



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:18 pm GMT

PDB ID : 4H0T  
Title : Crystal structure of Ia-ADPR-actin complex  
Authors : Tsurumura, T.; Oda, M.; Nagahama, M.; Tsuge, H.  
Deposited on : 2012-09-10  
Resolution : 2.20 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  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

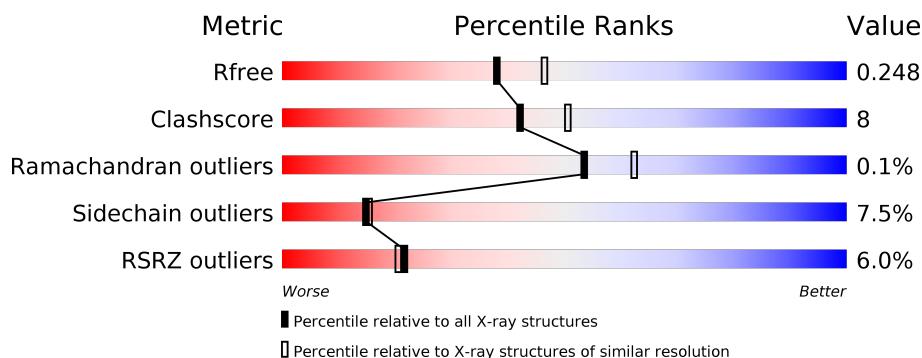
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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	418	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>• •</div> </div> </div>
2	B	375	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• • 5%</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6542 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 Iota toxin component Ia.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3371	2151	554	662	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ARG	-	EXPRESSION TAG	UNP Q46220
A	-3	GLY	-	EXPRESSION TAG	UNP Q46220
A	-2	SER	-	EXPRESSION TAG	UNP Q46220
A	-1	HIS	-	EXPRESSION TAG	UNP Q46220
A	0	MET	-	EXPRESSION TAG	UNP Q46220

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	358	Total	C	N	O	S	0	0	0
			2799	1774	469	537	19			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



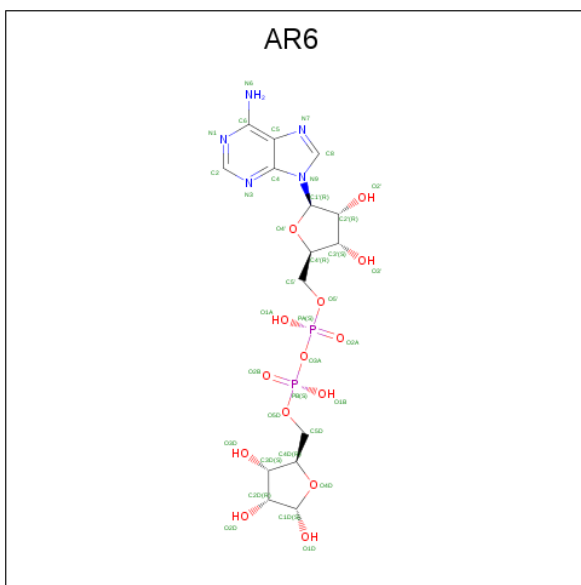
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).

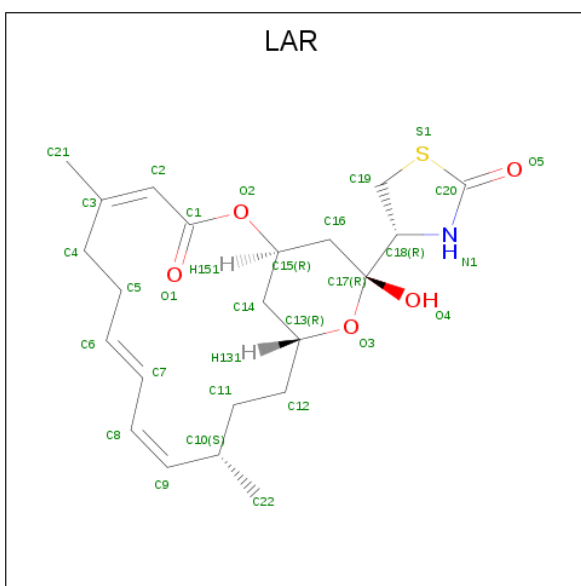


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

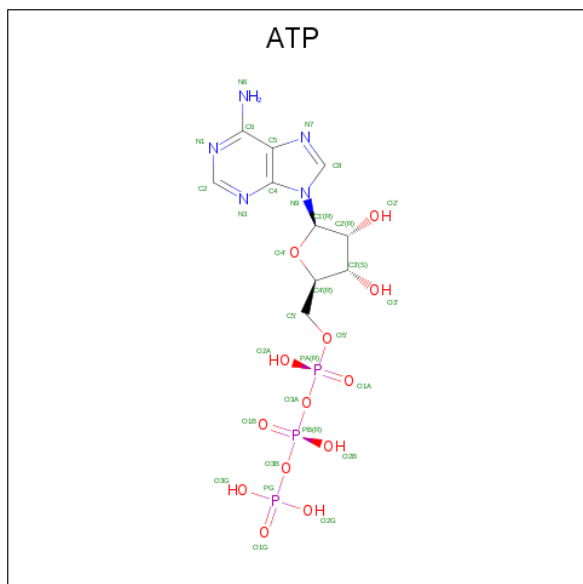
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0

- Molecule 7 is LATRUNCULIN A (three-letter code: LAR) (formula:  $C_{22}H_{31}NO_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

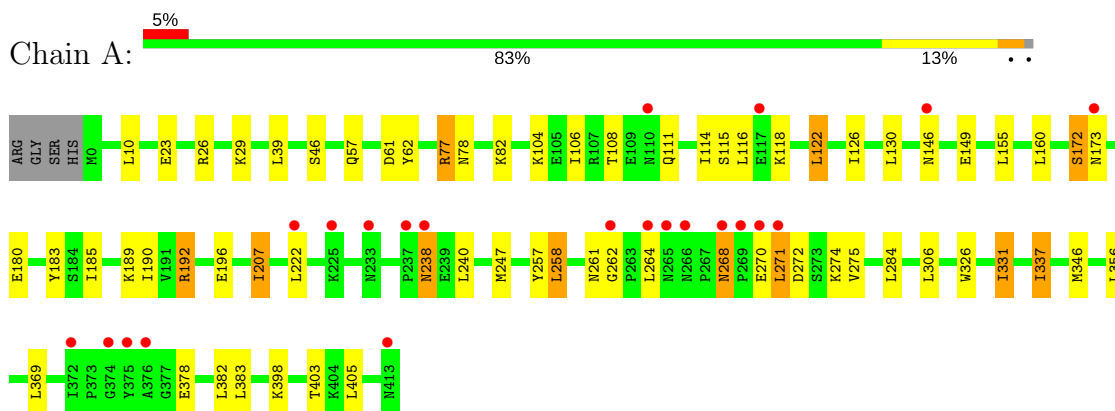
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	104	Total	O	0	0
			104	104		
9	B	95	Total	O	0	0
			95	95		

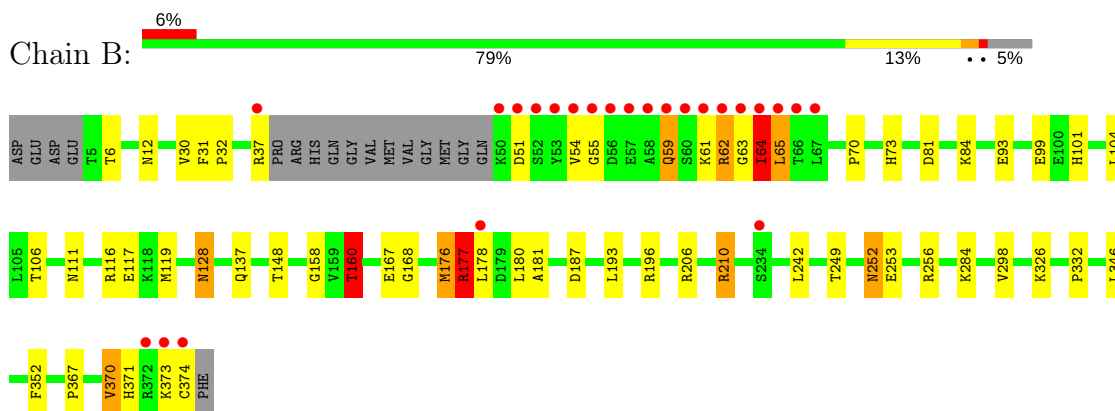
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Iota toxin component Ia



- Molecule 2: Actin, alpha skeletal muscle





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.02Å 134.17Å 151.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.20 33.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.54-2.20) 99.8 (33.54-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.22 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.212 , 0.240 0.223 , 0.248	Depositor DCC
$R_{free}$ test set	2873 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

Bond lengths and bond angles in the following residue types are not validated in this section: AR6, PO4, EDO, ATP, CA, LAR

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	0.35	0/3440	0.65	1/4647 (0.0%)
2	B	0.38	1/2858 (0.0%)	0.80	8/3873 (0.2%)
All	All	0.36	1/6298 (0.0%)	0.72	9/8520 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	160	THR	CB-OG1	5.59	1.54	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	177	ARG	C-N-CA	15.08	159.41	121.70
2	B	177	ARG	O-C-N	-14.20	99.97	122.70
2	B	176	MET	C-N-CA	9.76	146.09	121.70
2	B	177	ARG	NE-CZ-NH1	-9.68	115.46	120.30
2	B	210	ARG	NE-CZ-NH2	-7.87	116.36	120.30
2	B	177	ARG	CA-C-N	6.80	132.15	117.20
2	B	176	MET	O-C-N	-6.21	112.76	122.70
1	A	356	LEU	CA-CB-CG	5.49	127.93	115.30
2	B	210	ARG	NE-CZ-NH1	5.32	122.96	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	176	MET	Mainchain
2	B	177	ARG	Mainchain

## 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	3371	0	3355	36	0
2	B	2799	0	2771	58	0
3	A	5	0	0	0	0
4	A	36	0	54	1	0
4	B	36	0	54	2	0
5	B	35	0	19	0	0
6	B	1	0	0	0	0
7	B	29	0	31	4	0
8	B	31	0	12	0	0
9	A	104	0	0	1	0
9	B	95	0	0	0	0
All	All	6542	0	6296	95	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 8.

All (95) 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:114:ILE:O	1:A:192:ARG:NH1	2.01	0.93
2:B:63:GLY:C	2:B:65:LEU:H	1.65	0.92
2:B:346:LEU:HD21	2:B:352:PHE:CE1	2.06	0.90
2:B:346:LEU:HD21	2:B:352:PHE:CD1	2.07	0.90
2:B:37:ARG:O	2:B:65:LEU:HD12	1.72	0.89
2:B:37:ARG:C	2:B:65:LEU:CD1	2.42	0.88
2:B:37:ARG:C	2:B:65:LEU:HD12	1.94	0.88
1:A:326:TRP:CE3	1:A:331:ILE:HD11	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:LEU:HD23	2:B:346:LEU:C	1.98	0.84
2:B:6:THR:O	2:B:101:HIS:HD2	1.63	0.80
2:B:117:GLU:OE2	2:B:371:HIS:HE1	1.67	0.78
2:B:63:GLY:C	2:B:65:LEU:N	2.36	0.75
1:A:146:ASN:OD1	1:A:196:GLU:HG2	1.88	0.73
2:B:61:LYS:HE3	2:B:64:ILE:HD11	1.71	0.73
2:B:160:THR:HG23	2:B:180:LEU:O	1.88	0.72
2:B:61:LYS:CE	2:B:64:ILE:HD11	2.20	0.70
2:B:37:ARG:C	2:B:65:LEU:HD11	2.11	0.70
2:B:62:ARG:CG	2:B:62:ARG:O	2.40	0.69
2:B:54:VAL:HG12	2:B:55:GLY:N	2.09	0.67
2:B:111:ASN:HD21	2:B:119:MET:HE1	1.60	0.66
2:B:177:ARG:HG3	2:B:177:ARG:O	1.95	0.64
2:B:62:ARG:CD	2:B:62:ARG:O	2.45	0.64
2:B:210:ARG:NH2	7:B:403:LAR:H213	2.12	0.63
2:B:62:ARG:HG2	2:B:62:ARG:O	1.99	0.63
1:A:172:SER:OG	1:A:173:ASN:N	2.31	0.62
2:B:346:LEU:C	2:B:346:LEU:CD2	2.69	0.61
1:A:160:LEU:HD23	1:A:207:ILE:HD12	1.82	0.60
1:A:77:ARG:HG3	1:A:180:GLU:OE1	2.02	0.59
1:A:398:LYS:NZ	1:A:403:THR:OG1	2.31	0.58
2:B:62:ARG:HD3	2:B:62:ARG:O	2.04	0.57
2:B:6:THR:O	2:B:101:HIS:CD2	2.52	0.57
1:A:326:TRP:CZ3	1:A:331:ILE:HD11	2.40	0.57
1:A:271:LEU:HA	1:A:274:LYS:HB2	1.89	0.55
2:B:346:LEU:HD23	2:B:346:LEU:O	2.08	0.54
2:B:160:THR:CG2	2:B:180:LEU:O	2.55	0.54
2:B:62:ARG:HA	2:B:65:LEU:O	2.08	0.53
1:A:337:ILE:CD1	1:A:383:LEU:HB2	2.38	0.53
1:A:337:ILE:HD12	1:A:383:LEU:HB2	1.90	0.53
2:B:61:LYS:HE2	2:B:64:ILE:HD11	1.91	0.53
1:A:57:GLN:NE2	9:A:651:HOH:O	2.35	0.53
2:B:64:ILE:N	2:B:64:ILE:HD12	2.24	0.53
1:A:183:TYR:CZ	1:A:207:ILE:HD11	2.43	0.53
2:B:180:LEU:C	2:B:180:LEU:HD23	2.29	0.52
2:B:111:ASN:ND2	2:B:119:MET:HE1	2.24	0.52
2:B:298:VAL:CG1	4:B:407:EDO:H21	2.40	0.51
1:A:257:TYR:CE2	1:A:271:LEU:HD21	2.46	0.50
2:B:332:PRO:HG2	4:B:407:EDO:H12	1.93	0.50
7:B:403:LAR:O2	7:B:403:LAR:H42	2.12	0.50
2:B:54:VAL:CG1	2:B:55:GLY:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:THR:OG1	1:A:111:GLN:HG3	2.11	0.49
2:B:367:PRO:O	2:B:370:VAL:HG22	2.13	0.48
1:A:257:TYR:CE1	1:A:262:GLY:HA3	2.49	0.47
2:B:99:GLU:HG3	2:B:128:ASN:HB3	1.94	0.47
2:B:63:GLY:CA	2:B:65:LEU:H	2.26	0.47
1:A:26:ARG:O	1:A:29:LYS:HG2	2.14	0.47
1:A:258:LEU:HD11	1:A:275:VAL:HG21	1.96	0.47
2:B:346:LEU:CD2	2:B:352:PHE:CD1	2.90	0.47
2:B:116:ARG:HA	2:B:119:MET:HE2	1.96	0.47
1:A:106:ILE:O	1:A:118:LYS:HG2	2.15	0.46
2:B:111:ASN:HD21	2:B:119:MET:CE	2.26	0.46
2:B:187:ASP:OD1	2:B:206:ARG:HD2	2.16	0.45
1:A:369:LEU:HD22	1:A:382:LEU:HB2	1.97	0.45
1:A:268:ASN:HD22	1:A:268:ASN:C	2.21	0.44
2:B:148:THR:OG1	2:B:168:GLY:N	2.50	0.44
2:B:37:ARG:CA	2:B:65:LEU:HD11	2.46	0.44
2:B:116:ARG:HA	2:B:119:MET:CE	2.48	0.44
1:A:264:LEU:HD23	1:A:264:LEU:C	2.38	0.44
2:B:59:GLN:HB2	7:B:403:LAR:H91	2.00	0.44
1:A:183:TYR:CD2	1:A:207:ILE:HG12	2.54	0.43
2:B:117:GLU:OE2	2:B:371:HIS:CE1	2.58	0.43
2:B:111:ASN:ND2	2:B:119:MET:CE	2.81	0.43
1:A:346:MET:CE	1:A:378:GLU:HG3	2.49	0.43
1:A:122:LEU:HD22	1:A:126:ILE:HD13	2.01	0.43
1:A:115:SER:OG	1:A:118:LYS:HB2	2.18	0.43
1:A:23:GLU:OE2	1:A:26:ARG:NH1	2.51	0.43
1:A:247:MET:HE2	1:A:247:MET:HB3	1.88	0.43
2:B:73:HIS:HD2	2:B:158:GLY:O	2.01	0.43
2:B:180:LEU:HD23	2:B:181:ALA:N	2.34	0.43
2:B:252:ASN:ND2	2:B:256:ARG:HH21	2.17	0.42
1:A:238:ASN:N	1:A:238:ASN:OD1	2.51	0.42
2:B:65:LEU:HD12	2:B:65:LEU:HA	1.53	0.42
1:A:146:ASN:HA	1:A:196:GLU:CG	2.50	0.42
2:B:252:ASN:HD22	2:B:253:GLU:N	2.18	0.42
2:B:31:PHE:CE2	2:B:93:GLU:HG3	2.55	0.41
1:A:61:ASP:OD1	1:A:62:TYR:N	2.54	0.41
1:A:271:LEU:C	1:A:271:LEU:HD23	2.40	0.41
2:B:32:PRO:HB3	7:B:403:LAR:H141	2.01	0.41
2:B:106:THR:HB	2:B:137:GLN:HG3	2.03	0.41
1:A:126:ILE:HD11	1:A:190:ILE:HG21	2.02	0.41
1:A:271:LEU:HD23	1:A:272:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:PRO:HG3	2:B:81:ASP:HB3	2.03	0.40
1:A:26:ARG:HH11	1:A:26:ARG:HB3	1.86	0.40
2:B:196:ARG:HH21	2:B:249:THR:HG22	1.86	0.40
4:A:504:EDO:O1	2:B:284:LYS:HD2	2.20	0.40
1:A:257:TYR:CD1	1:A:262:GLY:HA3	2.56	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	412/418 (99%)	400 (97%)	12 (3%)	0	100	100
2	B	354/375 (94%)	345 (98%)	8 (2%)	1 (0%)	43	48
All	All	766/793 (97%)	745 (97%)	20 (3%)	1 (0%)	53	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	64	ILE

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/380 (99%)	347 (92%)	30 (8%)	13	13
2	B	304/318 (96%)	283 (93%)	21 (7%)	17	18
All	All	681/698 (98%)	630 (92%)	51 (8%)	15	15

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	39	LEU
1	A	46	SER
1	A	77	ARG
1	A	78	ASN
1	A	82	LYS
1	A	104	LYS
1	A	116	LEU
1	A	122	LEU
1	A	130	LEU
1	A	149	GLU
1	A	155	LEU
1	A	172	SER
1	A	185	ILE
1	A	189	LYS
1	A	192	ARG
1	A	207	ILE
1	A	222	LEU
1	A	238	ASN
1	A	240	LEU
1	A	258	LEU
1	A	261	ASN
1	A	268	ASN
1	A	270	GLU
1	A	271	LEU
1	A	284	LEU
1	A	306	LEU
1	A	331	ILE
1	A	337	ILE
1	A	405	LEU
2	B	12	ASN
2	B	30	VAL

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Mol	Chain	Res	Type
2	B	51	ASP
2	B	59	GLN
2	B	62	ARG
2	B	64	ILE
2	B	65	LEU
2	B	84	LYS
2	B	104	LEU
2	B	128	ASN
2	B	160	THR
2	B	167	GLU
2	B	177	ARG
2	B	178	LEU
2	B	193	LEU
2	B	242	LEU
2	B	252	ASN
2	B	326	LYS
2	B	370	VAL
2	B	373	LYS
2	B	374	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	51	ASN
1	A	90	ASN
1	A	111	GLN
1	A	157	HIS
1	A	209	ASN
1	A	227	ASN
1	A	256	ASN
1	A	261	ASN
1	A	268	ASN
1	A	300	GLN
1	A	392	ASN
2	B	73	HIS
2	B	87	HIS
2	B	88	HIS
2	B	101	HIS
2	B	111	ASN
2	B	162	ASN
2	B	246	GLN

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Mol	Chain	Res	Type
2	B	252	ASN
2	B	371	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	$\# Z  > 2$
3	PO4	A	501	-	4,4,4	0.75	0	6,6,6	0.42	0
4	EDO	A	502	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	A	503	-	3,3,3	0.42	0	2,2,2	0.63	0
4	EDO	A	504	-	3,3,3	0.48	0	2,2,2	0.12	0
4	EDO	A	505	-	3,3,3	0.53	0	2,2,2	0.17	0
4	EDO	A	506	-	3,3,3	0.45	0	2,2,2	0.32	0
4	EDO	A	507	-	3,3,3	0.48	0	2,2,2	0.49	0
4	EDO	A	508	-	3,3,3	0.51	0	2,2,2	0.42	0
4	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.26	0
4	EDO	A	510	-	3,3,3	0.48	0	2,2,2	0.28	0
5	AR6	B	401	2	33,38,39	2.44	7 (21%)	34,58,60	4.16	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	LAR	B	403	-	30,31,31	1.71	4 (13%)	36,43,43	2.37	10 (27%)
8	ATP	B	404	-	27,33,33	1.00	1 (3%)	27,52,52	1.70	3 (11%)
4	EDO	B	405	-	3,3,3	0.50	0	2,2,2	0.09	0
4	EDO	B	406	-	3,3,3	0.46	0	2,2,2	0.37	0
4	EDO	B	407	-	3,3,3	0.51	0	2,2,2	0.49	0
4	EDO	B	408	-	3,3,3	0.44	0	2,2,2	0.18	0
4	EDO	B	409	-	3,3,3	0.47	0	2,2,2	0.26	0
4	EDO	B	410	-	3,3,3	0.52	0	2,2,2	0.16	0
4	EDO	B	411	-	3,3,3	0.47	0	2,2,2	0.40	0
4	EDO	B	412	-	3,3,3	0.50	0	2,2,2	0.31	0
4	EDO	B	413	-	3,3,3	0.43	0	2,2,2	0.50	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
3	PO4	A	501	-	-	0/0/0/0	0/0/0/0
4	EDO	A	502	-	-	0/1/1/1	0/0/0/0
4	EDO	A	503	-	-	0/1/1/1	0/0/0/0
4	EDO	A	504	-	-	0/1/1/1	0/0/0/0
4	EDO	A	505	-	-	0/1/1/1	0/0/0/0
4	EDO	A	506	-	-	0/1/1/1	0/0/0/0
4	EDO	A	507	-	-	0/1/1/1	0/0/0/0
4	EDO	A	508	-	-	0/1/1/1	0/0/0/0
4	EDO	A	509	-	-	0/1/1/1	0/0/0/0
4	EDO	A	510	-	-	0/1/1/1	0/0/0/0
5	AR6	B	401	2	-	0/18/51/54	0/4/4/4
7	LAR	B	403	-	-	0/23/51/51	0/2/3/3
8	ATP	B	404	-	-	0/18/38/38	0/3/3/3
4	EDO	B	405	-	-	0/1/1/1	0/0/0/0
4	EDO	B	406	-	-	0/1/1/1	0/0/0/0
4	EDO	B	407	-	-	0/1/1/1	0/0/0/0
4	EDO	B	408	-	-	0/1/1/1	0/0/0/0
4	EDO	B	409	-	-	0/1/1/1	0/0/0/0
4	EDO	B	410	-	-	0/1/1/1	0/0/0/0
4	EDO	B	411	-	-	0/1/1/1	0/0/0/0
4	EDO	B	412	-	-	0/1/1/1	0/0/0/0
4	EDO	B	413	-	-	0/1/1/1	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	403	LAR	C20-S1	-4.91	1.66	1.78
5	B	401	AR6	C5-C4	-3.31	1.33	1.40
5	B	401	AR6	C8-N9	-3.18	1.33	1.36
7	B	403	LAR	C20-N1	-2.81	1.32	1.36
7	B	403	LAR	C19-S1	-2.05	1.77	1.81
5	B	401	AR6	O4'-C1'	2.18	1.44	1.41
5	B	401	AR6	O4D-C1D	2.34	1.49	1.43
5	B	401	AR6	O4D-C4D	2.41	1.48	1.44
8	B	404	ATP	C5-C4	2.97	1.47	1.40
7	B	403	LAR	O2-C1	6.00	1.47	1.34
5	B	401	AR6	C2-N1	7.98	1.48	1.33
5	B	401	AR6	C2-N3	8.25	1.45	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	AR6	N3-C2-N1	-23.16	109.04	128.86
7	B	403	LAR	C4-C5-C6	-8.03	95.18	112.63
8	B	404	ATP	N3-C2-N1	-6.47	123.32	128.86
7	B	403	LAR	C8-C7-C6	-5.75	101.62	124.64
5	B	401	AR6	PB-O3A-PA	-4.01	119.16	132.63
7	B	403	LAR	O1-C1-C2	-3.04	118.35	126.20
8	B	404	ATP	C4-C5-N7	-2.92	106.59	109.41
7	B	403	LAR	O2-C1-O1	-2.79	118.54	123.31
5	B	401	AR6	C1'-N9-C4	-2.50	122.32	126.64
8	B	404	ATP	PA-O3A-PB	-2.40	124.57	132.63
5	B	401	AR6	C2-N1-C6	2.13	122.37	118.75
7	B	403	LAR	C18-N1-C20	2.17	116.44	113.20
7	B	403	LAR	C5-C4-C3	2.32	120.52	112.85
7	B	403	LAR	C5-C6-C7	2.40	137.83	126.08
7	B	403	LAR	O2-C15-C16	2.40	113.53	107.58
7	B	403	LAR	C19-S1-C20	3.13	93.67	92.00
7	B	403	LAR	O2-C1-C2	5.17	123.10	111.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	EDO	1	0
7	B	403	LAR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	407	EDO	2	0

## 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	414/418 (99%)	0.15	22 (5%) 26 25	27, 43, 80, 97	0
2	B	358/375 (95%)	0.14	24 (6%) 18 17	19, 28, 73, 126	0
All	All	772/793 (97%)	0.14	46 (5%) 22 20	19, 36, 80, 126	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	60	SER	12.0
2	B	63	GLY	9.7
2	B	56	ASP	7.0
2	B	52	SER	7.0
2	B	53	TYR	6.7
2	B	374	CYS	6.0
2	B	51	ASP	5.6
2	B	59	GLN	5.5
2	B	61	LYS	5.3
2	B	57	GLU	5.1
2	B	54	VAL	4.6
2	B	62	ARG	4.3
1	A	237	PRO	4.0
2	B	66	THR	4.0
2	B	64	ILE	3.8
1	A	269	PRO	3.7
1	A	372	ILE	3.6
1	A	262	GLY	3.6
1	A	376	ALA	3.5
1	A	264	LEU	3.5
1	A	233	ASN	3.4
1	A	270	GLU	3.3
2	B	55	GLY	3.3
2	B	372	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	265	ASN	3.2
2	B	37	ARG	3.1
1	A	173	ASN	3.1
1	A	238	ASN	2.9
1	A	225	LYS	2.8
2	B	178	LEU	2.7
1	A	146	ASN	2.7
1	A	268	ASN	2.7
1	A	117	GLU	2.7
1	A	271	LEU	2.7
1	A	266	ASN	2.6
1	A	413	ASN	2.6
1	A	110	ASN	2.5
2	B	234	SER	2.5
2	B	58	ALA	2.4
2	B	50	LYS	2.4
1	A	222	LEU	2.4
1	A	374	GLY	2.2
2	B	65	LEU	2.2
2	B	373	LYS	2.2
2	B	67	LEU	2.1
1	A	375	TYR	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	508	4/4	0.82	0.23	43,43,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	407	4/4	0.83	0.24	32,33,33,33	0
4	EDO	B	411	4/4	0.84	0.17	38,38,38,38	0
4	EDO	A	509	4/4	0.85	0.21	40,41,41,41	0
4	EDO	A	503	4/4	0.85	0.34	33,34,34,34	0
4	EDO	B	410	4/4	0.88	0.14	41,41,41,42	0
5	AR6	B	401	35/36	0.89	0.14	52,62,77,77	0
4	EDO	B	406	4/4	0.91	0.15	45,45,45,45	0
7	LAR	B	403	29/29	0.91	0.14	29,32,38,39	0
4	EDO	B	413	4/4	0.91	0.19	41,42,43,43	0
4	EDO	A	502	4/4	0.92	0.16	41,42,42,42	0
4	EDO	A	507	4/4	0.92	0.15	44,44,44,44	0
4	EDO	A	510	4/4	0.93	0.17	43,43,43,43	0
4	EDO	B	405	4/4	0.93	0.15	42,43,43,43	0
4	EDO	B	412	4/4	0.94	0.11	34,34,34,35	0
4	EDO	B	408	4/4	0.94	0.17	43,44,44,44	0
4	EDO	A	505	4/4	0.94	0.12	30,30,30,30	0
4	EDO	B	409	4/4	0.95	0.16	43,44,44,44	0
4	EDO	A	506	4/4	0.95	0.15	46,47,47,47	0
4	EDO	A	504	4/4	0.97	0.17	32,32,32,32	0
3	PO4	A	501	5/5	0.97	0.19	56,56,56,56	0
8	ATP	B	404	31/31	0.98	0.11	20,20,20,20	0
6	CA	B	402	1/1	0.99	0.07	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.