



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:39 PM GMT

PDB ID : 3UK7  
Title : Crystal Structure of Arabidopsis thaliana DJ-1D  
Authors : Seo, K.H.; Zhuang, N.N.; Son, D.Y.; Lee, K.H.  
Deposited on : 2011-11-09  
Resolution : 2.05 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

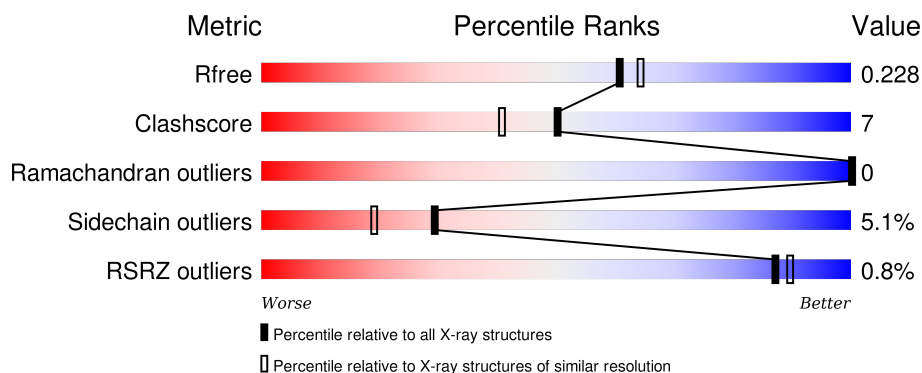
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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.

Mol	Chain	Length	Quality of chain
1	A	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 84%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>84%</span> <span>10%</span> <span>• •</span> </div> </div>
1	B	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 84%, yellow 10%, orange 1%, red 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>84%</span> <span>10%</span> <span>• •</span> </div> </div>
1	C	396	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 86%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>86%</span> <span>11%</span> <span>•</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9152 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 Class I glutamine amidotransferase-like domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	Se	0	0	0
			2916	1857	484	556	14	5			
1	B	386	Total	C	N	O	S	Se	0	0	0
			2916	1857	484	556	14	5			
1	C	396	Total	C	N	O	S	Se	0	0	0
			2984	1895	499	569	15	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP Q9M8R4
A	-6	GLN	-	EXPRESSION TAG	UNP Q9M8R4
A	-5	GLN	-	EXPRESSION TAG	UNP Q9M8R4
A	-4	MET	-	EXPRESSION TAG	UNP Q9M8R4
A	-3	GLY	-	EXPRESSION TAG	UNP Q9M8R4
A	-2	ARG	-	EXPRESSION TAG	UNP Q9M8R4
A	-1	GLY	-	EXPRESSION TAG	UNP Q9M8R4
A	0	SER	-	EXPRESSION TAG	UNP Q9M8R4
B	-7	GLY	-	EXPRESSION TAG	UNP Q9M8R4
B	-6	GLN	-	EXPRESSION TAG	UNP Q9M8R4
B	-5	GLN	-	EXPRESSION TAG	UNP Q9M8R4
B	-4	MET	-	EXPRESSION TAG	UNP Q9M8R4
B	-3	GLY	-	EXPRESSION TAG	UNP Q9M8R4
B	-2	ARG	-	EXPRESSION TAG	UNP Q9M8R4
B	-1	GLY	-	EXPRESSION TAG	UNP Q9M8R4
B	0	SER	-	EXPRESSION TAG	UNP Q9M8R4
C	-7	GLY	-	EXPRESSION TAG	UNP Q9M8R4
C	-6	GLN	-	EXPRESSION TAG	UNP Q9M8R4
C	-5	GLN	-	EXPRESSION TAG	UNP Q9M8R4
C	-4	MET	-	EXPRESSION TAG	UNP Q9M8R4
C	-3	GLY	-	EXPRESSION TAG	UNP Q9M8R4
C	-2	ARG	-	EXPRESSION TAG	UNP Q9M8R4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP Q9M8R4
C	0	SER	-	EXPRESSION TAG	UNP Q9M8R4

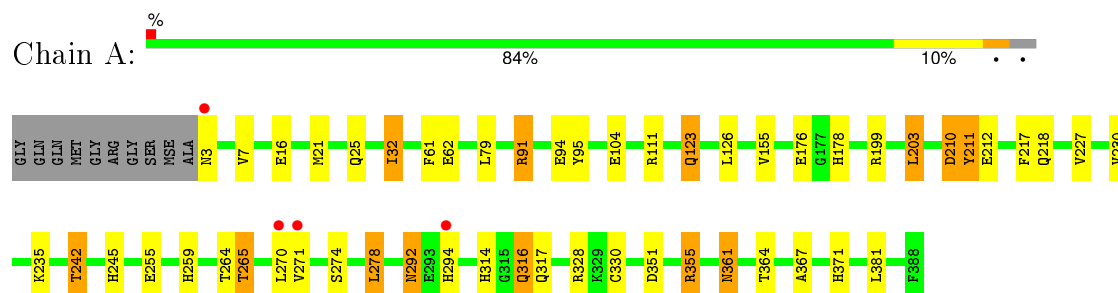
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	117	Total	O	0	0
			117	117		
2	B	103	Total	O	0	0
			103	103		
2	C	116	Total	O	0	0
			116	116		

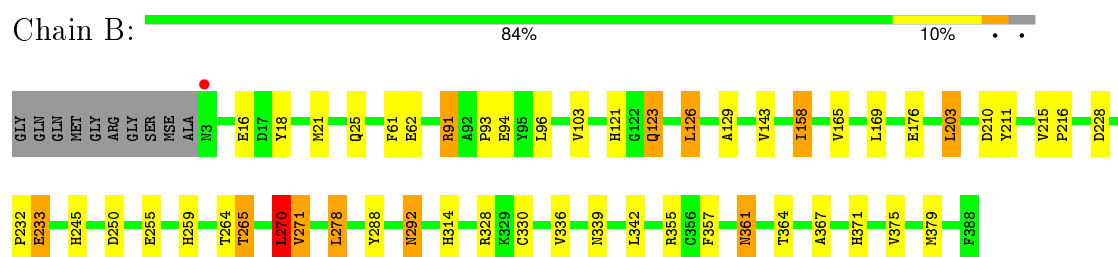
### 3 Residue-property plots [i](#)

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.

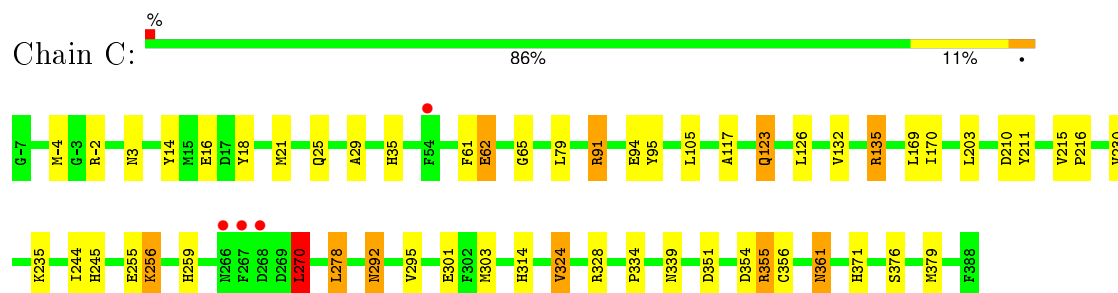
- Molecule 1: Class I glutamine amidotransferase-like domain-containing protein



- Molecule 1: Class I glutamine amidotransferase-like domain-containing protein



- Molecule 1: Class I glutamine amidotransferase-like domain-containing protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.78 Å 75.21 Å 141.67 Å 90.00° 96.87° 90.00°	Depositor
Resolution (Å)	45.10 – 2.05 45.11 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.10-2.05) 99.5 (45.11-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.05 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.174 , 0.225 0.181 , 0.228	Depositor DCC
$R_{free}$ test set	3722 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 73931 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: CSD, CSX

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	1.15	7/2964 (0.2%)	1.05	8/4025 (0.2%)
1	B	1.10	2/2964 (0.1%)	1.04	7/4025 (0.2%)
1	C	1.09	4/3031 (0.1%)	0.98	8/4110 (0.2%)
All	All	1.11	13/8959 (0.1%)	1.02	23/12160 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	CG-CD	6.32	1.61	1.51
1	A	61	PHE	CE1-CZ	6.20	1.49	1.37
1	A	211	TYR	CE2-CZ	6.10	1.46	1.38
1	A	367	ALA	CA-CB	5.98	1.65	1.52
1	C	62	GLU	CB-CG	5.74	1.63	1.52
1	C	95	TYR	CD2-CE2	5.60	1.47	1.39
1	A	211	TYR	CG-CD2	5.57	1.46	1.39
1	A	95	TYR	CD2-CE2	5.37	1.47	1.39
1	C	14	TYR	CD1-CE1	5.36	1.47	1.39
1	B	367	ALA	CA-CB	5.33	1.63	1.52
1	B	61	PHE	CE1-CZ	5.26	1.47	1.37
1	C	356	CYS	CB-SG	-5.05	1.73	1.81
1	A	155	VAL	CB-CG1	5.03	1.63	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ARG	NE-CZ-NH2	-21.95	109.33	120.30
1	A	91	ARG	NE-CZ-NH2	-19.90	110.35	120.30
1	B	91	ARG	NE-CZ-NH1	19.89	130.24	120.30
1	A	91	ARG	NE-CZ-NH1	16.87	128.74	120.30
1	C	91	ARG	NE-CZ-NH2	-16.24	112.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ARG	NE-CZ-NH1	-12.64	113.98	120.30
1	C	91	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	355	ARG	NE-CZ-NH2	9.24	124.92	120.30
1	B	91	ARG	CD-NE-CZ	7.76	134.47	123.60
1	C	278	LEU	CA-CB-CG	6.76	130.86	115.30
1	C	270	LEU	CA-CB-CG	6.74	130.79	115.30
1	A	91	ARG	CD-NE-CZ	6.68	132.95	123.60
1	A	210	ASP	CB-CG-OD1	6.60	124.24	118.30
1	C	91	ARG	CG-CD-NE	-5.97	99.27	111.80
1	C	354	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	278	LEU	CB-CG-CD2	5.74	120.76	111.00
1	B	126	LEU	CB-CG-CD1	5.67	120.64	111.00
1	B	250	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	342	LEU	CB-CG-CD1	-5.44	101.76	111.00
1	A	91	ARG	CG-CD-NE	-5.38	100.51	111.80
1	B	270	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	211	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	C	91	ARG	CD-NE-CZ	5.02	130.63	123.60

There are no chirality outliers.

There are no planarity outliers.

## 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	2916	0	2861	45	0
1	B	2916	0	2861	40	0
1	C	2984	0	2930	41	0
2	A	117	0	0	3	0
2	B	103	0	0	3	0
2	C	116	0	0	4	0
All	All	9152	0	8652	123	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 7.

All (123) 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:C:376:SER:HA	1:C:379:MSE:HE2	1.08	1.06
1:A:25:GLN:HE22	1:A:371:HIS:HD2	1.07	0.99
1:C:376:SER:HA	1:C:379:MSE:CE	1.97	0.93
1:A:328:ARG:HH22	1:A:361:ASN:ND2	1.68	0.91
1:B:62:GLU:OE1	1:B:91:ARG:HD3	1.74	0.86
1:A:16:GLU:OE2	1:A:259:HIS:HE1	1.60	0.85
1:A:328:ARG:HH22	1:A:361:ASN:HD21	1.26	0.84
1:A:210:ASP:OD1	1:A:259:HIS:HD2	1.59	0.84
1:A:25:GLN:HE22	1:A:371:HIS:CD2	1.95	0.84
1:C:62:GLU:OE1	1:C:91:ARG:HD3	1.79	0.83
1:A:123:GLN:N	1:A:123:GLN:HE21	1.79	0.80
1:A:25:GLN:NE2	1:A:371:HIS:HD2	1.78	0.80
1:C:25:GLN:HE22	1:C:371:HIS:HD2	1.30	0.78
1:A:245:HIS:HE1	1:A:255:GLU:OE2	1.66	0.78
1:C:18:TYR:OH	1:C:210:ASP:OD2	2.03	0.77
1:B:210:ASP:OD2	1:B:259:HIS:HD2	1.69	0.76
1:C:245:HIS:HE1	1:C:255:GLU:OE2	1.67	0.76
1:A:62:GLU:OE1	1:A:91:ARG:HD3	1.85	0.76
1:A:203:LEU:HD22	1:A:278:LEU:HD21	1.66	0.76
1:B:123:GLN:N	1:B:123:GLN:HE21	1.85	0.74
1:C:376:SER:CA	1:C:379:MSE:HE2	2.03	0.74
1:C:16:GLU:OE2	1:C:259:HIS:HE1	1.71	0.73
1:A:351:ASP:O	1:A:355:ARG:NH1	2.20	0.73
1:A:230:VAL:HG21	1:A:270:LEU:HD11	1.70	0.73
1:A:123:GLN:H	1:A:123:GLN:HE21	1.36	0.72
1:A:316:GLN:N	1:A:316:GLN:HE21	1.88	0.72
1:B:176:GLU:HG2	2:B:490:HOH:O	1.90	0.71
1:B:328:ARG:HH22	1:B:361:ASN:ND2	1.91	0.68
1:B:16:GLU:OE2	1:B:259:HIS:HE1	1.76	0.67
1:C:25:GLN:HE22	1:C:371:HIS:CD2	2.11	0.67
1:B:245:HIS:HE1	1:B:255:GLU:OE2	1.78	0.67
1:B:94:GLU:OE1	1:C:314:HIS:HE1	1.80	0.64
1:B:25:GLN:HE22	1:B:371:HIS:HD2	1.44	0.64
1:A:203:LEU:HD22	1:A:278:LEU:CD2	2.27	0.64
1:A:94:GLU:OE1	1:B:314:HIS:HE1	1.81	0.64
1:C:328:ARG:HH22	1:C:361:ASN:ND2	1.96	0.64
1:A:123:GLN:H	1:A:123:GLN:NE2	1.95	0.63
1:A:210:ASP:OD2	1:A:242:THR:HG21	1.99	0.62
1:C:25:GLN:NE2	1:C:371:HIS:HD2	1.97	0.61
1:A:314:HIS:HE1	1:C:94:GLU:OE1	1.84	0.61
1:C:123:GLN:HE21	1:C:123:GLN:N	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLU:OE2	1:C:259:HIS:CE1	2.56	0.58
1:A:292:ASN:ND2	1:A:294:HIS:H	2.02	0.58
1:A:25:GLN:NE2	1:A:371:HIS:CD2	2.63	0.57
1:A:7:VAL:HB	1:A:32:ILE:HD11	1.86	0.57
1:C:379:MSE:HE1	2:C:476:HOH:O	2.03	0.57
1:A:292:ASN:HD22	1:A:294:HIS:H	1.53	0.56
1:B:328:ARG:HH22	1:B:361:ASN:HD22	1.54	0.56
1:A:210:ASP:OD1	1:A:259:HIS:CD2	2.50	0.55
1:B:264:THR:C	1:B:265:THR:HG22	2.26	0.55
1:C:210:ASP:OD1	1:C:259:HIS:HD2	1.91	0.54
1:A:264:THR:O	1:A:265:THR:HG22	2.07	0.54
1:C:361:ASN:HD22	1:C:361:ASN:H	1.55	0.54
1:B:25:GLN:NE2	1:B:371:HIS:HD2	2.06	0.54
1:C:-4:MET:CE	1:C:35:HIS:CD2	2.91	0.54
1:B:21:MSE:HE2	1:B:211:TYR:CE1	2.42	0.54
1:B:228:ASP:CG	1:B:265:THR:HG21	2.28	0.53
1:A:361:ASN:HD22	1:A:361:ASN:H	1.56	0.53
1:C:21:MSE:HE2	1:C:211:TYR:CE1	2.44	0.52
1:B:103:VAL:HG13	1:B:129:ALA:HA	1.90	0.52
1:B:232:PRO:C	1:B:233:GLU:HG2	2.31	0.51
1:A:330:CYS:HB2	1:A:364:THR:HG21	1.91	0.51
1:B:245:HIS:HD2	2:B:476:HOH:O	1.92	0.51
1:A:316:GLN:H	1:A:316:GLN:NE2	2.09	0.51
1:B:264:THR:C	1:B:265:THR:CG2	2.79	0.50
1:B:25:GLN:HE22	1:B:371:HIS:CD2	2.27	0.50
1:C:256:LYS:HE3	2:C:445:HOH:O	2.12	0.50
1:B:270:LEU:HD23	1:B:271:VAL:N	2.25	0.50
1:A:178:HIS:HD2	1:A:218:GLN:OE1	1.95	0.50
1:C:351:ASP:O	1:C:355:ARG:NH1	2.45	0.49
1:B:375:VAL:O	1:B:379:MSE:HG3	2.12	0.49
1:A:264:THR:C	1:A:265:THR:HG22	2.32	0.49
1:B:330:CYS:HB2	1:B:364:THR:HG21	1.93	0.49
1:A:203:LEU:CD2	1:A:278:LEU:HD21	2.37	0.49
1:C:105:LEU:C	1:C:105:LEU:HD23	2.33	0.49
1:B:292:ASN:HD22	1:B:292:ASN:C	2.16	0.49
1:A:199:ARG:HD3	1:A:274:SER:O	2.13	0.49
1:B:361:ASN:HD22	1:B:361:ASN:H	1.61	0.48
1:B:270:LEU:C	1:B:270:LEU:HD23	2.34	0.48
1:C:29:ALA:O	1:C:379:MSE:HE1	2.13	0.48
1:A:292:ASN:HD22	1:A:294:HIS:N	2.12	0.48
1:C:245:HIS:HD2	2:C:482:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:ASN:HD22	1:C:339:ASN:H	1.61	0.48
1:A:328:ARG:NH2	1:A:361:ASN:ND2	2.51	0.48
1:C:123:GLN:HE21	1:C:123:GLN:H	1.62	0.48
1:A:316:GLN:N	1:A:316:GLN:NE2	2.60	0.48
1:C:-4:MET:HE1	1:C:35:HIS:CD2	2.50	0.47
1:C:25:GLN:NE2	1:C:371:HIS:CD2	2.78	0.47
1:A:316:GLN:H	1:A:316:GLN:HE21	1.57	0.47
1:A:21:MSE:HE2	1:A:211:TYR:CE1	2.50	0.47
1:B:123:GLN:N	1:B:123:GLN:NE2	2.60	0.47
1:B:215:VAL:HB	1:B:216:PRO:HD3	1.97	0.47
1:C:230:VAL:HG11	1:C:270:LEU:HD12	1.97	0.46
1:B:336:VAL:HA	1:B:339:ASN:HD22	1.80	0.46
1:B:93:PRO:HA	1:B:96:LEU:HB2	1.97	0.45
1:B:264:THR:O	1:B:265:THR:HG22	2.16	0.45
1:A:264:THR:C	1:A:265:THR:CG2	2.84	0.45
1:A:217:PHE:CE1	1:A:227:VAL:HG12	2.52	0.45
1:C:65:GLY:HA2	1:C:244:ILE:CD1	2.46	0.44
1:C:379:MSE:HE3	2:C:452:HOH:O	2.18	0.44
1:C:215:VAL:HB	1:C:216:PRO:HD3	2.00	0.44
1:C:328:ARG:HH22	1:C:361:ASN:HD22	1.63	0.44
1:B:355:ARG:HD3	1:B:357:PHE:CZ	2.53	0.44
1:B:158:ILE:HG12	1:B:158:ILE:H	1.40	0.44
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.72	0.43
1:B:121:HIS:HA	1:B:143:VAL:HG21	2.01	0.42
1:B:264:THR:OG1	1:B:265:THR:HG23	2.20	0.42
1:C:292:ASN:HD22	1:C:295:VAL:H	1.67	0.42
1:B:203:LEU:HD22	1:B:278:LEU:HD21	2.01	0.42
1:B:123:GLN:NE2	1:B:123:GLN:H	2.18	0.42
1:C:132:VAL:HA	1:C:135:ARG:HG3	2.02	0.42
1:B:176:GLU:CG	2:B:490:HOH:O	2.59	0.42
1:C:245:HIS:CE1	1:C:255:GLU:OE2	2.58	0.41
1:A:176:GLU:HG2	2:A:503:HOH:O	2.19	0.41
1:A:212:GLU:HA	1:A:371:HIS:CE1	2.55	0.41
1:C:292:ASN:HD22	1:C:292:ASN:C	2.23	0.41
1:B:210:ASP:OD2	1:B:259:HIS:CD2	2.60	0.41
1:A:317:GLN:NE2	2:A:398:HOH:O	2.45	0.41
1:A:245:HIS:HD2	2:A:483:HOH:O	2.02	0.41
1:C:303:MSE:HE2	1:C:324:VAL:HG13	2.03	0.41
1:B:18:TYR:CE1	1:B:259:HIS:CG	3.09	0.41
1:C:117:ALA:HA	1:C:170:ILE:O	2.21	0.41
1:C:292:ASN:ND2	1:C:295:VAL:H	2.19	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	382/396 (96%)	377 (99%)	5 (1%)	0	100	100
1	B	382/396 (96%)	374 (98%)	8 (2%)	0	100	100
1	C	392/396 (99%)	388 (99%)	4 (1%)	0	100	100
All	All	1156/1188 (97%)	1139 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	310/310 (100%)	295 (95%)	15 (5%)	31	22
1	B	310/310 (100%)	296 (96%)	14 (4%)	34	25
1	C	316/310 (102%)	297 (94%)	19 (6%)	24	13
All	All	936/930 (101%)	888 (95%)	48 (5%)	29	19

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	32	ILE

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Mol	Chain	Res	Type
1	A	79	LEU
1	A	111	ARG
1	A	123	GLN
1	A	126	LEU
1	A	203	LEU
1	A	235	LYS
1	A	242	THR
1	A	265	THR
1	A	271	VAL
1	A	278	LEU
1	A	292	ASN
1	A	316	GLN
1	A	361	ASN
1	B	123	GLN
1	B	126	LEU
1	B	158	ILE
1	B	165	VAL
1	B	169	LEU
1	B	203	LEU
1	B	233	GLU
1	B	265	THR
1	B	270	LEU
1	B	271	VAL
1	B	278	LEU
1	B	288	TYR
1	B	292	ASN
1	B	361	ASN
1	C	-2	ARG
1	C	3	ASN
1	C	61	PHE
1	C	79	LEU
1	C	123	GLN
1	C	126	LEU
1	C	135	ARG
1	C	169	LEU
1	C	203	LEU
1	C	235	LYS
1	C	256	LYS
1	C	270	LEU
1	C	278	LEU
1	C	292	ASN
1	C	301	GLU

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Mol	Chain	Res	Type
1	C	324	VAL
1	C	334	PRO
1	C	355	ARG
1	C	361	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	123	GLN
1	A	178	HIS
1	A	245	HIS
1	A	259	HIS
1	A	292	ASN
1	A	314	HIS
1	A	316	GLN
1	A	317	GLN
1	A	339	ASN
1	A	361	ASN
1	A	371	HIS
1	B	25	GLN
1	B	123	GLN
1	B	178	HIS
1	B	245	HIS
1	B	259	HIS
1	B	292	ASN
1	B	314	HIS
1	B	317	GLN
1	B	339	ASN
1	B	361	ASN
1	B	371	HIS
1	C	3	ASN
1	C	25	GLN
1	C	57	HIS
1	C	123	GLN
1	C	178	HIS
1	C	245	HIS
1	C	259	HIS
1	C	292	ASN
1	C	314	HIS
1	C	339	ASN
1	C	361	ASN

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Mol	Chain	Res	Type
1	C	371	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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$
1	CSX	A	120	1	3,6,7	0.84	0	3,6,8	2.01	2 (66%)
1	CSD	A	313	1	3,7,8	1.44	1 (33%)	3,8,10	3.86	2 (66%)
1	CSX	B	120	1	3,6,7	1.20	0	3,6,8	1.88	1 (33%)
1	CSD	B	313	1	3,7,8	1.25	0	3,8,10	4.18	1 (33%)
1	CSX	C	120	1	3,6,7	1.19	0	3,6,8	2.43	2 (66%)
1	CSD	C	313	1	3,7,8	1.24	0	3,8,10	5.88	3 (100%)

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
1	CSX	A	120	1	-	0/1/5/7	0/0/0/0
1	CSD	A	313	1	-	0/2/6/8	0/0/0/0
1	CSX	B	120	1	-	0/1/5/7	0/0/0/0
1	CSD	B	313	1	-	0/2/6/8	0/0/0/0
1	CSX	C	120	1	-	0/1/5/7	0/0/0/0
1	CSD	C	313	1	-	0/2/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	CSD	CB-SG	-2.00	1.67	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	313	CSD	O-C-CA	-2.42	119.19	125.49
1	A	120	CSX	O-C-CA	-2.32	119.45	125.49
1	A	313	CSD	O-C-CA	-2.15	119.90	125.49
1	C	120	CSX	O-C-CA	-2.11	119.99	125.49
1	B	120	CSX	CB-CA-C	2.01	116.96	111.46
1	A	120	CSX	CB-CA-C	2.43	118.13	111.46
1	C	313	CSD	CB-CA-C	2.77	119.05	111.46
1	C	120	CSX	CB-CA-C	3.35	120.65	111.46
1	A	313	CSD	OD1-SG-CB	6.20	115.74	105.40
1	B	313	CSD	OD1-SG-CB	6.81	116.75	105.40
1	C	313	CSD	OD1-SG-CB	9.50	121.24	105.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	379/396 (95%)	-0.40	4 (1%) 82 86	9, 18, 34, 45	0
1	B	379/396 (95%)	-0.41	1 (0%) 94 95	10, 20, 34, 47	0
1	C	388/396 (97%)	-0.44	4 (1%) 84 87	12, 21, 40, 51	2 (0%)
All	All	1146/1188 (96%)	-0.42	9 (0%) 87 90	9, 20, 36, 51	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	ASN	4.9
1	C	268	ASP	2.8
1	C	267	PHE	2.3
1	A	294	HIS	2.3
1	A	3	ASN	2.2
1	A	270	LEU	2.2
1	C	54	PHE	2.1
1	A	271	VAL	2.1
1	C	266	ASN	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSX	C	120	7/8	0.97	0.07	-	12,14,23,23	0
1	CSD	B	313	8/9	0.93	0.12	-	9,11,16,23	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSD	C	313	8/9	0.93	0.13	-	12,14,18,23	8
1	CSX	A	120	7/8	0.96	0.09	-	14,15,19,21	0
1	CSD	A	313	8/9	0.96	0.14	-	8,10,12,23	8
1	CSX	B	120	7/8	0.97	0.10	-	19,19,28,28	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.