



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:28 AM BST

PDB ID : 6LBJ  
Title : Structure of mouse GLD-2 (Terminal nucleotidyltransferase 2, TENT2)  
Authors : Ma, X.Y.; Gao, S.  
Deposited on : 2019-11-14  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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) : 1.13  
EDS : 2.14.4.dev1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

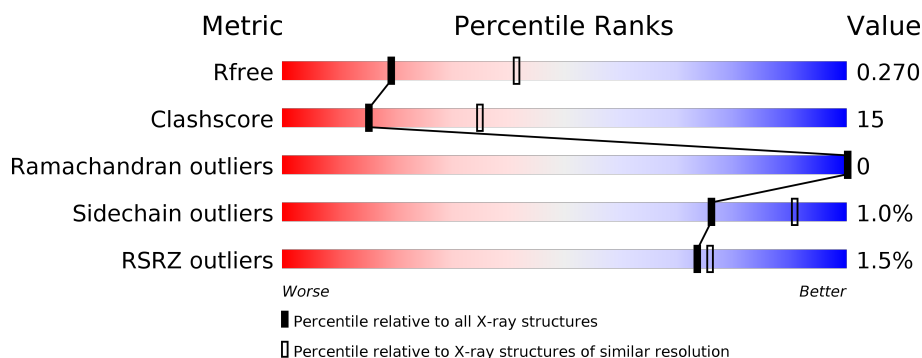
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	368	<div> <div> <div></div> <div>58%</div> <div>30%</div> <div>12%</div> </div> </div>
1	B	368	<div> <div> <div></div> <div>64%</div> <div>25%</div> <div>11%</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5322 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 Poly(A) RNA polymerase GLD2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2628	1682	465	470	11			
1	B	328	Total	C	N	O	S	0	0	0
			2664	1703	474	476	11			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	MET	-	expression tag	UNP Q91YI6
A	118	GLY	-	expression tag	UNP Q91YI6
A	119	SER	-	expression tag	UNP Q91YI6
A	120	SER	-	expression tag	UNP Q91YI6
A	121	HIS	-	expression tag	UNP Q91YI6
A	122	HIS	-	expression tag	UNP Q91YI6
A	123	HIS	-	expression tag	UNP Q91YI6
A	124	HIS	-	expression tag	UNP Q91YI6
A	125	HIS	-	expression tag	UNP Q91YI6
A	126	HIS	-	expression tag	UNP Q91YI6
A	127	SER	-	expression tag	UNP Q91YI6
A	128	SER	-	expression tag	UNP Q91YI6
A	129	GLY	-	expression tag	UNP Q91YI6
A	130	LEU	-	expression tag	UNP Q91YI6
A	131	GLU	-	expression tag	UNP Q91YI6
A	132	VAL	-	expression tag	UNP Q91YI6
A	133	LEU	-	expression tag	UNP Q91YI6
A	134	PHE	-	expression tag	UNP Q91YI6
A	135	GLN	-	expression tag	UNP Q91YI6
A	136	GLY	-	expression tag	UNP Q91YI6
A	137	PRO	-	expression tag	UNP Q91YI6
A	138	HIS	-	expression tag	UNP Q91YI6
A	139	MET	-	expression tag	UNP Q91YI6
A	140	GLY	-	expression tag	UNP Q91YI6
A	141	GLY	-	expression tag	UNP Q91YI6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	-	expression tag	UNP Q91YI6
A	213	ALA	ASP	engineered mutation	UNP Q91YI6
A	279	ALA	ASP	engineered mutation	UNP Q91YI6
B	117	MET	-	expression tag	UNP Q91YI6
B	118	GLY	-	expression tag	UNP Q91YI6
B	119	SER	-	expression tag	UNP Q91YI6
B	120	SER	-	expression tag	UNP Q91YI6
B	121	HIS	-	expression tag	UNP Q91YI6
B	122	HIS	-	expression tag	UNP Q91YI6
B	123	HIS	-	expression tag	UNP Q91YI6
B	124	HIS	-	expression tag	UNP Q91YI6
B	125	HIS	-	expression tag	UNP Q91YI6
B	126	HIS	-	expression tag	UNP Q91YI6
B	127	SER	-	expression tag	UNP Q91YI6
B	128	SER	-	expression tag	UNP Q91YI6
B	129	GLY	-	expression tag	UNP Q91YI6
B	130	LEU	-	expression tag	UNP Q91YI6
B	131	GLU	-	expression tag	UNP Q91YI6
B	132	VAL	-	expression tag	UNP Q91YI6
B	133	LEU	-	expression tag	UNP Q91YI6
B	134	PHE	-	expression tag	UNP Q91YI6
B	135	GLN	-	expression tag	UNP Q91YI6
B	136	GLY	-	expression tag	UNP Q91YI6
B	137	PRO	-	expression tag	UNP Q91YI6
B	138	HIS	-	expression tag	UNP Q91YI6
B	139	MET	-	expression tag	UNP Q91YI6
B	140	GLY	-	expression tag	UNP Q91YI6
B	141	GLY	-	expression tag	UNP Q91YI6
B	142	SER	-	expression tag	UNP Q91YI6
B	213	ALA	ASP	engineered mutation	UNP Q91YI6
B	279	ALA	ASP	engineered mutation	UNP Q91YI6

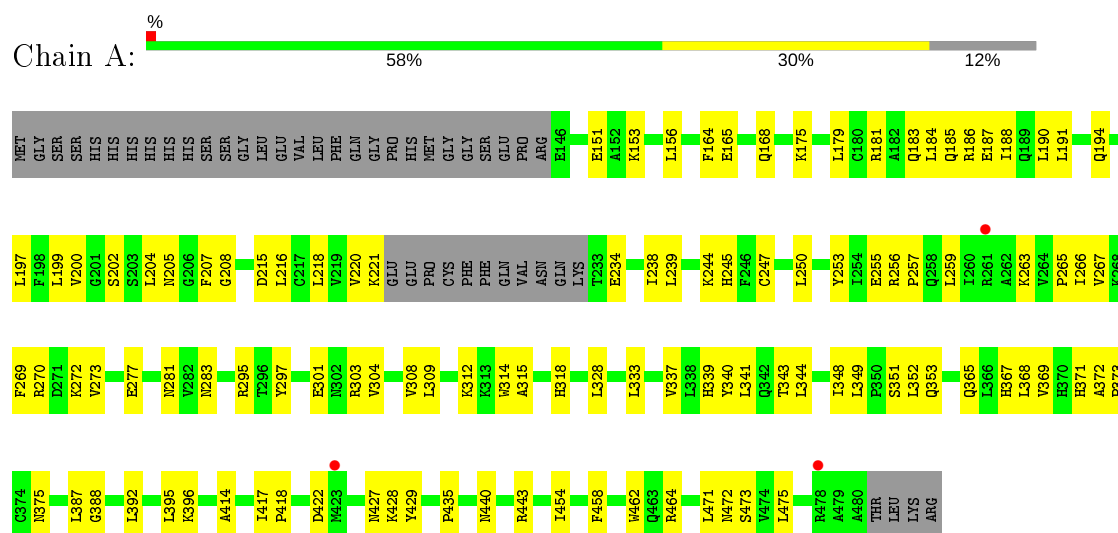
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	13	Total O 13 13	0	0

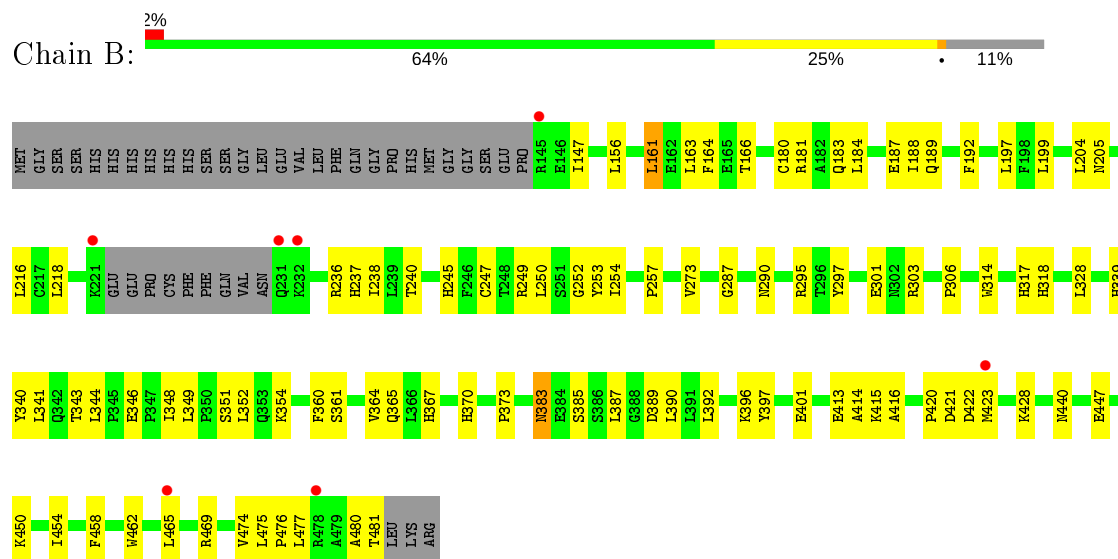
### 3 Residue-property plots [i](#)

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 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: Poly(A) RNA polymerase GLD2



#### • Molecule 1: Poly(A) RNA polymerase GLD2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.28Å 47.14Å 105.45Å 87.38° 88.06° 63.81°	Depositor
Resolution (Å)	35.51 – 2.70 35.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	80.3 (35.51-2.70) 80.3 (35.51-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.253 , 0.271 0.253 , 0.270	Depositor DCC
$R_{free}$ test set	925 reflections (5.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.106 for h,h-k,-l 0.006 for -h,-k,l 0.005 for -h,-h+k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.45	0/2684	0.59	0/3631
1	B	0.43	0/2720	0.59	0/3678
All	All	0.44	0/5404	0.59	0/7309

There are no bond length outliers.

There are no bond angle outliers.

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	2628	0	2688	81	10
1	B	2664	0	2729	87	0
2	A	17	0	0	0	0
2	B	13	0	0	0	0
All	All	5322	0	5417	160	10

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 15.

All (160) 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:263:LYS:HG3	1:A:443:ARG:HH21	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:NH2	1:B:180:CYS:HA	1.91	0.85
1:A:304:VAL:O	1:A:308:VAL:HG23	1.76	0.84
1:B:339:HIS:CE1	1:B:343:THR:HG21	2.14	0.82
1:A:303:ARG:HG2	1:A:387:LEU:HD21	1.61	0.82
1:A:428:LYS:HD3	1:A:440:ASN:HD22	1.45	0.80
1:B:475:LEU:O	1:B:475:LEU:HD12	1.80	0.80
1:A:234:GLU:O	1:A:238:ILE:HG13	1.82	0.80
1:A:464:ARG:HB3	1:A:473:SER:OG	1.84	0.77
1:B:317:HIS:NE2	1:B:476:PRO:CD	2.47	0.77
1:B:317:HIS:CD2	1:B:476:PRO:HD2	2.20	0.77
1:B:156:LEU:HD21	1:B:465:LEU:HD11	1.67	0.76
1:A:197:LEU:HD11	1:A:216:LEU:HB3	1.67	0.75
1:B:187:GLU:HG2	1:B:250:LEU:HD11	1.68	0.74
1:A:207:PHE:CE1	1:A:308:VAL:HG21	2.22	0.73
1:A:263:LYS:HG3	1:A:443:ARG:NH2	2.03	0.72
1:A:351:SER:HB2	1:A:414:ALA:HB2	1.72	0.72
1:B:317:HIS:NE2	1:B:476:PRO:HD3	2.04	0.71
1:B:247:CYS:SG	1:B:257:PRO:HG2	2.31	0.71
1:A:339:HIS:CE1	1:A:343:THR:HG21	2.26	0.70
1:A:200:VAL:O	1:A:215:ASP:HB2	1.92	0.69
1:B:317:HIS:CE1	1:B:476:PRO:HG3	2.28	0.68
1:A:239:LEU:C	1:A:239:LEU:HD23	2.13	0.68
1:B:237:HIS:O	1:B:240:THR:CG2	2.43	0.66
1:A:164:PHE:O	1:A:168:GLN:HB2	1.97	0.65
1:A:301:GLU:HB3	1:A:304:VAL:HG23	1.78	0.65
1:B:314:TRP:CD1	1:B:474:VAL:HG12	2.31	0.65
1:B:301:GLU:OE2	1:B:303:ARG:NH2	2.28	0.65
1:B:465:LEU:HD13	1:B:474:VAL:HG21	1.78	0.63
1:A:396:LYS:HB2	1:A:462:TRP:CD1	2.34	0.63
1:B:475:LEU:C	1:B:475:LEU:HD12	2.19	0.63
1:A:341:LEU:HD22	1:A:348:ILE:HD12	1.82	0.62
1:B:237:HIS:HA	1:B:240:THR:CG2	2.30	0.62
1:B:245:HIS:CE1	1:B:249:ARG:HG3	2.34	0.62
1:A:273:VAL:HG13	1:B:249:ARG:HD2	1.81	0.62
1:B:188:ILE:HD13	1:B:218:LEU:HD22	1.82	0.62
1:A:186:ARG:HH21	1:B:180:CYS:HA	1.63	0.61
1:B:317:HIS:CE1	1:B:476:PRO:CG	2.83	0.61
1:B:237:HIS:O	1:B:240:THR:HG23	2.01	0.60
1:B:317:HIS:CD2	1:B:476:PRO:CD	2.83	0.60
1:A:202:SER:HB3	1:A:208:GLY:HA2	1.83	0.59
1:A:185:GLN:HB2	1:A:197:LEU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HD13	1:B:163:LEU:C	2.22	0.59
1:B:447:GLU:HB2	1:B:450:LYS:HG2	1.84	0.59
1:B:187:GLU:OE2	1:B:250:LEU:HD21	2.02	0.59
1:B:465:LEU:HD13	1:B:474:VAL:CG2	2.33	0.59
1:B:197:LEU:HD11	1:B:216:LEU:HB3	1.84	0.59
1:B:341:LEU:HD22	1:B:348:ILE:HD12	1.84	0.58
1:A:239:LEU:HD21	1:A:259:LEU:HG	1.85	0.58
1:A:396:LYS:HB2	1:A:462:TRP:NE1	2.19	0.58
1:B:396:LYS:HB2	1:B:462:TRP:CD1	2.39	0.58
1:A:303:ARG:HG2	1:A:387:LEU:CD2	2.33	0.58
1:A:372:ALA:N	1:A:373:PRO:HD2	2.19	0.57
1:B:297:TYR:HD1	1:B:349:LEU:HD22	1.69	0.57
1:A:190:LEU:HD11	1:B:273:VAL:HG13	1.85	0.56
1:B:166:THR:HG21	1:B:481:THR:CG2	2.36	0.56
1:A:164:PHE:HD1	1:A:309:LEU:HD23	1.71	0.56
1:B:237:HIS:O	1:B:240:THR:HG22	2.05	0.56
1:B:396:LYS:HB2	1:B:462:TRP:NE1	2.21	0.55
1:A:297:TYR:HD1	1:A:349:LEU:HD22	1.71	0.55
1:A:244:LYS:O	1:A:244:LYS:HD3	2.07	0.55
1:B:389:ASP:OD1	1:B:469:ARG:NH2	2.39	0.54
1:B:184:LEU:HD21	1:B:254:ILE:HD11	1.89	0.54
1:B:237:HIS:HA	1:B:240:THR:HG22	1.88	0.54
1:A:186:ARG:HH22	1:B:180:CYS:HA	1.71	0.54
1:B:317:HIS:CE1	1:B:476:PRO:CD	2.90	0.54
1:A:188:ILE:O	1:A:191:LEU:N	2.42	0.53
1:A:194:GLN:O	1:A:221:LYS:NZ	2.31	0.53
1:A:340:TYR:O	1:A:344:LEU:HG	2.10	0.52
1:B:245:HIS:CE1	1:B:249:ARG:HB2	2.45	0.52
1:A:396:LYS:HD2	1:A:462:TRP:NE1	2.24	0.52
1:B:183:GLN:HA	1:B:183:GLN:OE1	2.10	0.51
1:B:303:ARG:HH12	1:B:385:SER:H	1.57	0.51
1:B:339:HIS:O	1:B:343:THR:HG23	2.10	0.51
1:A:314:TRP:NE1	1:A:318:HIS:CD2	2.79	0.51
1:B:189:GLN:HA	1:B:192:PHE:O	2.10	0.51
1:A:165:GLU:OE1	1:A:165:GLU:HA	2.10	0.51
1:A:188:ILE:HD13	1:A:218:LEU:HD22	1.93	0.51
1:B:354:LYS:HE3	1:B:413:GLU:HA	1.94	0.50
1:A:314:TRP:CD1	1:A:318:HIS:CD2	2.99	0.50
1:B:236:ARG:O	1:B:240:THR:HG22	2.12	0.50
1:B:204:LEU:O	1:B:295:ARG:HD2	2.11	0.49
1:B:192:PHE:CZ	1:B:238:ILE:HD12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:O	1:A:295:ARG:HD2	2.13	0.49
1:A:250:LEU:HD22	1:A:253:TYR:CE1	2.47	0.49
1:A:472:ASN:HA	1:A:475:LEU:O	2.13	0.48
1:B:237:HIS:CA	1:B:240:THR:HG22	2.42	0.48
1:A:396:LYS:HD2	1:A:462:TRP:CE2	2.48	0.48
1:B:163:LEU:O	1:B:163:LEU:HD13	2.14	0.48
1:B:188:ILE:HG21	1:B:218:LEU:HD11	1.96	0.48
1:B:428:LYS:HD3	1:B:440:ASN:HD22	1.79	0.48
1:A:266:ILE:HG22	1:A:281:ASN:HB3	1.95	0.47
1:A:250:LEU:HD22	1:A:253:TYR:HE1	1.79	0.47
1:B:187:GLU:HG2	1:B:250:LEU:HD21	1.96	0.47
1:A:270:ARG:HA	1:A:277:GLU:HA	1.96	0.47
1:B:352:LEU:HB3	1:B:360:PHE:CE2	2.50	0.47
1:B:187:GLU:CD	1:B:250:LEU:HD21	2.35	0.47
1:A:220:VAL:HG22	1:A:283:ASN:HD21	1.79	0.47
1:A:351:SER:HB2	1:A:414:ALA:CB	2.44	0.46
1:B:205:ASN:O	1:B:295:ARG:HA	2.16	0.46
1:A:392:LEU:O	1:A:392:LEU:HD23	2.16	0.46
1:B:351:SER:HB2	1:B:414:ALA:HB2	1.98	0.46
1:B:344:LEU:HD13	1:B:383:ASN:ND2	2.30	0.46
1:A:184:LEU:HD11	1:A:269:PHE:CZ	2.52	0.45
1:B:415:LYS:HE2	1:B:416:ALA:O	2.16	0.45
1:B:361:SER:HB3	1:B:364:VAL:HG23	1.98	0.45
1:A:353:GLN:HE22	1:A:435:PRO:HB2	1.81	0.45
1:A:191:LEU:HD11	1:A:245:HIS:CB	2.47	0.45
1:B:420:PRO:C	1:B:422:ASP:H	2.20	0.45
1:B:318:HIS:CE1	1:B:474:VAL:O	2.70	0.45
1:A:263:LYS:O	1:A:265:PRO:HD3	2.17	0.44
1:A:205:ASN:O	1:A:295:ARG:HA	2.17	0.44
1:A:156:LEU:HD23	1:A:388:GLY:HA3	1.98	0.44
1:A:199:LEU:HA	1:A:199:LEU:HD12	1.83	0.44
1:A:175:LYS:O	1:A:175:LYS:HD3	2.17	0.44
1:B:328:LEU:HG	1:B:454:ILE:HD13	2.00	0.43
1:A:301:GLU:HB3	1:A:304:VAL:CG2	2.47	0.43
1:B:164:PHE:CD1	1:B:306:PRO:HA	2.52	0.43
1:A:471:LEU:HD12	1:A:471:LEU:O	2.19	0.43
1:B:237:HIS:C	1:B:240:THR:HG22	2.39	0.43
1:A:183:GLN:NE2	1:B:253:TYR:CG	2.87	0.43
1:A:207:PHE:O	1:A:312:LYS:NZ	2.48	0.43
1:B:370:HIS:O	1:B:373:PRO:HD2	2.19	0.43
1:A:417:ILE:HG23	1:A:418:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HE	1:B:236:ARG:HB2	1.45	0.42
1:A:253:TYR:HB3	1:B:252:GLY:HA3	2.01	0.42
1:A:187:GLU:HG3	1:A:253:TYR:OH	2.19	0.42
1:B:392:LEU:HD12	1:B:392:LEU:C	2.40	0.42
1:B:477:LEU:HD12	1:B:480:ALA:HB3	2.01	0.42
1:A:328:LEU:HG	1:A:454:ILE:HD13	2.01	0.42
1:B:287:GLY:HA2	1:B:290:ASN:ND2	2.35	0.42
1:B:340:TYR:O	1:B:344:LEU:HG	2.20	0.42
1:B:346:GLU:O	1:B:383:ASN:HB2	2.20	0.42
1:B:147:ILE:HG22	1:B:147:ILE:O	2.19	0.42
1:A:315:ALA:CB	1:A:333:LEU:HD11	2.50	0.42
1:A:365:GLN:O	1:A:369:VAL:HG23	2.19	0.42
1:A:181:ARG:HD3	1:A:199:LEU:HB2	2.02	0.42
1:A:333:LEU:O	1:A:337:VAL:HG23	2.20	0.42
1:A:367:HIS:CE1	1:A:368:LEU:HG	2.55	0.41
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.82	0.41
1:A:314:TRP:NE1	1:A:318:HIS:HD2	2.18	0.41
1:B:184:LEU:HD23	1:B:184:LEU:HA	1.87	0.41
1:B:341:LEU:HB2	1:B:349:LEU:HD12	2.03	0.41
1:A:239:LEU:HG	1:A:267:VAL:HG23	2.02	0.41
1:A:247:CYS:SG	1:A:257:PRO:HG2	2.60	0.41
1:B:387:LEU:HD23	1:B:390:LEU:HD12	2.02	0.41
1:B:423:MET:HG3	1:B:423:MET:H	1.62	0.41
1:A:191:LEU:HG	1:A:245:HIS:ND1	2.35	0.41
1:B:365:GLN:HG2	1:B:367:HIS:NE2	2.35	0.41
1:B:306:PRO:HB2	1:B:387:LEU:HD11	2.02	0.41
1:A:239:LEU:O	1:A:239:LEU:HD23	2.20	0.41
1:A:263:LYS:CG	1:A:443:ARG:HH21	2.12	0.41
1:B:181:ARG:HD3	1:B:199:LEU:HB2	2.03	0.41
1:A:188:ILE:HG21	1:A:218:LEU:HD21	2.03	0.40
1:A:314:TRP:CH2	1:A:395:LEU:HD21	2.56	0.40
1:B:397:TYR:HA	1:B:401:GLU:HB2	2.03	0.40
1:A:297:TYR:CZ	1:A:352:LEU:HG	2.56	0.40
1:B:187:GLU:HG3	1:B:245:HIS:NE2	2.35	0.40
1:A:255:GLU:HG3	1:A:272:LYS:HD2	2.02	0.40
1:A:179:LEU:HD22	1:B:187:GLU:OE1	2.22	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:CZ	1:A:375:ASN:ND2[1_655]	1.10	1.10
1:A:256:ARG:NE	1:A:375:ASN:ND2[1_655]	1.44	0.76
1:A:256:ARG:NH2	1:A:375:ASN:ND2[1_655]	1.73	0.47
1:A:151:GLU:OE2	1:A:427:ASN:ND2[1_465]	1.81	0.39
1:A:256:ARG:NH1	1:A:371:HIS:O[1_655]	1.84	0.36
1:A:256:ARG:NH2	1:A:371:HIS:O[1_655]	1.91	0.29
1:A:153:LYS:NZ	1:A:429:TYR:OH[1_465]	1.94	0.26
1:A:256:ARG:NH1	1:A:375:ASN:ND2[1_655]	1.96	0.24
1:A:256:ARG:CZ	1:A:371:HIS:O[1_655]	2.12	0.08
1:A:256:ARG:CZ	1:A:375:ASN:CG[1_655]	2.19	0.01

## 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	320/368 (87%)	315 (98%)	5 (2%)	0	100	100
1	B	324/368 (88%)	316 (98%)	8 (2%)	0	100	100
All	All	644/736 (88%)	631 (98%)	13 (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	295/334 (88%)	293 (99%)	2 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	299/334 (90%)	295 (99%)	4 (1%)	69	87
All	All	594/668 (89%)	588 (99%)	6 (1%)	76	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	ASP
1	A	458	PHE
1	B	161	LEU
1	B	383	ASN
1	B	421	ASP
1	B	458	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	318	HIS
1	B	318	HIS

### 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](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	324/368 (88%)	-0.17	3 (0%) 84 85	41, 85, 140, 209	0
1	B	328/368 (89%)	-0.16	7 (2%) 63 65	38, 87, 150, 200	0
All	All	652/736 (88%)	-0.16	10 (1%) 73 76	38, 85, 147, 209	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	478	ARG	3.6
1	B	465	LEU	3.1
1	B	231	GLN	2.7
1	A	423	MET	2.7
1	A	261	ARG	2.5
1	B	221	LYS	2.5
1	B	232	LYS	2.4
1	B	423	MET	2.1
1	A	478	ARG	2.1
1	B	145	ARG	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.