Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 11:27 AM EDT

PDB ID	:	2J3K
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 (i) 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 (1)) were used in the production of this report:

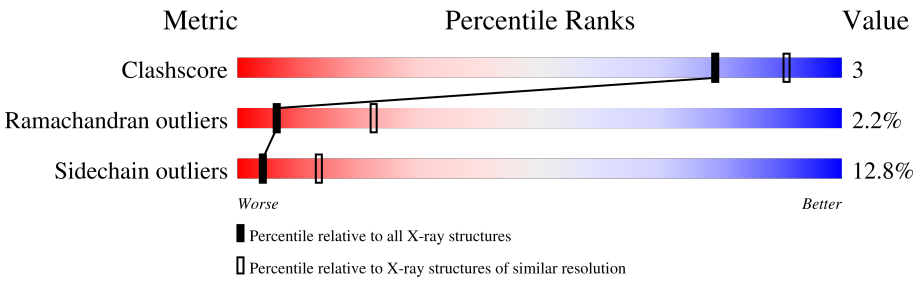
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	63% 27% 7% •
1	B	345	62% 31% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5556 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.

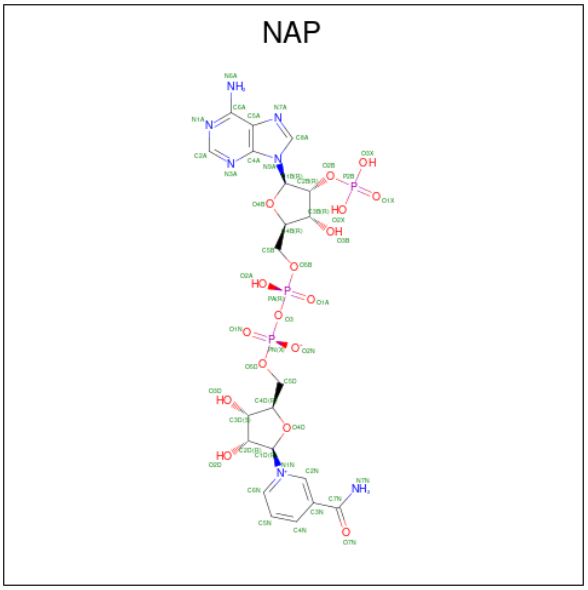
- Molecule 1 is a protein called NADPH-dependent oxidoreductase 2-alkenal reductase.

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 (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

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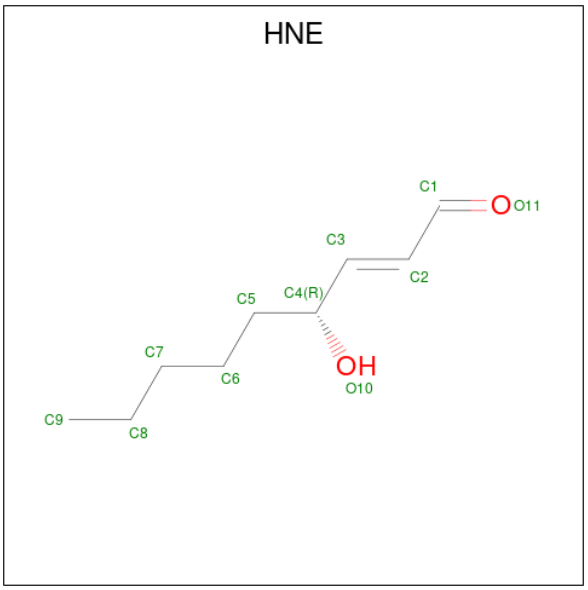
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	48	21	7	17	3	0	0

- Molecule 3 is (2E,4R)-4-HYDROXYNON-2-ENAL (three-letter code: HNE) (formula: $C_9H_{16}O_2$).



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

- Molecule 4 is water.

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

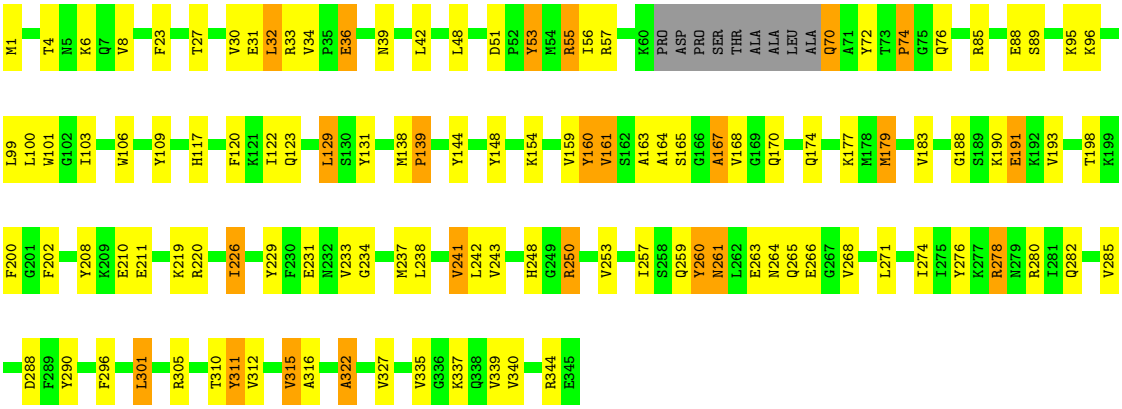
3 Residue-property plots (i)

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.

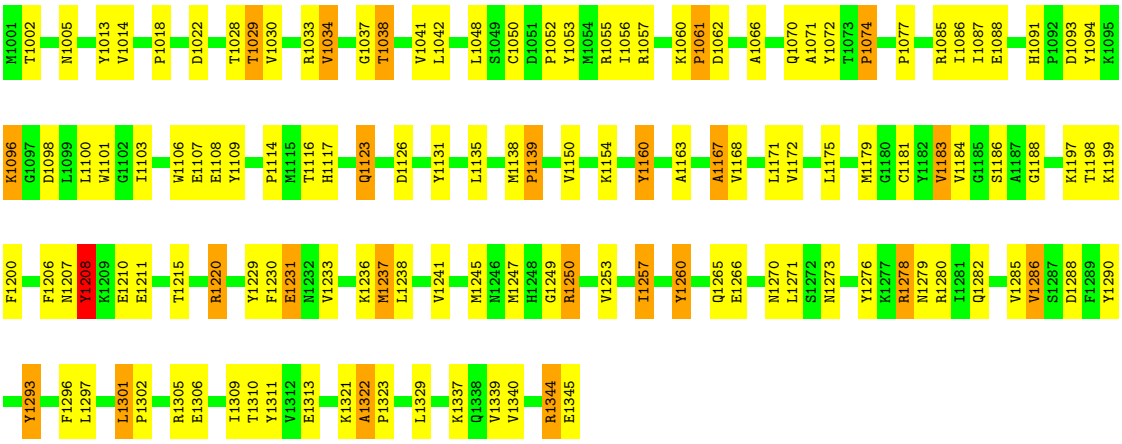
• Molecule 1: NADPH-dependent oxidoreductase 2-alkenal reductase

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

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	49.08Å 122.45Å 147.84Å 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 (i)

5.1 Standard geometry (i)

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

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	1.30	4/2681 (0.1%)	2.09	107/3625 (3.0%)
1	B	1.29	2/2742 (0.1%)	2.10	116/3713 (3.1%)
All	All	1.30	6/5423 (0.1%)	2.10	223/7338 (3.0%)

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	4
1	B	0	6
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	TYR	CG-CD2	5.48	1.46	1.39
1	A	53	TYR	CG-CD1	5.25	1.46	1.39
1	A	148	TYR	CG-CD2	5.22	1.46	1.39
1	B	1276	TYR	CG-CD2	5.11	1.45	1.39
1	B	1053	TYR	CG-CD1	5.04	1.45	1.39
1	A	72	TYR	CG-CD2	5.01	1.45	1.39

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	ARG	NE-CZ-NH1	11.99	126.29	120.30
1	A	72	TYR	CB-CG-CD1	-11.74	113.95	121.00
1	A	312	VAL	CG1-CB-CG2	-11.06	93.20	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1055	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	B	1253	VAL	CG1-CB-CG2	-10.44	94.20	110.90
1	A	57	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	B	1055	ARG	NE-CZ-NH2	-9.87	115.37	120.30
1	A	274	ILE	CG1-CB-CG2	-9.77	89.91	111.40
1	B	1072	TYR	CB-CG-CD1	-9.25	115.45	121.00
1	A	129	LEU	CA-CB-CG	9.15	136.35	115.30
1	A	278	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	1057	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	1101	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	160	TYR	CB-CG-CD2	-8.64	115.81	121.00
1	A	101	TRP	CD1-CG-CD2	8.63	113.20	106.30
1	B	1285	VAL	CG1-CB-CG2	-8.62	97.10	110.90
1	B	1029	THR	CA-CB-CG2	8.57	124.40	112.40
1	A	99	LEU	CA-CB-CG	8.57	135.00	115.30
1	B	1100	LEU	CA-CB-CG	8.42	134.67	115.30
1	A	280	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	290	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	A	198	THR	CA-CB-CG2	8.20	123.88	112.40
1	A	85	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	B	1168	VAL	CG1-CB-CG2	-8.13	97.89	110.90
1	B	1237	MET	CG-SD-CE	-8.07	87.30	100.20
1	B	1094	TYR	CB-CG-CD1	-7.98	116.21	121.00
1	A	290	TYR	CB-CG-CD1	7.98	125.79	121.00
1	B	1260	TYR	CB-CG-CD1	7.92	125.75	121.00
1	A	260	TYR	CB-CG-CD2	7.90	125.74	121.00
1	A	101	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	A	305	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	250	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	1101	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	B	1086	ILE	CG1-CB-CG2	-7.84	94.15	111.40
1	A	30	VAL	CG1-CB-CG2	-7.77	98.47	110.90
1	A	163	ALA	CA-C-N	-7.75	100.16	117.20
1	B	1160	TYR	CB-CG-CD2	-7.73	116.36	121.00
1	A	296	PHE	CB-CG-CD2	-7.71	115.41	120.80
1	A	55	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	B	1260	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	B	1231	GLU	CA-CB-CG	7.61	130.14	113.40
1	B	1160	TYR	CB-CG-CD1	7.58	125.55	121.00
1	B	1339	VAL	CG1-CB-CG2	-7.57	98.78	110.90
1	A	268	VAL	CG1-CB-CG2	-7.57	98.79	110.90
1	B	1200	PHE	CB-CG-CD2	-7.52	115.54	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1286	VAL	CA-CB-CG1	-7.45	99.72	110.90
1	B	1290	TYR	CB-CG-CD1	-7.44	116.54	121.00
1	A	311	TYR	CB-CG-CD1	-7.44	116.54	121.00
1	A	100	LEU	CA-CB-CG	7.42	132.35	115.30
1	B	1030	VAL	CG1-CB-CG2	-7.40	99.06	110.90
1	B	1280	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	72	TYR	CB-CG-CD2	7.40	125.44	121.00
1	A	106	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	B	1028	THR	CA-CB-CG2	7.33	122.66	112.40
1	A	131	TYR	CB-CG-CD1	-7.27	116.64	121.00
1	B	1106	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	B	1163	ALA	CA-C-N	-7.23	101.29	117.20
1	B	1220	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	160	TYR	CB-CG-CD1	7.21	125.32	121.00
1	A	103	ILE	CA-C-N	-7.20	101.36	117.20
1	A	327	VAL	CA-CB-CG2	-7.20	100.11	110.90
1	A	340	VAL	CG1-CB-CG2	-7.14	99.48	110.90
1	B	1048	LEU	CB-CG-CD2	-7.12	98.90	111.00
1	B	1033	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	131	TYR	CB-CG-CD2	7.05	125.23	121.00
1	A	253	VAL	CG1-CB-CG2	-7.04	99.63	110.90
1	B	1139	PRO	CA-N-CD	-6.96	101.75	111.50
1	A	168	VAL	CG1-CB-CG2	-6.90	99.86	110.90
1	B	1072	TYR	CB-CG-CD2	6.89	125.13	121.00
1	A	106	TRP	CD1-CG-CD2	6.87	111.79	106.30
1	A	231	GLU	CA-CB-CG	6.86	128.49	113.40
1	A	219	LYS	CA-CB-CG	6.83	128.43	113.40
1	B	1150	VAL	CG1-CB-CG2	-6.81	100.00	110.90
1	A	312	VAL	CA-CB-CG1	6.73	121.00	110.90
1	B	1236	LYS	CA-CB-CG	6.69	128.13	113.40
1	A	211	GLU	CA-C-N	-6.69	102.49	117.20
1	A	264	ASN	CA-C-N	-6.67	102.52	117.20
1	A	8	VAL	CG1-CB-CG2	-6.64	100.28	110.90
1	A	33	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	1253	VAL	CA-C-N	-6.62	102.64	117.20
1	A	200	PHE	CB-CG-CD2	-6.61	116.17	120.80
1	A	202	PHE	CB-CG-CD1	-6.61	116.18	120.80
1	B	1245	MET	CG-SD-CE	-6.57	89.69	100.20
1	B	1257	ILE	CB-CA-C	-6.57	98.47	111.60
1	A	101	TRP	CB-CG-CD1	-6.56	118.47	127.00
1	A	202	PHE	CB-CG-CD2	6.52	125.36	120.80
1	A	327	VAL	CA-CB-CG1	6.50	120.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	B	1138	MET	CA-C-O	-6.47	106.50	120.10
1	B	1048	LEU	CA-CB-CG	6.44	130.10	115.30
1	A	285	VAL	CG1-CB-CG2	-6.42	100.62	110.90
1	B	1265	GLN	CA-CB-CG	-6.39	99.33	113.40
1	B	1106	TRP	CD1-CG-CD2	6.39	111.41	106.30
1	B	1266	GLU	CA-CB-CG	6.37	127.42	113.40
1	A	288	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	101	TRP	CG-CD2-CE3	6.34	139.60	133.90
1	B	1313	GLU	CA-CB-CG	6.33	127.33	113.40
1	A	237	MET	CA-CB-CG	-6.33	102.55	113.30
1	A	276	TYR	CA-CB-CG	6.32	125.41	113.40
1	A	101	TRP	CA-CB-CG	6.28	125.63	113.70
1	B	1301	LEU	CA-C-O	-6.28	106.91	120.10
1	B	1167	ALA	N-CA-C	6.26	127.90	111.00
1	B	1184	VAL	CG1-CB-CG2	-6.26	100.89	110.90
1	B	1344	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	312	VAL	CA-CB-CG2	-6.25	101.53	110.90
1	B	1175	LEU	CB-CG-CD2	-6.22	100.42	111.00
1	A	193	VAL	CG1-CB-CG2	-6.22	100.95	110.90
1	A	6	LYS	CA-CB-CG	6.21	127.07	113.40
1	A	243	VAL	CG1-CB-CG2	-6.18	101.01	110.90
1	A	296	PHE	CB-CG-CD1	6.18	125.12	120.80
1	B	1057	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	260	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	A	335	VAL	CA-C-N	-6.08	104.04	116.20
1	B	1297	LEU	CB-CG-CD1	-6.07	100.68	111.00
1	A	179	MET	CG-SD-CE	-6.06	90.50	100.20
1	B	1172	VAL	CG1-CB-CG2	-6.06	101.21	110.90
1	A	74	PRO	CA-N-CD	-6.04	103.04	111.50
1	B	1345	GLU	CA-CB-CG	6.02	126.64	113.40
1	B	1135	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	248	HIS	CA-C-N	-6.01	104.18	116.20
1	B	1114	PRO	CA-C-N	-6.01	103.98	117.20
1	B	1271	LEU	CA-CB-CG	6.01	129.12	115.30
1	B	1131	TYR	CA-CB-CG	6.01	124.81	113.40
1	A	55	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	1311	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	A	234	GLY	CA-C-N	-5.94	104.32	116.20
1	B	1220	ARG	CA-CB-CG	5.94	126.46	113.40
1	A	36	GLU	CA-CB-CG	5.92	126.42	113.40
1	A	32	LEU	CA-C-N	-5.90	104.22	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	GLN	CA-CB-CG	5.85	126.27	113.40
1	B	1183	VAL	CG1-CB-CG2	-5.84	101.55	110.90
1	B	1311	TYR	CA-CB-CG	5.83	124.48	113.40
1	A	305	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	117	HIS	CA-C-N	-5.81	104.42	117.20
1	A	315	VAL	N-CA-C	5.80	126.66	111.00
1	B	1029	THR	CA-CB-OG1	-5.79	96.83	109.00
1	B	1123	GLN	CA-CB-CG	5.79	126.14	113.40
1	B	1167	ALA	N-CA-CB	-5.78	102.00	110.10
1	B	1050	CYS	CA-C-N	-5.78	104.49	117.20
1	A	263	GLU	CA-CB-CG	5.78	126.11	113.40
1	B	1278	ARG	CG-CD-NE	5.77	123.92	111.80
1	B	1041	VAL	CG1-CB-CG2	-5.76	101.68	110.90
1	B	1053	TYR	CA-CB-CG	5.76	124.35	113.40
1	A	109	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	A	27	THR	CA-CB-CG2	5.75	120.45	112.40
1	A	48	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	B	1103	ILE	CA-C-N	-5.74	104.58	117.20
1	B	1181	CYS	N-CA-C	5.71	126.43	111.00
1	B	1175	LEU	CA-CB-CG	5.71	128.43	115.30
1	B	1138	MET	CA-C-N	5.71	133.07	117.10
1	B	1018	PRO	CA-C-N	-5.70	104.67	117.20
1	A	161	VAL	CA-CB-CG1	-5.69	102.37	110.90
1	B	1014	VAL	CG1-CB-CG2	-5.67	101.82	110.90
1	B	1233	VAL	CA-C-N	5.67	127.54	116.20
1	A	233	VAL	CA-CB-CG1	5.66	119.40	110.90
1	B	1114	PRO	O-C-N	5.66	131.75	122.70
1	B	1329	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	282	GLN	CA-CB-CG	5.64	125.81	113.40
1	B	1290	TYR	CB-CG-CD2	5.64	124.38	121.00
1	A	193	VAL	CA-CB-CG1	5.64	119.36	110.90
1	B	1233	VAL	CG1-CB-CG2	-5.63	101.89	110.90
1	A	191	GLU	CA-CB-CG	5.63	125.78	113.40
1	B	1230	PHE	CA-C-N	-5.62	104.83	117.20
1	B	1305	ARG	CB-CG-CD	-5.62	97.00	111.60
1	A	103	ILE	CG1-CB-CG2	-5.61	99.06	111.40
1	B	1131	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	B	1260	TYR	CA-CB-CG	5.58	124.01	113.40
1	B	1094	TYR	CB-CG-CD2	5.58	124.35	121.00
1	B	1278	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	122	ILE	CA-C-N	-5.56	104.98	117.20
1	A	241	VAL	CG1-CB-CG2	-5.53	102.05	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1013	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	B	1002	THR	CA-CB-CG2	5.52	120.12	112.40
1	A	198	THR	CA-CB-OG1	-5.51	97.44	109.00
1	B	1208	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	B	1296	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	A	226	ILE	CA-CB-CG2	-5.46	99.99	110.90
1	B	1293	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	B	1101	TRP	CA-CB-CG	5.44	124.03	113.70
1	A	159	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	B	1215	THR	CA-CB-CG2	5.41	119.97	112.40
1	B	1286	VAL	CB-CA-C	-5.40	101.14	111.40
1	B	1301	LEU	CA-C-N	5.39	132.20	117.10
1	B	1286	VAL	CA-CB-CG2	5.38	118.97	110.90
1	A	301	LEU	CA-CB-CG	5.38	127.67	115.30
1	B	1309	ILE	CA-C-N	-5.38	105.37	117.20
1	A	315	VAL	CA-CB-CG1	-5.36	102.86	110.90
1	A	260	TYR	CA-CB-CG	5.35	123.57	113.40
1	B	1305	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	253	VAL	CA-C-N	-5.34	105.46	117.20
1	B	1276	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	B	1085	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	220	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	1106	TRP	CG-CD2-CE3	5.27	138.64	133.90
1	B	1098	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	1271	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	A	55	ARG	CB-CG-CD	5.25	125.26	111.60
1	B	1101	TRP	CG-CD2-CE3	5.25	138.63	133.90
1	B	1337	LYS	CB-CG-CD	5.22	125.18	111.60
1	A	30	VAL	CA-C-N	-5.21	105.73	117.20
1	A	139	PRO	CA-N-CD	-5.18	104.25	111.50
1	B	1037	GLY	C-N-CA	5.18	134.65	121.70
1	A	276	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	A	226	ILE	CA-CB-CG1	5.15	120.79	111.00
1	B	1197	LYS	CA-CB-CG	5.14	124.71	113.40
1	B	1087	ILE	CA-C-N	-5.13	105.92	117.20
1	B	1199	LYS	CA-CB-CG	5.11	124.65	113.40
1	A	120	PHE	CB-CG-CD2	-5.11	117.23	120.80
1	A	42	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	B	1313	GLU	N-CA-CB	-5.06	101.48	110.60
1	B	1096	LYS	N-CA-C	5.06	124.66	111.00
1	A	164	ALA	C-N-CA	5.05	134.33	121.70
1	A	89	SER	N-CA-C	5.05	124.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1061	PRO	CA-N-CD	-5.04	104.44	111.50
1	B	1077	PRO	N-CA-C	5.04	125.21	112.10
1	A	190	LYS	CA-CB-CG	5.04	124.48	113.40
1	B	1038	THR	CA-CB-CG2	5.03	119.45	112.40
1	B	1052	PRO	N-CA-C	5.03	125.18	112.10
1	A	161	VAL	CA-CB-CG2	5.02	118.44	110.90
1	A	74	PRO	N-CA-C	5.02	125.15	112.10
1	A	167	ALA	N-CA-CB	-5.02	103.08	110.10
1	B	1077	PRO	CA-N-CD	-5.02	104.48	111.50
1	B	1179	MET	CB-CG-SD	-5.01	97.36	112.40

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2623	0	2594	15	0
1	B	2681	0	2648	15	0
2	A	48	0	25	6	0
2	B	48	0	25	5	0
3	A	11	0	16	1	0
3	B	11	0	16	0	0
4	A	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	72	0	0	1	0
All	All	5556	0	5324	30	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 (30) 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: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
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%)	10 33
1	B	343/345 (99%)	305 (89%)	28 (8%)	10 (3%)	4 15
All	All	675/690 (98%)	598 (89%)	62 (9%)	15 (2%)	6 22

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 (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	283/289 (98%)	247 (87%)	36 (13%)	4 14
1	B	289/289 (100%)	252 (87%)	37 (13%)	4 13
All	All	572/578 (99%)	499 (87%)	73 (13%)	4 13

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	23	PHE
1	A	31	GLU
1	A	39	ASN
1	A	51	ASP
1	A	55	ARG
1	A	56	ILE
1	A	70	GLN
1	A	76	GLN
1	A	88	GLU
1	A	95	LYS
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
1	A	242	LEU
1	A	250	ARG
1	A	257	ILE
1	A	261	ASN
1	A	271	LEU
1	A	278	ARG
1	A	301	LEU
1	A	311	TYR
1	A	315	VAL
1	A	337	LYS
1	A	339	VAL

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Mol	Chain	Res	Type
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	1070	GLN
1	B	1074	PRO
1	B	1116	THR
1	B	1117	HIS
1	B	1123	GLN
1	B	1139	PRO
1	B	1154	LYS
1	B	1171	LEU
1	B	1183	VAL
1	B	1186	SER
1	B	1198	THR
1	B	1207	ASN
1	B	1210	GLU
1	B	1211	GLU
1	B	1231	GLU
1	B	1237	MET
1	B	1238	LEU
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	1301	LEU
1	B	1302	PRO
1	B	1306	GLU
1	B	1310	THR
1	B	1321	LYS
1	B	1323	PRO
1	B	1344	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	45	ASN
1	A	174	GLN
1	A	244	ASN
1	A	246	ASN
1	A	259	GLN
1	A	261	ASN
1	B	1005	ASN
1	B	1007	GLN
1	B	1170	GLN
1	B	1207	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	HNE	A	1347	-	10,10,10	1.48	2 (20%)	9,10,10	1.23	1 (11%)
2	NAP	B	2346	-	46,52,52	1.71	11 (23%)	61,80,80	2.46	17 (27%)
3	HNE	B	2347	-	10,10,10	1.47	2 (20%)	9,10,10	1.22	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	A	1346	-	46,52,52	2.04	9 (19%)	61,80,80	2.35	12 (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
3	HNE	A	1347	-	-	6/9/9/9	-
2	NAP	B	2346	-	-	13/31/67/67	0/5/5/5
3	HNE	B	2347	-	-	6/9/9/9	-
2	NAP	A	1346	-	-	16/31/67/67	0/5/5/5

All (24) 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	O4B-C1B	4.02	1.46	1.40
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	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
2	A	1346	NAP	O4B-C1B	2.34	1.44	1.40
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	C5A-N7A	-2.28	1.31	1.39
2	B	2346	NAP	C5N-C4N	2.27	1.42	1.38
2	B	2346	NAP	C4N-C3N	2.17	1.42	1.39
2	A	1346	NAP	C2A-N3A	2.17	1.35	1.32
2	B	2346	NAP	C2A-N3A	2.14	1.35	1.32
2	A	1346	NAP	C5A-N7A	-2.07	1.32	1.39
2	B	2346	NAP	P2B-O2X	-2.03	1.47	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2346	NAP	C4B-O4B-C1B	-9.90	100.86	109.92
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	O4B-C1B-N9A	6.03	116.74	108.75
2	A	1346	NAP	N3A-C2A-N1A	-5.92	120.63	128.67
2	B	2346	NAP	N3A-C2A-N1A	-5.75	120.87	128.67
2	A	1346	NAP	O4D-C4D-C3D	-5.45	94.34	105.15
2	B	2346	NAP	O3X-P2B-O2B	4.61	123.82	105.85
2	A	1346	NAP	C4A-C5A-N7A	4.55	114.14	109.34
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	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	B	2346	NAP	O5D-C5D-C4D	3.61	121.30	108.99
2	A	1346	NAP	C2B-C1B-N9A	3.52	120.37	112.56
2	B	2346	NAP	C4A-C5A-N7A	3.42	112.95	109.34
2	B	2346	NAP	C5N-C4N-C3N	3.17	123.48	120.36
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	B	2346	NAP	O4B-C1B-C2B	-2.99	101.51	106.61
2	A	1346	NAP	C5D-C4D-C3D	2.97	125.89	115.21
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	B	2346	NAP	C1B-N9A-C4A	2.12	130.37	126.64

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

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Mol	Chain	Res	Type	Atoms
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
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
3	A	1347	HNE	1	0

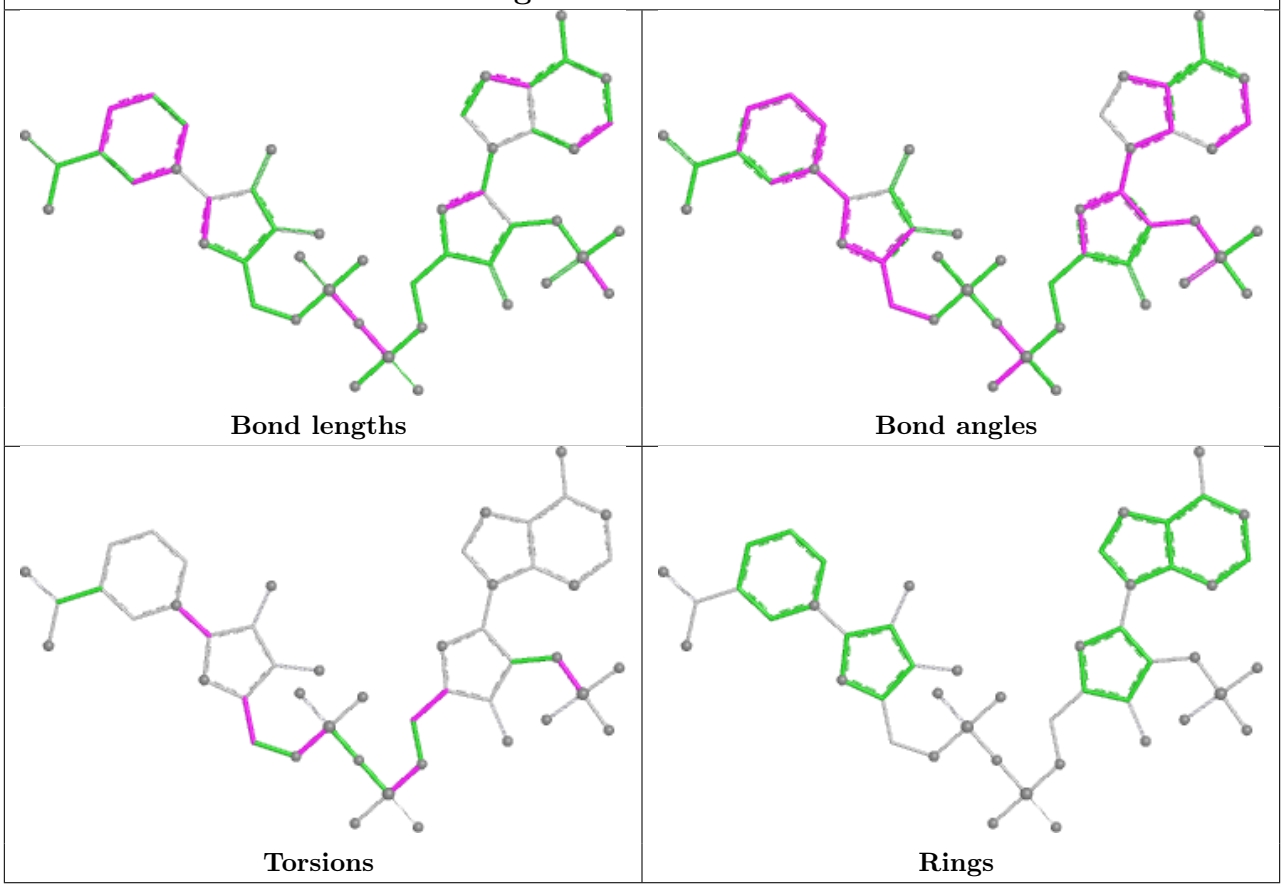
Continued on next page...

Continued from previous page...

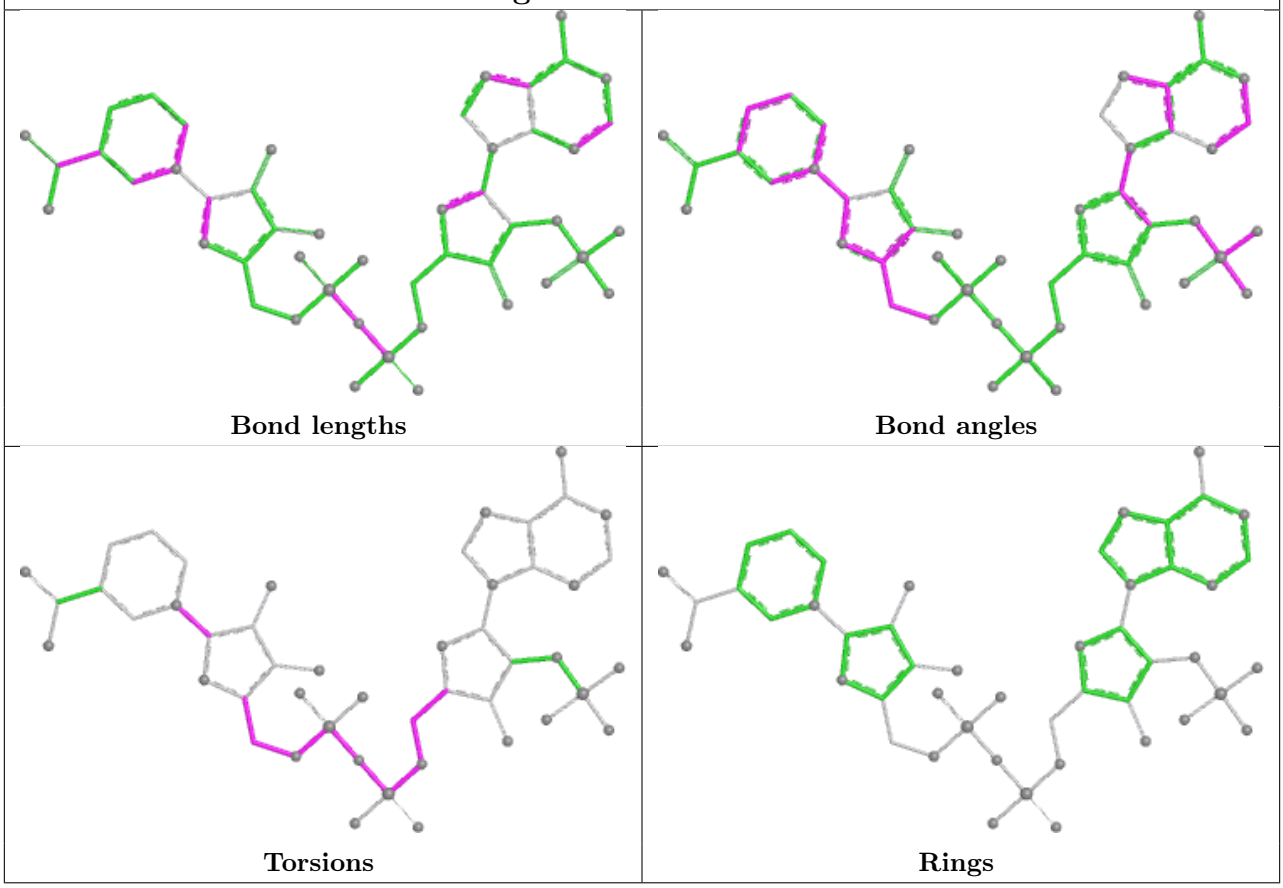
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2346	NAP	5	0
2	A	1346	NAP	6	0

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 then 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.

Ligand NAP B 2346



Ligand NAP A 1346



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.