



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:42 pm GMT

PDB ID : 2J3H  
Title : CRYSTAL STRUCTURE OF ARABIDOPSIS THALIANA DOUBLE BOND  
REDUCTASE (AT5G16970)-APO FORM  
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Deposited on : 2006-08-21  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

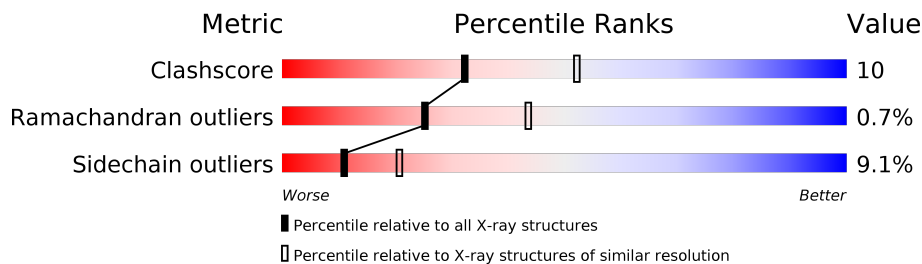
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	345	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5437 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 water.

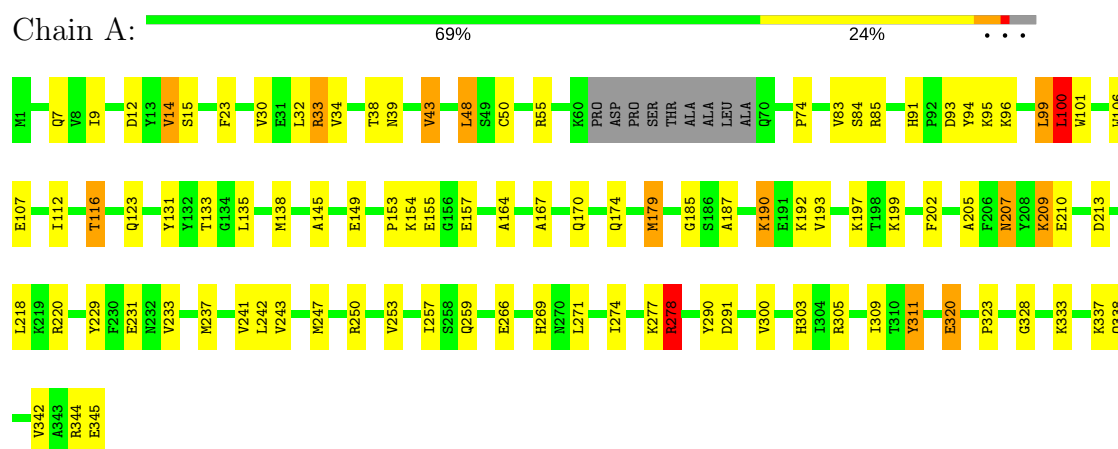
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	71	Total	O	0	0
			71	71		
2	B	62	Total	O	0	0
			62	62		

### 3 Residue-property plots

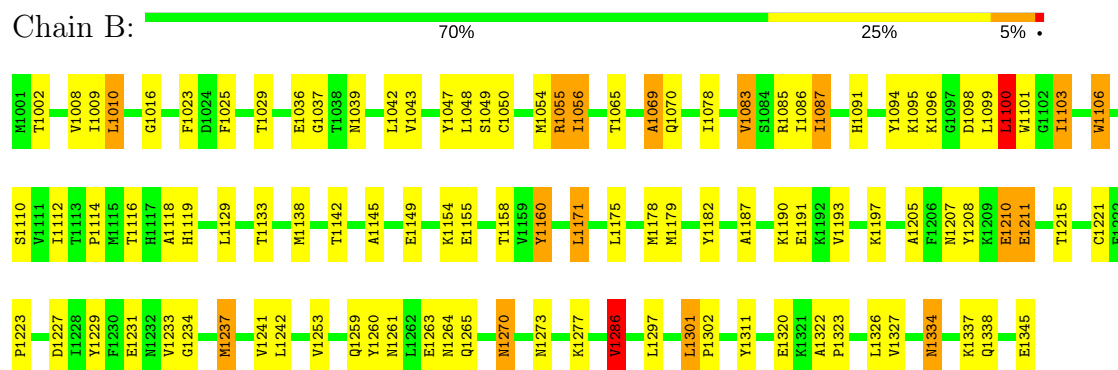
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



#### • Molecule 1: NADP-DEPENDENT OXIDOREDUCTASE P1



## 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, $\alpha$ , $\beta$ , $\gamma$	49.46 Å 122.98 Å 148.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.5 (15.00-2.50)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5437	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.77	0/2681	1.49	27/3625 (0.7%)
1	B	0.78	0/2742	1.44	18/3713 (0.5%)
All	All	0.78	0/5423	1.47	45/7338 (0.6%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1311	TYR	CB-CG-CD2	-9.06	115.56	121.00
1	B	1106	TRP	CD1-CG-CD2	8.50	113.10	106.30
1	B	1101	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	A	311	TYR	CB-CG-CD1	-8.44	115.94	121.00
1	A	100	LEU	CA-CB-CG	8.31	134.42	115.30
1	A	101	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	101	TRP	CE2-CD2-CG	-8.04	100.87	107.30
1	B	1101	TRP	CE2-CD2-CG	-7.99	100.91	107.30
1	A	344	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	106	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	B	1106	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	A	106	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	A	290	TYR	CB-CG-CD2	-7.45	116.53	121.00
1	B	1311	TYR	CB-CG-CD1	7.20	125.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1286	VAL	CB-CA-C	-7.03	98.05	111.40
1	B	1094	TYR	CB-CG-CD1	-6.94	116.83	121.00
1	A	33	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	1100	LEU	CA-CB-CG	6.91	131.18	115.30
1	A	179	MET	CG-SD-CE	-6.71	89.46	100.20
1	A	193	VAL	CG1-CB-CG2	-6.55	100.41	110.90
1	A	39	ASN	CA-C-N	-6.24	103.48	117.20
1	A	101	TRP	CG-CD2-CE3	6.23	139.51	133.90
1	A	94	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	A	250	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	116	THR	N-CA-C	5.76	126.56	111.00
1	A	55	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	250	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	1054	MET	CG-SD-CE	-5.55	91.32	100.20
1	A	99	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	1010	LEU	CA-CB-CG	5.49	127.93	115.30
1	B	1208	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	B	1160	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	1211	GLU	CA-C-N	-5.40	105.31	117.20
1	A	220	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	1178	MET	CA-CB-CG	5.29	122.30	113.30
1	A	85	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	131	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	A	311	TYR	CB-CG-CD2	5.21	124.12	121.00
1	A	278	ARG	CA-CB-CG	5.15	124.73	113.40
1	A	101	TRP	CA-CB-CG	5.12	123.44	113.70
1	A	277	LYS	CA-CB-CG	-5.07	102.24	113.40
1	B	1327	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	A	243	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	B	1106	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	B	1260	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	VAL	Peptide
1	B	1160	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2623	0	2594	48	0
1	B	2681	0	2648	58	0
2	A	71	0	0	3	0
2	B	62	0	0	3	0
All	All	5437	0	5242	105	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 10.

All (105) 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:274:ILE:HD11	1:B:1253:VAL:HG21	1.67	0.77
1:B:1171:LEU:HD22	1:B:1175:LEU:HD13	1.66	0.76
1:B:1103:ILE:HB	2:B:2016:HOH:O	1.89	0.71
1:B:1334:ASN:H	1:B:1334:ASN:HD22	1.39	0.69
1:B:1055:ARG:HH11	1:B:1261:ASN:HD22	1.41	0.66
1:B:1055:ARG:HD3	1:B:1261:ASN:ND2	2.10	0.66
1:B:1050:CYS:SG	2:B:2060:HOH:O	2.50	0.66
1:A:303:HIS:HB3	1:A:309:ILE:HG12	1.77	0.65
1:B:1025:PHE:HZ	1:B:1320:GLU:HA	1.60	0.65
1:A:207:ASN:HD22	1:A:209:LYS:H	1.43	0.65
1:A:48:LEU:HD22	1:A:342:VAL:HG21	1.78	0.64
1:A:170:GLN:O	1:A:174:GLN:HG3	1.99	0.63
1:A:231:GLU:HG2	1:A:253:VAL:HG22	1.81	0.62
1:A:23:PHE:CD2	1:A:323:PRO:HB3	2.35	0.61
1:B:1099:LEU:HD13	1:B:1129:LEU:HD11	1.82	0.61
1:A:154:LYS:O	1:A:157:GLU:HG2	2.01	0.60
1:B:1002:THR:HG22	1:B:1029:THR:HG22	1.83	0.60
1:B:1334:ASN:ND2	1:B:1334:ASN:H	1.99	0.60
1:A:259:GLN:HE22	1:A:266:GLU:H	1.49	0.60
1:B:1242:LEU:O	1:B:1277:LYS:HE3	2.02	0.60
1:B:1025:PHE:CZ	1:B:1320:GLU:HA	2.36	0.59
1:A:12:ASP:HA	1:A:74:PRO:HB3	1.84	0.58
1:B:1190:LYS:HG2	1:B:1207:ASN:HD22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1229:TYR:CE2	1:B:1231:GLU:HG2	2.37	0.58
1:B:1155:GLU:HG2	1:B:1179:MET:HG3	1.86	0.58
1:B:1085:ARG:HH21	1:B:1087:ILE:HD13	1.69	0.57
1:B:1338:GLN:HG2	2:B:2060:HOH:O	2.04	0.57
1:B:1297:LEU:O	1:B:1301:LEU:HB2	2.05	0.57
1:A:207:ASN:HB3	1:A:210:GLU:HG2	1.86	0.56
1:B:1270:ASN:HB3	1:B:1273:ASN:ND2	2.20	0.56
1:A:259:GLN:NE2	1:A:266:GLU:H	2.03	0.56
1:A:274:ILE:O	1:A:278:ARG:HA	2.07	0.55
1:B:1103:ILE:HD11	1:B:1118:ALA:HB1	1.89	0.55
1:A:199:LYS:HG2	2:A:2065:HOH:O	2.06	0.54
1:A:207:ASN:ND2	1:A:209:LYS:H	2.04	0.54
1:B:1016:GLY:H	1:B:1263:GLU:CD	2.10	0.54
1:B:1138:MET:HG2	1:B:1286:VAL:HG21	1.90	0.54
1:A:190:LYS:HE2	1:A:190:LYS:HA	1.89	0.53
1:A:138:MET:C	1:A:138:MET:SD	2.87	0.53
1:B:1056:ILE:HG12	1:B:1069:ALA:HB2	1.91	0.53
1:A:303:HIS:CB	1:A:309:ILE:HG12	2.38	0.53
1:B:1049:SER:HB2	1:B:1133:THR:HB	1.90	0.52
1:B:1047:TYR:HB2	1:B:1083:VAL:HG13	1.92	0.51
1:B:1055:ARG:HD3	1:B:1261:ASN:HD21	1.74	0.51
1:A:247:MET:HE1	2:A:2057:HOH:O	2.11	0.51
1:A:135:LEU:HD22	1:A:311:TYR:HB2	1.93	0.50
1:B:1233:VAL:HG23	1:B:1234:GLY:H	1.76	0.50
1:A:187:ALA:HB1	1:A:192:LYS:HB3	1.94	0.50
1:B:1270:ASN:HB3	1:B:1273:ASN:HD22	1.76	0.50
1:B:1039:ASN:HB3	1:B:1091:HIS:CD2	2.48	0.49
1:A:167:ALA:HB2	1:A:337:LYS:HG3	1.93	0.49
1:B:1103:ILE:O	1:B:1119:HIS:HE1	1.95	0.49
1:A:30:VAL:HG12	1:A:32:LEU:HD12	1.94	0.49
1:A:83:VAL:HG23	1:A:133:THR:HG23	1.94	0.49
1:B:1207:ASN:HB3	1:B:1210:GLU:HB3	1.95	0.48
1:A:229:TYR:CD2	1:A:241:VAL:HG11	2.48	0.48
1:A:48:LEU:HD22	1:A:342:VAL:CG2	2.42	0.48
1:B:1016:GLY:O	1:B:1055:ARG:NH1	2.47	0.48
1:B:1237:MET:O	1:B:1241:VAL:HG13	2.13	0.48
1:A:153:PRO:HB2	1:A:179:MET:CE	2.44	0.47
1:B:1145:ALA:O	1:B:1149:GLU:HB2	2.15	0.47
1:B:1221:CYS:O	1:B:1223:PRO:HD3	2.14	0.47
1:B:1190:LYS:HA	1:B:1193:VAL:HB	1.97	0.47
1:B:1036:GLU:HG2	1:B:1037:GLY:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1322:ALA:HB3	1:B:1323:PRO:HD3	1.97	0.47
1:A:164:ALA:HB1	1:A:202:PHE:CE1	2.50	0.46
1:A:320:GLU:HB2	2:A:2067:HOH:O	2.16	0.46
1:B:1114:PRO:HA	1:B:1119:HIS:CD2	2.50	0.46
1:A:164:ALA:HB1	1:A:202:PHE:HE1	1.80	0.46
1:B:1043:VAL:HG22	1:B:1110:SER:O	2.16	0.45
1:B:1233:VAL:HG23	1:B:1234:GLY:N	2.31	0.45
1:B:1016:GLY:HA2	1:B:1261:ASN:O	2.17	0.45
1:A:50:CYS:HB2	1:A:338:GLN:HB3	1.99	0.44
1:B:1231:GLU:HB3	1:B:1253:VAL:HA	1.99	0.44
1:A:14:VAL:HG12	1:A:15:SER:H	1.83	0.44
1:A:7:GLN:HG2	1:A:107:GLU:HG2	1.99	0.44
1:A:100:LEU:HD11	1:A:112:ILE:HD11	1.98	0.44
1:A:43:VAL:HG22	1:A:84:SER:HB3	2.00	0.44
1:A:145:ALA:O	1:A:149:GLU:HB2	2.18	0.44
1:B:1106:TRP:CH2	1:B:1326:LEU:HD22	2.53	0.43
1:B:1100:LEU:HD11	1:B:1112:ILE:HD11	1.99	0.43
1:B:1055:ARG:HH11	1:B:1261:ASN:ND2	2.12	0.43
1:B:1158:THR:HG22	1:B:1182:TYR:HB3	2.00	0.43
1:B:1103:ILE:HG13	1:B:1103:ILE:H	1.66	0.42
1:B:1187:ALA:O	1:B:1207:ASN:HA	2.19	0.42
1:A:305:ARG:HH11	1:A:305:ARG:HD2	1.73	0.42
1:A:91:HIS:ND1	1:A:93:ASP:HB2	2.34	0.42
1:A:328:GLY:HA2	1:A:333:LYS:NZ	2.35	0.42
1:B:1087:ILE:O	1:B:1096:LYS:HG2	2.19	0.42
1:B:1085:ARG:HD3	1:B:1345:GLU:OE2	2.20	0.42
1:A:233:VAL:HA	1:A:257:ILE:HG12	2.01	0.42
1:A:229:TYR:CE2	1:A:231:GLU:HB2	2.54	0.42
1:A:311:TYR:OH	1:A:337:LYS:HD2	2.20	0.42
1:A:185:GLY:O	1:A:205:ALA:HA	2.20	0.41
1:B:1142:THR:HA	1:B:1286:VAL:HG13	2.01	0.41
1:A:153:PRO:HB2	1:A:179:MET:HE1	2.02	0.41
1:A:199:LYS:HA	1:A:199:LYS:HD2	1.86	0.41
1:A:197:LYS:HB2	1:A:197:LYS:HE3	1.82	0.41
1:B:1259:GLN:HB3	1:B:1265:GLN:HE22	1.85	0.41
1:B:1043:VAL:HG12	1:B:1086:ILE:HD13	2.03	0.41
1:A:271:LEU:HA	1:A:271:LEU:HD12	1.89	0.41
1:B:1036:GLU:HG2	1:B:1037:GLY:N	2.36	0.40
1:A:233:VAL:HG21	1:A:237:MET:HG2	2.04	0.40
1:B:1023:PHE:HD2	1:B:1078:ILE:HD11	1.85	0.40
1:B:1197:LYS:HG3	1:B:1205:ALA:HB3	2.04	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%)	314 (95%)	16 (5%)	2 (1%)	28	48
1	B	343/345 (99%)	314 (92%)	26 (8%)	3 (1%)	20	36
All	All	675/690 (98%)	628 (93%)	42 (6%)	5 (1%)	25	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	THR
1	B	1069	ALA
1	A	38	THR
1	B	1087	ILE
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%)	260 (92%)	23 (8%)	14	26
1	B	289/289 (100%)	260 (90%)	29 (10%)	9	17
All	All	572/578 (99%)	520 (91%)	52 (9%)	11	21

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	14	VAL
1	A	33	ARG
1	A	43	VAL
1	A	48	LEU
1	A	95	LYS
1	A	96	LYS
1	A	99	LEU
1	A	100	LEU
1	A	123	GLN
1	A	155	GLU
1	A	190	LYS
1	A	207	ASN
1	A	209	LYS
1	A	213	ASP
1	A	218	LEU
1	A	242	LEU
1	A	269	HIS
1	A	278	ARG
1	A	291	ASP
1	A	300	VAL
1	A	320	GLU
1	A	345	GLU
1	B	1008	VAL
1	B	1009	ILE
1	B	1010	LEU
1	B	1042	LEU
1	B	1048	LEU
1	B	1055	ARG
1	B	1056	ILE
1	B	1065	THR
1	B	1070	GLN
1	B	1083	VAL
1	B	1095	LYS
1	B	1098	ASP
1	B	1100	LEU
1	B	1103	ILE
1	B	1116	THR
1	B	1154	LYS
1	B	1171	LEU
1	B	1191	GLU
1	B	1210	GLU
1	B	1211	GLU

*Continued on next page...*

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Mol	Chain	Res	Type
1	B	1215	THR
1	B	1227	ASP
1	B	1237	MET
1	B	1264	ASN
1	B	1286	VAL
1	B	1301	LEU
1	B	1302	PRO
1	B	1334	ASN
1	B	1337	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	207	ASN
1	A	244	ASN
1	A	259	GLN
1	A	279	ASN
1	B	1070	GLN
1	B	1119	HIS
1	B	1232	ASN
1	B	1244	ASN
1	B	1261	ASN
1	B	1264	ASN
1	B	1265	GLN
1	B	1269	HIS
1	B	1273	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

There are no ligands in this entry.

## 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 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.