



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:08 am GMT

PDB ID : 1AJ8  
Title : CITRATE SYNTHASE FROM PYROCOCCLUS FURIOSUS  
Authors : Russell, R.J.M.; Ferguson, J.M.C.; Hough, D.W.; Danson, M.J.; Taylor, G.L.  
Deposited on : 1997-05-16  
Resolution : 1.90 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

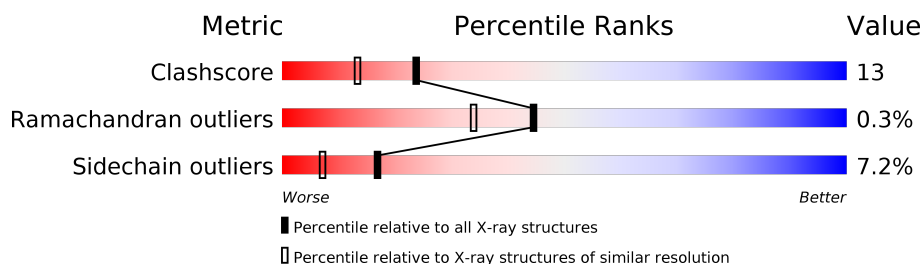
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	371	 74% 23% .
1	B	371	 78% 19% .

## 2 Entry composition [i](#)

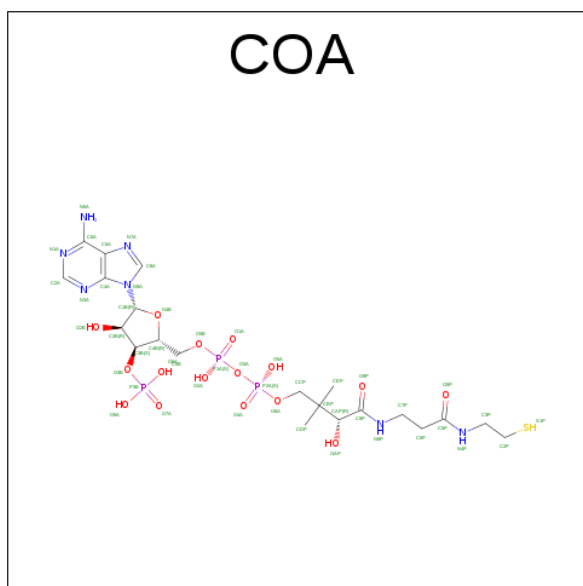
There are 4 unique types of molecules in this entry. The entry contains 6562 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2987	1943	492	542	10			
1	B	370	Total	C	N	O	S	0	0	0
			2975	1937	488	540	10			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			46	20	7	16	3		
2	B	1	Total	C	N	O	P	0	0
			46	20	7	16	3		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

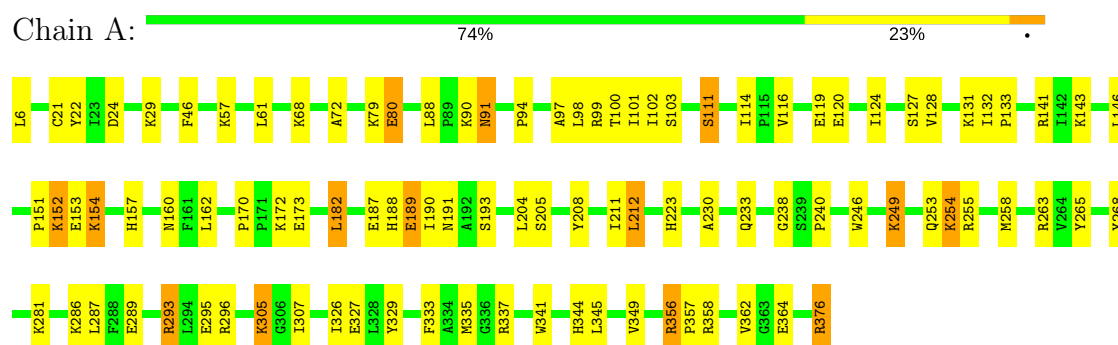
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total	O	0	0
			248	248		
4	B	234	Total	O	0	0
			234	234		

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

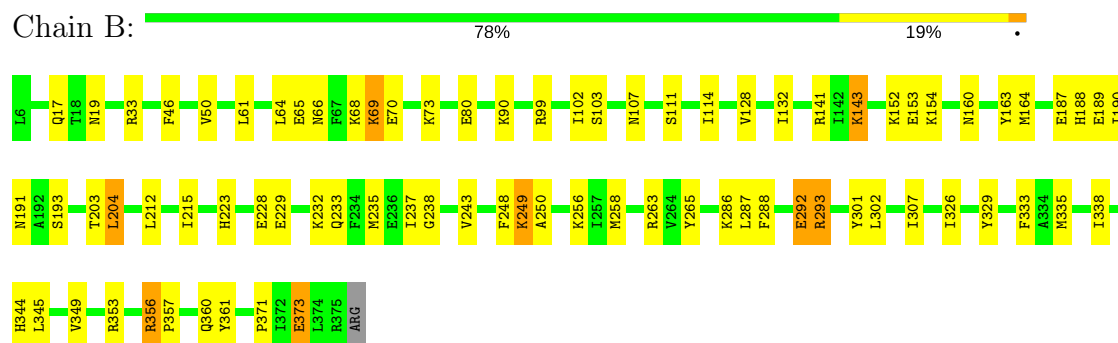
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: CITRATE SYNTHASE



#### • Molecule 1: CITRATE SYNTHASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.29Å 98.29Å 238.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 1.90	Depositor
% Data completeness (in resolution range)	98.5 (100.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.191 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.34	0/3059	0.58	0/4133
1	B	0.32	0/3047	0.56	0/4119
All	All	0.33	0/6106	0.57	0/8252

There are no bond length outliers.

There are no bond angle outliers.

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	2987	0	3035	96	0
1	B	2975	0	3022	77	0
2	A	46	0	27	1	0
2	B	46	0	27	2	0
3	A	13	0	5	2	0
3	B	13	0	5	2	0
4	A	248	0	0	10	0
4	B	234	0	0	4	0
All	All	6562	0	6121	154	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 13.

All (154) 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:152:LYS:H	1:A:160:ASN:ND2	1.71	0.88
1:A:99:ARG:HD3	1:B:212:LEU:HD13	1.63	0.80
1:A:249:LYS:HD2	4:A:3120:HOH:O	1.82	0.78
1:A:80:GLU:HG3	4:A:3198:HOH:O	1.84	0.76
1:A:376:ARG:H	1:A:376:ARG:HH11	1.35	0.74
1:B:102:ILE:HD12	1:B:215:ILE:CD1	2.18	0.73
1:A:376:ARG:HD3	1:A:376:ARG:N	2.04	0.73
1:A:99:ARG:HD2	1:B:103:SER:OG	1.89	0.72
1:A:233:GLN:HE22	1:A:258:MET:H	1.36	0.71
1:A:187:GLU:OE2	1:A:344:HIS:HE1	1.74	0.71
1:B:152:LYS:H	1:B:160:ASN:ND2	1.89	0.71
1:B:152:LYS:H	1:B:160:ASN:HD21	1.39	0.69
1:B:102:ILE:HD12	1:B:215:ILE:HD13	1.73	0.69
1:A:152:LYS:H	1:A:160:ASN:HD21	1.39	0.67
1:A:99:ARG:HD3	1:B:212:LEU:CD1	2.26	0.66
1:B:90:LYS:HD2	1:B:143:LYS:HA	1.79	0.64
1:A:356:ARG:HG2	1:B:263:ARG:HG2	1.80	0.64
1:B:102:ILE:CD1	1:B:215:ILE:HD11	2.28	0.64
1:A:88:LEU:HD11	1:A:101:ILE:HD11	1.80	0.64
1:A:111:SER:HB3	1:A:114:ILE:HD12	1.78	0.63
1:A:344:HIS:HD2	4:A:3040:HOH:O	1.80	0.63
1:B:256:LYS:HE2	4:B:4012:HOH:O	1.99	0.62
1:B:356:ARG:HG3	1:B:356:ARG:O	2.00	0.62
1:A:356:ARG:HD2	1:B:191:ASN:HA	1.80	0.62
1:A:356:ARG:O	1:A:356:ARG:HG3	2.01	0.61
1:A:356:ARG:NH2	1:B:189:GLU:OE1	2.34	0.61
1:A:263:ARG:HG2	1:B:356:ARG:HG2	1.83	0.60
1:B:248:PHE:HZ	1:B:301:TYR:CZ	2.19	0.60
1:B:187:GLU:OE2	1:B:344:HIS:HE1	1.83	0.60
1:A:263:ARG:HG2	1:B:356:ARG:CG	2.32	0.60
1:A:154:LYS:H	1:A:154:LYS:HE2	1.67	0.59
1:A:376:ARG:H	1:A:376:ARG:HD3	1.67	0.59
1:A:103:SER:OG	1:B:99:ARG:HD2	2.03	0.59
1:B:233:GLN:HE22	1:B:258:MET:H	1.51	0.58
1:A:356:ARG:CG	1:B:263:ARG:HG2	2.34	0.58
1:B:102:ILE:CD1	1:B:215:ILE:CD1	2.81	0.58
1:B:188:HIS:HD2	3:B:2000:CIT:O1	1.87	0.58
1:B:152:LYS:HD3	1:B:154:LYS:HE2	1.87	0.57
1:A:249:LYS:NZ	1:A:253:GLN:HE22	2.02	0.57
1:A:238:GLY:O	1:A:286:LYS:HE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASN:HA	1:B:356:ARG:HD2	1.86	0.57
1:A:376:ARG:H	1:A:376:ARG:CD	2.14	0.56
1:B:237:ILE:HG21	1:B:243:VAL:HG22	1.86	0.56
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.70	0.56
1:A:154:LYS:H	1:A:154:LYS:CE	2.19	0.55
1:B:344:HIS:HD2	4:B:4040:HOH:O	1.88	0.55
1:A:72:ALA:HB1	1:A:153:GLU:HG3	1.87	0.55
2:B:4000:COA:HN4	2:B:4000:COA:H131	1.73	0.55
1:A:188:HIS:HD2	3:A:1000:CIT:O1	1.91	0.54
1:A:376:ARG:CD	1:A:376:ARG:N	2.70	0.54
1:B:132:ILE:HG22	1:B:335:MET:HG3	1.88	0.54
1:B:238:GLY:O	1:B:286:LYS:HE2	2.08	0.54
1:B:66:ASN:O	1:B:70:GLU:HG3	2.08	0.54
1:A:91:ASN:H	1:A:91:ASN:HD22	1.54	0.53
1:A:255:ARG:HD3	4:A:3020:HOH:O	2.08	0.53
1:A:376:ARG:HG2	1:A:376:ARG:NH1	2.23	0.53
1:A:230:ALA:O	1:A:233:GLN:HB3	2.09	0.53
1:A:6:LEU:HD11	1:B:17:GLN:HG3	1.89	0.52
1:B:288:PHE:CE1	1:B:292:GLU:HG3	2.44	0.52
1:B:345:LEU:O	1:B:349:VAL:HG22	2.09	0.52
1:A:376:ARG:H	1:A:376:ARG:NH1	2.06	0.52
1:A:91:ASN:HD22	1:A:91:ASN:N	2.09	0.51
1:A:356:ARG:HD3	3:B:2000:CIT:O2	2.10	0.50
1:A:293:ARG:HH11	1:A:293:ARG:HG2	1.77	0.50
1:A:190:ILE:O	1:A:190:ILE:HG23	2.12	0.50
1:B:73:LYS:HD3	1:B:153:GLU:OE2	2.12	0.49
1:A:293:ARG:HH11	1:A:293:ARG:CG	2.25	0.49
1:B:111:SER:CB	1:B:114:ILE:HD12	2.43	0.49
1:B:249:LYS:HE3	1:B:250:ALA:CA	2.43	0.49
1:A:189:GLU:OE1	1:B:356:ARG:NH2	2.45	0.49
1:B:188:HIS:HE1	1:B:265:TYR:OH	1.95	0.49
1:A:212:LEU:HD23	1:B:99:ARG:HD3	1.94	0.48
1:B:249:LYS:HE3	1:B:250:ALA:N	2.29	0.48
1:A:46:PHE:CD1	1:A:182:LEU:HB3	2.49	0.48
1:B:190:ILE:O	1:B:190:ILE:HG23	2.13	0.48
1:B:326:ILE:HA	1:B:329:TYR:CZ	2.49	0.48
1:B:373:GLU:H	1:B:373:GLU:CD	2.17	0.48
1:A:111:SER:CB	1:A:114:ILE:HD12	2.44	0.47
1:B:46:PHE:O	1:B:50:VAL:HG23	2.14	0.47
1:A:111:SER:HA	1:A:114:ILE:HD12	1.96	0.47
1:B:371:PRO:HB3	1:B:373:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:HG23	1:A:362:VAL:O	2.14	0.47
1:B:193:SER:H	1:B:223:HIS:CE1	2.32	0.47
1:A:356:ARG:HG2	1:B:263:ARG:CB	2.44	0.46
1:A:249:LYS:HZ2	1:A:253:GLN:HE22	1.62	0.46
1:A:132:ILE:HG22	1:A:335:MET:HG2	1.97	0.46
1:A:193:SER:H	1:A:223:HIS:CE1	2.33	0.46
1:A:193:SER:H	1:A:223:HIS:HE1	1.62	0.46
1:B:193:SER:H	1:B:223:HIS:HE1	1.63	0.46
1:B:258:MET:SD	2:B:4000:COA:H61	2.55	0.46
1:A:97:ALA:O	1:A:101:ILE:HG12	2.15	0.46
1:A:253:GLN:O	1:A:254:LYS:HB2	2.15	0.46
2:A:3000:COA:H131	2:A:3000:COA:HN4	1.81	0.46
1:A:263:ARG:HG2	1:B:356:ARG:HG3	1.98	0.46
1:B:64:LEU:O	1:B:68:LYS:HG3	2.16	0.46
1:A:240:PRO:HG3	1:A:289:GLU:HB3	1.98	0.46
1:A:22:TYR:HB2	1:B:361:TYR:CD2	2.50	0.46
1:A:120:GLU:O	1:A:124:ILE:HG12	2.15	0.46
1:B:302:LEU:HB3	1:B:307:ILE:HB	1.98	0.46
1:A:151:PRO:HA	1:A:160:ASN:HD21	1.81	0.45
1:B:228:GLU:O	1:B:232:LYS:HG3	2.16	0.45
1:A:188:HIS:HE1	1:A:265:TYR:OH	1.99	0.45
1:A:356:ARG:HG2	1:B:263:ARG:CG	2.45	0.45
1:B:360:GLN:HG3	4:B:4105:HOH:O	2.17	0.44
1:A:80:GLU:HG3	1:A:80:GLU:H	1.50	0.44
1:B:293:ARG:HD3	4:B:4109:HOH:O	2.16	0.44
3:A:1000:CIT:O2	1:B:356:ARG:HD3	2.17	0.44
1:A:170:PRO:HD2	4:A:3188:HOH:O	2.17	0.44
1:A:100:THR:OG1	1:B:107:ASN:ND2	2.50	0.44
1:A:249:LYS:HZ3	1:A:255:ARG:HH21	1.66	0.44
1:A:249:LYS:NZ	1:A:255:ARG:HH21	2.15	0.44
1:A:345:LEU:O	1:A:349:VAL:HG22	2.18	0.44
1:A:133:PRO:HG2	1:A:157:HIS:CE1	2.53	0.44
1:A:233:GLN:HE22	1:A:258:MET:N	2.09	0.44
1:B:69:LYS:O	1:B:73:LYS:HG2	2.18	0.44
1:A:337:ARG:HG3	1:A:341:TRP:CE2	2.53	0.43
1:A:154:LYS:HE2	1:A:154:LYS:N	2.33	0.43
1:A:263:ARG:CB	1:B:356:ARG:HG2	2.48	0.43
1:A:358:ARG:NH1	4:A:3066:HOH:O	2.52	0.43
1:B:191:ASN:H	1:B:191:ASN:ND2	2.17	0.43
1:A:305:LYS:HD3	1:A:307:ILE:HD12	2.00	0.43
1:B:203:THR:O	1:B:204:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:MET:HE2	1:B:235:MET:HB2	1.88	0.43
1:B:19:ASN:O	1:B:33:ARG:HD3	2.19	0.43
1:A:152:LYS:N	1:A:160:ASN:HD21	2.11	0.43
1:A:173:GLU:H	1:A:173:GLU:CD	2.21	0.43
1:B:111:SER:HB3	1:B:114:ILE:HD12	2.00	0.42
1:B:329:TYR:N	1:B:329:TYR:CD1	2.85	0.42
1:A:263:ARG:CG	1:B:356:ARG:HG2	2.49	0.42
1:A:24:ASP:HB3	1:A:29:LYS:HB2	2.01	0.42
1:A:94:PRO:HG2	1:A:327:GLU:O	2.19	0.42
1:B:249:LYS:HE3	1:B:250:ALA:HA	2.01	0.42
1:B:338:ILE:HG13	1:B:338:ILE:O	2.20	0.42
1:A:293:ARG:NH1	1:A:293:ARG:CG	2.83	0.42
1:A:128:VAL:O	1:A:132:ILE:HG13	2.20	0.42
1:B:229:GLU:HB3	1:B:258:MET:HG3	2.02	0.42
1:A:116:VAL:HG22	1:A:205:SER:O	2.20	0.42
1:A:98:LEU:HG	1:A:102:ILE:CD1	2.50	0.41
1:B:111:SER:HA	1:B:114:ILE:HD12	2.02	0.41
1:A:208:TYR:O	1:A:212:LEU:HD22	2.21	0.41
1:A:344:HIS:CD2	4:A:3040:HOH:O	2.64	0.41
1:A:98:LEU:HD11	1:A:102:ILE:HD11	2.03	0.41
1:B:152:LYS:HE3	1:B:163:TYR:CZ	2.56	0.41
1:B:141:ARG:HD2	1:B:164:MET:O	2.21	0.41
1:A:141:ARG:HB3	1:A:146:LEU:HB2	2.02	0.41
1:A:246:TRP:O	1:A:249:LYS:HD3	2.21	0.41
1:B:102:ILE:HD13	1:B:215:ILE:HD11	2.02	0.41
1:A:326:ILE:HA	1:A:329:TYR:CZ	2.56	0.41
1:B:233:GLN:HE22	1:B:258:MET:N	2.18	0.41
1:B:128:VAL:O	1:B:132:ILE:HG13	2.21	0.40
1:A:29:LYS:HD3	4:A:3225:HOH:O	2.21	0.40
1:A:68:LYS:HD2	4:A:3175:HOH:O	2.22	0.40
1:A:127:SER:O	1:A:131:LYS:HG3	2.22	0.40
1:A:296:ARG:HD2	4:A:3177:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/371 (100%)	357 (97%)	11 (3%)	1 (0%)	44	34
1	B	368/371 (99%)	357 (97%)	10 (3%)	1 (0%)	44	34
All	All	737/742 (99%)	714 (97%)	21 (3%)	2 (0%)	44	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	357	PRO
1	A	357	PRO

### 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	314/314 (100%)	283 (90%)	31 (10%)	9	3
1	B	313/314 (100%)	299 (96%)	14 (4%)	32	21
All	All	627/628 (100%)	582 (93%)	45 (7%)	17	7

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	CYS
1	A	57	LYS
1	A	61	LEU
1	A	79	LYS
1	A	80	GLU
1	A	90	LYS
1	A	91	ASN
1	A	111	SER
1	A	119	GLU
1	A	143	LYS

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Mol	Chain	Res	Type
1	A	152	LYS
1	A	154	LYS
1	A	162	LEU
1	A	172	LYS
1	A	182	LEU
1	A	189	GLU
1	A	204	LEU
1	A	211	ILE
1	A	212	LEU
1	A	249	LYS
1	A	254	LYS
1	A	268	TYR
1	A	281	LYS
1	A	287	LEU
1	A	293	ARG
1	A	295	GLU
1	A	305	LYS
1	A	333	PHE
1	A	356	ARG
1	A	364	GLU
1	A	376	ARG
1	B	61	LEU
1	B	65	GLU
1	B	69	LYS
1	B	80	GLU
1	B	143	LYS
1	B	204	LEU
1	B	249	LYS
1	B	287	LEU
1	B	292	GLU
1	B	293	ARG
1	B	333	PHE
1	B	353	ARG
1	B	356	ARG
1	B	373	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	107	ASN
1	A	160	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	188	HIS
1	A	223	HIS
1	A	233	GLN
1	A	253	GLN
1	A	344	HIS
1	B	107	ASN
1	B	144	ASN
1	B	160	ASN
1	B	188	HIS
1	B	223	HIS
1	B	233	GLN
1	B	253	GLN
1	B	344	HIS

### 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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	CIT	A	1000	-	3,12,12	3.96	2 (66%)	3,17,17	5.48	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	COA	A	3000	-	41,48,50	1.81	9 (21%)	47,73,75	1.45	5 (10%)
3	CIT	B	2000	-	3,12,12	3.75	2 (66%)	3,17,17	4.67	2 (66%)
2	COA	B	4000	-	41,48,50	1.99	9 (21%)	47,73,75	1.49	5 (10%)

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	CIT	A	1000	-	-	0/6/16/16	0/0/0/0
2	COA	A	3000	-	-	0/42/62/64	0/3/3/3
3	CIT	B	2000	-	-	0/6/16/16	0/0/0/0
2	COA	B	4000	-	-	1/42/62/64	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	CIT	C4-C3	-5.97	1.45	1.54
3	B	2000	CIT	C4-C3	-5.31	1.46	1.54
2	B	4000	COA	C5A-N7A	-3.68	1.26	1.39
2	A	3000	COA	C5A-N7A	-3.56	1.27	1.39
2	A	3000	COA	O9P-C9P	2.00	1.27	1.23
2	A	3000	COA	O4B-C1B	2.08	1.44	1.41
2	B	4000	COA	O4B-C1B	2.20	1.44	1.41
2	B	4000	COA	O9P-C9P	2.31	1.27	1.23
2	A	3000	COA	C3P-N4P	2.54	1.50	1.45
2	A	3000	COA	C2A-N3A	2.79	1.36	1.32
2	B	4000	COA	C3P-N4P	2.80	1.50	1.45
2	A	3000	COA	CCP-CBP	3.04	1.56	1.52
2	B	4000	COA	C2A-N3A	3.20	1.37	1.32
2	A	3000	COA	P3B-O7A	3.30	1.62	1.50
2	B	4000	COA	P3B-O7A	3.34	1.62	1.50
3	A	1000	CIT	C2-C3	3.36	1.59	1.54
2	B	4000	COA	CCP-CBP	3.38	1.57	1.52
3	B	2000	CIT	C2-C3	3.56	1.60	1.54
2	A	3000	COA	C8A-N7A	3.81	1.41	1.34
2	B	4000	COA	C8A-N7A	4.13	1.42	1.34
2	A	3000	COA	P3B-O3B	6.42	1.70	1.59
2	B	4000	COA	P3B-O3B	7.27	1.72	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	CIT	C3-C4-C5	-9.01	100.87	114.95
3	B	2000	CIT	C3-C4-C5	-7.53	103.19	114.95
2	B	4000	COA	N3A-C2A-N1A	-4.28	125.13	128.86
2	A	3000	COA	C1B-N9A-C4A	-4.20	119.38	126.64
2	B	4000	COA	C1B-N9A-C4A	-4.01	119.71	126.64
2	A	3000	COA	N3A-C2A-N1A	-4.00	125.37	128.86
2	B	4000	COA	C4B-O4B-C1B	2.17	112.08	109.77
2	A	3000	COA	C4B-O4B-C1B	2.49	112.42	109.77
3	A	1000	CIT	C4-C3-C2	2.77	116.65	109.75
3	B	2000	CIT	C4-C3-C2	2.79	116.69	109.75
2	A	3000	COA	N6A-C6A-N1A	2.82	124.35	118.77
2	B	4000	COA	N6A-C6A-N1A	3.12	124.94	118.77
2	A	3000	COA	C4A-C5A-N7A	4.74	113.98	109.41
2	B	4000	COA	C4A-C5A-N7A	5.27	114.50	109.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4000	COA	C6P-C5P-N4P-C3P

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	CIT	2	0
2	A	3000	COA	1	0
3	B	2000	CIT	2	0
2	B	4000	COA	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.