Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:51 AM GMT

PDB ID	:	2J3J
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

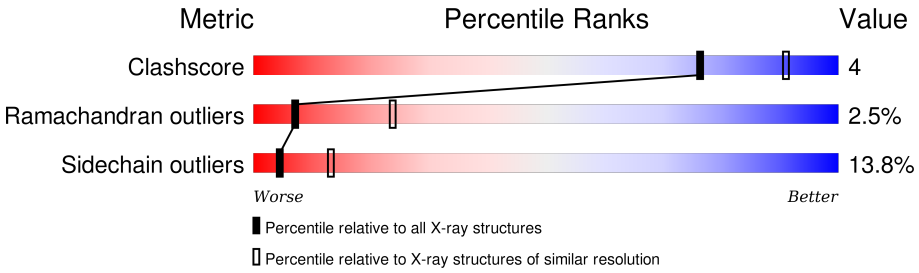
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	63% 28% 6% ·
1	B	345	66% 29% · ·

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.

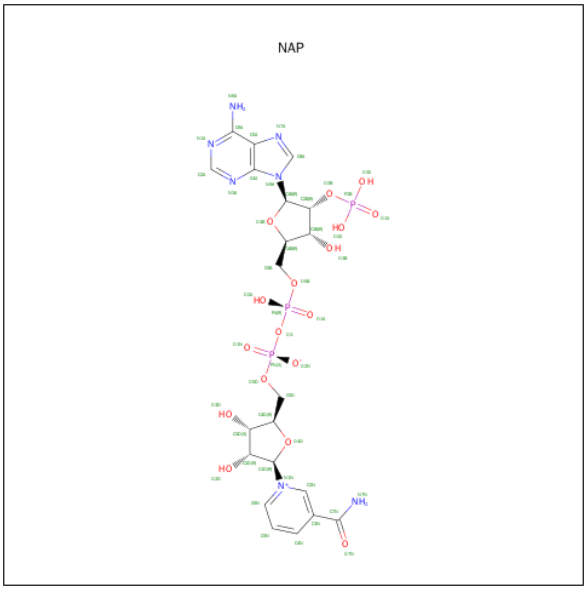
- Molecule 1 is a protein called NADP-DEPENDENT OXIDOREDUCTASE P1.

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

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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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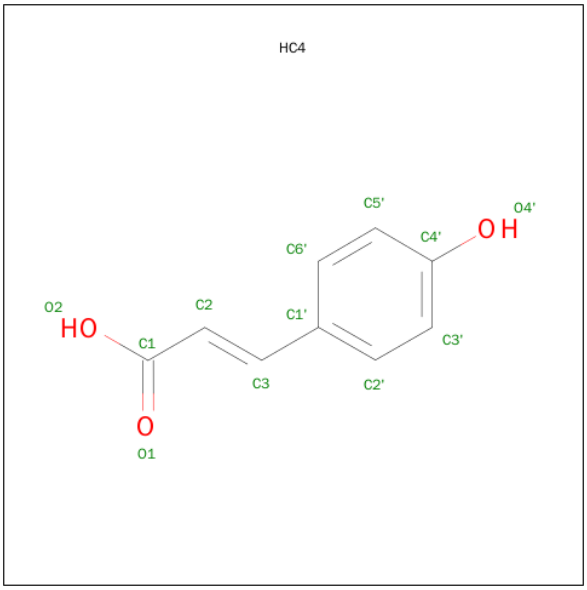
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 4'-HYDROXYCINNAMIC ACID (three-letter code: HC4) (formula: $C_9H_8O_3$).



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		

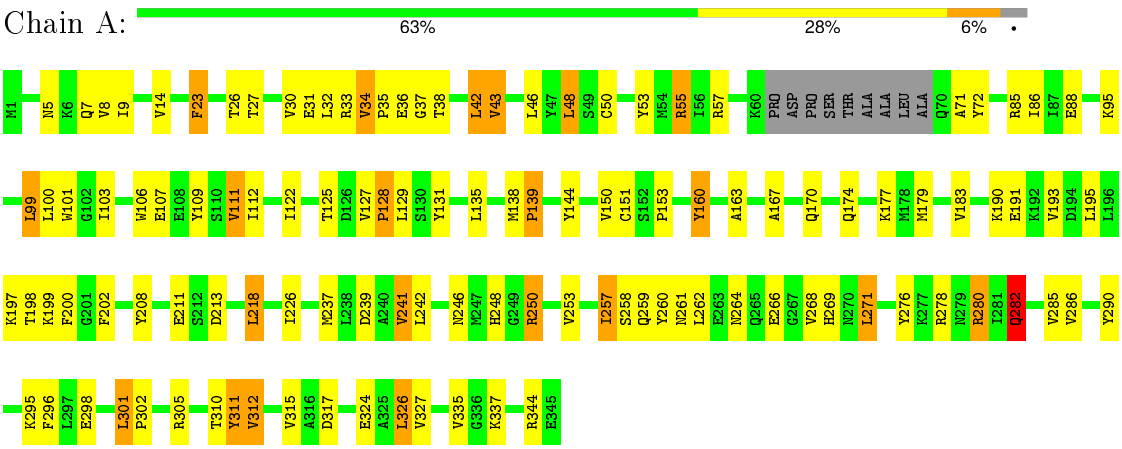
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

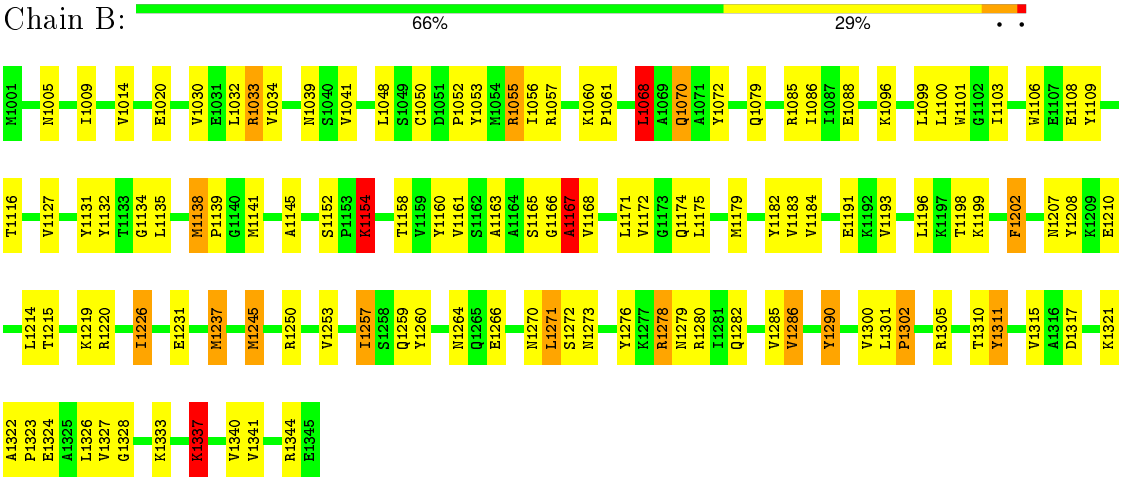
- Molecule 1: NADP-DEPENDENT OXIDOREDUCTASE P1

Chain A:



- Molecule 1: NADP-DEPENDENT OXIDOREDUCTASE P1

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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: NAP, HC4

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	1.27	2/2681 (0.1%)	2.04	97/3625 (2.7%)
1	B	1.26	5/2742 (0.2%)	2.03	97/3713 (2.6%)
All	All	1.27	7/5423 (0.1%)	2.03	194/7338 (2.6%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1290	TYR	C-N	-5.82	1.20	1.34
1	B	1341	VAL	CA-CB	5.64	1.66	1.54
1	A	53	TYR	CG-CD1	5.18	1.45	1.39
1	B	1127	VAL	CA-CB	5.08	1.65	1.54
1	A	144	TYR	CG-CD2	5.08	1.45	1.39
1	B	1053	TYR	CG-CD1	5.04	1.45	1.39
1	B	1276	TYR	CG-CD2	5.03	1.45	1.39

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	B	1085	ARG	NE-CZ-NH2	-9.81	115.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1305	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	A	241	VAL	CG1-CB-CG2	-9.63	95.49	110.90
1	A	99	LEU	CA-CB-CG	9.40	136.93	115.30
1	A	278	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	B	1253	VAL	CG1-CB-CG2	-9.28	96.05	110.90
1	B	1245	MET	CG-SD-CE	-9.12	85.60	100.20
1	A	160	TYR	CB-CG-CD2	-8.98	115.61	121.00
1	A	280	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	B	1280	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	B	1099	LEU	CA-CB-CG	8.78	135.50	115.30
1	B	1085	ARG	NE-CZ-NH1	8.77	124.69	120.30
1	A	131	TYR	CB-CG-CD1	-8.73	115.76	121.00
1	A	305	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	55	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	290	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	A	106	TRP	CE2-CD2-CG	-8.26	100.69	107.30
1	B	1057	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	A	250	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	85	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	B	1311	TYR	CB-CG-CD2	-8.07	116.16	121.00
1	B	1055	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	1260	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	A	86	ILE	CG1-CB-CG2	-7.95	93.92	111.40
1	B	1290	TYR	C-N-CA	7.95	141.57	121.70
1	A	290	TYR	CB-CG-CD1	7.86	125.72	121.00
1	A	160	TYR	CB-CG-CD1	7.76	125.66	121.00
1	B	1160	TYR	CB-CG-CD2	-7.72	116.37	121.00
1	A	131	TYR	CB-CG-CD2	7.65	125.59	121.00
1	B	1033	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	1237	MET	CG-SD-CE	-7.60	88.05	100.20
1	A	253	VAL	CG1-CB-CG2	-7.59	98.75	110.90
1	A	106	TRP	CD1-CG-CD2	7.59	112.37	106.30
1	B	1100	LEU	CA-CB-CG	7.56	132.70	115.30
1	A	260	TYR	CB-CG-CD1	-7.54	116.47	121.00
1	B	1048	LEU	CB-CG-CD2	-7.48	98.28	111.00
1	B	1101	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	A	55	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	1101	TRP	CD1-CG-CD2	7.37	112.20	106.30
1	B	1276	TYR	CB-CG-CD2	7.29	125.37	121.00
1	B	1103	ILE	CA-C-N	-7.25	101.24	117.20
1	B	1163	ALA	CA-C-N	-7.20	101.36	117.20
1	B	1086	ILE	CG1-CB-CG2	-7.16	95.64	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	101	TRP	CA-CB-CG	7.13	127.25	113.70
1	A	33	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	57	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	B	1053	TYR	CA-CB-CG	7.02	126.74	113.40
1	B	1131	TYR	CB-CG-CD2	-7.01	116.79	121.00
1	B	1165	SER	CA-C-N	-6.97	102.25	116.20
1	A	312	VAL	CG1-CB-CG2	-6.84	99.96	110.90
1	B	1301	LEU	CA-C-O	-6.83	105.75	120.10
1	B	1278	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	53	TYR	CA-CB-CG	6.75	126.23	113.40
1	A	100	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	101	TRP	CG-CD2-CE3	6.73	139.96	133.90
1	B	1220	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	32	LEU	CA-C-N	-6.68	102.50	117.20
1	B	1344	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	1160	TYR	CB-CG-CD1	6.68	125.01	121.00
1	A	101	TRP	CD1-CG-CD2	6.67	111.64	106.30
1	A	327	VAL	CA-CB-CG2	-6.65	100.93	110.90
1	A	88	GLU	CA-CB-CG	6.63	127.98	113.40
1	A	128	PRO	N-CA-C	6.62	129.31	112.10
1	B	1220	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	327	VAL	CA-CB-CG1	6.45	120.58	110.90
1	B	1285	VAL	CG1-CB-CG2	-6.43	100.61	110.90
1	B	1337	LYS	CA-CB-CG	6.43	127.54	113.40
1	B	1041	VAL	CG1-CB-CG2	-6.42	100.63	110.90
1	B	1068	LEU	CA-CB-CG	6.42	130.06	115.30
1	B	1324	GLU	CA-CB-CG	6.41	127.51	113.40
1	B	1168	VAL	CG1-CB-CG2	-6.41	100.65	110.90
1	B	1276	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	B	1280	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	1290	TYR	O-C-N	-6.34	112.56	122.70
1	B	1057	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	1131	TYR	CA-CB-CG	6.33	125.42	113.40
1	A	50	CYS	CA-C-N	-6.31	103.31	117.20
1	B	1191	GLU	CA-CB-CG	6.29	127.23	113.40
1	B	1048	LEU	CA-CB-CG	6.27	129.73	115.30
1	B	1301	LEU	CA-C-N	6.24	134.57	117.10
1	A	46	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	200	PHE	CB-CG-CD2	-6.22	116.44	120.80
1	B	1072	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	A	139	PRO	CA-N-CD	-6.19	102.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1172	VAL	CG1-CB-CG2	-6.17	101.02	110.90
1	B	1276	TYR	CA-CB-CG	6.16	125.10	113.40
1	B	1202	PHE	CB-CG-CD2	6.15	125.11	120.80
1	B	1106	TRP	CE2-CD2-CG	-6.13	102.39	107.30
1	A	33	ARG	CB-CG-CD	-6.13	95.66	111.60
1	B	1323	PRO	CA-N-CD	-6.12	102.93	111.50
1	A	101	TRP	CB-CG-CD1	-6.12	119.05	127.00
1	A	208	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	B	1167	ALA	N-CA-C	6.11	127.49	111.00
1	A	163	ALA	CA-C-N	-6.08	103.83	117.20
1	A	218	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	260	TYR	CB-CG-CD2	6.07	124.64	121.00
1	B	1337	LYS	CB-CG-CD	6.04	127.31	111.60
1	B	1257	ILE	CB-CA-C	-6.03	99.54	111.60
1	A	296	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	B	1328	GLY	CA-C-N	-5.99	104.03	117.20
1	B	1341	VAL	CG1-CB-CG2	-5.98	101.33	110.90
1	B	1106	TRP	CD1-CG-CD2	5.97	111.08	106.30
1	B	1193	VAL	CA-CB-CG1	5.97	119.86	110.90
1	B	1305	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	1327	VAL	CA-CB-CG2	-5.91	102.04	110.90
1	A	311	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	A	122	ILE	CA-C-N	-5.89	104.24	117.20
1	B	1014	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	A	86	ILE	CA-C-N	-5.79	104.45	117.20
1	A	282	GLN	CA-CB-CG	5.78	126.12	113.40
1	B	1154	LYS	CA-CB-CG	5.75	126.06	113.40
1	A	202	PHE	CB-CG-CD1	-5.72	116.79	120.80
1	A	72	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	B	1193	VAL	CA-CB-CG2	-5.70	102.35	110.90
1	B	1311	TYR	CB-CG-CD1	5.69	124.41	121.00
1	B	1161	VAL	CG1-CB-CG2	-5.68	101.81	110.90
1	B	1237	MET	CA-CB-CG	-5.66	103.67	113.30
1	B	1138	MET	CA-CB-CG	5.65	122.91	113.30
1	A	150	VAL	CG1-CB-CG2	-5.64	101.87	110.90
1	B	1030	VAL	CG1-CB-CG2	-5.64	101.88	110.90
1	A	285	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	B	1327	VAL	CA-CB-CG1	5.62	119.32	110.90
1	A	106	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	A	48	LEU	CA-CB-CG	5.59	128.15	115.30
1	A	268	VAL	CG1-CB-CG2	-5.59	101.96	110.90
1	B	1009	ILE	CA-CB-CG1	-5.57	100.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	37	GLY	C-N-CA	5.57	135.62	121.70
1	B	1179	MET	CG-SD-CE	-5.54	91.33	100.20
1	B	1141	MET	CA-CB-CG	5.54	122.72	113.30
1	A	302	PRO	CA-N-CD	-5.51	103.78	111.50
1	B	1302	PRO	CA-N-CD	-5.50	103.80	111.50
1	B	1260	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	344	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	248	HIS	CA-C-N	-5.48	105.24	116.20
1	B	1132	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	128	PRO	CA-N-CD	-5.47	103.84	111.50
1	A	43	VAL	N-CA-CB	-5.47	99.47	111.50
1	B	1344	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	42	LEU	CA-CB-CG	5.47	127.87	115.30
1	A	296	PHE	CB-CG-CD1	5.47	124.63	120.80
1	A	151	CYS	CA-CB-SG	5.44	123.80	114.00
1	A	257	ILE	CB-CA-C	-5.44	100.71	111.60
1	A	111	VAL	CA-CB-CG1	-5.44	102.74	110.90
1	B	1103	ILE	O-C-N	5.44	131.40	122.70
1	A	55	ARG	CB-CG-CD	5.41	125.67	111.60
1	A	106	TRP	CA-C-N	-5.40	105.32	117.20
1	B	1315	VAL	N-CA-CB	-5.39	99.63	111.50
1	A	250	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	1055	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	14	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	B	1050	CYS	CA-C-N	-5.38	105.36	117.20
1	A	198	THR	CA-CB-CG2	5.38	119.93	112.40
1	B	1215	THR	CA-CB-CG2	5.36	119.90	112.40
1	A	27	THR	CA-CB-CG2	5.33	119.87	112.40
1	A	193	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	A	33	ARG	CA-CB-CG	5.31	125.09	113.40
1	A	7	GLN	CA-CB-CG	5.31	125.08	113.40
1	A	211	GLU	CA-CB-CG	5.30	125.05	113.40
1	B	1286	VAL	CA-CB-CG1	-5.25	103.02	110.90
1	A	177	LYS	CA-C-N	-5.25	105.65	117.20
1	B	1135	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	99	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	A	237	MET	CA-CB-CG	5.22	122.18	113.30
1	B	1166	GLY	CA-C-N	-5.18	105.81	117.20
1	A	262	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	1055	ARG	CB-CG-CD	5.17	125.04	111.60
1	B	1052	PRO	N-CA-C	5.16	125.52	112.10
1	A	326	LEU	CB-CG-CD1	-5.16	102.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1231	GLU	CA-CB-CG	5.16	124.75	113.40
1	A	107	GLU	CA-CB-CG	5.15	124.73	113.40
1	B	1175	LEU	CB-CG-CD2	-5.15	102.25	111.00
1	B	1184	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	B	1116	THR	N-CA-C	5.13	124.85	111.00
1	A	23	PHE	CA-CB-CG	5.13	126.20	113.90
1	A	30	VAL	CA-C-N	-5.11	105.97	117.20
1	A	103	ILE	CA-C-N	-5.11	105.97	117.20
1	A	295	LYS	CA-CB-CG	5.10	124.63	113.40
1	B	1226	ILE	CA-CB-CG2	-5.09	100.72	110.90
1	A	8	VAL	CG1-CB-CG2	-5.09	102.75	110.90
1	B	1198	THR	CA-CB-CG2	5.09	119.52	112.40
1	A	276	TYR	CA-CB-CG	5.08	123.04	113.40
1	A	190	LYS	CA-C-N	-5.07	106.04	117.20
1	A	276	TYR	CB-CG-CD2	5.06	124.03	121.00
1	B	1145	ALA	CA-C-N	-5.05	106.09	116.20
1	B	1290	TYR	CA-C-N	5.05	128.32	117.20
1	A	257	ILE	N-CA-CB	5.04	122.40	110.80
1	A	335	VAL	CA-CB-CG2	-5.04	103.34	110.90
1	B	1138	MET	CA-C-O	-5.04	109.52	120.10
1	A	153	PRO	N-CA-C	5.01	125.13	112.10
1	A	301	LEU	CA-C-O	-5.01	109.58	120.10
1	A	271	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	B	1053	TYR	CB-CG-CD2	-5.01	118.00	121.00

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 (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	13	0
1	B	2681	0	2647	18	0
2	A	48	0	25	9	0
2	B	48	0	25	7	0
3	A	11	0	7	0	0
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	41	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 (41) 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:C2B	2:B:2346:NAP:P2B	2.11	1.38
2:A:1346:NAP:C2B	2:A:1346:NAP:P2B	2.15	1.34
2:A:1346:NAP:P2B	2:A:1346:NAP:O2B	0.86	1.26
2:B:2346:NAP:O2B	2:B:2346:NAP:P2B	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:O2X	2:A:1346:NAP:O2B	1.87	0.91
1:B:1174:GLN:HE22	1:B:1310:THR:H	1.27	0.81
2:B:2346:NAP:H2B	2:B:2346:NAP:P2B	2.21	0.80
1:A:282:GLN:NE2	1:B:1278:ARG:HH21	1.82	0.78
2:B:2346:NAP:O3X	2:B:2346:NAP:O2B	1.99	0.75
2:B:2346:NAP:O2X	2:B:2346:NAP:O2B	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1167:ALA:HB3	2:B:2346:NAP:O2N	2.20	0.42
1:B:1134:GLY:HA3	1:B:1311:TYR:OH	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%)	6	21
1	B	343/345 (99%)	302 (88%)	33 (10%)	8 (2%)	8	26
All	All	675/690 (98%)	601 (89%)	57 (8%)	17 (2%)	7	24

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ALA
1	A	128	PRO
1	A	129	LEU

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Mol	Chain	Res	Type
1	A	167	ALA
1	B	1039	ASN
1	B	1070	GLN
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 (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%)	242 (86%)	41 (14%)	4	11
1	B	289/289 (100%)	251 (87%)	38 (13%)	5	15
All	All	572/578 (99%)	493 (86%)	79 (14%)	4	13

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
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
1	A	55	ARG

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Mol	Chain	Res	Type
1	A	95	LYS
1	A	99	LEU
1	A	111	VAL
1	A	112	ILE
1	A	125	THR
1	A	127	VAL
1	A	135	LEU
1	A	139	PRO
1	A	179	MET
1	A	183	VAL
1	A	197	LYS
1	A	199	LYS
1	A	213	ASP
1	A	218	LEU
1	A	239	ASP
1	A	242	LEU
1	A	246	ASN
1	A	250	ARG
1	A	257	ILE
1	A	261	ASN
1	A	264	ASN
1	A	269	HIS
1	A	280	ARG
1	A	282	GLN
1	A	298	GLU
1	A	301	LEU
1	A	311	TYR
1	A	315	VAL
1	A	317	ASP
1	A	324	GLU
1	A	326	LEU
1	A	337	LYS
1	B	1020	GLU
1	B	1033	ARG
1	B	1034	VAL
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	1139	PRO

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Mol	Chain	Res	Type
1	B	1154	LYS
1	B	1171	LEU
1	B	1183	VAL
1	B	1196	LEU
1	B	1199	LYS
1	B	1202	PHE
1	B	1207	ASN
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	1326	LEU
1	B	1333	LYS
1	B	1337	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	45	ASN
1	A	170	GLN
1	A	174	GLN
1	A	244	ASN
1	A	246	ASN
1	A	259	GLN
1	A	265	GLN
1	A	282	GLN
1	B	1005	ASN

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Mol	Chain	Res	Type
1	B	1076	GLN
1	B	1174	GLN
1	B	1207	ASN
1	B	1259	GLN
1	B	1270	ASN
1	B	1273	ASN
1	B	1279	ASN
1	B	1334	ASN

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 carbohydrates 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	-	42,52,52	3.97	6 (14%)	54,80,80	2.63	13 (24%)
3	HC4	A	1347	-	11,11,12	3.02	8 (72%)	12,13,15	2.12	1 (8%)
2	NAP	B	2346	-	42,52,52	3.97	6 (14%)	54,80,80	2.55	15 (27%)
3	HC4	B	2347	-	11,11,12	2.97	8 (72%)	12,13,15	2.08	1 (8%)

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	-	-	0/27/67/67	0/5/5/5
3	HC4	A	1347	-	-	0/4/4/5	0/1/1/1
2	NAP	B	2346	-	-	0/27/67/67	0/5/5/5
3	HC4	B	2347	-	-	0/4/4/5	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2346	NAP	P2B-O2B	-24.52	0.85	1.60
2	A	1346	NAP	P2B-O2B	-24.21	0.86	1.60
3	B	2347	HC4	C2-C3	-6.95	1.21	1.34
3	A	1347	HC4	C2-C3	-6.81	1.21	1.34
2	A	1346	NAP	C5A-N7A	-2.13	1.32	1.39
2	B	2346	NAP	C5A-N7A	-2.11	1.32	1.39
3	B	2347	HC4	C3'-C2'	2.12	1.42	1.38
3	B	2347	HC4	C2'-C1'	2.14	1.43	1.39
2	B	2346	NAP	O4B-C1B	2.15	1.43	1.41
2	B	2346	NAP	C3N-C7N	2.16	1.53	1.50
3	A	1347	HC4	C3'-C2'	2.25	1.42	1.38
3	A	1347	HC4	C2'-C1'	2.30	1.43	1.39
3	B	2347	HC4	C2-C1	2.34	1.50	1.44
2	A	1346	NAP	C3N-C7N	2.41	1.54	1.50
2	B	2346	NAP	O4D-C1D	2.41	1.44	1.41
3	A	1347	HC4	C2-C1	2.48	1.51	1.44
3	B	2347	HC4	C6'-C5'	2.75	1.43	1.38
2	A	1346	NAP	C6N-N1N	2.78	1.42	1.35
3	B	2347	HC4	C6'-C1'	2.82	1.44	1.39
3	B	2347	HC4	C5'-C4'	2.86	1.44	1.38
3	B	2347	HC4	C3'-C4'	2.86	1.44	1.38
3	A	1347	HC4	C6'-C5'	2.88	1.43	1.38
3	A	1347	HC4	C3'-C4'	2.91	1.44	1.38
2	A	1346	NAP	O4D-C1D	2.93	1.44	1.41
3	A	1347	HC4	C5'-C4'	2.94	1.44	1.38
3	A	1347	HC4	C6'-C1'	2.94	1.45	1.39
2	B	2346	NAP	C6N-N1N	3.05	1.43	1.35
2	A	1346	NAP	O4B-C1B	3.68	1.45	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1346	NAP	N3A-C2A-N1A	-10.22	121.07	128.89
2	B	2346	NAP	N3A-C2A-N1A	-10.21	121.08	128.89
3	A	1347	HC4	C1'-C3-C2	-6.98	116.24	127.26
3	B	2347	HC4	C1'-C3-C2	-6.69	116.70	127.26
2	B	2346	NAP	O2B-P2B-O1X	-4.62	95.56	107.11
2	A	1346	NAP	O4D-C4D-C3D	-4.23	96.63	105.15
2	B	2346	NAP	C4B-O4B-C1B	-3.45	105.93	109.72
2	B	2346	NAP	O4B-C4B-C3B	-3.11	98.88	105.15
2	B	2346	NAP	O4B-C1B-C2B	-2.71	101.70	106.60
2	A	1346	NAP	C3N-C7N-N7N	-2.67	114.90	117.82
2	B	2346	NAP	O4B-C4B-C5B	-2.49	100.42	109.32
2	A	1346	NAP	O2B-P2B-O1X	-2.11	101.84	107.11
2	A	1346	NAP	O4D-C4D-C5D	2.01	116.50	109.32
2	B	2346	NAP	C5N-C4N-C3N	2.06	122.93	120.33
2	B	2346	NAP	O3-PA-O5B	2.13	108.59	102.94
2	B	2346	NAP	O4D-C4D-C5D	2.35	117.71	109.32
2	A	1346	NAP	O3B-C3B-C2B	2.45	118.23	111.16
2	B	2346	NAP	C4D-O4D-C1D	2.53	112.50	109.72
2	B	2346	NAP	P2B-O2B-C2B	2.81	128.31	121.56
2	B	2346	NAP	O4B-C1B-N9A	3.21	114.81	108.10
2	A	1346	NAP	C4D-O4D-C1D	3.34	113.39	109.72
2	A	1346	NAP	O7N-C7N-C3N	3.41	123.31	119.59
2	A	1346	NAP	O3-PN-O5D	3.67	112.67	102.94
2	B	2346	NAP	C4A-C5A-N7A	3.97	113.14	109.48
2	A	1346	NAP	P2B-O2B-C2B	4.24	131.74	121.56
2	B	2346	NAP	O5D-C5D-C4D	4.27	124.88	109.12
2	A	1346	NAP	C4A-C5A-N7A	4.48	113.60	109.48
2	A	1346	NAP	O5D-C5D-C4D	6.37	132.59	109.12
2	A	1346	NAP	O4D-C1D-N1N	8.92	117.94	108.13
2	B	2346	NAP	O4D-C1D-N1N	9.15	118.19	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 17 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.