



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:14 PM GMT

PDB ID : 1JED  
Title : Crystal Structure of ATP Sulfurylase in complex with ADP  
Authors : Ullrich, T.C.; Huber, R.  
Deposited on : 2001-06-17  
Resolution : 2.95 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.

---

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

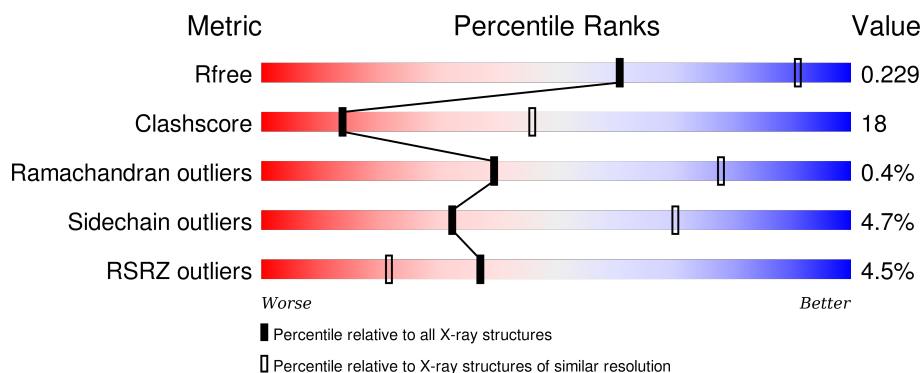
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	510	<div> <div>5%</div> <div>65%</div> <div>32%</div> <div>.</div> </div>
1	B	510	<div> <div>5%</div> <div>68%</div> <div>30%</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
2	CD	B	533	-	-	X	-
5	MG	A	521	-	-	-	X
7	TRS	A	1415	-	X	-	-
7	TRS	B	1416	-	X	-	-
8	ACY	A	551	-	-	-	X
8	ACY	A	557	-	-	-	X
8	ACY	B	558	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8877 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 SULFATE ADENYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	21	0	0
			4075	2598	706	766	5			
1	B	510	Total	C	N	O	S	8	0	0
			4075	2598	706	766	5			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Cd	0	0
			5	5		
2	A	6	Total	Cd	0	0
			6	6		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

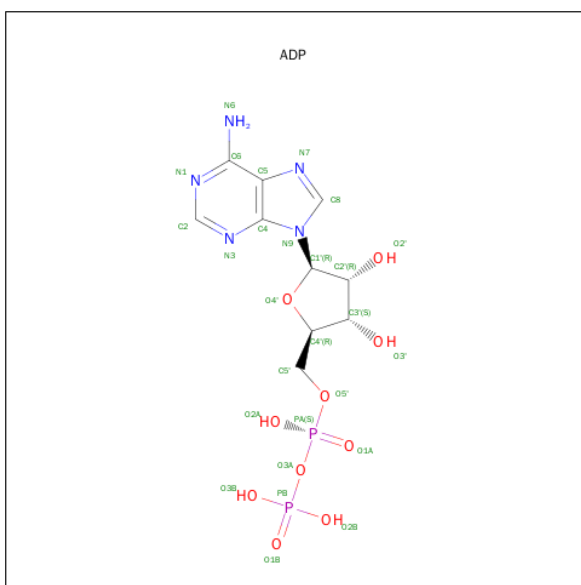
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	Na	0	0
			6	6		
4	A	6	Total	Na	0	0
			6	6		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

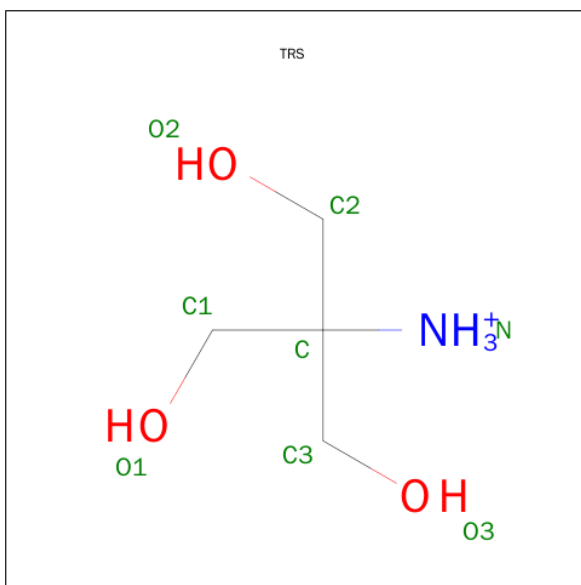
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mg 2 2	0	0
5	A	2	Total Mg 2 2	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



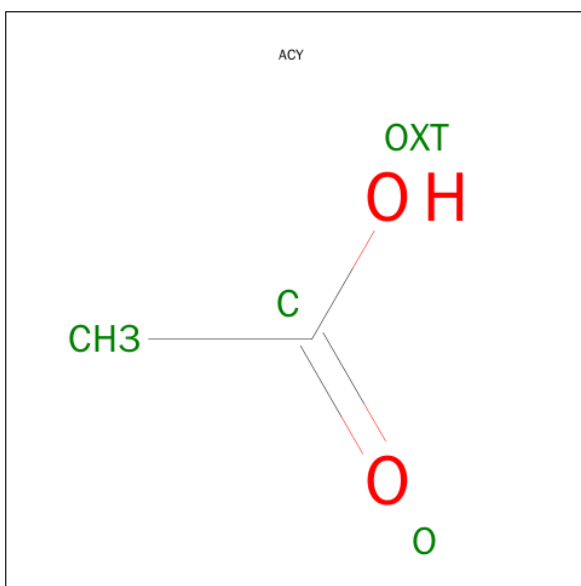
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
6	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

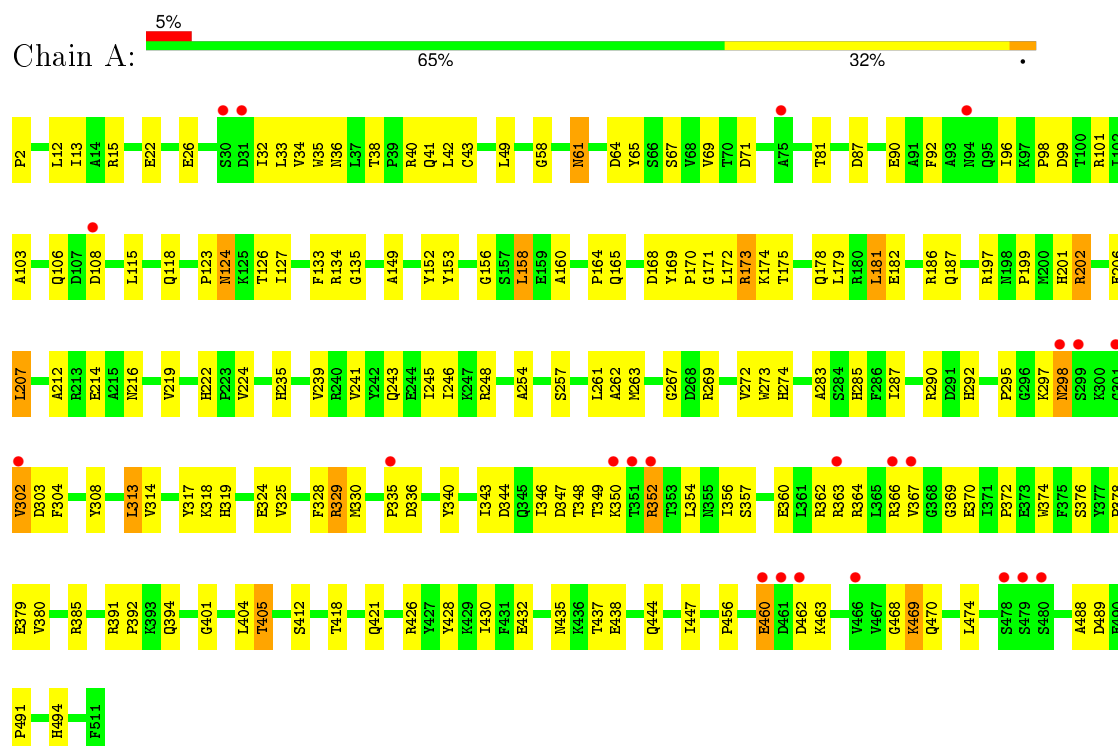
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	278	Total O 278 278	0	0
9	B	286	Total O 286 286	0	0

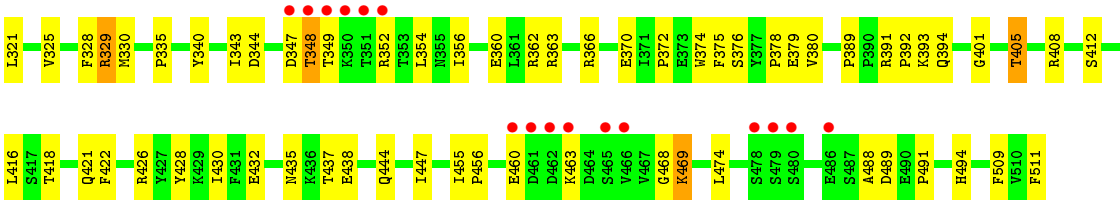
### 3 Residue-property plots

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







## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.13Å 186.13Å 223.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.81 – 2.95 24.81 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.81-2.95) 99.9 (24.81-2.95)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 2.94Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.192 , 0.227 0.192 , 0.229	Depositor DCC
$R_{free}$ test set	1616 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 78.6	EDS
Estimated twinning fraction	0.024 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.010 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.000 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31381 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8877	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, NA, CA, CD, ACY, TRS

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	0.41	0/4171	0.67	3/5667 (0.1%)
1	B	0.42	0/4171	0.68	3/5667 (0.1%)
All	All	0.42	0/8342	0.68	6/11334 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	A	352	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	352	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	B	352	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	B	135	GLY	N-CA-C	5.51	126.88	113.10
1	A	135	GLY	N-CA-C	5.47	126.79	113.10

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	4075	0	4035	157	2
1	B	4075	0	4035	146	1
2	A	6	0	0	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	4
3	A	3	0	0	0	1
3	B	3	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	27	0	12	1	0
6	B	27	0	12	0	0
7	A	8	0	10	0	0
7	B	8	0	7	2	0
8	A	32	0	24	0	0
8	B	28	0	21	0	0
9	A	278	0	0	10	0
9	B	286	0	0	6	0
All	All	8877	0	8156	303	5

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 18.

All (303) 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:435:ASN:HD21	1:B:460:GLU:HB2	1.34	0.92
1:A:435:ASN:HD21	1:A:460:GLU:HB2	1.33	0.91
1:B:469:LYS:H	1:B:469:LYS:HD3	1.36	0.90
1:A:364:ARG:HG2	9:A:663:HOH:O	1.72	0.89
1:B:329:ARG:HH21	1:B:329:ARG:CA	1.88	0.86
1:A:329:ARG:HH21	1:A:329:ARG:CA	1.89	0.84
1:B:469:LYS:N	1:B:469:LYS:HD3	1.90	0.83
1:A:35:TRP:HE1	1:A:41:GLN:HE22	1.27	0.83
1:A:169:TYR:N	1:A:170:PRO:HD3	1.94	0.82
1:A:469:LYS:HD3	1:A:469:LYS:N	1.95	0.82
1:B:61:ASN:ND2	1:B:64:ASP:H	1.79	0.81
1:A:469:LYS:HD3	1:A:469:LYS:H	1.47	0.80
1:A:437:THR:HG22	1:A:463:LYS:HD2	1.63	0.78
1:B:35:TRP:HE1	1:B:41:GLN:HE22	1.29	0.78
1:A:61:ASN:ND2	1:A:64:ASP:H	1.81	0.78
1:B:437:THR:HG22	1:B:463:LYS:HD2	1.65	0.77
1:A:366:ARG:HH21	1:A:366:ARG:HG2	1.51	0.76
1:A:314:VAL:CG1	1:A:325:VAL:HG21	2.16	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HH21	1:A:329:ARG:CB	1.99	0.75
1:A:42:LEU:HD11	1:A:106:GLN:HG3	1.66	0.75
1:B:169:TYR:N	1:B:170:PRO:HD3	2.01	0.75
1:B:314:VAL:CG1	1:B:325:VAL:HG21	2.17	0.74
1:B:366:ARG:HH21	1:B:366:ARG:HG2	1.52	0.74
1:A:61:ASN:C	1:A:61:ASN:HD22	1.91	0.73
1:A:98:PRO:O	1:A:99:ASP:HB2	1.89	0.72
1:B:329:ARG:HH21	1:B:329:ARG:CB	2.02	0.72
1:A:124:ASN:HD21	1:A:126:THR:HB	1.53	0.71
1:A:362:ARG:HG2	1:A:363:ARG:N	2.06	0.71
1:A:298:ASN:C	1:A:298:ASN:HD22	1.94	0.70
1:B:61:ASN:HD21	1:B:64:ASP:H	1.37	0.70
1:B:42:LEU:HD11	1:B:106:GLN:HG3	1.72	0.70
1:B:98:PRO:O	1:B:99:ASP:HB2	1.90	0.70
1:B:106:GLN:HE22	1:B:165:GLN:H	1.39	0.70
1:B:469:LYS:CD	1:B:469:LYS:H	2.05	0.70
1:A:61:ASN:HD21	1:A:64:ASP:H	1.37	0.70
1:B:61:ASN:HD22	1:B:61:ASN:C	1.94	0.69
1:A:444:GLN:NE2	1:A:447:ILE:HD12	2.06	0.69
1:A:274:HIS:ND1	1:A:292:HIS:HE1	1.90	0.69
1:A:175:THR:H	1:A:178:GLN:NE2	1.91	0.69
1:A:175:THR:H	1:A:178:GLN:HE21	1.40	0.68
1:A:366:ARG:HG3	1:A:394:GLN:HE22	1.59	0.67
1:A:106:GLN:HE22	1:A:165:GLN:H	1.42	0.67
1:B:175:THR:H	1:B:178:GLN:HE21	1.40	0.67
1:B:329:ARG:HG2	1:B:344:ASP:HB3	1.75	0.67
1:B:362:ARG:HG2	1:B:363:ARG:N	2.09	0.66
1:B:175:THR:H	1:B:178:GLN:NE2	1.93	0.66
1:A:460:GLU:HG2	9:A:651:HOH:O	1.95	0.66
1:A:58:GLY:HA2	1:A:158:LEU:HD22	1.77	0.66
1:B:295:PRO:HG2	1:B:304:PHE:CD1	2.31	0.66
1:B:298:ASN:C	1:B:298:ASN:HD22	2.00	0.66
1:A:405:THR:HG22	1:A:489:ASP:HA	1.78	0.65
1:B:274:HIS:ND1	1:B:292:HIS:HE1	1.94	0.65
1:A:329:ARG:HG2	1:A:344:ASP:HB3	1.78	0.65
1:A:314:VAL:HG11	1:A:325:VAL:HG21	1.78	0.65
1:B:444:GLN:NE2	1:B:447:ILE:HD12	2.12	0.65
1:A:469:LYS:CD	1:A:469:LYS:H	2.09	0.65
1:A:49:LEU:HD22	1:A:160:ALA:HB2	1.77	0.65
1:B:314:VAL:HG11	1:B:325:VAL:HG21	1.78	0.64
1:B:347:ASP:C	1:B:349:THR:H	2.02	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ASN:HD21	1:B:302:VAL:HG13	1.63	0.63
1:B:366:ARG:HG3	1:B:394:GLN:HE22	1.61	0.63
1:A:357:SER:HB2	9:A:1097:HOH:O	1.98	0.63
1:A:295:PRO:HG2	1:A:304:PHE:CD1	2.33	0.63
1:A:435:ASN:ND2	1:A:460:GLU:HB2	2.12	0.62
1:B:49:LEU:HD22	1:B:160:ALA:HB2	1.81	0.62
1:B:12:LEU:HD22	1:B:15:ARG:CZ	2.30	0.61
1:A:243:GLN:O	1:A:246:ILE:HG22	1.99	0.61
1:B:298:ASN:ND2	1:B:302:VAL:HG13	2.15	0.61
1:B:318:LYS:HE3	1:B:319:HIS:CE1	2.35	0.61
1:B:67:SER:O	1:B:71:ASP:HB2	2.01	0.61
1:A:67:SER:O	1:A:71:ASP:HB2	2.00	0.61
1:A:343:ILE:HD12	1:A:346:ILE:HD11	1.83	0.60
1:B:243:GLN:O	1:B:246:ILE:HG22	2.01	0.60
1:B:115:LEU:HD23	1:B:158:LEU:HD13	1.82	0.60
1:A:298:ASN:HD21	1:A:302:VAL:HG13	1.66	0.60
1:B:248:ARG:CZ	9:B:1109:HOH:O	2.50	0.60
1:A:298:ASN:ND2	1:A:302:VAL:HG13	2.17	0.60
1:A:347:ASP:C	1:A:349:THR:H	2.05	0.60
1:A:372:PRO:HB3	1:A:374:TRP:NE1	2.17	0.60
1:A:329:ARG:HB2	1:A:329:ARG:NH2	2.16	0.59
1:B:239:VAL:O	1:B:243:GLN:HG3	2.02	0.59
1:B:124:ASN:HD21	1:B:126:THR:HB	1.65	0.59
1:A:378:PRO:HG2	1:A:379:GLU:OE1	2.03	0.59
1:A:115:LEU:HD23	1:A:158:LEU:HD13	1.85	0.58
1:A:169:TYR:N	1:A:170:PRO:CD	2.66	0.58
1:A:239:VAL:O	1:A:243:GLN:HG3	2.04	0.58
1:A:347:ASP:OD1	1:A:350:LYS:HG2	2.03	0.58
1:B:491:PRO:HG2	1:B:494:HIS:CG	2.38	0.58
1:B:118:GLN:HG3	1:B:156:GLY:HA2	1.86	0.57
1:B:58:GLY:HA2	1:B:158:LEU:HD22	1.86	0.57
1:B:329:ARG:HH21	1:B:329:ARG:N	2.03	0.57
1:A:329:ARG:HH21	1:A:329:ARG:HB2	1.64	0.57
1:A:118:GLN:HG3	1:A:156:GLY:HA2	1.86	0.56
1:B:372:PRO:HB3	1:B:374:TRP:NE1	2.20	0.56
1:B:235:HIS:HD1	7:B:1416:TRS:C1	2.18	0.56
1:B:298:ASN:HD21	1:B:302:VAL:H	1.52	0.56
1:A:356:ILE:HG23	1:A:360:GLU:HG3	1.88	0.56
1:B:405:THR:HG22	1:B:489:ASP:HA	1.87	0.55
1:A:272:VAL:HG21	1:A:313:LEU:HD13	1.88	0.55
1:A:329:ARG:N	1:A:329:ARG:HH21	2.05	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLU:OE2	1:A:22:GLU:N	2.39	0.55
1:B:272:VAL:HG21	1:B:313:LEU:HD13	1.88	0.54
1:A:173:ARG:HB2	9:A:726:HOH:O	2.07	0.54
1:A:207:LEU:HD12	1:A:207:LEU:C	2.27	0.54
1:B:432:GLU:HG2	1:B:456:PRO:HG3	1.89	0.54
1:A:329:ARG:CB	1:A:329:ARG:NH2	2.71	0.54
1:B:38:THR:H	1:B:41:GLN:NE2	2.05	0.54
1:A:469:LYS:CD	1:A:469:LYS:N	2.68	0.54
1:B:216:ASN:ND2	9:B:656:HOH:O	2.40	0.54
1:A:329:ARG:HG3	1:A:343:ILE:CG2	2.38	0.53
1:A:491:PRO:HG2	1:A:494:HIS:CG	2.44	0.53
1:A:224:VAL:HG11	1:A:263:MET:HG3	1.89	0.53
1:A:12:LEU:HD22	1:A:15:ARG:CZ	2.38	0.53
1:A:418:THR:O	1:A:421:GLN:HG3	2.08	0.53
1:A:43:CYS:CB	1:A:262:ALA:HB2	2.39	0.53
1:B:272:VAL:CG2	1:B:313:LEU:HD13	2.38	0.52
1:B:329:ARG:HB2	1:B:329:ARG:NH2	2.24	0.52
1:B:491:PRO:HG2	1:B:494:HIS:CD2	2.45	0.52
1:B:169:TYR:N	1:B:170:PRO:CD	2.72	0.52
1:B:378:PRO:HG2	1:B:379:GLU:OE1	2.09	0.52
1:A:372:PRO:HB3	1:A:374:TRP:CD1	2.45	0.52
1:B:207:LEU:HD12	1:B:207:LEU:C	2.30	0.52
1:B:343:ILE:HD11	1:B:348:THR:HG22	1.92	0.52
1:A:470:GLN:NE2	9:A:745:HOH:O	2.42	0.52
1:B:435:ASN:ND2	1:B:460:GLU:HB2	2.14	0.52
1:A:318:LYS:HE3	1:A:319:HIS:CE1	2.45	0.52
1:B:329:ARG:HG3	1:B:343:ILE:CG2	2.40	0.51
1:A:308:TYR:CE2	1:A:329:ARG:HD3	2.46	0.51
1:B:343:ILE:HD11	1:B:348:THR:CG2	2.40	0.51
1:B:22:GLU:N	1:B:22:GLU:OE2	2.40	0.50
1:A:298:ASN:HD21	1:A:302:VAL:H	1.57	0.50
1:B:298:ASN:C	1:B:298:ASN:ND2	2.64	0.50
1:A:92:PHE:CE2	1:A:96:ILE:HD11	2.47	0.50
1:B:224:VAL:HG11	1:B:263:MET:HG3	1.94	0.50
1:B:43:CYS:CB	1:B:262:ALA:HB2	2.42	0.50
1:B:422:PHE:HB2	9:B:676:HOH:O	2.12	0.50
1:A:437:THR:CG2	1:A:463:LYS:HD2	2.39	0.50
1:A:298:ASN:C	1:A:298:ASN:ND2	2.61	0.50
1:B:298:ASN:HD21	1:B:302:VAL:CG1	2.25	0.50
1:B:298:ASN:ND2	1:B:302:VAL:H	2.10	0.50
1:B:172:LEU:N	1:B:172:LEU:HD23	2.27	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLN:NE2	1:A:468:GLY:O	2.45	0.49
1:A:272:VAL:CG2	1:A:313:LEU:HD13	2.41	0.49
1:B:261:LEU:HG	1:B:262:ALA:N	2.28	0.49
1:B:188:TRP:CE2	1:B:218:LYS:HG3	2.48	0.49
1:B:329:ARG:HH21	1:B:329:ARG:HB2	1.72	0.49
1:A:261:LEU:HG	1:A:262:ALA:N	2.27	0.49
1:B:36:ASN:OD1	1:B:108:ASP:N	2.41	0.49
1:A:426:ARG:HD2	1:A:428:TYR:CZ	2.48	0.49
1:A:124:ASN:ND2	1:A:126:THR:HB	2.26	0.49
1:B:35:TRP:HE1	1:B:41:GLN:NE2	2.05	0.49
1:B:347:ASP:C	1:B:349:THR:N	2.65	0.49
1:B:356:ILE:HG23	1:B:360:GLU:HG3	1.95	0.49
1:B:207:LEU:HD13	1:B:328:PHE:CD2	2.48	0.49
1:A:261:LEU:HD11	1:A:273:TRP:CH2	2.47	0.48
1:A:329:ARG:HA	1:A:329:ARG:HD3	1.65	0.48
1:A:335:PRO:HG3	1:A:354:LEU:HD12	1.95	0.48
1:A:356:ILE:HG23	1:A:360:GLU:CG	2.42	0.48
1:B:379:GLU:H	1:B:379:GLU:CD	2.16	0.48
1:A:329:ARG:HG3	1:A:343:ILE:HG22	1.96	0.48
1:A:61:ASN:ND2	1:A:61:ASN:C	2.64	0.48
1:A:186:ARG:O	1:A:187:GLN:HB2	2.13	0.48
1:A:172:LEU:HD23	1:A:172:LEU:N	2.29	0.48
1:A:38:THR:H	1:A:41:GLN:NE2	2.11	0.48
1:A:362:ARG:CG	1:A:363:ARG:N	2.77	0.47
1:B:444:GLN:HG3	1:B:468:GLY:HA3	1.96	0.47
1:A:347:ASP:C	1:A:349:THR:N	2.67	0.47
1:A:33:LEU:HG	1:A:92:PHE:CE1	2.49	0.47
1:B:61:ASN:ND2	1:B:61:ASN:C	2.67	0.47
1:B:372:PRO:HB3	1:B:374:TRP:CD1	2.49	0.47
1:A:366:ARG:CG	1:A:366:ARG:NH2	2.77	0.47
1:A:356:ILE:HD11	1:A:372:PRO:HG2	1.97	0.47
1:B:313:LEU:HD22	1:B:317:TYR:CE1	2.49	0.47
1:B:412:SER:HB3	1:B:430:ILE:HD12	1.97	0.47
1:A:241:VAL:HG13	1:A:380:VAL:HG13	1.97	0.47
1:B:87:ASP:OD1	1:B:149:ALA:HA	2.14	0.47
1:B:426:ARG:HD2	1:B:428:TYR:CZ	2.49	0.47
1:A:42:LEU:CD1	1:A:106:GLN:HG3	2.38	0.47
1:A:298:ASN:HD21	1:A:302:VAL:CG1	2.27	0.47
1:A:379:GLU:H	1:A:379:GLU:CD	2.18	0.47
1:B:356:ILE:HG23	1:B:360:GLU:CG	2.44	0.47
1:A:366:ARG:HG2	1:A:366:ARG:NH2	2.26	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:SER:HB3	1:A:430:ILE:HD12	1.97	0.47
1:B:38:THR:H	1:B:41:GLN:HE21	1.63	0.47
1:B:261:LEU:HD11	1:B:273:TRP:CH2	2.50	0.46
1:A:216:ASN:ND2	9:A:894:HOH:O	2.48	0.46
1:B:366:ARG:CG	1:B:366:ARG:HH21	2.21	0.46
1:B:106:GLN:HE21	1:B:112:ILE:HD11	1.80	0.46
1:B:418:THR:O	1:B:421:GLN:HG3	2.14	0.46
1:A:405:THR:HB	1:A:488:ALA:HB1	1.97	0.46
1:A:40:ARG:HG3	1:A:262:ALA:HB1	1.98	0.46
1:B:201:HIS:ND1	1:B:376:SER:HB2	2.30	0.46
1:A:124:ASN:HD22	1:A:124:ASN:C	2.19	0.46
1:B:212:ALA:HB2	1:B:219:VAL:CG2	2.46	0.46
1:B:437:THR:CG2	1:B:463:LYS:HD2	2.42	0.46
1:B:444:GLN:NE2	1:B:468:GLY:O	2.49	0.46
1:A:347:ASP:O	1:A:349:THR:N	2.49	0.46
1:A:432:GLU:HG2	1:A:456:PRO:HG3	1.96	0.46
1:B:405:THR:HB	1:B:488:ALA:HB1	1.98	0.46
1:A:391:ARG:N	1:A:392:PRO:HD2	2.31	0.46
1:A:34:VAL:HG22	1:A:103:ALA:HB3	1.98	0.46
1:A:366:ARG:HH21	1:A:366:ARG:CG	2.19	0.45
1:B:227:LEU:HA	7:B:1416:TRS:H31	1.98	0.45
1:B:347:ASP:O	1:B:349:THR:N	2.50	0.45
1:A:36:ASN:OD1	1:A:108:ASP:N	2.37	0.45
1:B:32:ILE:HD13	1:B:103:ALA:HB2	1.99	0.45
1:A:222:HIS:HD2	1:A:257:SER:O	2.00	0.45
1:B:308:TYR:CE2	1:B:329:ARG:HD3	2.52	0.45
1:B:366:ARG:NH2	1:B:366:ARG:HG2	2.26	0.45
1:A:313:LEU:HD22	1:A:317:TYR:CE1	2.52	0.45
1:B:241:VAL:HG13	1:B:380:VAL:HG13	1.99	0.45
1:A:26:GLU:OE1	1:A:101:ARG:NE	2.43	0.45
1:B:329:ARG:CB	1:B:329:ARG:NH2	2.74	0.45
1:B:329:ARG:HG3	1:B:343:ILE:HG22	1.99	0.44
1:A:298:ASN:ND2	1:A:302:VAL:H	2.15	0.44
1:A:444:GLN:HG3	1:A:468:GLY:HA3	1.98	0.44
1:A:81:THR:HB	1:A:269:ARG:HD3	1.98	0.44
1:B:290:ARG:HD2	1:B:330:MET:HB2	1.99	0.44
1:A:298:ASN:OD1	1:A:302:VAL:HG13	2.17	0.44
1:A:207:LEU:HD13	1:A:328:PHE:CD2	2.51	0.44
1:B:33:LEU:HG	1:B:92:PHE:CE1	2.51	0.44
1:A:171:GLY:O	1:A:174:LYS:HE2	2.18	0.44
1:B:42:LEU:CD1	1:B:106:GLN:HG3	2.43	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HD13	1:A:103:ALA:HB2	1.99	0.44
1:A:87:ASP:OD1	1:A:149:ALA:HA	2.16	0.44
1:A:2:PRO:HD2	1:A:283:ALA:O	2.17	0.44
1:B:223:PRO:HD2	1:B:257:SER:O	2.17	0.44
1:B:81:THR:HB	1:B:269:ARG:HD3	1.99	0.44
1:A:343:ILE:CD1	1:A:346:ILE:HD11	2.48	0.44
1:B:60:LEU:HA	9:B:796:HOH:O	2.17	0.44
1:B:202:ARG:HB3	1:B:340:TYR:CE1	2.52	0.44
1:A:133:PHE:O	1:A:134:ARG:HB2	2.17	0.44
1:B:298:ASN:OD1	1:B:302:VAL:HG13	2.18	0.44
1:A:367:VAL:HG23	1:A:369:GLY:H	1.83	0.43
1:B:362:ARG:CG	1:B:363:ARG:N	2.80	0.43
1:A:35:TRP:HE1	1:A:41:GLN:NE2	2.05	0.43
1:B:455:ILE:HA	1:B:456:PRO:HD2	1.68	0.43
1:A:124:ASN:ND2	1:A:127:ILE:H	2.16	0.43
1:A:297:LYS:HG2	1:A:303:ASP:OD2	2.19	0.43
1:A:42:LEU:HD22	1:A:164:PRO:HB3	2.00	0.43
1:A:292:HIS:CD2	6:A:635:ADP:O3'	2.72	0.43
1:A:199:PRO:HG2	9:A:655:HOH:O	2.19	0.43
1:B:310:ALA:O	1:B:314:VAL:HG23	2.18	0.43
1:B:202:ARG:HB2	1:B:375:PHE:O	2.19	0.43
1:B:42:LEU:HD22	1:B:164:PRO:HB3	1.99	0.42
1:A:367:VAL:HG23	1:A:369:GLY:N	2.34	0.42
1:B:92:PHE:CE2	1:B:96:ILE:HD11	2.54	0.42
1:B:171:GLY:O	1:B:174:LYS:HE2	2.19	0.42
1:A:201:HIS:ND1	1:A:376:SER:HB2	2.34	0.42
1:A:219:VAL:O	1:A:254:ALA:HA	2.19	0.42
1:B:509:PHE:HB3	1:B:511:PHE:CE1	2.54	0.42
1:B:174:LYS:HB2	1:B:257:SER:OG	2.19	0.42
1:B:186:ARG:O	1:B:187:GLN:HB2	2.19	0.42
1:A:401:GLY:O	1:A:404:LEU:HB2	2.19	0.42
1:B:401:GLY:O	1:B:408:ARG:NH1	2.42	0.42
1:B:329:ARG:HH21	1:B:329:ARG:HA	1.75	0.42
1:A:287:ILE:HB	9:A:777:HOH:O	2.20	0.42
1:A:65:TYR:O	1:A:69:VAL:HG23	2.20	0.42
1:A:13:ILE:HD13	1:A:160:ALA:HB1	2.01	0.42
1:A:207:LEU:HD12	1:A:207:LEU:O	2.20	0.42
1:A:418:THR:O	1:A:421:GLN:CG	2.68	0.42
1:A:123:PRO:HG3	1:A:153:TYR:CZ	2.55	0.42
1:A:290:ARG:NH2	9:A:712:HOH:O	2.52	0.42
1:B:354:LEU:HA	1:B:354:LEU:HD23	1.88	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:HIS:O	1:A:239:VAL:HG23	2.20	0.41
1:B:356:ILE:HD11	1:B:372:PRO:HG2	2.02	0.41
1:A:391:ARG:HD3	1:A:391:ARG:HA	1.85	0.41
1:A:385:ARG:HH21	1:A:385:ARG:HG2	1.85	0.41
1:B:393:LYS:NZ	9:B:1124:HOH:O	2.53	0.41
1:B:366:ARG:CG	1:B:366:ARG:NH2	2.79	0.41
1:A:426:ARG:HD2	1:A:428:TYR:CE2	2.55	0.41
1:B:335:PRO:HG3	1:B:354:LEU:HD12	2.02	0.41
1:A:363:ARG:CZ	9:A:663:HOH:O	2.67	0.41
1:A:168:ASP:C	1:A:170:PRO:HD3	2.41	0.41
1:B:46:GLU:HB2	1:B:164:PRO:HD2	2.00	0.41
1:A:336:ASP:OD1	1:A:352:ARG:NH2	2.52	0.41
1:B:266:SER:O	1:B:267:GLY:C	2.59	0.41
1:B:123:PRO:HG3	1:B:153:TYR:CZ	2.55	0.41
1:B:391:ARG:N	1:B:392:PRO:HD2	2.35	0.41
1:B:298:ASN:CG	1:B:302:VAL:HG13	2.41	0.41
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.92	0.41
1:A:90:GLU:HB2	1:A:152:TYR:CE1	2.55	0.41
1:A:202:ARG:HB3	1:A:340:TYR:CE1	2.56	0.41
1:A:298:ASN:CG	1:A:302:VAL:HG13	2.41	0.41
1:A:40:ARG:HG3	1:A:262:ALA:CB	2.50	0.41
1:B:248:ARG:NE	9:B:1109:HOH:O	2.54	0.41
1:B:219:VAL:O	1:B:254:ALA:HA	2.21	0.41
1:B:389:PRO:HB2	1:B:393:LYS:HB2	2.03	0.41
1:A:245:ILE:O	1:A:248:ARG:HG2	2.21	0.41
1:A:285:HIS:HA	1:A:324:GLU:O	2.20	0.41
1:B:235:HIS:O	1:B:239:VAL:HG23	2.21	0.41
1:B:416:LEU:HB2	1:B:430:ILE:HD11	2.02	0.41
1:A:491:PRO:HG2	1:A:494:HIS:CD2	2.56	0.40
1:B:221:ILE:HG22	1:B:223:PRO:HD3	2.04	0.40
1:A:212:ALA:HB2	1:A:219:VAL:CG2	2.51	0.40
1:B:2:PRO:HD2	1:B:283:ALA:O	2.22	0.40
1:B:329:ARG:HD3	1:B:329:ARG:HA	1.60	0.40
1:A:40:ARG:O	1:A:43:CYS:HB2	2.21	0.40
1:A:181:LEU:HA	1:A:181:LEU:HD23	1.86	0.40
1:B:90:GLU:HB2	1:B:152:TYR:CE1	2.57	0.40
1:B:329:ARG:N	1:B:329:ARG:NH2	2.69	0.40
1:A:290:ARG:HD2	1:A:330:MET:HB2	2.04	0.40
1:B:391:ARG:HD3	1:B:391:ARG:HA	1.87	0.40

All (5) 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)
2:A:515:CD:CD	2:B:533:CD:CD[2_765]	1.23	0.97
3:A:520:CA:CA	3:A:520:CA:CA[10_456]	1.69	0.51
1:A:319:HIS:NE2	2:B:532:CD:CD[10_556]	2.14	0.06
1:A:182:GLU:OE1	2:B:533:CD:CD[2_765]	2.17	0.03
1:B:494:HIS:NE2	2:B:534:CD:CD[3_675]	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	508/510 (100%)	481 (95%)	25 (5%)	2 (0%)	39	78
1	B	508/510 (100%)	483 (95%)	23 (4%)	2 (0%)	39	78
All	All	1016/1020 (100%)	964 (95%)	48 (5%)	4 (0%)	39	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	GLY
1	A	267	GLY
1	A	348	THR
1	B	348	THR

### 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	445/445 (100%)	423 (95%)	22 (5%)	31	68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	445/445 (100%)	425 (96%)	20 (4%)	34	72
All	All	890/890 (100%)	848 (95%)	42 (5%)	32	70

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	124	ASN
1	A	158	LEU
1	A	173	ARG
1	A	179	LEU
1	A	181	LEU
1	A	197	ARG
1	A	202	ARG
1	A	206	GLU
1	A	207	LEU
1	A	214	GLU
1	A	298	ASN
1	A	302	VAL
1	A	313	LEU
1	A	329	ARG
1	A	370	GLU
1	A	405	THR
1	A	438	GLU
1	A	460	GLU
1	A	462	ASP
1	A	469	LYS
1	A	474	LEU
1	B	61	ASN
1	B	124	ASN
1	B	158	LEU
1	B	173	ARG
1	B	179	LEU
1	B	181	LEU
1	B	197	ARG
1	B	202	ARG
1	B	206	GLU
1	B	207	LEU
1	B	214	GLU
1	B	298	ASN
1	B	302	VAL
1	B	313	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	329	ARG
1	B	370	GLU
1	B	405	THR
1	B	438	GLU
1	B	469	LYS
1	B	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	21	ASN
1	A	41	GLN
1	A	61	ASN
1	A	63	ASN
1	A	94	ASN
1	A	106	GLN
1	A	118	GLN
1	A	124	ASN
1	A	147	ASN
1	A	165	GLN
1	A	178	GLN
1	A	198	ASN
1	A	216	ASN
1	A	243	GLN
1	A	292	HIS
1	A	298	ASN
1	A	319	HIS
1	A	345	GLN
1	A	470	GLN
1	A	471	ASN
1	A	484	GLN
1	A	506	ASN
1	B	10	GLN
1	B	21	ASN
1	B	41	GLN
1	B	61	ASN
1	B	63	ASN
1	B	94	ASN
1	B	106	GLN
1	B	118	GLN
1	B	124	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	147	ASN
1	B	178	GLN
1	B	198	ASN
1	B	216	ASN
1	B	243	GLN
1	B	292	HIS
1	B	298	ASN
1	B	345	GLN
1	B	470	GLN
1	B	471	ASN
1	B	484	GLN
1	B	506	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 33 are monoatomic - leaving 19 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	$\# Z  > 2$
7	TRS	A	1415	-	7,7,7	5.24	7 (100%)	9,9,9	7.92	6 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ACY	A	551	2	1,3,3	4.72	1 (100%)	0,3,3	0.00	-
8	ACY	A	552	2	1,3,3	4.84	1 (100%)	0,3,3	0.00	-
8	ACY	A	553	-	1,3,3	6.17	1 (100%)	0,3,3	0.00	-
8	ACY	A	554	-	1,3,3	4.94	1 (100%)	0,3,3	0.00	-
8	ACY	A	555	2	1,3,3	4.56	1 (100%)	0,3,3	0.00	-
8	ACY	A	556	2	1,3,3	4.82	1 (100%)	0,3,3	0.00	-
8	ACY	A	557	2	1,3,3	3.67	1 (100%)	0,3,3	0.00	-
8	ACY	A	565	2	1,3,3	4.69	1 (100%)	0,3,3	0.00	-
6	ADP	A	635	-	22,29,29	1.33	3 (13%)	27,45,45	2.69	2 (7%)
7	TRS	B	1416	-	7,7,7	7.98	3 (42%)	9,9,9	5.91	7 (77%)
8	ACY	B	558	2	1,3,3	4.86	1 (100%)	0,3,3	0.00	-
8	ACY	B	559	2	1,3,3	5.00	1 (100%)	0,3,3	0.00	-
8	ACY	B	560	-	1,3,3	5.24	1 (100%)	0,3,3	0.00	-
8	ACY	B	561	-	1,3,3	5.62	1 (100%)	0,3,3	0.00	-
8	ACY	B	562	-	1,3,3	4.30	1 (100%)	0,3,3	0.00	-
8	ACY	B	563	2	1,3,3	5.08	1 (100%)	0,3,3	0.00	-
8	ACY	B	564	2	1,3,3	5.05	1 (100%)	0,3,3	0.00	-
6	ADP	B	636	-	22,29,29	1.37	3 (13%)	27,45,45	2.68	2 (7%)

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
7	TRS	A	1415	-	-	0/9/9/9	0/0/0/0
8	ACY	A	551	2	-	0/0/0/0	0/0/0/0
8	ACY	A	552	2	-	0/0/0/0	0/0/0/0
8	ACY	A	553	-	-	0/0/0/0	0/0/0/0
8	ACY	A	554	-	-	0/0/0/0	0/0/0/0
8	ACY	A	555	2	-	0/0/0/0	0/0/0/0
8	ACY	A	556	2	-	0/0/0/0	0/0/0/0
8	ACY	A	557	2	-	0/0/0/0	0/0/0/0
8	ACY	A	565	2	-	0/0/0/0	0/0/0/0
6	ADP	A	635	-	-	0/12/32/32	0/3/3/3
7	TRS	B	1416	-	-	0/9/9/9	0/0/0/0
8	ACY	B	558	2	-	0/0/0/0	0/0/0/0
8	ACY	B	559	2	-	0/0/0/0	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ACY	B	560	-	-	0/0/0/0	0/0/0/0
8	ACY	B	561	-	-	0/0/0/0	0/0/0/0
8	ACY	B	562	-	-	0/0/0/0	0/0/0/0
8	ACY	B	563	2	-	0/0/0/0	0/0/0/0
8	ACY	B	564	2	-	0/0/0/0	0/0/0/0
6	ADP	B	636	-	-	0/12/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1416	TRS	C-N	-16.01	1.26	1.50
7	B	1416	TRS	C1-C	-12.64	1.28	1.53
7	A	1415	TRS	C3-C	-7.20	1.39	1.53
7	A	1415	TRS	C1-C	-7.12	1.39	1.53
7	A	1415	TRS	C2-C	-5.15	1.43	1.53
7	A	1415	TRS	O3-C3	-4.71	1.26	1.42
7	A	1415	TRS	O1-C1	-3.16	1.31	1.42
6	A	635	ADP	C5-N7	-2.27	1.31	1.39
6	B	636	ADP	C5-N7	-2.23	1.31	1.39
7	A	1415	TRS	O2-C2	2.09	1.49	1.42
6	A	635	ADP	PB-O2B	2.19	1.62	1.54
6	B	636	ADP	PB-O2B	2.38	1.63	1.54
8	A	557	ACY	CH3-C	3.67	1.53	1.48
6	A	635	ADP	O4'-C1'	3.69	1.45	1.41
6	B	636	ADP	O4'-C1'	3.95	1.46	1.41
8	B	562	ACY	CH3-C	4.30	1.54	1.48
8	A	555	ACY	CH3-C	4.56	1.55	1.48
8	A	565	ACY	CH3-C	4.69	1.55	1.48
8	A	551	ACY	CH3-C	4.72	1.55	1.48
8	A	556	ACY	CH3-C	4.82	1.55	1.48
8	A	552	ACY	CH3-C	4.84	1.55	1.48
8	B	558	ACY	CH3-C	4.86	1.55	1.48
8	A	554	ACY	CH3-C	4.94	1.55	1.48
8	B	559	ACY	CH3-C	5.00	1.55	1.48
7	B	1416	TRS	C3-C	5.00	1.62	1.53
8	B	564	ACY	CH3-C	5.05	1.55	1.48
8	B	563	ACY	CH3-C	5.08	1.55	1.48
7	A	1415	TRS	C-N	5.15	1.58	1.50
8	B	560	ACY	CH3-C	5.24	1.56	1.48
8	B	561	ACY	CH3-C	5.62	1.56	1.48
8	A	553	ACY	CH3-C	6.17	1.57	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1415	TRS	C3-C-C2	-13.93	80.63	110.78
6	A	635	ADP	N3-C2-N1	-13.25	118.75	128.89
6	B	636	ADP	N3-C2-N1	-13.21	118.78	128.89
7	B	1416	TRS	C1-C-N	-10.04	89.81	108.09
7	B	1416	TRS	C3-C-N	-4.26	100.33	108.09
6	A	635	ADP	C4-C5-N7	-2.59	107.10	109.48
6	B	636	ADP	C4-C5-N7	-2.56	107.12	109.48
7	B	1416	TRS	C3-C-C2	2.81	116.87	110.78
7	A	1415	TRS	C3-C-N	2.87	113.31	108.09
7	A	1415	TRS	O1-C1-C	5.61	122.54	111.18
7	B	1416	TRS	O2-C2-C	5.94	123.21	111.18
7	B	1416	TRS	O1-C1-C	6.44	124.22	111.18
7	A	1415	TRS	O3-C3-C	6.84	125.03	111.18
7	B	1416	TRS	C3-C-C1	7.06	126.08	110.78
7	B	1416	TRS	O3-C3-C	7.47	126.30	111.18
7	A	1415	TRS	C3-C-C1	8.69	129.59	110.78
7	A	1415	TRS	O2-C2-C	14.20	139.92	111.18

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
6	A	635	ADP	1	0
7	B	1416	TRS	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	510/510 (100%)	-0.02	23 (4%)	37 21	14, 28, 50, 62	9 (1%)
1	B	510/510 (100%)	0.01	23 (4%)	37 21	14, 28, 49, 63	6 (1%)
All	All	1020/1020 (100%)	-0.01	46 (4%)	37 21	14, 28, 50, 63	15 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	SER	4.1
1	B	479	SER	4.0
1	B	348	THR	3.6
1	B	298	ASN	3.4
1	A	350	LYS	3.4
1	B	462	ASP	3.4
1	A	479	SER	3.3
1	B	480	SER	3.2
1	A	462	ASP	3.2
1	B	349	THR	3.1
1	A	31	ASP	3.1
1	A	367	VAL	3.1
1	A	460	GLU	3.1
1	B	302	VAL	2.9
1	B	465	SER	2.9
1	B	299	SER	2.8
1	A	480	SER	2.8
1	B	350	LYS	2.8
1	A	75	ALA	2.6
1	A	298	ASN	2.6
1	B	478	SER	2.5
1	A	301	GLY	2.5
1	A	478	SER	2.5
1	B	460	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	302	VAL	2.4
1	A	94	ASN	2.4
1	B	301	GLY	2.3
1	A	351	THR	2.3
1	A	352	ARG	2.3
1	B	461	ASP	2.3
1	B	351	THR	2.3
1	A	461	ASP	2.2
1	B	300	LYS	2.2
1	B	486	GLU	2.2
1	A	30	SER	2.2
1	B	466	VAL	2.2
1	B	352	ARG	2.2
1	A	108	ASP	2.1
1	B	297	LYS	2.1
1	A	363	ARG	2.1
1	A	366	ARG	2.1
1	B	347	ASP	2.1
1	B	31	ASP	2.0
1	B	463	LYS	2.0
1	A	466	VAL	2.0
1	A	335	PRO	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
8	ACY	A	557	4/4	0.98	0.25	5.07	17,19,20,21	0
5	MG	A	521	1/1	0.95	0.24	3.49	54,54,54,54	0
8	ACY	B	558	4/4	0.98	0.38	2.95	28,29,29,29	0
8	ACY	A	551	4/4	0.97	0.38	2.22	26,26,26,27	0
2	CD	B	531	1/1	0.81	0.26	1.97	92,92,92,92	1
8	ACY	B	560	4/4	0.93	0.34	1.45	44,45,46,47	0
8	ACY	B	561	4/4	0.91	0.20	1.13	23,26,26,28	0
8	ACY	A	553	4/4	0.89	0.24	0.36	27,31,31,31	0
8	ACY	B	564	4/4	0.99	0.17	0.31	18,19,20,21	0
7	TRS	A	1415	8/8	0.93	0.21	0.24	30,30,30,30	0
7	TRS	B	1416	8/8	0.94	0.19	0.13	30,30,30,30	0
8	ACY	A	554	4/4	0.96	0.15	-0.09	23,24,24,24	0
6	ADP	A	635	27/27	0.97	0.16	-0.30	24,31,34,35	0
6	ADP	B	636	27/27	0.97	0.16	-0.52	26,29,30,32	0
8	ACY	B	562	4/4	0.99	0.14	-0.61	20,21,21,22	0
8	ACY	A	555	4/4	0.98	0.13	-0.80	20,22,23,23	0
5	MG	B	547	1/1	0.97	0.14	-0.97	47,47,47,47	0
2	CD	A	513	1/1	0.96	0.11	-1.86	74,74,74,74	1
2	CD	A	514	1/1	1.00	0.03	-4.48	34,34,34,34	0
2	CD	A	515	1/1	1.00	0.05	-4.82	34,34,34,34	0
2	CD	B	532	1/1	0.99	0.04	-4.87	33,33,33,33	0
4	NA	B	541	1/1	0.92	0.08	-	27,27,27,27	0
2	CD	B	534	1/1	1.00	0.03	-	12,12,12,12	1
2	CD	B	530	1/1	0.99	0.04	-	30,30,30,30	0
4	NA	A	525	1/1	0.98	0.14	-	2,2,2,2	0
3	CA	B	535	1/1	0.98	0.06	-	30,30,30,30	0
4	NA	A	518	1/1	0.41	0.20	-	47,47,47,47	0
5	MG	A	539	1/1	0.74	0.34	-	34,34,34,34	0
4	NA	B	543	1/1	0.61	0.19	-	45,45,45,45	0
8	ACY	A	565	4/4	0.98	0.20	-	32,33,33,33	0
4	NA	B	545	1/1	0.83	0.17	-	23,23,23,23	0
2	CD	A	516	1/1	1.00	0.03	-	13,13,13,13	1
2	CD	A	512	1/1	0.99	0.04	-	29,29,29,29	0
8	ACY	A	556	4/4	0.99	0.22	-	24,25,25,26	0
3	CA	B	538	1/1	0.98	0.10	-	17,17,17,17	0
3	CA	A	519	1/1	0.89	0.17	-	83,83,83,83	0
8	ACY	A	552	4/4	0.99	0.11	-	17,18,18,19	0
4	NA	B	542	1/1	0.95	0.11	-	24,24,24,24	0
4	NA	A	526	1/1	0.92	0.17	-	34,34,34,34	0
4	NA	A	522	1/1	0.65	0.11	-	30,30,30,30	0
8	ACY	B	563	4/4	0.99	0.28	-	26,28,28,29	0
3	CA	A	520	1/1	0.97	0.05	-	29,29,29,29	0
3	CA	B	537	1/1	0.78	0.18	-	89,89,89,89	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	B	544	1/1	0.87	0.13	-	35,35,35,35	0
3	CA	A	517	1/1	0.90	0.06	-	31,31,31,31	0
4	NA	A	527	1/1	0.88	0.07	-	22,22,22,22	0
5	MG	B	546	1/1	0.91	0.43	-	28,28,28,28	0
4	NA	B	540	1/1	0.79	0.12	-	35,35,35,35	0
2	CD	A	524	1/1	0.99	0.04	-	43,43,43,43	0
4	NA	A	523	1/1	0.84	0.13	-	43,43,43,43	0
2	CD	B	533	1/1	1.00	0.06	-	45,45,45,45	1
8	ACY	B	559	4/4	0.99	0.15	-	17,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.