



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:03 PM GMT

PDB ID : 4WQ4  
Title : E. coli YgjD(E12A)-YeaZ heterodimer in complex with ATP  
Authors : Zhang, W.; Collinet, B.  
Deposited on : 2014-10-21  
Resolution : 2.33 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

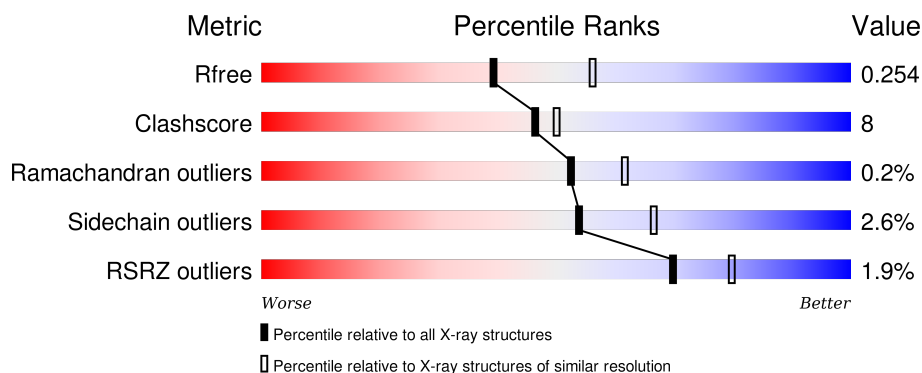
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	343	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	343	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
2	C	237	<div> <div></div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>
2	D	237	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	B	403	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8711 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 tRNA N6-adenosine threonylcarbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2476	1575	419	468	14			
1	B	336	Total	C	N	O	S	0	0	0
			2459	1565	419	461	14			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	GLU	engineered mutation	UNP P05852
A	338	HIS	-	expression tag	UNP P05852
A	339	HIS	-	expression tag	UNP P05852
A	340	HIS	-	expression tag	UNP P05852
A	341	HIS	-	expression tag	UNP P05852
A	342	HIS	-	expression tag	UNP P05852
A	343	HIS	-	expression tag	UNP P05852
B	12	ALA	GLU	engineered mutation	UNP P05852
B	338	HIS	-	expression tag	UNP P05852
B	339	HIS	-	expression tag	UNP P05852
B	340	HIS	-	expression tag	UNP P05852
B	341	HIS	-	expression tag	UNP P05852
B	342	HIS	-	expression tag	UNP P05852
B	343	HIS	-	expression tag	UNP P05852

- Molecule 2 is a protein called tRNA threonylcarbamoyladenosine biosynthesis protein Tsab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	229	Total	C	N	O	S	0	0	0
			1707	1084	290	321	12			
2	D	229	Total	C	N	O	S	0	0	0
			1695	1078	290	316	11			

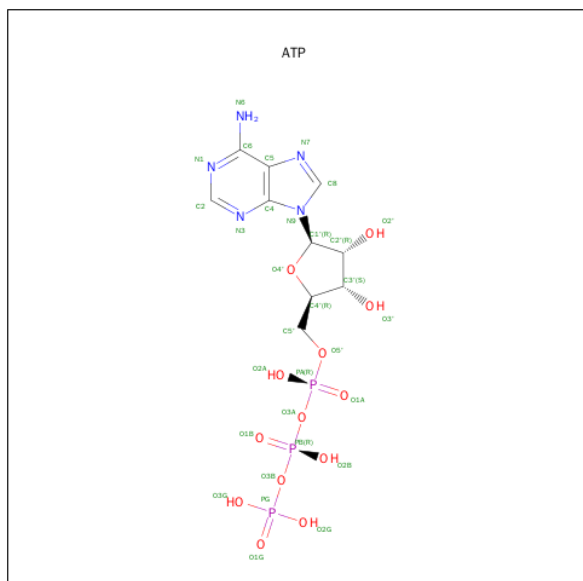
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	232	HIS	-	expression tag	UNP P76256
C	233	HIS	-	expression tag	UNP P76256
C	234	HIS	-	expression tag	UNP P76256
C	235	HIS	-	expression tag	UNP P76256
C	236	HIS	-	expression tag	UNP P76256
C	237	HIS	-	expression tag	UNP P76256
D	232	HIS	-	expression tag	UNP P76256
D	233	HIS	-	expression tag	UNP P76256
D	234	HIS	-	expression tag	UNP P76256
D	235	HIS	-	expression tag	UNP P76256
D	236	HIS	-	expression tag	UNP P76256
D	237	HIS	-	expression tag	UNP P76256

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe 1 1	0	0
3	A	1	Total Fe 1 1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



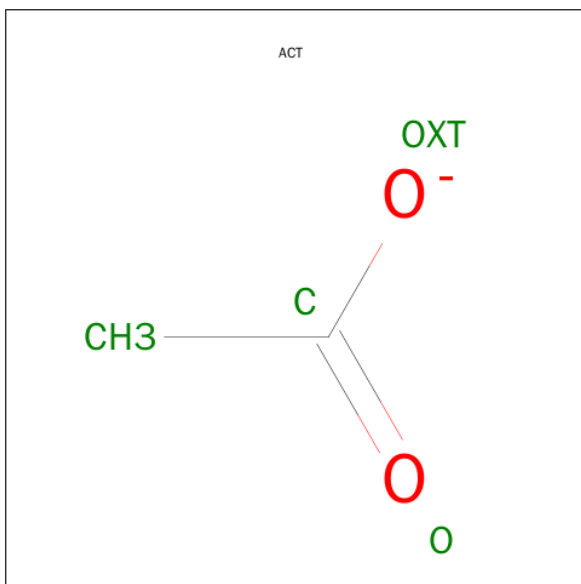
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 31 10 5 13 3	0	0

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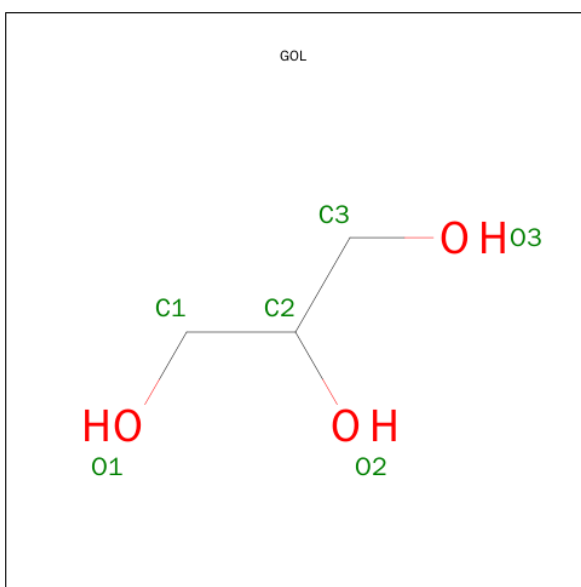
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



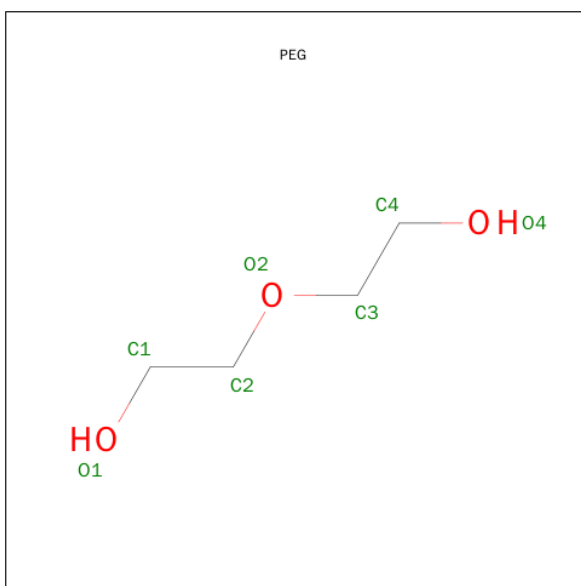
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

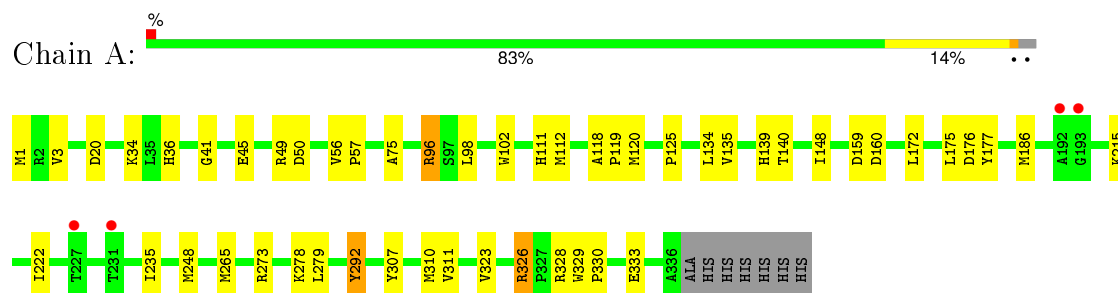
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	91	Total 91	O 91	0	0
8	B	72	Total 72	O 72	0	0
8	C	63	Total 63	O 63	0	0
8	D	56	Total 56	O 56	0	0

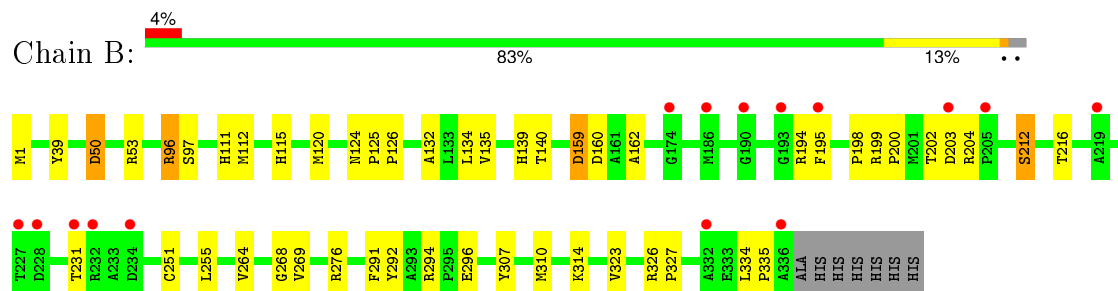
### 3 Residue-property plots [i](#)

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.

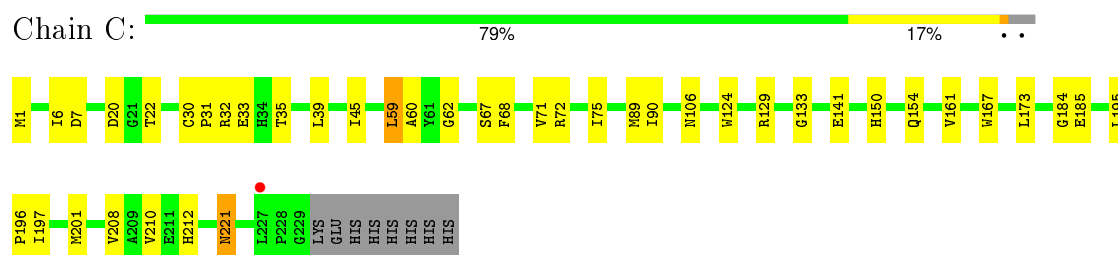
- Molecule 1: tRNA N6-adenosine threonylcarbamoyltransferase



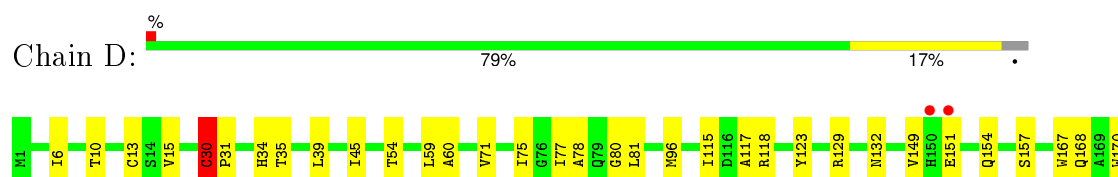
- Molecule 1: tRNA N6-adenosine threonylcarbamoyltransferase



- Molecule 2: tRNA threonylcarbamoyladenosine biosynthesis protein TsAB



- Molecule 2: tRNA threonylcarbamoyladenosine biosynthesis protein TsAB



L173	L187	L195	P196	P215	R219	A223	G229	LYS	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.27Å 68.07Å 87.13Å 109.30° 92.98° 117.23°	Depositor
Resolution (Å)	49.04 – 2.33 49.04 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.04-2.33) 82.4 (49.04-2.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.202 , 0.253 0.207 , 0.254	Depositor DCC
$R_{free}$ test set	2451 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 49013 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.41% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, FE, ATP, ACT

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	0.71	0/2525	0.75	2/3429 (0.1%)
1	B	0.70	1/2508 (0.0%)	0.74	3/3409 (0.1%)
2	C	0.76	0/1744	0.71	0/2380
2	D	0.70	0/1731	0.74	1/2363 (0.0%)
All	All	0.72	1/8508 (0.0%)	0.74	6/11581 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	PRO	N-CD	5.73	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	273	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	276	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	96	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	334	LEU	C-N-CD	5.24	139.41	128.40
2	D	219	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	2476	0	2442	43	0
1	B	2459	0	2410	35	0
2	C	1707	0	1656	27	0
2	D	1695	0	1632	25	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	4	0
5	A	4	0	3	0	0
5	B	4	0	3	3	0
6	C	6	0	8	1	0
7	C	7	0	10	2	0
7	D	7	0	10	1	0
8	A	91	0	0	3	1
8	B	72	0	0	0	1
8	C	63	0	0	0	0
8	D	56	0	0	1	0
All	All	8711	0	8198	126	1

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 8.

All (126) 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:53:ARG:HD3	5:B:403:ACT:O	1.71	0.90
1:B:112:MET:HE1	1:B:115:HIS:HD2	1.42	0.84
1:A:265:MET:HE3	1:A:292:TYR:HD2	1.40	0.84
1:B:50:ASP:OD1	5:B:403:ACT:OXT	2.01	0.78
2:C:197:ILE:HG22	2:C:201:MET:HE1	1.67	0.76
1:B:135:VAL:HG22	1:B:269:VAL:HB	1.70	0.73
1:A:265:MET:HE2	1:A:279:LEU:HD12	1.73	0.71
1:A:159:ASP:OD1	1:A:160:ASP:N	2.26	0.68
1:B:199:ARG:HB3	1:B:202:THR:HG21	1.75	0.68
1:A:265:MET:HE3	1:A:292:TYR:CD2	2.28	0.66
1:A:323:VAL:HB	2:C:35:THR:HB	1.77	0.66
1:B:135:VAL:HG23	1:B:162:ALA:HB3	1.77	0.66
2:C:197:ILE:HG22	2:C:201:MET:CE	2.27	0.63
1:A:265:MET:CE	1:A:292:TYR:HD2	2.09	0.63
2:C:195:LEU:HB2	2:C:196:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:7:ASP:OD1	2:C:62:GLY:HA3	2.00	0.62
2:C:221:ASN:H	2:C:221:ASN:HD22	1.50	0.60
2:D:71:VAL:O	2:D:75:ILE:HG13	2.03	0.59
2:D:75:ILE:HD12	2:D:215:PRO:HB3	1.84	0.58
1:A:172:LEU:HD11	1:A:215:LYS:HE3	1.84	0.57
2:D:96:MET:SD	2:D:197:ILE:HD13	2.45	0.57
2:C:67:SER:HA	7:C:302:PEG:H41	1.88	0.56
2:C:32:ARG:HA	6:C:301:GOL:H11	1.87	0.56
1:A:36:HIS:HB3	1:A:41:GLY:O	2.05	0.56
1:A:34:LYS:HG2	8:A:582:HOH:O	2.06	0.55
1:A:139:HIS:HD2	4:A:402:ATP:O1G	1.89	0.55
1:B:323:VAL:HB	2:D:35:THR:HB	1.88	0.54
1:B:203:ASP:OD1	1:B:204:ARG:N	2.40	0.54
2:D:117:ALA:O	2:D:118:ARG:HB2	2.06	0.54
1:B:194:ARG:HG3	1:B:195:PHE:CD2	2.43	0.54
2:C:72:ARG:HA	2:C:75:ILE:HG22	1.90	0.54
1:A:175:LEU:HD21	1:A:186:MET:CE	2.38	0.53
1:A:1:MET:HE2	1:A:310:MET:SD	2.49	0.53
1:A:326:ARG:NH2	8:A:560:HOH:O	2.41	0.53
2:C:67:SER:O	2:C:71:VAL:HG23	2.08	0.53
2:D:34:HIS:H	7:D:301:PEG:H42	1.74	0.52
2:C:161:VAL:HG13	2:C:184:GLY:CA	2.39	0.52
2:D:30:CYS:N	2:D:31:PRO:CD	2.72	0.52
1:A:326:ARG:HE	1:A:326:ARG:CA	2.21	0.52
1:A:330:PRO:HG2	1:A:333:GLU:OE2	2.10	0.52
1:B:134:LEU:O	1:B:140:THR:HA	2.09	0.52
2:D:167:TRP:CZ3	2:D:173:LEU:HB3	2.45	0.51
2:D:168:GLN:NE2	2:D:187:LEU:HD21	2.25	0.51
2:C:90:ILE:HG22	2:C:201:MET:HE3	1.91	0.51
1:B:120:MET:HA	1:B:125:PRO:HB3	1.92	0.50
2:C:90:ILE:CG2	2:C:201:MET:HE3	2.41	0.50
1:A:120:MET:HA	1:A:125:PRO:HB3	1.94	0.49
1:A:139:HIS:CD2	4:A:402:ATP:O1G	2.66	0.49
1:B:139:HIS:CD2	4:B:402:ATP:O3G	2.66	0.49
1:A:326:ARG:HE	1:A:326:ARG:HA	1.76	0.49
2:C:106:ASN:ND2	2:C:185:GLU:OE1	2.45	0.49
2:D:59:LEU:HD12	2:D:60:ALA:N	2.28	0.48
1:B:53:ARG:CD	5:B:403:ACT:O	2.51	0.48
1:A:98:LEU:HD11	1:A:102:TRP:CE2	2.49	0.48
1:A:248:MET:CE	1:A:278:LYS:NZ	2.76	0.48
1:B:199:ARG:HB3	1:B:202:THR:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE2	1:B:310:MET:SD	2.54	0.48
2:C:124:TRP:O	2:C:141:GLU:HA	2.14	0.48
1:B:111:HIS:HD2	1:B:112:MET:CE	2.27	0.47
2:C:59:LEU:HD12	2:C:60:ALA:N	2.29	0.47
2:D:132:ASN:N	2:D:132:ASN:OD1	2.48	0.47
1:B:159:ASP:OD1	1:B:160:ASP:N	2.47	0.47
2:C:208:VAL:HB	2:C:212:HIS:HB2	1.97	0.46
1:B:132:ALA:HA	1:B:264:VAL:O	2.14	0.46
1:A:111:HIS:HD2	1:A:112:MET:CE	2.28	0.46
2:D:13:CYS:SG	2:D:34:HIS:HA	2.56	0.46
1:B:96:ARG:HA	1:B:96:ARG:HD2	1.79	0.46
2:C:221:ASN:H	2:C:221:ASN:ND2	2.13	0.46
2:C:30:CYS:O	2:C:31:PRO:C	2.54	0.46
1:A:175:LEU:HD21	1:A:186:MET:HE3	1.97	0.46
1:A:134:LEU:O	1:A:140:THR:HA	2.16	0.46
1:B:294:ARG:HG3	1:B:296:GLU:HG2	1.97	0.46
1:A:326:ARG:CZ	1:A:328:ARG:O	2.64	0.45
1:A:177:TYR:C	1:A:177:TYR:CD1	2.89	0.45
1:B:39:TYR:CE1	2:D:223:ALA:HB1	2.51	0.45
2:D:129:ARG:NE	8:D:441:HOH:O	2.49	0.45
8:A:531:HOH:O	2:C:39:LEU:HB2	2.16	0.45
1:B:268:GLY:HA3	4:B:402:ATP:O5'	2.17	0.45
1:B:135:VAL:CG2	1:B:162:ALA:HB3	2.44	0.45
1:A:45:GLU:O	1:A:49:ARG:HG3	2.16	0.44
2:D:151:GLU:O	2:D:154:GLN:HB2	2.17	0.44
2:C:89:MET:SD	2:C:210:VAL:HA	2.57	0.44
2:D:115:ILE:HB	2:D:123:TYR:HB2	2.00	0.44
1:A:248:MET:HE2	1:A:278:LYS:NZ	2.33	0.43
1:B:126:PRO:HB3	1:B:291:PHE:CD1	2.53	0.43
2:C:30:CYS:N	2:C:31:PRO:CD	2.81	0.43
1:B:139:HIS:HD2	4:B:402:ATP:O3G	2.02	0.43
1:A:222:ILE:HG12	1:A:235:ILE:HD13	2.00	0.43
2:D:6:ILE:HD11	2:D:78:ALA:HB2	2.00	0.43
1:A:20:ASP:HB3	1:A:310:MET:HE3	2.01	0.43
1:A:118:ALA:N	1:A:119:PRO:CD	2.82	0.43
2:C:129:ARG:CZ	2:C:133:GLY:HA2	2.49	0.42
2:C:59:LEU:O	2:C:89:MET:HA	2.19	0.42
2:C:150:HIS:O	2:C:154:GLN:HG2	2.19	0.42
2:D:170:TRP:O	2:D:173:LEU:HB2	2.19	0.42
1:B:310:MET:SD	1:B:314:LYS:HE3	2.59	0.42
2:C:167:TRP:CZ3	2:C:173:LEU:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:HG2	1:A:323:VAL:HG22	2.02	0.42
1:A:56:VAL:HB	1:A:57:PRO:HD3	2.02	0.42
1:B:326:ARG:HA	1:B:327:PRO:HD2	1.90	0.42
1:A:148:ILE:HD12	1:A:311:VAL:HG11	2.03	0.41
2:D:77:ILE:O	2:D:81:LEU:HG	2.20	0.41
2:D:15:VAL:HG23	2:D:45:ILE:HG13	2.01	0.41
1:A:111:HIS:HD2	1:A:112:MET:HE3	1.85	0.41
1:B:111:HIS:CD2	1:B:112:MET:CE	3.04	0.41
1:A:96:ARG:HD2	1:A:96:ARG:HA	1.86	0.41
1:A:175:LEU:HD21	1:A:186:MET:HE1	2.02	0.41
1:A:326:ARG:HB3	1:A:329:TRP:HB2	2.02	0.41
1:B:307:TYR:O	1:B:310:MET:HB3	2.21	0.41
1:B:112:MET:HE3	4:B:402:ATP:O2G	2.20	0.41
1:A:265:MET:CE	1:A:279:LEU:HD12	2.47	0.41
1:A:3:VAL:HG22	1:A:75:ALA:HB3	2.02	0.41
1:B:198:PRO:O	1:B:200:PRO:HD3	2.21	0.41
1:A:248:MET:HE3	1:A:278:LYS:NZ	2.36	0.41
2:D:39:LEU:HA	2:D:39:LEU:HD23	1.90	0.41
1:B:112:MET:HB3	1:B:134:LEU:HD21	2.03	0.40
1:A:307:TYR:O	1:A:310:MET:HB3	2.21	0.40
1:A:135:VAL:HG12	1:A:140:THR:HG23	2.03	0.40
1:B:97:SER:OG	2:D:80:GLY:HA3	2.22	0.40
1:B:160:ASP:OD2	1:B:212:SER:HB3	2.21	0.40
2:D:10:THR:O	2:D:34:HIS:HE1	2.05	0.40
1:B:251:CYS:O	1:B:255:LEU:HG	2.21	0.40
2:C:68:PHE:H	7:C:302:PEG:H42	1.87	0.40
2:D:149:VAL:HG11	2:D:173:LEU:HG	2.03	0.40
1:A:248:MET:CE	1:A:278:LYS:HZ1	2.35	0.40
2:D:195:LEU:HB2	2:D:196:PRO:HD3	2.04	0.40

All (1) 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)
8:A:511:HOH:O	8:B:508:HOH:O[1_665]	0.57	1.63

## 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	334/343 (97%)	326 (98%)	8 (2%)	0	100	100
1	B	334/343 (97%)	321 (96%)	12 (4%)	1 (0%)	46	54
2	C	227/237 (96%)	217 (96%)	10 (4%)	0	100	100
2	D	227/237 (96%)	217 (96%)	9 (4%)	1 (0%)	39	45
All	All	1122/1160 (97%)	1081 (96%)	39 (4%)	2 (0%)	52	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	ASP
2	D	30	CYS

### 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	244/263 (93%)	240 (98%)	4 (2%)	70	82
1	B	239/263 (91%)	233 (98%)	6 (2%)	55	68
2	C	168/187 (90%)	160 (95%)	8 (5%)	31	39
2	D	163/187 (87%)	160 (98%)	3 (2%)	66	79
All	All	814/900 (90%)	793 (97%)	21 (3%)	54	66

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	176	ASP
1	A	292	TYR
1	A	326	ARG
1	B	50	ASP
1	B	124	ASN
1	B	212	SER
1	B	216	THR
1	B	231	THR
1	B	292	TYR
2	C	1	MET
2	C	6	ILE
2	C	20	ASP
2	C	22	THR
2	C	33	GLU
2	C	45	ILE
2	C	59	LEU
2	C	221	ASN
2	D	30	CYS
2	D	54	THR
2	D	157	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	139	HIS
1	B	111	HIS
1	B	139	HIS
1	B	150	GLN
2	C	155	GLN
2	C	168	GLN
2	C	221	ASN
2	D	34	HIS
2	D	36	GLN
2	D	168	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z  > 2$
4	ATP	A	402	3	24,33,33	1.13	2 (8%)	31,52,52	1.72	9 (29%)
5	ACT	A	403	-	1,3,3	1.77	0	0,3,3	0.00	-
4	ATP	B	402	3	24,33,33	1.33	2 (8%)	31,52,52	2.17	9 (29%)
5	ACT	B	403	-	1,3,3	0.41	0	0,3,3	0.00	-
6	GOL	C	301	-	5,5,5	0.34	0	5,5,5	0.33	0
7	PEG	C	302	-	6,6,6	0.70	0	5,5,5	0.46	0
7	PEG	D	301	-	6,6,6	0.63	0	5,5,5	0.51	0

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
4	ATP	A	402	3	-	0/18/38/38	0/3/3/3
5	ACT	A	403	-	-	0/0/0/0	0/0/0/0
4	ATP	B	402	3	-	0/18/38/38	0/3/3/3
5	ACT	B	403	-	-	0/0/0/0	0/0/0/0
6	GOL	C	301	-	-	0/4/4/4	0/0/0/0
7	PEG	C	302	-	-	0/4/4/4	0/0/0/0
7	PEG	D	301	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	ATP	C2-N1	2.50	1.38	1.33
4	B	402	ATP	C5-C4	3.29	1.47	1.40
4	A	402	ATP	C5-C4	3.33	1.48	1.40
4	B	402	ATP	O4'-C1'	3.73	1.45	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	ATP	N3-C2-N1	-7.69	123.01	128.89
4	B	402	ATP	PA-O3A-PB	-4.38	120.43	132.73
4	A	402	ATP	N3-C2-N1	-3.55	126.18	128.89
4	A	402	ATP	C2'-C1'-N9	-3.28	109.28	114.29
4	A	402	ATP	C4-C5-N7	-3.17	106.57	109.48
4	A	402	ATP	PA-O3A-PB	-3.01	124.29	132.73
4	B	402	ATP	C1'-N9-C4	-2.78	122.75	126.94
4	B	402	ATP	PB-O3B-PG	-2.73	123.53	132.67
4	B	402	ATP	C4'-O4'-C1'	-2.65	106.80	109.72
4	A	402	ATP	O3'-C3'-C2'	-2.46	103.82	111.83
4	B	402	ATP	C4-C5-N7	-2.32	107.34	109.48
4	A	402	ATP	PB-O3B-PG	-2.16	125.44	132.67
4	B	402	ATP	C2'-C1'-N9	-2.04	111.18	114.29
4	A	402	ATP	O2G-PG-O1G	2.21	117.69	110.58
4	B	402	ATP	C2-N1-C6	2.25	122.79	118.77
4	B	402	ATP	O3G-PG-O2G	2.27	116.03	107.38
4	A	402	ATP	O2B-PB-O3B	2.60	116.90	105.09
4	A	402	ATP	O3G-PG-O2G	2.78	117.98	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	ATP	2	0
4	B	402	ATP	4	0
5	B	403	ACT	3	0
6	C	301	GOL	1	0
7	C	302	PEG	2	0
7	D	301	PEG	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	336/343 (97%)	-0.17	4 (1%) 81 88	16, 29, 48, 62	0
1	B	336/343 (97%)	0.04	15 (4%) 37 50	18, 35, 57, 76	0
2	C	229/237 (96%)	-0.22	1 (0%) 93 97	18, 29, 48, 66	0
2	D	229/237 (96%)	-0.06	2 (0%) 85 91	20, 32, 51, 64	0
All	All	1130/1160 (97%)	-0.10	22 (1%) 70 80	16, 31, 52, 76	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	GLY	4.5
1	B	219	ALA	4.0
1	A	193	GLY	3.7
1	B	203	ASP	3.2
1	B	186	MET	3.1
1	B	190	GLY	3.1
1	B	227	THR	3.0
1	B	332	ALA	2.7
1	A	231	THR	2.7
2	D	151	GLU	2.6
1	A	227	THR	2.5
1	B	205	PRO	2.5
1	B	234	ASP	2.4
2	C	227	LEU	2.3
1	B	232	ARG	2.3
1	B	195	PHE	2.3
1	B	228	ASP	2.3
2	D	150	HIS	2.3
1	A	192	ALA	2.2
1	B	174	GLY	2.1
1	B	231	THR	2.1
1	B	336	ALA	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 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(Å <sup>2</sup> )	Q<0.9
7	PEG	C	302	7/7	0.83	0.14	0.90	32,38,42,46	0
7	PEG	D	301	7/7	0.84	0.14	0.49	39,42,50,51	0
4	ATP	A	402	31/31	0.94	0.11	-0.09	23,34,52,61	0
4	ATP	B	402	31/31	0.94	0.12	-0.26	25,35,59,67	0
6	GOL	C	301	6/6	0.93	0.11	-1.00	26,35,36,37	0
3	FE	B	401	1/1	0.86	0.08	-	51,51,51,51	0
5	ACT	B	403	4/4	0.79	0.27	-	26,28,29,32	0
3	FE	A	401	1/1	0.96	0.06	-	48,48,48,48	0
5	ACT	A	403	4/4	0.80	0.18	-	27,27,29,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.