



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:37 pm GMT

PDB ID : 1JEE  
Title : Crystal Structure of ATP Sulfurylase in complex with chlorate  
Authors : Ullrich, T.C.; Huber, R.  
Deposited on : 2001-06-17  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

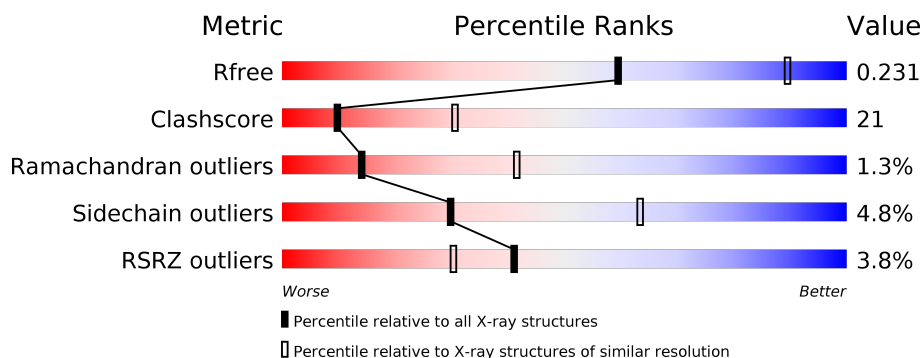
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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>4%</div> <div> <div></div> <div>64%</div> <div>32%</div> <div>.</div> </div> </div>
1	B	510	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>32%</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
10	ACY	A	556	-	-	-	X
10	ACY	B	561	-	-	-	X
10	ACY	B	563	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8941 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	2	0	0
			4075	2598	706	766	5			
1	B	510	Total	C	N	O	S	3	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		

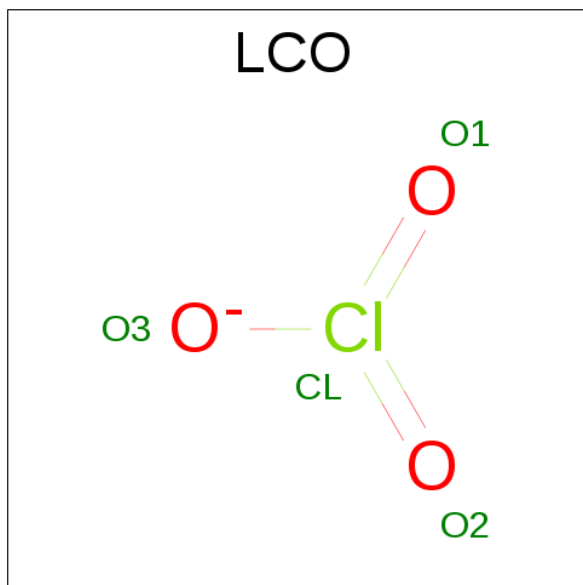
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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).

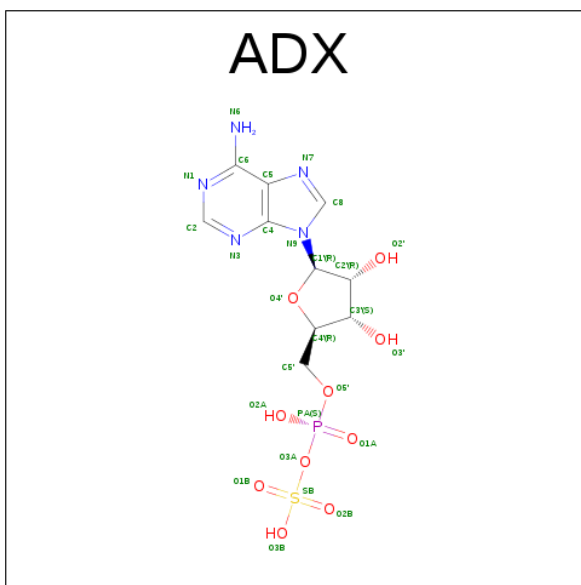
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORATE ION (three-letter code: LCO) (formula:  $\text{ClO}_3$ ).



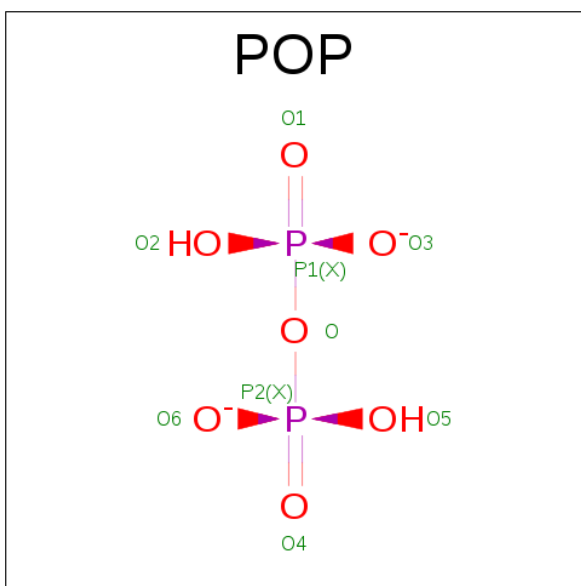
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Cl	O	0	0
			4	1	3		
6	B	1	Total	Cl	O	0	0
			4	1	3		

- Molecule 7 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula:  $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_{10}\text{PS}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
7	B	2	Total	C	N	O	P	S	0	0
			54	20	10	20	2	2		

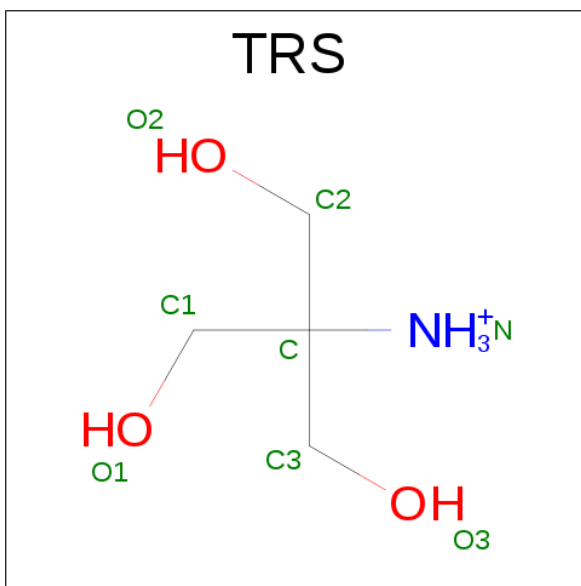
- Molecule 8 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 9	O 7	P 2	0	0
8	B	1	Total 9	O 7	P 2	0	0

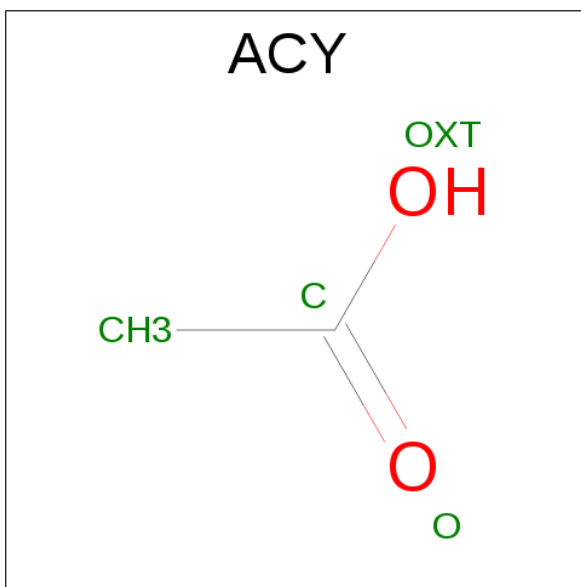
- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code:

TRS) (formula:  $C_4H_{12}NO_3$ ).



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

- Molecule 10 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



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

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

- Molecule 11 is water.

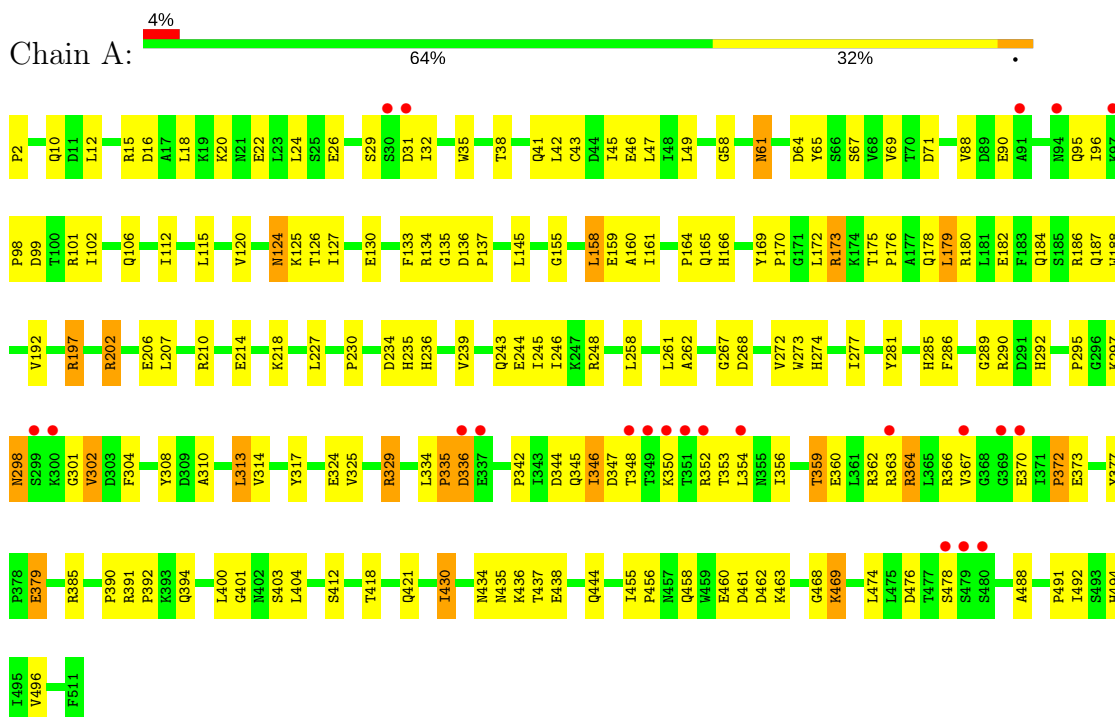
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	300	Total O 300 300	0	0
11	B	304	Total O 304 304	0	0



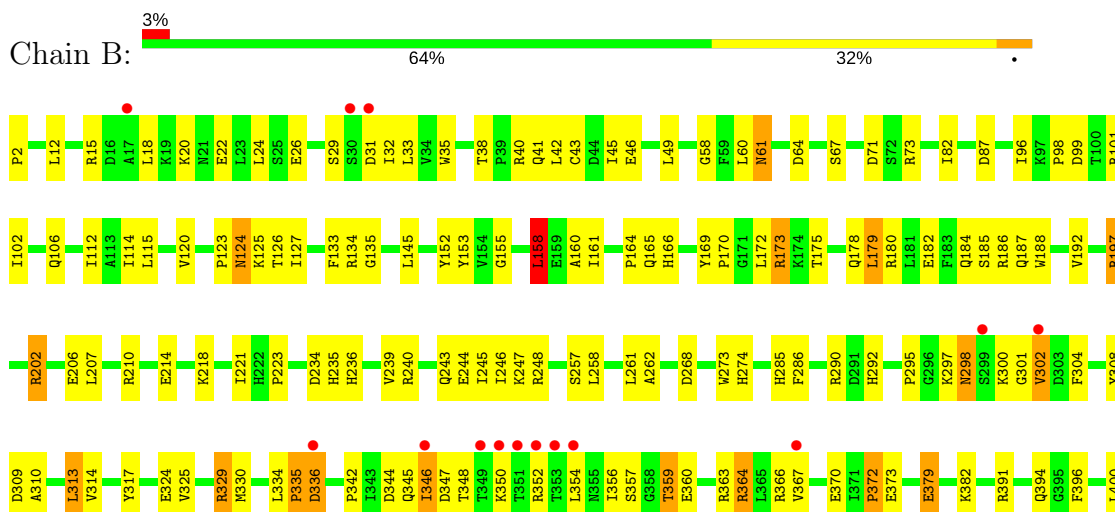
### 3 Residue-property plots

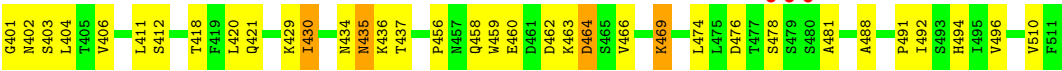
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: SULFATE ADENYLYLTRANSFERASE



#### • Molecule 1: SULFATE ADENYLYLTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.94Å 185.94Å 223.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.87 – 2.80 24.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.87-2.80) 95.4 (24.87-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.184 , 0.232 0.184 , 0.231	Depositor DCC
$R_{free}$ test set	1800 reflections (5.15%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 63.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 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 0.015 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.007 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8941	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.35% 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: MG, NA, CA, ADX, CD, POP, LCO, 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	0.51	0/4171	0.72	4/5667 (0.1%)
1	B	0.52	0/4171	0.72	5/5667 (0.1%)
All	All	0.52	0/8342	0.72	9/11334 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	B	135	GLY	N-CA-C	6.26	128.75	113.10
1	A	364	ARG	NE-CZ-NH1	-6.11	117.24	120.30
1	B	364	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	430	ILE	N-CA-C	-5.65	95.76	111.00
1	B	364	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	135	GLY	N-CA-C	5.37	126.52	113.10
1	A	430	ILE	N-CA-C	-5.36	96.52	111.00
1	B	158	LEU	CA-CB-CG	5.11	127.04	115.30

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	4075	0	4035	176	0
1	B	4075	0	4035	174	0
2	A	6	0	0	0	1
2	B	5	0	0	0	1
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
7	B	54	0	26	8	0
8	A	9	0	0	1	0
8	B	9	0	0	2	0
9	A	8	0	12	1	0
9	B	8	0	12	0	0
10	A	32	0	24	1	0
10	B	28	0	21	3	0
11	A	300	0	0	15	0
11	B	304	0	0	16	0
All	All	8941	0	8165	353	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 21.

All (353) 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:329:ARG:H	1:B:329:ARG:HD2	1.09	1.07
1:B:469:LYS:H	1:B:469:LYS:HD3	1.08	1.06
1:A:329:ARG:HD2	1:A:329:ARG:H	1.07	1.05
1:A:469:LYS:HD3	1:A:469:LYS:H	1.19	1.05
1:A:58:GLY:HA2	1:A:158:LEU:HD22	1.45	0.98
1:B:106:GLN:HE22	1:B:165:GLN:H	1.01	0.94
1:A:106:GLN:HE22	1:A:165:GLN:H	1.09	0.92
1:B:58:GLY:HA2	1:B:158:LEU:HD22	1.52	0.91
1:A:202:ARG:HH21	1:A:202:ARG:HG3	1.36	0.90
1:A:329:ARG:HD2	1:A:329:ARG:N	1.88	0.88
1:B:329:ARG:N	1:B:329:ARG:HD2	1.90	0.87
1:A:352:ARG:HH21	1:A:352:ARG:HB3	1.39	0.86
1:B:352:ARG:HB3	1:B:352:ARG:HH21	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:TRP:HE1	1:B:41:GLN:HE22	1.27	0.82
1:B:469:LYS:N	1:B:469:LYS:HD3	1.91	0.82
1:A:329:ARG:CD	1:A:329:ARG:H	1.91	0.81
1:A:61:ASN:ND2	1:A:64:ASP:H	1.79	0.80
1:B:202:ARG:HG3	1:B:202:ARG:HH21	1.44	0.80
1:B:329:ARG:CD	1:B:329:ARG:H	1.93	0.80
1:A:352:ARG:HB3	1:A:352:ARG:NH2	1.97	0.80
1:A:175:THR:H	1:A:178:GLN:HE21	1.30	0.80
1:B:412:SER:HB3	1:B:430:ILE:HD12	1.65	0.79
1:A:96:ILE:HG21	1:A:102:ILE:HD11	1.63	0.78
1:A:352:ARG:HA	11:A:649:HOH:O	1.82	0.78
1:A:364:ARG:HA	1:A:367:VAL:HG22	1.66	0.78
1:A:175:THR:H	1:A:178:GLN:NE2	1.81	0.77
1:B:61:ASN:ND2	1:B:64:ASP:H	1.82	0.77
1:B:366:ARG:HH21	1:B:366:ARG:HG2	1.49	0.77
1:B:175:THR:H	1:B:178:GLN:HE21	1.32	0.77
1:A:412:SER:HB3	1:A:430:ILE:HD12	1.67	0.77
1:A:469:LYS:HD3	1:A:469:LYS:N	1.98	0.76
1:B:61:ASN:HD22	1:B:61:ASN:C	1.90	0.75
1:A:366:ARG:HH21	1:A:366:ARG:HG2	1.52	0.74
1:A:35:TRP:HE1	1:A:41:GLN:HE22	1.31	0.74
1:B:290:ARG:HD2	11:B:1001:HOH:O	1.86	0.74
1:A:61:ASN:C	1:A:61:ASN:HD22	1.89	0.74
1:A:356:ILE:HD13	1:A:364:ARG:NH1	2.03	0.73
1:A:58:GLY:HA2	1:A:158:LEU:CD2	2.16	0.73
1:B:352:ARG:NH2	1:B:352:ARG:HB3	2.02	0.73
1:B:364:ARG:HA	1:B:367:VAL:HG22	1.70	0.73
1:A:352:ARG:HH21	1:A:352:ARG:CB	2.00	0.73
1:A:61:ASN:HD21	1:A:64:ASP:H	1.35	0.72
1:B:175:THR:H	1:B:178:GLN:NE2	1.87	0.72
1:B:96:ILE:HG21	1:B:102:ILE:HD11	1.71	0.71
1:A:295:PRO:HG2	1:A:304:PHE:CD1	2.26	0.70
1:A:335:PRO:HG3	1:A:354:LEU:HD12	1.74	0.70
1:A:314:VAL:CG1	1:A:325:VAL:HG21	2.22	0.70
1:B:210:ARG:O	1:B:214:GLU:HG2	1.90	0.70
1:B:352:ARG:CB	1:B:352:ARG:HH21	2.05	0.70
1:B:61:ASN:HD21	1:B:64:ASP:H	1.40	0.70
1:B:295:PRO:HG2	1:B:304:PHE:CD1	2.28	0.69
1:A:462:ASP:OD1	1:A:463:LYS:HG2	1.94	0.67
1:B:314:VAL:CG1	1:B:325:VAL:HG21	2.24	0.67
1:B:363:ARG:O	1:B:367:VAL:HG13	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:C	1:A:298:ASN:HD22	1.98	0.67
1:A:329:ARG:HG2	1:A:344:ASP:HB3	1.77	0.67
1:A:46:GLU:HB2	1:A:164:PRO:HD2	1.77	0.67
1:B:240:ARG:HD2	11:B:878:HOH:O	1.95	0.67
1:A:202:ARG:HG3	1:A:202:ARG:NH2	2.09	0.66
1:B:46:GLU:HB2	1:B:164:PRO:HD2	1.77	0.66
1:B:166:HIS:HD2	11:B:646:HOH:O	1.79	0.66
1:B:106:GLN:NE2	1:B:165:GLN:H	1.86	0.65
1:A:169:TYR:N	1:A:170:PRO:HD3	2.11	0.65
1:A:243:GLN:O	1:A:246:ILE:HG22	1.97	0.65
1:B:356:ILE:HD13	1:B:364:ARG:HH12	1.62	0.65
1:A:106:GLN:NE2	1:A:165:GLN:H	1.90	0.65
1:B:329:ARG:HG2	1:B:344:ASP:HB3	1.79	0.65
1:B:437:THR:HG22	1:B:463:LYS:HD2	1.79	0.65
1:A:210:ARG:O	1:A:214:GLU:HG2	1.97	0.64
1:B:335:PRO:HG3	1:B:354:LEU:HD12	1.80	0.64
1:A:274:HIS:ND1	1:A:292:HIS:HE1	1.96	0.63
1:A:227:LEU:HA	9:A:602:TRS:H21	1.80	0.63
1:A:363:ARG:O	1:A:367:VAL:HG13	1.99	0.63
1:B:348:THR:C	1:B:350:LYS:H	2.02	0.63
1:B:469:LYS:CD	1:B:469:LYS:H	1.92	0.63
1:B:58:GLY:HA2	1:B:158:LEU:CD2	2.27	0.63
1:A:329:ARG:HD3	1:A:342:PRO:HB3	1.81	0.62
1:A:437:THR:HG22	1:A:463:LYS:HD2	1.81	0.62
1:B:172:LEU:N	1:B:172:LEU:HD12	2.15	0.62
1:A:348:THR:C	1:A:350:LYS:H	2.03	0.62
1:A:20:LYS:HB3	10:A:550:ACY:H2	1.81	0.62
1:B:298:ASN:HD21	1:B:302:VAL:HG13	1.64	0.62
1:A:2:PRO:HD2	11:A:1105:HOH:O	2.00	0.61
1:B:274:HIS:ND1	1:B:292:HIS:HE1	1.99	0.61
1:B:20:LYS:HB3	10:B:557:ACY:H2	1.83	0.60
1:A:124:ASN:HD21	1:A:126:THR:HB	1.66	0.60
1:A:166:HIS:HD2	11:A:705:HOH:O	1.84	0.60
1:B:462:ASP:OD1	1:B:463:LYS:HG2	2.02	0.60
1:B:247:LYS:HE3	11:B:1031:HOH:O	2.01	0.60
1:B:335:PRO:HD2	1:B:352:ARG:O	2.01	0.59
1:B:169:TYR:N	1:B:170:PRO:HD3	2.18	0.59
1:B:188:TRP:CE2	1:B:218:LYS:HG3	2.37	0.59
1:B:366:ARG:HD3	11:B:1029:HOH:O	2.02	0.59
1:A:173:ARG:HG2	1:A:173:ARG:HH21	1.68	0.59
1:B:510:VAL:HA	11:B:841:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HD11	1:A:372:PRO:HG2	1.84	0.58
1:A:289:GLY:HA3	7:B:635:ADX:N3	2.19	0.58
1:A:172:LEU:HD12	1:A:172:LEU:N	2.19	0.57
1:B:2:PRO:HD2	11:B:658:HOH:O	2.03	0.57
1:B:418:THR:O	1:B:421:GLN:HG2	2.03	0.57
1:B:124:ASN:HD22	1:B:127:ILE:H	1.52	0.57
1:B:329:ARG:HD3	1:B:342:PRO:HB3	1.86	0.57
1:A:379:GLU:HB3	11:A:1045:HOH:O	2.04	0.57
1:B:46:GLU:OE2	1:B:166:HIS:HE1	1.87	0.57
1:A:234:ASP:OD2	1:A:236:HIS:HB2	2.05	0.57
1:A:362:ARG:NH1	11:A:1243:HOH:O	2.25	0.57
1:B:26:GLU:OE1	1:B:101:ARG:NE	2.30	0.57
1:A:173:ARG:NH2	1:A:173:ARG:HG2	2.20	0.56
1:A:61:ASN:HA	1:A:155:GLY:HA3	1.86	0.56
1:B:298:ASN:C	1:B:298:ASN:HD22	2.09	0.56
1:B:180:ARG:O	1:B:184:GLN:HG3	2.06	0.56
1:A:356:ILE:HD13	1:A:364:ARG:HH11	1.71	0.56
1:B:207:LEU:HD23	1:B:207:LEU:C	2.27	0.56
1:B:22:GLU:N	1:B:22:GLU:OE2	2.32	0.56
1:A:492:ILE:O	1:A:496:VAL:HG23	2.06	0.55
1:A:335:PRO:HD2	1:A:352:ARG:O	2.05	0.55
1:A:438:GLU:HG2	11:A:1100:HOH:O	2.05	0.55
1:B:49:LEU:HD22	1:B:160:ALA:HB2	1.88	0.55
1:B:261:LEU:HG	1:B:262:ALA:N	2.22	0.55
1:A:345:GLN:O	1:A:346:ILE:HG23	2.06	0.55
1:B:243:GLN:O	1:B:246:ILE:HG22	2.07	0.55
1:B:179:LEU:O	1:B:182:GLU:HB2	2.08	0.54
1:A:366:ARG:HH21	1:A:366:ARG:CG	2.18	0.54
1:A:244:GLU:HG3	1:A:379:GLU:OE2	2.07	0.54
1:A:347:ASP:CG	1:A:348:THR:H	2.09	0.54
1:B:106:GLN:HE21	1:B:112:ILE:HD11	1.71	0.54
1:A:178:GLN:O	1:A:182:GLU:HG2	2.07	0.54
1:B:435:ASN:HD21	1:B:460:GLU:H	1.55	0.54
1:A:418:THR:O	1:A:421:GLN:HG2	2.08	0.54
1:B:244:GLU:HG3	1:B:379:GLU:OE2	2.08	0.54
1:A:26:GLU:OE1	1:A:101:ARG:NE	2.27	0.53
1:A:67:SER:O	1:A:71:ASP:HB2	2.09	0.53
1:A:245:ILE:O	1:A:248:ARG:HG2	2.08	0.53
1:A:400:LEU:HG	1:A:456:PRO:HA	1.90	0.53
1:B:290:ARG:HG3	1:B:308:TYR:CZ	2.44	0.53
1:B:61:ASN:HA	1:B:155:GLY:HA3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD22	1:A:164:PRO:HB3	1.91	0.53
1:A:366:ARG:HG3	1:A:394:GLN:HE22	1.72	0.53
1:A:347:ASP:CG	1:A:348:THR:N	2.62	0.53
1:A:348:THR:HG21	1:A:350:LYS:HZ2	1.74	0.53
1:A:385:ARG:HA	11:A:760:HOH:O	2.08	0.53
1:B:98:PRO:O	1:B:99:ASP:HB2	2.08	0.53
1:A:336:ASP:CG	1:A:352:ARG:HH22	2.12	0.52
1:B:12:LEU:HD22	1:B:15:ARG:CZ	2.39	0.52
1:B:297:LYS:HD3	1:B:301:GLY:O	2.08	0.52
1:A:46:GLU:OE2	1:A:166:HIS:HE1	1.92	0.52
1:B:366:ARG:CG	1:B:366:ARG:HH21	2.17	0.52
1:B:67:SER:O	1:B:71:ASP:HB2	2.09	0.52
1:A:314:VAL:HG11	1:A:325:VAL:HG21	1.91	0.52
1:A:235:HIS:O	1:A:239:VAL:HG23	2.10	0.52
1:B:434:ASN:O	1:B:436:LYS:HG3	2.10	0.52
1:A:22:GLU:OE2	1:A:22:GLU:N	2.40	0.51
1:A:285:HIS:HA	1:A:324:GLU:O	2.10	0.51
1:A:98:PRO:O	1:A:99:ASP:HB2	2.11	0.51
1:B:314:VAL:HG11	1:B:325:VAL:HG21	1.92	0.51
1:A:298:ASN:HD21	1:A:302:VAL:HG13	1.74	0.51
1:A:329:ARG:HG2	1:A:344:ASP:CB	2.40	0.51
1:A:49:LEU:HD22	1:A:160:ALA:HB2	1.92	0.51
1:A:12:LEU:HD22	1:A:15:ARG:CZ	2.41	0.51
1:A:335:PRO:HG3	1:A:354:LEU:CD1	2.39	0.51
1:A:95:GLN:NE2	11:A:1177:HOH:O	2.44	0.51
1:A:272:VAL:HG21	1:A:313:LEU:HD13	1.93	0.50
1:B:202:ARG:NH2	1:B:202:ARG:HG3	2.16	0.50
1:B:115:LEU:HD23	1:B:158:LEU:HD13	1.94	0.50
1:B:124:ASN:HD21	1:B:126:THR:HB	1.77	0.50
1:B:207:LEU:HD23	1:B:207:LEU:O	2.11	0.50
1:B:347:ASP:CG	1:B:348:THR:H	2.14	0.50
1:A:202:ARG:CG	1:A:202:ARG:NH2	2.73	0.50
1:A:298:ASN:C	1:A:298:ASN:ND2	2.64	0.50
1:B:357:SER:HA	11:B:1244:HOH:O	2.12	0.50
1:A:61:ASN:ND2	1:A:61:ASN:C	2.62	0.49
1:B:133:PHE:O	1:B:134:ARG:HB2	2.12	0.49
1:B:61:ASN:ND2	1:B:61:ASN:C	2.62	0.49
1:A:261:LEU:HG	1:A:262:ALA:N	2.26	0.49
1:B:178:GLN:O	1:B:182:GLU:HG2	2.12	0.49
1:B:268:ASP:HA	1:B:310:ALA:HA	1.95	0.49
1:A:179:LEU:O	1:A:182:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:HA3	1:A:476:ASP:OD1	2.13	0.49
1:B:202:ARG:CG	1:B:202:ARG:HH21	2.21	0.49
1:B:335:PRO:HG3	1:B:354:LEU:CD1	2.41	0.49
1:A:38:THR:H	1:A:41:GLN:NE2	2.10	0.49
1:B:336:ASP:CG	1:B:352:ARG:HH22	2.15	0.49
1:A:207:LEU:HD23	1:A:207:LEU:C	2.33	0.49
1:B:261:LEU:HD11	1:B:273:TRP:CH2	2.48	0.48
1:B:347:ASP:CG	1:B:348:THR:N	2.64	0.48
1:B:382:LYS:HD3	11:B:770:HOH:O	2.13	0.48
1:A:230:PRO:HD2	11:A:873:HOH:O	2.13	0.48
1:B:172:LEU:N	1:B:172:LEU:CD1	2.76	0.48
1:A:292:HIS:HD2	7:B:635:ADX:O3'	1.95	0.48
1:A:42:LEU:O	1:A:45:ILE:HG22	2.13	0.48
1:A:90:GLU:HG3	11:A:747:HOH:O	2.12	0.48
1:B:223:PRO:HD2	1:B:257:SER:O	2.12	0.48
1:A:96:ILE:HG13	1:A:120:VAL:HG21	1.95	0.48
1:A:42:LEU:HD11	1:A:106:GLN:HG3	1.95	0.48
1:A:379:GLU:HG3	1:A:379:GLU:H	1.34	0.48
1:A:292:HIS:CD2	7:B:635:ADX:O3'	2.67	0.48
1:A:297:LYS:HD3	1:A:301:GLY:O	2.13	0.48
1:B:356:ILE:HD11	1:B:372:PRO:HG2	1.94	0.48
1:A:418:THR:O	1:A:421:GLN:CG	2.62	0.48
1:B:124:ASN:ND2	1:B:127:ILE:H	2.12	0.48
1:B:12:LEU:HD22	1:B:15:ARG:NH2	2.29	0.48
1:A:169:TYR:N	1:A:170:PRO:CD	2.77	0.47
1:A:16:ASP:OD1	1:A:159:GLU:HA	2.13	0.47
1:A:346:ILE:HG13	1:A:347:ASP:N	2.30	0.47
1:A:435:ASN:HD21	1:A:460:GLU:H	1.61	0.47
1:B:245:ILE:O	1:B:248:ARG:HG2	2.14	0.47
1:A:124:ASN:ND2	1:A:127:ILE:H	2.13	0.47
1:B:125:LYS:HD3	1:B:145:LEU:HG	1.96	0.47
1:A:124:ASN:ND2	1:A:127:ILE:HG13	2.29	0.47
1:A:115:LEU:HD23	1:A:158:LEU:HD13	1.96	0.47
1:B:435:ASN:HD21	1:B:460:GLU:HB2	1.80	0.47
1:A:268:ASP:HA	1:A:310:ALA:HA	1.97	0.47
1:A:359:THR:HG22	1:A:360:GLU:N	2.28	0.47
1:A:403:SER:O	1:A:488:ALA:HB1	2.14	0.47
1:A:172:LEU:CD1	1:A:172:LEU:N	2.78	0.47
1:B:329:ARG:HG2	1:B:344:ASP:CB	2.44	0.47
1:B:345:GLN:O	1:B:346:ILE:HG23	2.15	0.47
1:A:391:ARG:N	1:A:392:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ASN:HD21	1:A:460:GLU:HB2	1.80	0.47
1:A:272:VAL:CG2	1:A:313:LEU:HD13	2.45	0.46
1:B:402:ASN:OD1	1:B:458:GLN:HG3	2.15	0.46
1:B:38:THR:H	1:B:41:GLN:NE2	2.13	0.46
1:A:35:TRP:CZ2	1:A:88:VAL:HG12	2.50	0.46
1:A:385:ARG:HH21	1:A:385:ARG:HG2	1.80	0.46
1:A:274:HIS:HB3	1:A:286:PHE:CZ	2.51	0.46
1:A:458:GLN:HB3	11:A:1190:HOH:O	2.16	0.46
7:B:636:ADX:N7	8:B:638:POP:P1	2.89	0.46
1:A:314:VAL:HG13	1:A:325:VAL:HG21	1.98	0.46
8:A:637:POP:O6	7:B:635:ADX:N7	2.49	0.46
1:B:173:ARG:HG2	1:B:173:ARG:NH2	2.31	0.46
1:B:404:LEU:HD12	1:B:406:VAL:HG22	1.97	0.46
1:B:197:ARG:HD3	7:B:636:ADX:O1B	2.16	0.46
1:A:45:ILE:O	1:A:49:LEU:HG	2.16	0.45
1:B:96:ILE:HG13	1:B:120:VAL:HG21	1.97	0.45
1:B:458:GLN:HE21	1:B:458:GLN:HB3	1.52	0.45
1:A:359:THR:HA	11:A:686:HOH:O	2.15	0.45
1:B:313:LEU:HD22	1:B:317:TYR:CE1	2.52	0.45
1:B:366:ARG:CG	1:B:366:ARG:NH2	2.79	0.45
1:B:240:ARG:CD	11:B:878:HOH:O	2.61	0.45
1:A:112:ILE:O	1:A:161:ILE:HB	2.17	0.45
1:B:112:ILE:O	1:B:161:ILE:HB	2.16	0.45
1:B:334:LEU:HD21	1:B:346:ILE:CD1	2.47	0.45
1:A:188:TRP:CE2	1:A:218:LYS:HG3	2.51	0.45
1:A:461:ASP:HB3	11:A:851:HOH:O	2.15	0.45
1:A:180:ARG:O	1:A:184:GLN:HG3	2.16	0.45
1:A:124:ASN:HD22	1:A:124:ASN:C	2.20	0.45
1:A:401:GLY:O	1:A:404:LEU:HB2	2.16	0.45
1:B:236:HIS:HE1	10:B:563:ACY:O	1.99	0.45
1:B:400:LEU:N	1:B:400:LEU:HD23	2.31	0.45
1:B:429:LYS:NZ	11:B:1206:HOH:O	2.49	0.45
1:B:466:VAL:HG12	1:B:466:VAL:O	2.17	0.45
1:A:133:PHE:O	1:A:134:ARG:HB2	2.17	0.44
1:B:285:HIS:HA	1:B:324:GLU:O	2.16	0.44
1:B:366:ARG:HG3	1:B:394:GLN:HE22	1.82	0.44
1:A:290:ARG:HG3	1:A:308:TYR:CZ	2.52	0.44
1:B:172:LEU:HB3	1:B:258:LEU:HG	1.99	0.44
1:A:403:SER:HB3	11:A:1228:HOH:O	2.16	0.44
1:A:469:LYS:CD	1:A:469:LYS:H	2.01	0.44
1:B:173:ARG:HG2	1:B:173:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:GLY:HA3	1:B:476:ASP:OD1	2.17	0.44
1:A:455:ILE:HA	1:A:456:PRO:HD2	1.88	0.44
1:A:126:THR:O	1:A:130:GLU:HG3	2.18	0.44
1:B:314:VAL:HG13	1:B:325:VAL:HG21	2.00	0.44
1:A:347:ASP:OD2	1:A:348:THR:N	2.51	0.43
1:A:360:GLU:OE2	1:A:364:ARG:HG3	2.18	0.43
1:A:363:ARG:O	1:A:367:VAL:HG22	2.18	0.43
1:B:40:ARG:HG3	1:B:262:ALA:HB1	2.01	0.43
1:B:459:TRP:NE1	1:B:464:ASP:HA	2.33	0.43
1:A:491:PRO:HG2	1:A:494:HIS:CG	2.53	0.43
1:B:82:ILE:HG13	1:B:273:TRP:CE3	2.53	0.43
1:B:184:GLN:C	1:B:186:ARG:N	2.71	0.43
1:B:400:LEU:HG	1:B:456:PRO:HA	1.99	0.43
1:B:71:ASP:O	1:B:73:ARG:HG3	2.18	0.43
1:B:42:LEU:HD22	1:B:164:PRO:HB3	1.99	0.43
1:B:274:HIS:HB3	1:B:286:PHE:CZ	2.53	0.43
1:B:418:THR:O	1:B:421:GLN:CG	2.66	0.43
1:B:42:LEU:HD11	1:B:106:GLN:HG3	2.00	0.43
1:A:35:TRP:CH2	1:A:88:VAL:HG12	2.54	0.43
1:B:184:GLN:O	1:B:185:SER:C	2.57	0.43
1:B:348:THR:C	1:B:350:LYS:N	2.69	0.43
1:B:391:ARG:HA	1:B:391:ARG:HD3	1.85	0.43
1:B:298:ASN:ND2	1:B:302:VAL:HG13	2.31	0.43
1:B:309:ASP:HB3	11:B:704:HOH:O	2.19	0.43
1:A:202:ARG:HG2	1:A:377:TYR:CE1	2.54	0.42
1:A:273:TRP:CE2	1:A:277:ILE:HD11	2.53	0.42
1:B:101:ARG:NH1	1:B:114:ILE:HG21	2.34	0.42
1:B:235:HIS:O	1:B:239:VAL:HG23	2.19	0.42
1:B:43:CYS:CB	1:B:262:ALA:HB2	2.49	0.42
1:A:172:LEU:HB3	1:A:258:LEU:HG	2.01	0.42
1:B:87:ASP:HA	1:B:152:TYR:O	2.20	0.42
1:B:359:THR:HG22	1:B:360:GLU:N	2.33	0.42
1:B:400:LEU:HD13	1:B:411:LEU:HD23	2.01	0.42
1:B:492:ILE:O	1:B:496:VAL:HG23	2.19	0.42
1:A:42:LEU:HA	1:A:45:ILE:HG22	2.01	0.42
1:A:444:GLN:NE2	1:A:468:GLY:O	2.46	0.42
1:B:234:ASP:OD2	1:B:236:HIS:HB2	2.19	0.42
1:B:290:ARG:HD3	1:B:330:MET:HB2	2.02	0.42
1:B:476:ASP:HB3	1:B:481:ALA:HB2	2.00	0.42
1:B:45:ILE:O	1:B:49:LEU:HG	2.19	0.42
1:B:186:ARG:NH1	10:B:561:ACY:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:CYS:CB	1:A:262:ALA:HB2	2.50	0.42
1:A:334:LEU:HD21	1:A:346:ILE:CD1	2.49	0.42
1:A:434:ASN:O	1:A:436:LYS:HG3	2.20	0.42
1:B:124:ASN:ND2	1:B:127:ILE:HG13	2.35	0.42
1:B:202:ARG:NH2	1:B:202:ARG:CG	2.80	0.42
1:B:298:ASN:C	1:B:298:ASN:ND2	2.72	0.42
1:B:391:ARG:HH21	1:B:391:ARG:HG3	1.84	0.42
1:B:491:PRO:HG2	1:B:494:HIS:CG	2.55	0.42
1:A:261:LEU:HD11	1:A:273:TRP:CH2	2.54	0.42
1:A:329:ARG:HG2	1:A:344:ASP:CG	2.40	0.42
1:A:346:ILE:CG1	1:A:347:ASP:H	2.31	0.42
1:A:192:VAL:HA	1:A:285:HIS:HB2	2.02	0.42
1:A:197:ARG:HD3	7:B:635:ADX:O2B	2.20	0.42
1:A:363:ARG:NH2	11:A:1179:HOH:O	2.52	0.42
1:B:298:ASN:HD21	1:B:302:VAL:H	1.66	0.42
1:B:300:LYS:HE2	11:B:871:HOH:O	2.20	0.42
1:B:166:HIS:CD2	11:B:711:HOH:O	2.73	0.41
1:A:125:LYS:HD3	1:A:145:LEU:HG	2.03	0.41
1:B:188:TRP:CD2	1:B:218:LYS:HG3	2.55	0.41
1:B:403:SER:O	1:B:488:ALA:HB1	2.21	0.41
1:B:346:ILE:HG13	1:B:347:ASP:N	2.36	0.41
1:B:274:HIS:ND1	1:B:292:HIS:CE1	2.85	0.41
1:A:186:ARG:O	1:A:187:GLN:HB2	2.19	0.41
1:B:123:PRO:HG3	1:B:153:TYR:CE1	2.56	0.41
1:A:176:PRO:HD3	1:A:281:TYR:CE1	2.55	0.41
1:A:348:THR:C	1:A:350:LYS:N	2.71	0.41
1:A:124:ASN:HD22	1:A:127:ILE:H	1.67	0.41
1:A:65:TYR:O	1:A:69:VAL:HG23	2.20	0.41
1:B:29:SER:O	1:B:32:ILE:HG22	2.21	0.41
1:B:33:LEU:HD12	11:B:1155:HOH:O	2.20	0.41
1:B:347:ASP:OD2	1:B:348:THR:N	2.54	0.41
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.84	0.41
1:A:313:LEU:HD22	1:A:317:TYR:CE1	2.56	0.41
1:B:192:VAL:HA	1:B:285:HIS:HB2	2.03	0.41
1:A:169:TYR:CE1	1:A:239:VAL:HG11	2.56	0.41
1:B:184:GLN:O	1:B:187:GLN:N	2.42	0.41
1:B:221:ILE:HG22	1:B:223:PRO:HD3	2.02	0.41
1:A:175:THR:N	1:A:178:GLN:HE21	2.09	0.41
1:A:274:HIS:ND1	1:A:292:HIS:CE1	2.83	0.41
1:A:29:SER:O	1:A:32:ILE:HG22	2.21	0.41
1:A:390:PRO:HB2	1:A:392:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD23	1:A:353:THR:HG22	2.03	0.40
1:A:366:ARG:CG	1:A:366:ARG:NH2	2.80	0.40
1:A:136:ASP:HA	1:A:137:PRO:HD2	1.95	0.40
1:A:356:ILE:HD13	1:A:364:ARG:HH12	1.82	0.40
1:B:169:TYR:N	1:B:170:PRO:CD	2.84	0.40
1:B:396:PHE:C	1:B:396:PHE:CD1	2.94	0.40
1:B:178:GLN:HE21	1:B:178:GLN:HB2	1.71	0.40
1:B:420:LEU:HA	1:B:420:LEU:HD23	1.88	0.40
7:B:636:ADX:N7	8:B:638:POP:O3	2.55	0.40
1:A:10:GLN:NE2	1:A:10:GLN:HA	2.36	0.40
1:B:26:GLU:CD	1:B:101:ARG:HE	2.22	0.40
1:B:60:LEU:HA	11:B:905:HOH:O	2.21	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)
2:A:515:CD:CD	2:B:533:CD:CD[2_765]	1.10	1.10

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/510 (100%)	473 (93%)	29 (6%)	6 (1%)	15	44
1	B	508/510 (100%)	470 (92%)	31 (6%)	7 (1%)	13	39
All	All	1016/1020 (100%)	943 (93%)	60 (6%)	13 (1%)	14	41

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ILE

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Mol	Chain	Res	Type
1	B	346	ILE
1	A	336	ASP
1	B	336	ASP
1	A	335	PRO
1	A	359	THR
1	B	335	PRO
1	B	359	THR
1	B	372	PRO
1	B	464	ASP
1	A	267	GLY
1	A	372	PRO
1	B	435	ASN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/445 (100%)	423 (95%)	22 (5%)	29	62
1	B	445/445 (100%)	424 (95%)	21 (5%)	30	64
All	All	890/890 (100%)	847 (95%)	43 (5%)	30	63

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	24	LEU
1	A	31	ASP
1	A	47	LEU
1	A	61	ASN
1	A	124	ASN
1	A	158	LEU
1	A	173	ARG
1	A	179	LEU
1	A	197	ARG
1	A	202	ARG

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Mol	Chain	Res	Type
1	A	206	GLU
1	A	298	ASN
1	A	302	VAL
1	A	313	LEU
1	A	329	ARG
1	A	370	GLU
1	A	373	GLU
1	A	379	GLU
1	A	469	LYS
1	A	474	LEU
1	A	478	SER
1	B	18	LEU
1	B	24	LEU
1	B	31	ASP
1	B	61	ASN
1	B	124	ASN
1	B	158	LEU
1	B	173	ARG
1	B	179	LEU
1	B	197	ARG
1	B	202	ARG
1	B	206	GLU
1	B	298	ASN
1	B	302	VAL
1	B	313	LEU
1	B	329	ARG
1	B	370	GLU
1	B	373	GLU
1	B	379	GLU
1	B	469	LYS
1	B	474	LEU
1	B	478	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) 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

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	106	GLN
1	A	118	GLN
1	A	124	ASN
1	A	147	ASN
1	A	166	HIS
1	A	178	GLN
1	A	184	GLN
1	A	198	ASN
1	A	292	HIS
1	A	298	ASN
1	A	434	ASN
1	A	435	ASN
1	A	471	ASN
1	A	484	GLN
1	B	10	GLN
1	B	21	ASN
1	B	41	GLN
1	B	61	ASN
1	B	94	ASN
1	B	106	GLN
1	B	118	GLN
1	B	124	ASN
1	B	147	ASN
1	B	166	HIS
1	B	178	GLN
1	B	184	GLN
1	B	198	ASN
1	B	236	HIS
1	B	292	HIS
1	B	298	ASN
1	B	434	ASN
1	B	435	ASN
1	B	471	ASN
1	B	484	GLN
1	B	506	ASN

### 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 54 ligands modelled in this entry, 31 are monoatomic - leaving 23 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	$\# Z  > 2$
10	ACY	A	550	2	1,3,3	5.26	1 (100%)	0,3,3	0.00	-
10	ACY	A	551	2	1,3,3	5.91	1 (100%)	0,3,3	0.00	-
10	ACY	A	552	-	1,3,3	6.21	1 (100%)	0,3,3	0.00	-
10	ACY	A	553	-	1,3,3	6.63	1 (100%)	0,3,3	0.00	-
10	ACY	A	554	2	1,3,3	5.19	1 (100%)	0,3,3	0.00	-
10	ACY	A	555	2	1,3,3	5.94	1 (100%)	0,3,3	0.00	-
10	ACY	A	556	2	1,3,3	4.36	1 (100%)	0,3,3	0.00	-
10	ACY	A	564	2	1,3,3	5.57	1 (100%)	0,3,3	0.00	-
6	LCO	A	600	-	2,3,3	0.47	0	1,3,3	0.08	0
9	TRS	A	602	-	7,7,7	0.92	0	9,9,9	2.59	3 (33%)
8	POP	A	637	-	8,8,8	1.26	0	8,13,13	1.27	2 (25%)
10	ACY	B	557	2	1,3,3	4.44	1 (100%)	0,3,3	0.00	-
10	ACY	B	558	2	1,3,3	5.83	1 (100%)	0,3,3	0.00	-
10	ACY	B	559	-	1,3,3	5.83	1 (100%)	0,3,3	0.00	-
10	ACY	B	560	-	1,3,3	5.81	1 (100%)	0,3,3	0.00	-
10	ACY	B	561	2	1,3,3	6.64	1 (100%)	0,3,3	0.00	-
10	ACY	B	562	2	1,3,3	5.72	1 (100%)	0,3,3	0.00	-
10	ACY	B	563	2	1,3,3	5.57	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	LCO	B	601	-	2,3,3	0.36	0	1,3,3	0.24	0
9	TRS	B	603	-	7,7,7	1.20	0	9,9,9	1.76	1 (11%)
7	ADX	B	635	-	24,29,29	1.34	3 (12%)	24,45,45	2.57	2 (8%)
7	ADX	B	636	-	24,29,29	1.56	4 (16%)	24,45,45	2.47	2 (8%)
8	POP	B	638	-	8,8,8	1.23	0	8,13,13	1.35	2 (25%)

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
10	ACY	A	550	2	-	0/0/0/0	0/0/0/0
10	ACY	A	551	2	-	0/0/0/0	0/0/0/0
10	ACY	A	552	-	-	0/0/0/0	0/0/0/0
10	ACY	A	553	-	-	0/0/0/0	0/0/0/0
10	ACY	A	554	2	-	0/0/0/0	0/0/0/0
10	ACY	A	555	2	-	0/0/0/0	0/0/0/0
10	ACY	A	556	2	-	0/0/0/0	0/0/0/0
10	ACY	A	564	2	-	0/0/0/0	0/0/0/0
6	LCO	A	600	-	-	0/0/0/0	0/0/0/0
9	TRS	A	602	-	-	0/9/9/9	0/0/0/0
8	POP	A	637	-	-	0/6/6/6	0/0/0/0
10	ACY	B	557	2	-	0/0/0/0	0/0/0/0
10	ACY	B	558	2	-	0/0/0/0	0/0/0/0
10	ACY	B	559	-	-	0/0/0/0	0/0/0/0
10	ACY	B	560	-	-	0/0/0/0	0/0/0/0
10	ACY	B	561	2	-	0/0/0/0	0/0/0/0
10	ACY	B	562	2	-	0/0/0/0	0/0/0/0
10	ACY	B	563	2	-	0/0/0/0	0/0/0/0
6	LCO	B	601	-	-	0/0/0/0	0/0/0/0
9	TRS	B	603	-	-	0/9/9/9	0/0/0/0
7	ADX	B	635	-	-	0/6/32/32	0/3/3/3
7	ADX	B	636	-	-	0/6/32/32	0/3/3/3
8	POP	B	638	-	-	0/6/6/6	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	636	ADX	C2'-C1'	-2.49	1.49	1.53
7	B	635	ADX	C5-N7	-2.47	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	636	ADX	C2-N3	2.12	1.35	1.32
7	B	635	ADX	O4'-C1'	2.15	1.44	1.41
7	B	636	ADX	O4'-C1'	2.63	1.44	1.41
7	B	635	ADX	O2B-SB	4.34	1.61	1.45
10	A	556	ACY	CH3-C	4.36	1.54	1.48
10	B	557	ACY	CH3-C	4.44	1.54	1.48
7	B	636	ADX	O2B-SB	5.07	1.64	1.45
10	A	554	ACY	CH3-C	5.19	1.55	1.48
10	A	550	ACY	CH3-C	5.26	1.55	1.48
10	B	563	ACY	CH3-C	5.57	1.55	1.48
10	A	564	ACY	CH3-C	5.57	1.55	1.48
10	B	562	ACY	CH3-C	5.72	1.56	1.48
10	B	560	ACY	CH3-C	5.81	1.56	1.48
10	B	559	ACY	CH3-C	5.83	1.56	1.48
10	B	558	ACY	CH3-C	5.83	1.56	1.48
10	A	551	ACY	CH3-C	5.91	1.56	1.48
10	A	555	ACY	CH3-C	5.94	1.56	1.48
10	A	552	ACY	CH3-C	6.21	1.56	1.48
10	A	553	ACY	CH3-C	6.63	1.57	1.48
10	B	561	ACY	CH3-C	6.64	1.57	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	635	ADX	N3-C2-N1	-11.56	118.79	128.86
7	B	636	ADX	N3-C2-N1	-11.23	119.08	128.86
9	A	602	TRS	C1-C-N	-3.57	100.14	107.73
7	B	636	ADX	C4-C5-N7	-2.98	106.53	109.41
7	B	635	ADX	C4-C5-N7	-2.95	106.56	109.41
9	A	602	TRS	C3-C-C2	-2.61	103.66	111.06
8	A	637	POP	O5-P2-O4	-2.47	100.83	110.50
8	B	638	POP	O5-P2-O4	-2.43	101.00	110.50
8	A	637	POP	O6-P2-O4	2.29	119.46	110.50
8	B	638	POP	O6-P2-O4	2.52	120.36	110.50
9	B	603	TRS	C2-C-N	4.66	117.64	107.73
9	A	602	TRS	C2-C-N	5.84	120.14	107.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	550	ACY	1	0
9	A	602	TRS	1	0
8	A	637	POP	1	0
10	B	557	ACY	1	0
10	B	561	ACY	1	0
10	B	563	ACY	1	0
7	B	635	ADX	5	0
7	B	636	ADX	3	0
8	B	638	POP	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	510/510 (100%)	-0.18	22 (4%)	36 26	14, 31, 68, 85	1 (0%)
1	B	510/510 (100%)	-0.24	17 (3%)	47 36	14, 31, 68, 85	2 (0%)
All	All	1020/1020 (100%)	-0.21	39 (3%)	41 30	14, 31, 68, 85	3 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	THR	4.4
1	A	349	THR	4.1
1	A	367	VAL	3.8
1	B	349	THR	3.5
1	A	369	GLY	3.3
1	A	480	SER	2.9
1	A	350	LYS	2.9
1	B	354	LEU	2.8
1	B	352	ARG	2.8
1	B	367	VAL	2.8
1	A	336	ASP	2.8
1	A	30	SER	2.6
1	B	479	SER	2.6
1	A	354	LEU	2.6
1	B	351	THR	2.6
1	A	299	SER	2.6
1	B	350	LYS	2.5
1	B	302	VAL	2.5
1	B	478	SER	2.5
1	A	300	LYS	2.4
1	A	363	ARG	2.4
1	B	480	SER	2.4
1	A	31	ASP	2.3
1	A	94	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	31	ASP	2.3
1	A	337	GLU	2.3
1	B	346	ILE	2.3
1	A	479	SER	2.2
1	B	299	SER	2.2
1	B	353	THR	2.2
1	B	30	SER	2.1
1	A	97	LYS	2.1
1	A	91	ALA	2.1
1	A	351	THR	2.1
1	B	336	ASP	2.1
1	A	352	ARG	2.1
1	B	17	ALA	2.1
1	A	370	GLU	2.1
1	A	478	SER	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
10	ACY	B	561	4/4	0.97	0.21	4.52	18,19,21,23	0
10	ACY	B	563	4/4	0.98	0.24	4.26	19,22,22,22	0
10	ACY	A	556	4/4	0.99	0.22	3.15	30,30,30,30	0
6	LCO	B	601	4/4	0.88	0.28	1.68	58,58,58,59	0
10	ACY	B	560	4/4	0.93	0.20	1.65	33,35,36,36	0
10	ACY	B	557	4/4	0.98	0.31	1.19	31,31,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
10	ACY	A	553	4/4	0.94	0.17	0.68	31,32,32,34	0
9	TRS	A	602	8/8	0.90	0.21	0.64	22,25,26,29	0
10	ACY	B	559	4/4	0.84	0.22	0.49	71,71,72,73	0
10	ACY	A	550	4/4	0.99	0.23	0.44	27,29,29,31	0
6	LCO	A	600	4/4	0.96	0.19	0.02	32,34,34,36	0
9	TRS	B	603	8/8	0.95	0.15	-0.01	29,31,32,33	0
8	POP	B	638	9/9	0.93	0.20	-0.30	90,90,91,91	0
7	ADX	B	636	27/27	0.97	0.16	-0.33	26,30,43,43	0
7	ADX	B	635	27/27	0.97	0.15	-0.61	20,32,38,39	0
10	ACY	A	552	4/4	0.95	0.13	-1.08	44,45,46,46	0
10	ACY	A	554	4/4	0.97	0.11	-1.25	23,25,26,27	0
8	POP	A	637	9/9	0.95	0.15	-2.16	46,49,50,51	0
2	CD	B	532	1/1	0.99	0.05	-2.26	39,39,39,39	0
2	CD	A	513	1/1	0.95	0.07	-3.04	66,66,66,66	1
2	CD	A	514	1/1	0.99	0.06	-3.91	36,36,36,36	0
2	CD	B	533	1/1	1.00	0.05	-4.22	64,64,64,64	0
2	CD	A	515	1/1	1.00	0.05	-4.68	58,58,58,58	0
2	CD	B	531	1/1	0.97	0.06	-7.46	65,65,65,65	1
10	ACY	A	551	4/4	0.98	0.21	-	31,32,33,33	0
2	CD	B	534	1/1	1.00	0.03	-	35,35,35,35	0
4	NA	A	526	1/1	0.97	0.06	-	22,22,22,22	0
2	CD	A	524	1/1	1.00	0.04	-	54,54,54,54	0
3	CA	A	519	1/1	0.89	0.06	-	68,68,68,68	0
10	ACY	B	562	4/4	0.97	0.44	-	65,66,66,66	0
2	CD	A	512	1/1	1.00	0.04	-	34,34,34,34	0
4	NA	B	542	1/1	0.96	0.09	-	53,53,53,53	0
4	NA	B	540	1/1	0.98	0.06	-	28,28,28,28	0
4	NA	B	543	1/1	0.92	0.13	-	36,36,36,36	0
4	NA	A	523	1/1	0.94	0.09	-	42,42,42,42	0
5	MG	A	521	1/1	0.95	0.12	-	26,26,26,26	0
3	CA	B	537	1/1	0.76	0.12	-	76,76,76,76	0
4	NA	A	527	1/1	0.92	0.09	-	33,33,33,33	0
10	ACY	A	555	4/4	0.98	0.25	-	47,48,49,49	0
4	NA	A	525	1/1	0.99	0.13	-	5,5,5,5	0
4	NA	B	541	1/1	0.97	0.07	-	19,19,19,19	0
3	CA	B	538	1/1	0.99	0.09	-	26,26,26,26	0
10	ACY	B	558	4/4	0.98	0.26	-	34,35,36,36	0
4	NA	A	518	1/1	0.96	0.07	-	45,45,45,45	0
3	CA	B	535	1/1	0.94	0.10	-	37,37,37,37	0
3	CA	A	517	1/1	0.99	0.04	-	32,32,32,32	0
4	NA	B	544	1/1	0.92	0.08	-	28,28,28,28	0
2	CD	A	516	1/1	1.00	0.02	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	B	536	1/1	0.95	0.09	-	44,44,44,44	0
5	MG	B	539	1/1	0.78	0.33	-	69,69,69,69	0
10	ACY	A	564	4/4	0.99	0.15	-	25,27,27,30	0
2	CD	B	530	1/1	1.00	0.04	-	39,39,39,39	0
4	NA	A	522	1/1	0.98	0.05	-	24,24,24,24	0
3	CA	A	520	1/1	0.95	0.05	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.