C-O	-5.42	115.12	120.70
1	B	1123	GLN	CA-C-N	5.41	130.05	121.72
1	B	1123	GLN	C-N-CA	5.41	130.05	121.72
1	B	1061	PRO	CA-N-CD	-5.40	104.44	112.00
1	B	1169	GLY	N-CA-C	5.39	119.20	112.73
1	B	1077	PRO	CA-N-CD	-5.37	104.48	112.00
1	A	260	TYR	CA-CB-CG	5.37	123.57	113.90
1	A	241	VAL	CA-C-O	-5.36	115.10	121.05
1	B	1322	ALA	CA-C-O	-5.36	112.82	120.16
1	A	33	ARG	N-CA-C	5.35	118.38	110.46
1	A	296	PHE	CA-C-O	-5.35	115.19	120.70
1	A	99	LEU	CA-CB-CG	5.34	135.00	116.30
1	B	1030	VAL	CG1-CB-CG2	-5.34	99.06	110.80
1	A	211	GLU	O-C-N	5.34	129.85	123.13
1	B	1130	SER	N-CA-C	5.34	119.27	112.87
1	B	1144	TYR	CA-C-N	5.34	127.69	120.65
1	B	1144	TYR	C-N-CA	5.34	127.69	120.65
1	A	70	GLN	CA-C-N	5.33	131.72	121.54
1	A	70	GLN	C-N-CA	5.33	131.72	121.54
1	B	1020	GLU	CA-C-N	5.33	131.04	121.66
1	B	1020	GLU	C-N-CA	5.33	131.04	121.66
1	A	240	ALA	CA-C-O	5.32	126.06	120.42
1	A	122	ILE	CA-C-O	5.32	126.26	120.57
1	B	1053	TYR	CA-C-N	5.32	128.15	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1053	TYR	C-N-CA	5.32	128.15	120.38
1	B	1055	ARG	CA-C-O	-5.31	114.79	120.42
1	A	189	SER	CA-C-N	5.31	127.39	120.28
1	A	189	SER	C-N-CA	5.31	127.39	120.28
1	B	1197	LYS	CA-CB-CG	5.30	124.71	114.10
1	A	103	ILE	CA-C-O	5.30	127.28	120.76
1	B	1226	ILE	CB-CG1-CD1	5.30	124.93	113.80
1	A	198	THR	O-C-N	5.30	127.81	122.09
1	A	233	VAL	CA-CB-CG1	5.29	119.40	110.40
1	B	1189	SER	CA-CB-OG	5.29	121.68	111.10
1	B	1210	GLU	CB-CG-CD	5.29	121.60	112.60
1	B	1213	ASP	N-CA-C	-5.29	99.78	108.41
1	A	76	GLN	CA-C-N	5.28	126.44	119.84
1	A	76	GLN	C-N-CA	5.28	126.44	119.84
1	B	1199	LYS	CA-CB-CG	5.27	124.65	114.10
1	A	193	VAL	CA-CB-CG1	5.27	119.36	110.40
1	A	13	TYR	N-CA-C	5.27	117.67	110.24
1	B	1038	THR	CA-CB-CG2	5.26	119.45	110.50
1	A	339	VAL	CB-CA-C	-5.26	103.84	111.68
1	A	86	ILE	CB-CG1-CD1	5.25	124.83	113.80
1	B	1100	LEU	CA-CB-CG	5.25	134.67	116.30
1	B	1324	GLU	O-C-N	5.25	128.36	122.22
1	A	138	MET	CA-C-O	-5.24	112.98	120.16
1	A	30	VAL	CA-C-N	5.22	129.35	122.30
1	A	30	VAL	C-N-CA	5.22	129.35	122.30
1	A	315	VAL	CA-C-N	5.22	131.51	121.54
1	A	315	VAL	C-N-CA	5.22	131.51	121.54
1	A	312	VAL	CA-CB-CG2	-5.22	101.53	110.40
1	A	341	VAL	N-CA-C	-5.21	100.39	107.99
1	B	1037	GLY	O-C-N	5.21	129.47	122.70
1	A	223	PRO	CA-C-N	5.20	130.10	121.99
1	A	223	PRO	C-N-CA	5.20	130.10	121.99
1	B	1084	SER	N-CA-C	5.20	116.84	108.32
1	B	1246	ASN	O-C-N	5.20	128.76	122.94
1	A	190	LYS	CA-CB-CG	5.19	124.48	114.10
1	A	257	ILE	CB-CA-C	-5.19	101.87	111.79
1	B	1124	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	A	101	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	166	GLY	O-C-N	5.18	129.23	122.91
1	A	286	VAL	N-CA-C	5.18	115.91	110.62
1	B	1254	CYS	O-C-N	5.17	128.11	122.11
1	B	1176	ALA	CA-C-O	-5.16	115.39	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	TYR	CA-C-N	5.15	127.70	120.28
1	A	53	TYR	C-N-CA	5.15	127.70	120.28
1	A	244	ASN	N-CA-C	5.15	119.43	113.20
1	A	340	VAL	CG1-CB-CG2	-5.14	99.48	110.80
1	B	1101	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	A	233	VAL	CA-C-O	-5.14	114.35	120.78
1	A	299	PHE	CA-CB-CG	5.13	118.93	113.80
1	A	87	ILE	CB-CG1-CD1	5.13	124.57	113.80
1	A	337	LYS	CA-CB-CG	5.13	124.36	114.10
1	B	1025	PHE	N-CA-C	5.13	117.76	109.40
1	B	1341	VAL	CA-C-O	-5.13	114.75	120.95
1	A	52	PRO	CA-C-N	5.12	128.80	120.60
1	A	52	PRO	C-N-CA	5.12	128.80	120.60
1	A	122	ILE	O-C-N	5.12	128.71	123.03
1	B	1011	LYS	CA-C-N	5.12	130.56	121.80
1	B	1011	LYS	C-N-CA	5.12	130.56	121.80
1	B	1141	MET	CA-C-O	-5.12	114.99	120.42
1	A	91	HIS	CA-C-N	5.12	124.43	118.85
1	A	91	HIS	C-N-CA	5.12	124.43	118.85
1	A	306	GLU	N-CA-C	5.12	119.79	113.50
1	A	115	MET	CA-C-N	5.11	128.49	120.82
1	A	115	MET	C-N-CA	5.11	128.49	120.82
1	B	1179	MET	CB-CG-SD	-5.11	97.36	112.70
1	B	1266	GLU	CA-C-N	5.11	126.53	121.62
1	B	1266	GLU	C-N-CA	5.11	126.53	121.62
1	A	127	VAL	CA-C-N	5.11	125.02	119.76
1	A	127	VAL	C-N-CA	5.11	125.02	119.76
1	B	1245	MET	CG-SD-CE	-5.10	89.69	100.90
1	B	1245	MET	N-CA-C	5.10	118.02	110.48
1	B	1009	ILE	CA-CB-CG1	-5.09	101.75	110.40
1	B	1050	CYS	O-C-N	5.09	129.63	123.01
1	A	45	ASN	O-C-N	5.09	129.28	123.02
1	B	1009	ILE	N-CA-CB	-5.08	102.38	112.24
1	B	1121	LYS	CG-CD-CE	-5.08	99.61	111.30
1	A	233	VAL	N-CA-C	5.08	119.91	109.34
1	A	302	PRO	CA-N-CD	-5.08	104.89	112.00
1	A	253	VAL	CG1-CB-CG2	-5.08	99.63	110.80
1	A	109	TYR	N-CA-C	5.05	116.53	107.80
1	B	1058	MET	CB-CG-SD	-5.05	97.56	112.70
1	B	1232	ASN	CA-C-O	-5.04	113.57	118.97
1	B	1286	VAL	CA-CB-CG2	5.04	118.97	110.40
1	B	1088	GLU	CA-C-N	5.04	131.27	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1088	GLU	C-N-CA	5.04	131.27	122.81
1	B	1257	ILE	N-CA-CB	5.04	120.75	110.78
1	A	30	VAL	CA-C-O	5.03	126.08	120.59
1	B	1221	CYS	N-CA-C	5.03	116.84	111.36
1	A	163	ALA	CA-C-O	5.03	127.91	122.03
1	A	95	LYS	CA-C-N	5.02	128.45	121.02
1	A	95	LYS	C-N-CA	5.02	128.45	121.02
1	B	1167	ALA	N-CA-CB	-5.02	102.00	110.49
1	B	1241	VAL	CA-C-O	-5.02	115.53	120.85
1	B	1049	SER	O-C-N	5.01	129.70	123.19
1	A	240	ALA	N-CA-C	5.00	116.81	111.36
1	A	274	ILE	CA-C-N	5.00	126.82	120.72
1	A	274	ILE	C-N-CA	5.00	126.82	120.72

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	TYR	Sidechain
1	A	260	TYR	Sidechain
1	A	322	ALA	Peptide
1	A	34	VAL	Peptide
1	B	1034	VAL	Peptide
1	B	1160	TYR	Sidechain
1	B	1208	TYR	Sidechain
1	B	1260	TYR	Sidechain
1	B	1293	TYR	Sidechain
1	B	1322	ALA	Peptide

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	16	0
1	B	2681	0	2648	15	0
2	A	48	0	25	6	0
2	B	48	0	25	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	16	1	0
3	B	11	0	16	0	0
4	A	62	0	0	0	0
4	B	72	0	0	1	0
All	All	5556	0	5324	31	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 3.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:TYR:HE2	2:A:1346:NAP:O3X	1.43	1.02
1:A:174:GLN:HE22	1:A:310:THR:H	1.41	0.68
1:A:208:TYR:CE2	2:A:1346:NAP:O3X	2.36	0.67
1:B:1208:TYR:OH	2:B:2346:NAP:O3X	2.15	0.64
1:A:208:TYR:HE2	2:A:1346:NAP:P2B	2.24	0.61
1:B:1208:TYR:HE1	2:B:2346:NAP:O2X	1.86	0.58
1:B:1005:ASN:HD22	1:B:1108:GLU:HB2	1.68	0.58
1:B:1322:ALA:HB2	1:B:1340:VAL:HG11	1.89	0.54
1:B:1208:TYR:CE1	2:B:2346:NAP:O2X	2.62	0.53
1:B:1279:ASN:HB3	4:B:2057:HOH:O	2.11	0.51
1:A:259:GLN:HE22	1:A:266:GLU:N	2.11	0.48
1:B:1188:GLY:N	2:B:2346:NAP:O2X	2.48	0.47
1:A:261:ASN:ND2	1:A:261:ASN:H	2.13	0.46
1:A:1:MET:HB2	1:A:32:LEU:HD22	1.98	0.46
1:A:259:GLN:NE2	1:A:265:GLN:HB2	2.31	0.46
1:A:53:TYR:CE1	3:A:1347:HNE:H8C1	2.50	0.46
1:A:208:TYR:CE2	2:A:1346:NAP:P2B	3.06	0.46
1:B:1005:ASN:HD21	1:B:1107:GLU:HB2	1.82	0.45
1:B:1091:HIS:HD2	1:B:1093:ASP:H	1.65	0.45
1:A:229:TYR:CD2	1:A:241:VAL:HG11	2.52	0.43
1:B:1249:GLY:HA2	1:B:1250:ARG:HH21	1.83	0.43
1:A:157:GLU:CD	1:A:250:ARG:HH22	2.28	0.42
1:B:1229:TYR:CD2	1:B:1241:VAL:HG11	2.54	0.42
1:A:138:MET:SD	2:A:1346:NAP:H5N	2.60	0.42
1:A:165:SER:O	1:A:170:GLN:NE2	2.53	0.42
1:B:1005:ASN:ND2	1:B:1109:TYR:H	2.18	0.41
1:A:188:GLY:N	2:A:1346:NAP:P2B	2.93	0.41
1:B:1270:ASN:HB2	1:B:1273:ASN:HD22	1.86	0.41
1:B:1188:GLY:HA3	2:B:2346:NAP:O1X	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1206:PHE:HB3	1:B:1220:ARG:HH12	1.86	0.40
1:A:261:ASN:H	1:A:261:ASN:HD22	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/345 (96%)	293 (88%)	34 (10%)	5 (2%)	8	28
1	B	343/345 (99%)	305 (89%)	28 (8%)	10 (3%)	3	13
All	All	675/690 (98%)	598 (89%)	62 (9%)	15 (2%)	5	19

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	322	ALA
1	B	1034	VAL
1	B	1096	LYS
1	B	1167	ALA
1	A	167	ALA
1	A	316	ALA
1	B	1038	THR
1	B	1071	ALA
1	B	1074	PRO
1	B	1066	ALA
1	A	74	PRO
1	B	1061	PRO
1	B	1088	GLU
1	B	1126	ASP

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%)	242 (86%)	41 (14%)	3	11
1	B	289/289 (100%)	246 (85%)	43 (15%)	3	10
All	All	572/578 (99%)	488 (85%)	84 (15%)	3	10

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	14	VAL
1	A	23	PHE
1	A	31	GLU
1	A	34	VAL
1	A	39	ASN
1	A	48	LEU
1	A	51	ASP
1	A	55	ARG
1	A	56	ILE
1	A	58	MET
1	A	70	GLN
1	A	76	GLN
1	A	88	GLU
1	A	96	LYS
1	A	123	GLN
1	A	129	LEU
1	A	139	PRO
1	A	154	LYS
1	A	161	VAL
1	A	177	LYS
1	A	179	MET
1	A	183	VAL
1	A	191	GLU
1	A	210	GLU
1	A	226	ILE
1	A	238	LEU

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Mol	Chain	Res	Type
1	A	242	LEU
1	A	247	MET
1	A	256	MET
1	A	257	ILE
1	A	261	ASN
1	A	264	ASN
1	A	271	LEU
1	A	301	LEU
1	A	308	LYS
1	A	311	TYR
1	A	315	VAL
1	A	337	LYS
1	A	339	VAL
1	A	344	ARG
1	B	1022	ASP
1	B	1029	THR
1	B	1042	LEU
1	B	1056	ILE
1	B	1060	LYS
1	B	1062	ASP
1	B	1068	LEU
1	B	1070	GLN
1	B	1074	PRO
1	B	1078	ILE
1	B	1103	ILE
1	B	1111	VAL
1	B	1112	ILE
1	B	1116	THR
1	B	1123	GLN
1	B	1139	PRO
1	B	1154	LYS
1	B	1171	LEU
1	B	1175	LEU
1	B	1183	VAL
1	B	1186	SER
1	B	1195	LEU
1	B	1198	THR
1	B	1207	ASN
1	B	1211	GLU
1	B	1231	GLU
1	B	1237	MET
1	B	1238	LEU

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Mol	Chain	Res	Type
1	B	1247	MET
1	B	1250	ARG
1	B	1257	ILE
1	B	1278	ARG
1	B	1282	GLN
1	B	1286	VAL
1	B	1288	ASP
1	B	1300	VAL
1	B	1301	LEU
1	B	1302	PRO
1	B	1306	GLU
1	B	1310	THR
1	B	1323	PRO
1	B	1337	LYS
1	B	1344	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	123	GLN
1	A	174	GLN
1	A	224	ASN
1	A	259	GLN
1	A	261	ASN
1	A	279	ASN
1	B	1005	ASN
1	B	1007	GLN
1	B	1123	GLN
1	B	1170	GLN
1	B	1207	ASN
1	B	1246	ASN
1	B	1248	HIS
1	B	1261	ASN
1	B	1264	ASN
1	B	1270	ASN
1	B	1334	ASN
1	B	1338	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	NAP	A	1346	-	50,52,52	2.02	7 (14%)	71,80,80	2.50	18 (25%)
3	HNE	A	1347	-	10,10,10	1.48	2 (20%)	9,10,10	1.23	1 (11%)
2	NAP	B	2346	-	50,52,52	1.68	10 (20%)	71,80,80	2.29	21 (29%)
3	HNE	B	2347	-	10,10,10	1.47	2 (20%)	9,10,10	1.22	1 (11%)

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	NAP	A	1346	-	-	16/35/67/67	0/5/5/5
3	HNE	A	1347	-	-	6/9/9/9	-
2	NAP	B	2346	-	-	13/35/67/67	0/5/5/5
3	HNE	B	2347	-	-	6/9/9/9	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1346	NAP	PN-O3	6.64	1.66	1.59
2	A	1346	NAP	C2N-N1N	6.29	1.41	1.35
2	B	2346	NAP	C2N-N1N	5.42	1.40	1.35
2	A	1346	NAP	PA-O3	4.59	1.64	1.59
2	B	2346	NAP	C5A-N7A	-4.06	1.31	1.39
2	B	2346	NAP	PA-O3	3.82	1.63	1.59
2	A	1346	NAP	C6N-N1N	3.81	1.44	1.35
2	A	1346	NAP	O4D-C1D	3.77	1.45	1.40
2	A	1346	NAP	C5A-N7A	-3.65	1.32	1.39
2	B	2346	NAP	C6N-N1N	3.64	1.43	1.35
3	A	1347	HNE	C2-C1	3.60	1.54	1.44
3	B	2347	HNE	C2-C1	3.57	1.54	1.44
2	B	2346	NAP	O4D-C1D	2.64	1.44	1.40
2	B	2346	NAP	PN-O3	2.58	1.62	1.59
3	A	1347	HNE	C4-C3	2.32	1.54	1.50
2	A	1346	NAP	C3N-C7N	2.31	1.54	1.50
3	B	2347	HNE	C4-C3	2.30	1.54	1.50
2	B	2346	NAP	C5N-C4N	2.27	1.42	1.38
2	B	2346	NAP	C8A-N9A	-2.18	1.33	1.37
2	B	2346	NAP	C4N-C3N	2.17	1.42	1.39
2	B	2346	NAP	P2B-O2X	-2.03	1.47	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1346	NAP	O5D-C5D-C4D	7.74	135.34	108.99
2	A	1346	NAP	C4D-O4D-C1D	7.53	116.82	109.92
2	B	2346	NAP	C5A-C4A-N3A	-6.76	117.41	126.72
2	A	1346	NAP	N3A-C4A-N9A	6.40	138.05	127.17
2	A	1346	NAP	C5A-C4A-N3A	-6.30	118.04	126.72
2	B	2346	NAP	N3A-C4A-N9A	6.20	137.72	127.17
2	A	1346	NAP	O4D-C4D-C3D	-5.45	94.34	105.15
2	A	1346	NAP	N3A-C2A-N1A	-5.25	120.63	128.58
2	B	2346	NAP	N3A-C2A-N1A	-5.09	120.87	128.58
2	B	2346	NAP	O3X-P2B-O2B	4.61	123.82	105.85
2	B	2346	NAP	O4B-C1B-N9A	4.51	116.74	108.09
2	A	1346	NAP	O2B-P2B-O1X	4.34	124.79	109.33
2	B	2346	NAP	C4D-O4D-C1D	4.09	113.67	109.92
2	A	1346	NAP	O2X-P2B-O2B	-4.07	90.00	105.85
2	A	1346	NAP	C2B-C1B-N9A	4.02	120.37	113.75
2	A	1346	NAP	C6A-C5A-N7A	-4.01	124.35	132.09
2	B	2346	NAP	C2A-N3A-C4A	3.96	121.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2346	NAP	C4B-O4B-C1B	-3.90	100.86	109.47
2	B	2346	NAP	C2N-N1N-C1D	-3.83	110.69	119.13
2	B	2346	NAP	C6N-N1N-C1D	3.71	127.01	119.73
2	A	1346	NAP	C2A-N3A-C4A	3.67	120.80	111.83
2	B	2346	NAP	O5D-C5D-C4D	3.61	121.30	108.99
2	B	2346	NAP	C6A-C5A-N7A	-3.36	125.61	132.09
2	B	2346	NAP	C5N-C4N-C3N	3.17	123.48	120.36
2	A	1346	NAP	C6A-C5A-C4A	3.17	121.50	117.18
2	B	2346	NAP	C6A-C5A-C4A	3.13	121.45	117.18
2	A	1346	NAP	C4A-C5A-N7A	3.11	114.14	110.58
2	A	1346	NAP	C6N-N1N-C1D	3.05	125.72	119.73
2	B	2346	NAP	P2B-O2B-C2B	3.04	131.55	123.43
2	A	1346	NAP	C5N-C4N-C3N	3.00	123.31	120.36
2	A	1346	NAP	C5D-C4D-C3D	2.97	125.89	115.21
2	B	2346	NAP	O4B-C1B-C2B	-2.95	101.51	106.59
2	B	2346	NAP	O4D-C4D-C3D	-2.92	99.36	105.15
2	B	2346	NAP	O3-PA-O1A	-2.91	101.94	110.70
2	B	2346	NAP	O4D-C4D-C5D	2.75	118.15	109.33
2	B	2346	NAP	C5N-C6N-N1N	-2.51	116.97	120.38
3	A	1347	HNE	C6-C5-C4	-2.48	109.87	114.94
2	A	1346	NAP	C2N-N1N-C1D	-2.47	113.67	119.13
3	B	2347	HNE	C6-C5-C4	-2.47	109.89	114.94
2	A	1346	NAP	C2A-N1A-C6A	2.40	122.67	118.73
2	B	2346	NAP	C4A-C5A-N7A	2.07	112.95	110.58

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1346	NAP	C5B-O5B-PA-O3
2	A	1346	NAP	C3B-C4B-C5B-O5B
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-C2N
2	A	1346	NAP	O4D-C1D-N1N-C6N
2	A	1346	NAP	C2D-C1D-N1N-C2N
2	A	1346	NAP	C2D-C1D-N1N-C6N
2	B	2346	NAP	C5B-O5B-PA-O1A
2	B	2346	NAP	C5B-O5B-PA-O2A
2	B	2346	NAP	C5B-O5B-PA-O3
2	B	2346	NAP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	B	2346	NAP	C5D-O5D-PN-O1N
2	B	2346	NAP	O4D-C4D-C5D-O5D
2	B	2346	NAP	O4D-C1D-N1N-C2N
2	B	2346	NAP	O4D-C1D-N1N-C6N
3	A	1347	HNE	C3-C4-C5-C6
3	A	1347	HNE	O10-C4-C5-C6
3	B	2347	HNE	C3-C4-C5-C6
3	B	2347	HNE	O10-C4-C5-C6
2	B	2346	NAP	O4B-C4B-C5B-O5B
2	B	2346	NAP	C3B-C4B-C5B-O5B
2	B	2346	NAP	C3D-C4D-C5D-O5D
2	A	1346	NAP	C4B-C5B-O5B-PA
2	A	1346	NAP	O4B-C4B-C5B-O5B
3	A	1347	HNE	C2-C3-C4-C5
3	B	2347	HNE	C2-C3-C4-C5
3	A	1347	HNE	C6-C7-C8-C9
3	B	2347	HNE	C6-C7-C8-C9
3	A	1347	HNE	C2-C3-C4-O10
3	B	2347	HNE	C2-C3-C4-O10
2	A	1346	NAP	PN-O3-PA-O5B
2	A	1346	NAP	PA-O3-PN-O2N
2	A	1346	NAP	C5B-O5B-PA-O1A
2	B	2346	NAP	C5D-O5D-PN-O2N
3	A	1347	HNE	C4-C5-C6-C7
3	B	2347	HNE	C4-C5-C6-C7
2	A	1346	NAP	PA-O3-PN-O1N
2	B	2346	NAP	C2B-O2B-P2B-O3X
2	A	1346	NAP	O4D-C4D-C5D-O5D

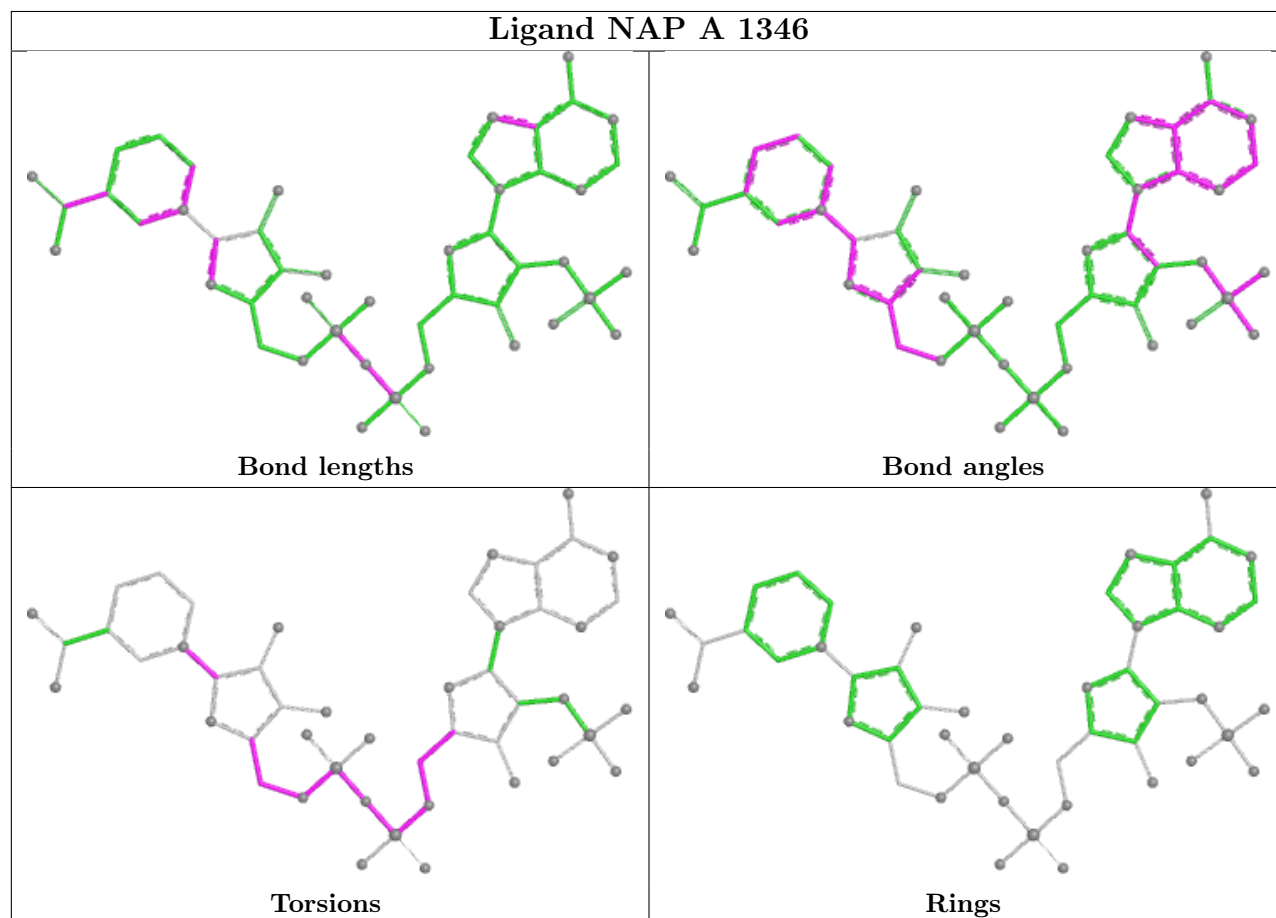
There are no ring outliers.

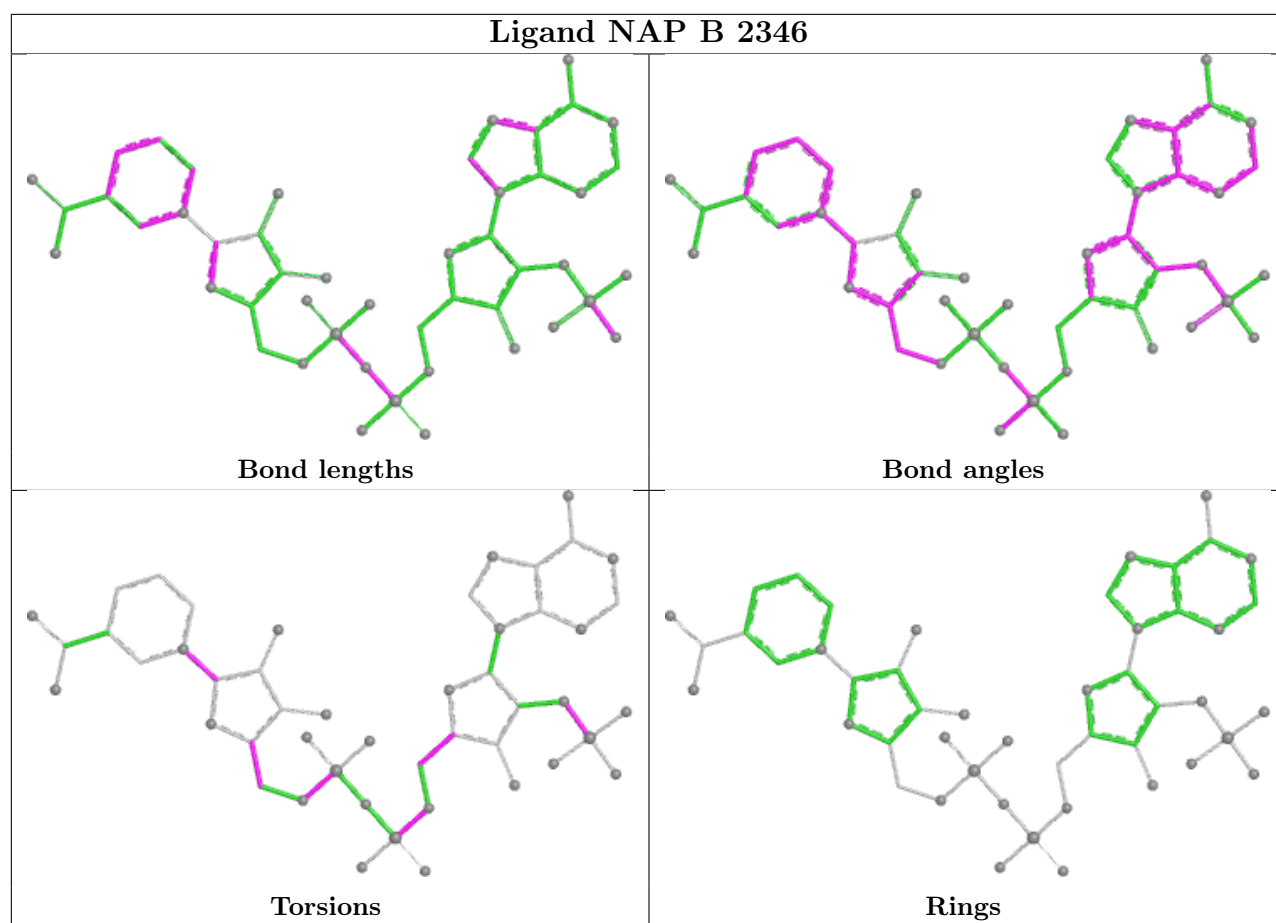
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1346	NAP	6	0
3	A	1347	HNE	1	0
2	B	2346	NAP	5	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.