



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:37 am GMT

PDB ID : 3BTS  
Title : Crystal structure of a ternary complex of the transcriptional repressor Gal80p (Gal80S0 [G301R]) and the acidic activation domain of Gal4p (aa 854-874) from *Saccharomyces cerevisiae* with NAD  
Authors : Kumar, P.R.; Joshua-Tor, L.  
Deposited on : 2007-12-30  
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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

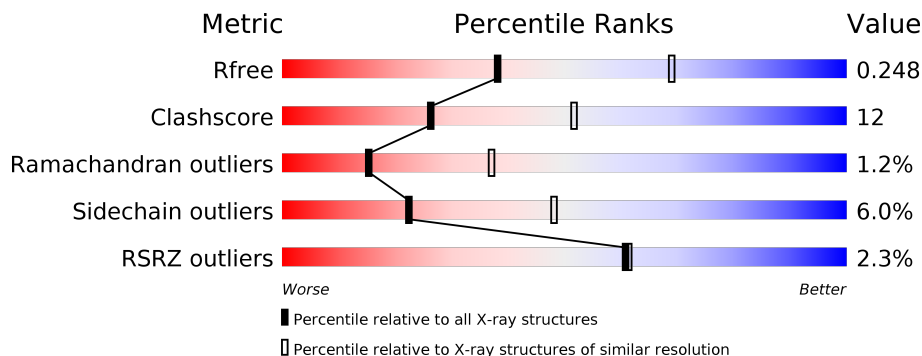
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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. 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	438	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 21%, green 64%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> <span>%</span> <span>64%</span> <span>21%</span> <span>•</span> <span>12%</span> </div> </div>
1	B	438	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 23%, green 63%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> <span>3%</span> <span>63%</span> <span>23%</span> <span>•</span> <span>11%</span> </div> </div>
2	E	21	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 43%, grey 57%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> <span>43%</span> <span>57%</span> </div> </div>
2	F	21	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 1%, yellow 24%, green 76%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> <span>5%</span> <span>24%</span> <span>76%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6432 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	3	0
			3050	1958	513	566	13			
1	B	390	Total	C	N	O	S	0	3	0
			3097	1990	519	576	12			

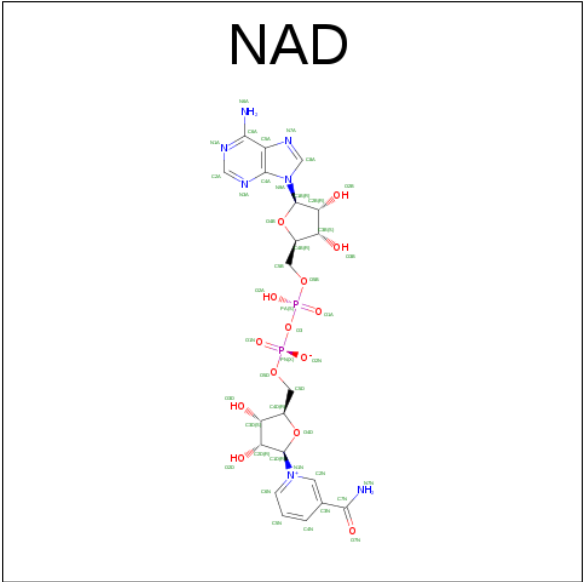
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P04387
A	-1	SER	-	EXPRESSION TAG	UNP P04387
A	0	HIS	-	EXPRESSION TAG	UNP P04387
A	301	ARG	GLY	ENGINEERED	UNP P04387
B	-2	GLY	-	EXPRESSION TAG	UNP P04387
B	-1	SER	-	EXPRESSION TAG	UNP P04387
B	0	HIS	-	EXPRESSION TAG	UNP P04387
B	301	ARG	GLY	ENGINEERED	UNP P04387

- Molecule 2 is a protein called Regulatory protein GAL4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			45	27	9	9			
2	F	5	Total	C	N	O	0	0	0
			25	15	5	5			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

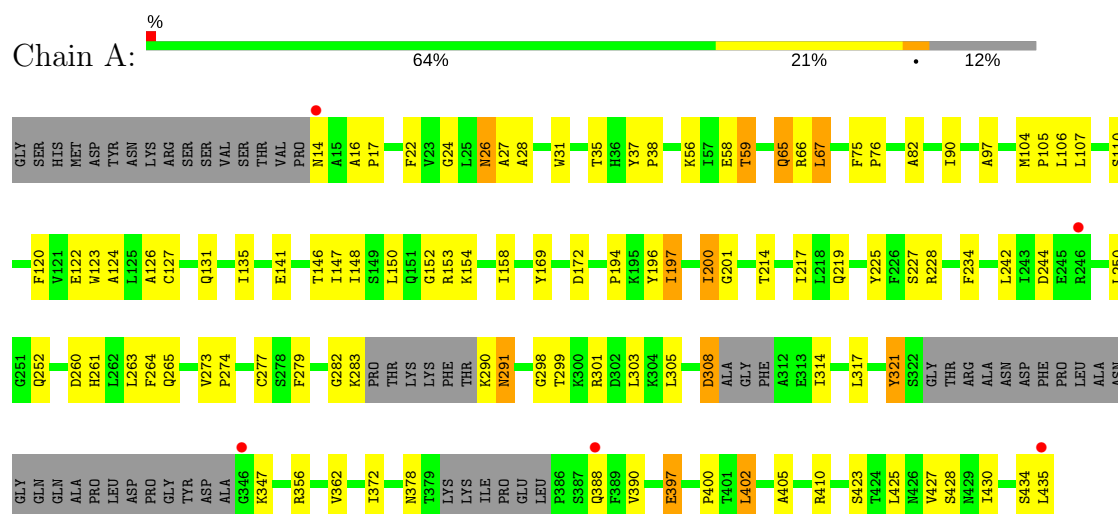
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	56	Total	O	0	0
			56	56		

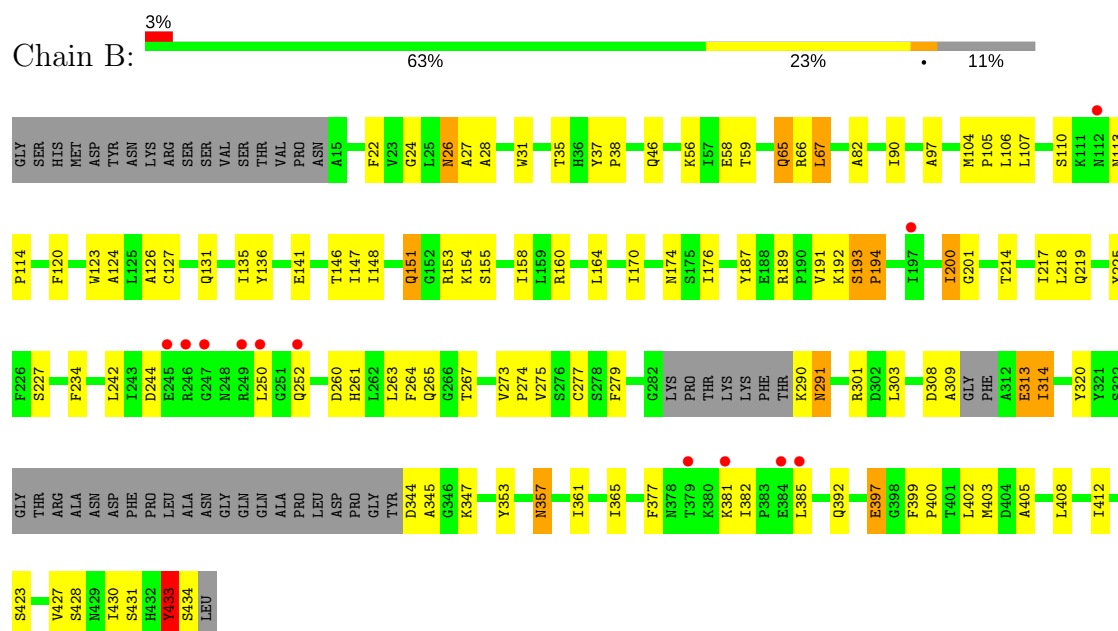
### 3 Residue-property plots

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.

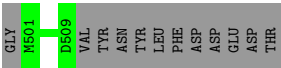
- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80



- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80



- Molecule 2: Regulatory protein GAL4



● Molecule 2: Regulatory protein GAL4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.07Å 103.43Å 106.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 2.70 46.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.57-2.70) 99.4 (46.55-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.69Å)	Xtriage
Refinement program	PHENIX.REFINE	Depositor
R, $R_{free}$	0.175 , 0.232 0.193 , 0.248	Depositor DCC
$R_{free}$ test set	1394 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.32	0/3114	0.52	0/4214
1	B	0.31	0/3164	0.52	1/4286 (0.0%)
2	E	0.23	0/44	0.27	0/60
2	F	0.21	0/24	0.26	0/32
All	All	0.32	0/6346	0.52	1/8592 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	TYR	N-CA-C	6.93	129.70	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3050	0	3046	76	0
1	B	3097	0	3091	82	0
2	E	45	0	17	0	0
2	F	25	0	9	0	0
3	A	44	0	26	2	0
3	B	44	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	71	0	0	3	0
4	B	56	0	0	0	0
All	All	6432	0	6215	147	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 12.

All (147) 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:B:153:ARG:HD2	1:B:400:PRO:HG3	1.65	0.76
1:B:403:MET:HE1	1:B:434:SER:HB3	1.69	0.74
1:B:344:ASP:N	1:B:345:ALA:HA	2.04	0.72
1:A:158:ILE:HD11	1:A:314:ILE:HD12	1.72	0.70
1:A:26:ASN:HD22	1:A:27:ALA:N	1.90	0.69
1:B:277[B]:CYS:SG	1:B:279:PHE:HE2	2.15	0.69
1:B:26:ASN:HD22	1:B:27:ALA:N	1.92	0.68
1:B:277[B]:CYS:HG	1:B:279:PHE:HE2	1.41	0.68
1:A:277[B]:CYS:SG	1:A:279:PHE:HE2	2.15	0.68
1:A:26:ASN:ND2	1:A:28:ALA:H	1.92	0.68
1:B:26:ASN:ND2	1:B:28:ALA:H	1.92	0.68
1:B:126:ALA:HB1	1:B:131:GLN:HE21	1.59	0.67
1:A:126:ALA:HB1	1:A:131:GLN:HE21	1.61	0.66
1:B:97:ALA:HA	1:B:127:CYS:SG	2.35	0.66
1:B:403:MET:HE3	1:B:433:TYR:O	1.96	0.66
1:A:291:ASN:HB2	1:A:308:ASP:HA	1.78	0.66
1:B:403:MET:CE	1:B:434:SER:HB3	2.26	0.66
1:A:97:ALA:HA	1:A:127:CYS:SG	2.38	0.64
1:A:104:MET:HB2	1:A:105:PRO:HD3	1.80	0.63
1:A:301:ARG:HG2	1:A:321:TYR:HB3	1.80	0.62
1:A:305:LEU:HD22	1:A:314:ILE:HD13	1.80	0.62
1:B:26:ASN:C	1:B:26:ASN:HD22	2.03	0.62
1:B:277[B]:CYS:SG	1:B:279:PHE:CE2	2.91	0.62
1:B:155:SER:HB3	1:B:158:ILE:HG12	1.83	0.61
1:A:277[B]:CYS:SG	1:A:279:PHE:CE2	2.93	0.61
1:B:123:TRP:CD2	1:B:124:ALA:HA	2.36	0.61
1:B:104:MET:HB2	1:B:105:PRO:HD3	1.83	0.60
1:A:26:ASN:C	1:A:26:ASN:HD22	2.05	0.60
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.37	0.59
1:A:158:ILE:CD1	1:A:314:ILE:HD12	2.33	0.58
1:B:191:VAL:HA	1:B:242:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PRO:HB3	1:A:196:TYR:CE1	2.38	0.58
1:A:131:GLN:O	1:A:135:ILE:HG13	2.04	0.58
1:A:90:ILE:HD13	1:A:106:LEU:HD21	1.85	0.57
1:B:427:VAL:HB	1:B:430:ILE:HD12	1.87	0.56
1:A:261[A]:HIS:HE1	1:B:174:ASN:OD1	1.89	0.56
1:A:56:LYS:HB3	1:A:58:GLU:OE1	2.05	0.56
1:B:347:LYS:HB3	1:B:347:LYS:NZ	2.21	0.55
1:B:136:TYR:CE2	1:B:434:SER:HB2	2.42	0.55
1:A:227:SER:HA	1:A:428:SER:HB3	1.89	0.54
1:B:146:THR:C	1:B:147:ILE:HG13	2.28	0.54
1:B:90:ILE:HD13	1:B:106:LEU:HD21	1.89	0.54
1:A:59:THR:HG22	4:A:499:HOH:O	2.08	0.54
1:B:303:LEU:HD23	1:B:303:LEU:C	2.28	0.54
1:B:313:GLU:HA	1:B:314:ILE:O	2.08	0.54
1:B:131:GLN:O	1:B:135:ILE:HG13	2.09	0.53
1:A:14:ASN:C	1:A:16:ALA:H	2.12	0.53
1:B:160:ARG:NH2	1:B:353[B]:TYR:HE1	2.08	0.52
1:A:263:LEU:HD13	1:B:265:GLN:HB2	1.91	0.52
1:B:65:GLN:HG3	1:B:66:ARG:N	2.25	0.52
1:A:146:THR:C	1:A:147:ILE:HG13	2.31	0.52
1:B:382:ILE:HD12	1:B:385:LEU:HD11	1.91	0.52
1:A:147:ILE:HD13	1:A:372:ILE:CD1	2.39	0.51
1:A:410:ARG:HB3	1:A:435:LEU:CD1	2.40	0.51
1:B:56:LYS:HB3	1:B:58:GLU:OE1	2.11	0.51
1:A:37:TYR:HB3	1:A:38:PRO:HD3	1.92	0.51
1:B:37:TYR:HB3	1:B:38:PRO:HD3	1.92	0.51
1:B:264:PHE:HB3	1:B:277[B]:CYS:HB3	1.92	0.50
1:B:24:GLY:HA2	3:B:436:NAD:O4B	2.12	0.49
1:A:65:GLN:HG3	1:A:66:ARG:N	2.27	0.49
1:B:58:GLU:H	1:B:58:GLU:CD	2.16	0.49
1:A:58:GLU:CD	1:A:58:GLU:H	2.16	0.49
1:B:26:ASN:HD22	1:B:28:ALA:H	1.60	0.49
1:A:305:LEU:HB3	1:A:314:ILE:HD13	1.95	0.49
1:A:214:THR:O	1:A:217:ILE:HG12	2.13	0.48
1:A:26:ASN:HD22	1:A:28:ALA:H	1.61	0.48
1:A:234:PHE:HE2	1:B:267:THR:CG2	2.26	0.48
1:A:225:TYR:HB3	4:A:442:HOH:O	2.12	0.48
1:B:214:THR:O	1:B:217:ILE:HG12	2.14	0.48
1:B:227:SER:HA	1:B:428:SER:HB3	1.96	0.48
1:B:189:ARG:O	1:B:242:LEU:HA	2.14	0.48
1:B:123:TRP:CG	1:B:124:ALA:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:SER:HA	1:B:423:SER:HA	1.96	0.48
1:A:234:PHE:HE2	1:B:267:THR:HG22	1.79	0.48
1:A:82:ALA:O	1:A:110:SER:HA	2.14	0.47
1:A:123:TRP:CG	1:A:124:ALA:HA	2.49	0.47
1:B:234:PHE:HB2	1:B:261[A]:HIS:HB2	1.95	0.47
1:B:219:GLN:HE21	1:B:225:TYR:HA	1.80	0.47
1:B:397:GLU:H	1:B:397:GLU:CD	2.18	0.47
1:A:264:PHE:HB3	1:A:277[B]:CYS:HB3	1.96	0.47
1:A:427:VAL:O	1:A:430:ILE:HG12	2.14	0.47
1:A:397:GLU:CD	1:A:397:GLU:H	2.18	0.46
1:A:234:PHE:HB2	1:A:261[A]:HIS:HB2	1.98	0.46
1:B:242:LEU:HD12	1:B:252:GLN:HB3	1.98	0.46
1:B:244:ASP:HB3	1:B:250:LEU:HD21	1.97	0.46
1:A:265:GLN:HB2	1:B:263:LEU:HD13	1.97	0.46
1:B:403:MET:HE1	1:B:434:SER:CB	2.44	0.46
1:A:169:TYR:O	1:A:301:ARG:HD2	2.16	0.45
1:A:244:ASP:HB3	1:A:250:LEU:HD21	1.97	0.45
1:A:172:ASP:O	1:A:298:GLY:HA2	2.17	0.45
1:B:273:VAL:HA	1:B:274:PRO:HD3	1.85	0.45
1:A:299:THR:HG22	1:B:187:TYR:HE1	1.81	0.45
1:A:234:PHE:CE2	1:B:267:THR:CG2	2.99	0.45
1:B:147:ILE:HG12	1:B:399:PHE:CE2	2.51	0.45
1:A:219:GLN:HE21	1:A:225:TYR:HA	1.82	0.45
1:A:148:ILE:HG12	1:A:405:ALA:HB2	1.99	0.45
1:B:430:ILE:O	1:B:431:SER:CB	2.65	0.44
1:A:299:THR:HG22	1:B:187:TYR:CE1	2.52	0.44
1:A:290:LYS:O	1:A:291:ASN:C	2.55	0.44
1:B:290:LYS:O	1:B:291:ASN:C	2.56	0.44
1:A:273:VAL:HA	1:A:274:PRO:HD3	1.80	0.44
1:B:82:ALA:O	1:B:110:SER:HA	2.17	0.44
1:A:228:ARG:HA	1:A:425:LEU:O	2.17	0.44
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.83	0.43
1:A:242:LEU:HD12	1:A:252:GLN:HB3	2.00	0.43
1:B:408:LEU:O	1:B:412:ILE:HG12	2.17	0.43
1:A:24:GLY:HA2	3:A:436:NAD:O4B	2.17	0.43
1:B:200:ILE:HG12	1:B:201:GLY:N	2.32	0.43
1:B:31:TRP:CZ2	1:B:35:THR:HG21	2.54	0.43
1:A:200:ILE:HG12	1:A:201:GLY:N	2.33	0.43
1:B:433:TYR:O	1:B:434:SER:HB3	2.19	0.43
1:A:430:ILE:HG22	1:A:435:LEU:HD12	2.00	0.43
1:A:234:PHE:CE2	1:B:267:THR:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLN:HB3	1:B:377:PHE:HE1	1.84	0.42
1:A:303:LEU:HD21	1:A:317:LEU:HD11	2.00	0.42
1:B:148:ILE:HG12	1:B:405:ALA:HB2	2.00	0.42
1:B:155:SER:HB3	1:B:158:ILE:CG1	2.48	0.42
1:B:170:ILE:HA	1:B:301:ARG:HB2	2.01	0.42
1:B:357:ASN:HA	1:B:357:ASN:HD22	1.62	0.42
1:A:153:ARG:CD	1:A:400:PRO:HG3	2.50	0.42
1:A:152:GLY:C	1:A:154:LYS:H	2.23	0.42
1:A:16:ALA:HA	1:A:17:PRO:HD3	1.90	0.42
1:A:261[A]:HIS:CE1	1:B:174:ASN:OD1	2.71	0.42
1:A:153:ARG:HD2	1:A:400:PRO:HG3	2.02	0.42
1:B:107:LEU:HA	1:B:107:LEU:HD23	1.83	0.42
1:B:308:ASP:O	1:B:309:ALA:C	2.56	0.42
1:B:164:LEU:HA	1:B:164:LEU:HD23	1.81	0.41
1:B:392:GLN:HB2	1:B:399:PHE:O	2.19	0.41
1:A:435:LEU:HD12	1:A:435:LEU:HA	1.91	0.41
1:B:403:MET:CE	1:B:433:TYR:O	2.66	0.41
1:A:147:ILE:HD13	1:A:372:ILE:HD13	2.01	0.41
1:A:402:LEU:HD12	1:A:402:LEU:HA	1.89	0.41
1:B:113:ASN:HA	1:B:114:PRO:HD3	1.89	0.41
1:A:265:GLN:NE2	4:A:445:HOH:O	2.48	0.41
1:B:193:SER:HA	1:B:194:PRO:HD3	1.79	0.41
1:B:27:ALA:HB2	1:B:67:LEU:CD2	2.50	0.41
1:B:151:GLN:H	1:B:151:GLN:HG3	1.49	0.41
1:A:75:PHE:HA	1:A:76:PRO:HD3	1.76	0.41
1:A:197:ILE:HG13	1:A:197:ILE:O	2.21	0.40
1:A:27:ALA:HB2	1:A:67:LEU:CD2	2.51	0.40
1:B:154:LYS:HA	1:B:154:LYS:HD3	1.90	0.40
1:B:176:ILE:HD13	1:B:218:LEU:HD11	2.03	0.40
1:B:265:GLN:HA	1:B:275:VAL:O	2.21	0.40
1:A:122:GLU:OE1	3:A:436:NAD:H2N	2.21	0.40
1:A:26:ASN:C	1:A:26:ASN:ND2	2.74	0.40
1:A:31:TRP:CZ2	1:A:35:THR:HG21	2.56	0.40
1:B:158:ILE:CD1	1:B:217:ILE:HD12	2.52	0.40

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	377/438 (86%)	358 (95%)	16 (4%)	3 (1%)	22	49
1	B	385/438 (88%)	360 (94%)	19 (5%)	6 (2%)	11	28
2	E	7/21 (33%)	4 (57%)	3 (43%)	0	100	100
2	F	3/21 (14%)	2 (67%)	1 (33%)	0	100	100
All	All	772/918 (84%)	724 (94%)	39 (5%)	9 (1%)	15	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	ILE
1	A	282	GLY
1	A	291	ASN
1	A	434	SER
1	B	291	ASN
1	B	433	TYR
1	B	381	LYS
1	B	192	LYS
1	B	194	PRO

### 5.3.2 Protein sidechains

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	335/376 (89%)	313 (93%)	22 (7%)	19	43
1	B	339/376 (90%)	321 (95%)	18 (5%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	674/752 (90%)	634 (94%)	40 (6%)	22	49

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	26	ASN
1	A	59	THR
1	A	65	GLN
1	A	67	LEU
1	A	120	PHE
1	A	141	GLU
1	A	150	LEU
1	A	197	ILE
1	A	200	ILE
1	A	260	ASP
1	A	283	LYS
1	A	308	ASP
1	A	321	TYR
1	A	347	LYS
1	A	356	ARG
1	A	362	VAL
1	A	378	ASN
1	A	388	GLN
1	A	390	VAL
1	A	397	GLU
1	A	402	LEU
1	B	22	PHE
1	B	26	ASN
1	B	59	THR
1	B	65	GLN
1	B	67	LEU
1	B	120	PHE
1	B	141	GLU
1	B	151	GLN
1	B	193	SER
1	B	200	ILE
1	B	260	ASP
1	B	313	GLU
1	B	320	TYR
1	B	357	ASN
1	B	361	ILE

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Mol	Chain	Res	Type
1	B	365	ILE
1	B	397	GLU
1	B	402	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	65	GLN
1	A	71	ASN
1	A	131	GLN
1	A	167	GLN
1	A	174	ASN
1	A	181	ASN
1	A	219	GLN
1	A	252	GLN
1	A	265	GLN
1	A	366	HIS
1	A	376	HIS
1	A	426	ASN
1	A	429	ASN
1	B	26	ASN
1	B	46	GLN
1	B	65	GLN
1	B	71	ASN
1	B	131	GLN
1	B	151	GLN
1	B	167	GLN
1	B	219	GLN
1	B	265	GLN
1	B	357	ASN
1	B	370	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAD	A	436	-	41,48,48	1.65	3 (7%)	43,73,73	1.64	1 (2%)
3	NAD	B	436	-	41,48,48	1.65	3 (7%)	43,73,73	1.73	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	436	-	-	0/22/62/62	0/5/5/5
3	NAD	B	436	-	-	0/22/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	436	NAD	C2A-N1A	2.48	1.38	1.33
3	B	436	NAD	C2A-N1A	2.56	1.38	1.33
3	A	436	NAD	C2A-N3A	3.68	1.38	1.32
3	B	436	NAD	C2A-N3A	3.86	1.38	1.32
3	B	436	NAD	O7N-C7N	8.25	1.41	1.24
3	A	436	NAD	O7N-C7N	8.28	1.41	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	436	NAD	N3A-C2A-N1A	-9.71	120.40	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	436	NAD	N3A-C2A-N1A	-9.35	120.71	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	436	NAD	2	0
3	B	436	NAD	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

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	384/438 (87%)	-0.15	5 (1%) 77 78	27, 59, 112, 153	0
1	B	390/438 (89%)	0.08	12 (3%) 49 49	32, 67, 123, 197	0
2	E	9/21 (42%)	0.25	0 100 100	76, 111, 146, 159	0
2	F	5/21 (23%)	1.38	1 (20%) 1 1	150, 153, 158, 166	0
All	All	788/918 (85%)	-0.02	18 (2%) 61 61	27, 63, 122, 197	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	GLY	5.5
1	B	245	GLU	4.4
1	A	435	LEU	3.2
1	B	252	GLN	3.0
1	B	379	THR	2.9
1	B	250	LEU	2.9
1	A	14	ASN	2.7
1	B	246	ARG	2.6
1	A	388	GLN	2.5
1	A	346	GLY	2.5
1	B	197	ILE	2.4
1	B	384	GLU	2.4
2	F	506	THR	2.3
1	B	381	LYS	2.2
1	B	385	LEU	2.1
1	B	249	ARG	2.0
1	B	112	ASN	2.0
1	A	246	ARG	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
3	NAD	A	436	44/44	0.97	0.16	-0.24	39,53,92,111	0
3	NAD	B	436	44/44	0.92	0.15	-0.52	58,78,121,138	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.