



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:49 PM GMT

PDB ID : 3CSC  
Title : STRUCTURE OF TERNARY COMPLEXES OF CITRATE SYNTHASE  
WITH D-AND L-MALATE: MECHANISTIC IMPLICATIONS  
Authors : Karpusas, M.; Holland, D.; Remington, S.J.  
Deposited on : 1990-05-07  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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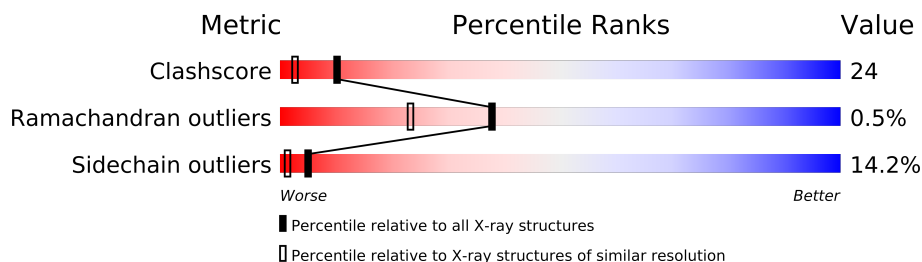
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	

## 2 Entry composition i

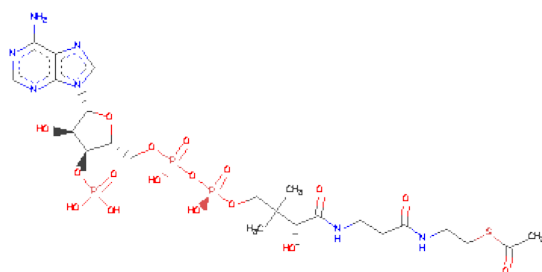
There are 4 unique types of molecules in this entry. The entry contains 3467 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

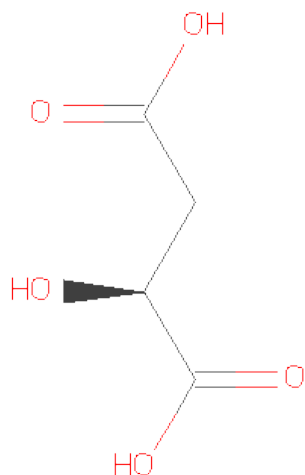
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3306	2115	571	603	17	0	0	0

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	51	23	7	17	3	1	0	0

- Molecule 3 is (2S)-2-HYDROXYBUTANEDIOICACID (three-letter code: LMR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		

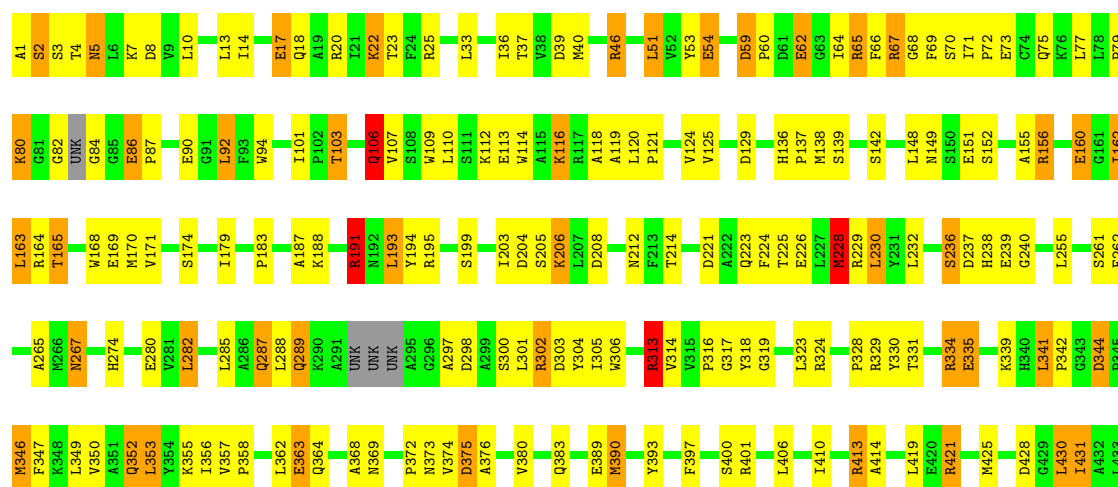
### 3 Residue-property plots

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.

Note EDS was not executed.

#### • Molecule 1: CITRATE SYNTHASE

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.00Å 78.10Å 58.30Å 90.00° 78.90° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 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: LMR, ACO

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	1.24	15/3386 (0.4%)	1.49	58/4598 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	GLU	CD-OE2	9.97	1.36	1.25
1	A	54	GLU	CD-OE2	9.74	1.36	1.25
1	A	226	GLU	CD-OE2	8.15	1.34	1.25
1	A	280	GLU	CD-OE2	8.11	1.34	1.25
1	A	160	GLU	CD-OE2	7.57	1.33	1.25
1	A	54	GLU	CG-CD	-7.08	1.41	1.51
1	A	363	GLU	CD-OE2	6.48	1.32	1.25
1	A	113	GLU	CD-OE2	6.37	1.32	1.25
1	A	335	GLU	CD-OE2	6.09	1.32	1.25
1	A	151	GLU	CD-OE2	5.53	1.31	1.25
1	A	103	THR	CB-OG1	5.46	1.54	1.43
1	A	90	GLU	CD-OE2	5.40	1.31	1.25
1	A	62	GLU	CD-OE2	5.26	1.31	1.25
1	A	165	THR	CB-OG1	5.26	1.53	1.43
1	A	17	GLU	CD-OE1	-5.12	1.20	1.25

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	NE-CZ-NH1	12.79	126.70	120.30
1	A	313	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	A	401	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	A	413	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	A	39	ASP	CB-CG-OD2	-8.71	110.47	118.30
1	A	46	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	A	228	MET	CG-SD-CE	-8.22	87.05	100.20
1	A	59	ASP	CB-CG-OD1	8.14	125.63	118.30
1	A	401	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	A	237	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	59	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	413	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	67	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	298	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	A	156	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	289	GLN	CB-CA-C	-7.10	96.20	110.40
1	A	33	LEU	CA-CB-CG	-7.02	99.15	115.30
1	A	303	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	A	1	ALA	N-CA-CB	6.81	119.63	110.10
1	A	174	SER	CB-CA-C	6.80	123.02	110.10
1	A	22	LYS	N-CA-CB	6.78	122.81	110.60
1	A	39	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	66	PHE	O-C-N	-6.60	112.14	122.70
1	A	33	LEU	CB-CG-CD1	-6.57	99.83	111.00
1	A	221	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	1	ALA	CB-CA-C	6.38	119.67	110.10
1	A	191	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	421	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	237	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	46	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	344	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	67	ARG	CB-CA-C	-5.80	98.79	110.40
1	A	119	ALA	N-CA-CB	5.80	118.22	110.10
1	A	54	GLU	CG-CD-OE2	-5.78	106.74	118.30
1	A	334	ARG	CD-NE-CZ	-5.70	115.62	123.60
1	A	25	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	368	ALA	CB-CA-C	5.66	118.59	110.10
1	A	68	GLY	N-CA-C	-5.64	98.99	113.10
1	A	8	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	302	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	239	GLU	CB-CA-C	5.52	121.45	110.40
1	A	65	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	106	GLN	N-CA-CB	5.47	120.44	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLU	CB-CG-CD	-5.45	99.48	114.20
1	A	67	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	297	ALA	CB-CA-C	-5.37	102.05	110.10
1	A	344	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	289	GLN	CB-CG-CD	-5.35	97.70	111.60
1	A	165	THR	CA-CB-CG2	-5.29	104.99	112.40
1	A	208	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	66	PHE	C-N-CA	-5.24	108.60	121.70
1	A	221	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	129	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	431	ILE	CA-CB-CG1	5.18	120.84	111.00
1	A	92	LEU	CA-CB-CG	-5.14	103.49	115.30
1	A	375	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	51	LEU	CB-CA-C	-5.04	100.62	110.20
1	A	191	ARG	NE-CZ-NH2	-5.01	117.80	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	ALA	CA
1	A	22	LYS	CA
1	A	174	SER	CA
1	A	431	ILE	CB

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3306	0	3297	153	1
2	A	51	0	34	8	0
3	A	9	0	4	3	0
4	A	101	0	0	5	0
All	All	3467	0	3335	158	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (158) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:301:LEU:HD23	1:A:356:ILE:HD13	1.47	0.94
1:A:109:TRP:HE3	1:A:110:LEU:HD23	1.34	0.93
1:A:163:LEU:HD12	1:A:165:THR:H	1.32	0.92
1:A:109:TRP:CE3	1:A:110:LEU:HD23	2.05	0.92
1:A:136:HIS:HD2	1:A:138:MET:H	1.09	0.91
1:A:301:LEU:HD23	1:A:356:ILE:CD1	2.03	0.87
1:A:136:HIS:CD2	1:A:138:MET:H	1.94	0.84
1:A:67:ARG:HA	4:A:548:HOH:O	1.82	0.80
1:A:350:VAL:CG1	1:A:380:VAL:HG21	2.14	0.77
1:A:287:GLN:HE21	1:A:287:GLN:N	1.82	0.77
1:A:350:VAL:HG11	1:A:380:VAL:HG21	1.67	0.75
1:A:335:GLU:O	1:A:339:LYS:HE2	1.88	0.73
1:A:323:LEU:O	1:A:324:ARG:HD3	1.87	0.73
1:A:14:ILE:HG12	1:A:414:ALA:HB1	1.71	0.72
1:A:282:LEU:HD23	1:A:390:MET:HE2	1.71	0.72
1:A:71:ILE:HG22	1:A:72:PRO:HD3	1.72	0.72
1:A:77:LEU:HB3	1:A:101:ILE:HD13	1.72	0.71
1:A:288:LEU:HD13	1:A:304:TYR:CD2	2.25	0.71
1:A:282:LEU:HD22	1:A:393:TYR:HE2	1.55	0.71
1:A:3:SER:OG	1:A:4:THR:N	2.24	0.70
1:A:125:VAL:HG13	1:A:188:LYS:HE2	1.74	0.69
1:A:67:ARG:HB2	1:A:69:PHE:CD1	2.30	0.67
1:A:267:ASN:HD22	1:A:267:ASN:N	1.93	0.67
1:A:339:LYS:N	1:A:339:LYS:HD3	2.08	0.67
1:A:346:MET:HG2	1:A:380:VAL:HG22	1.78	0.66
1:A:124:VAL:HG21	1:A:148:LEU:HD23	1.78	0.66
1:A:80:LYS:N	1:A:80:LYS:HD2	2.09	0.66
1:A:282:LEU:HD22	1:A:393:TYR:CE2	2.31	0.64
1:A:152:SER:HB3	1:A:155:ALA:HB3	1.79	0.64
1:A:64:ILE:HD13	1:A:238:HIS:CD2	2.33	0.64
1:A:5:ASN:HD22	1:A:7:LYS:H	1.45	0.63
1:A:77:LEU:HD13	1:A:101:ILE:CD1	2.29	0.62
1:A:106:GLN:CA	1:A:106:GLN:HE21	2.10	0.62
1:A:136:HIS:HD2	1:A:138:MET:N	1.91	0.62
1:A:79:PRO:HG2	1:A:107:VAL:HG21	1.81	0.61
1:A:302:ARG:NH2	1:A:363:GLU:OE1	2.34	0.61
1:A:287:GLN:HE21	1:A:287:GLN:CA	2.12	0.61
1:A:136:HIS:CD2	1:A:137:PRO:HD2	2.36	0.60
1:A:77:LEU:HD13	1:A:101:ILE:HD12	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:HIS:HD1	3:A:702:LMR:H2	1.65	0.60
1:A:305:ILE:HD13	1:A:357:VAL:HG22	1.81	0.60
1:A:112:LYS:O	1:A:116:LYS:HG3	2.02	0.60
1:A:75:GLN:NE2	1:A:86:GLU:HG3	2.16	0.60
1:A:288:LEU:HD13	1:A:304:TYR:CE2	2.36	0.60
1:A:274:HIS:HA	2:A:700:ACO:O	2.03	0.58
1:A:428:ASP:O	1:A:431:ILE:HG22	2.03	0.58
1:A:349:LEU:O	1:A:353:LEU:HD22	2.02	0.58
1:A:335:GLU:HG3	1:A:339:LYS:HE2	1.84	0.58
2:A:700:ACO:S1P	3:A:702:LMR:H3A	2.43	0.58
1:A:5:ASN:C	1:A:5:ASN:HD22	2.07	0.58
1:A:419:LEU:HD23	1:A:421:ARG:HB2	1.86	0.57
1:A:82:GLY:H	1:A:84:GLY:HA2	1.70	0.56
1:A:317:GLY:O	1:A:376:ALA:HB2	2.04	0.56
1:A:92:LEU:HD23	1:A:236:SER:OG	2.05	0.56
1:A:5:ASN:ND2	1:A:7:LYS:H	2.03	0.56
1:A:187:ALA:O	1:A:191:ARG:HB2	2.06	0.55
1:A:323:LEU:O	1:A:324:ARG:NH1	2.40	0.55
1:A:319:GLY:HA2	1:A:369:ASN:O	2.05	0.55
1:A:204:ASP:OD2	1:A:206:LYS:HE2	2.06	0.55
1:A:37:THR:OG1	1:A:40:MET:HG3	2.07	0.55
1:A:106:GLN:HA	1:A:106:GLN:HE21	1.72	0.55
1:A:109:TRP:HE3	1:A:110:LEU:CD2	2.12	0.54
1:A:109:TRP:CE3	1:A:110:LEU:CD2	2.84	0.54
1:A:77:LEU:CB	1:A:101:ILE:HD13	2.37	0.54
2:A:700:ACO:CDP	2:A:700:ACO:H21	2.38	0.54
1:A:288:LEU:HD13	1:A:304:TYR:CG	2.43	0.53
1:A:318:TYR:CE1	1:A:372:PRO:HD3	2.43	0.53
1:A:124:VAL:HG21	1:A:148:LEU:CD2	2.38	0.53
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.90	0.53
1:A:352:GLN:O	1:A:356:ILE:HD12	2.08	0.53
1:A:64:ILE:HG13	1:A:65:ARG:N	2.24	0.53
1:A:136:HIS:O	1:A:139:SER:HB2	2.10	0.52
1:A:375:ASP:OD1	2:A:700:ACO:HH33	2.10	0.52
1:A:287:GLN:NE2	1:A:287:GLN:CA	2.72	0.52
1:A:168:TRP:CZ2	1:A:169:GLU:HG2	2.45	0.52
1:A:194:TYR:CG	1:A:389:GLU:HG2	2.45	0.51
1:A:67:ARG:HB2	1:A:69:PHE:CE1	2.45	0.51
1:A:306:TRP:HZ2	1:A:363:GLU:CD	2.14	0.51
1:A:103:THR:H	1:A:106:GLN:HG2	1.74	0.51
1:A:71:ILE:CG2	1:A:72:PRO:HD3	2.41	0.50
1:A:71:ILE:HG22	1:A:72:PRO:CD	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:LEU:CD1	1:A:304:TYR:CG	2.95	0.50
2:A:700:ACO:H131	2:A:700:ACO:H21	1.93	0.50
1:A:419:LEU:CD2	1:A:421:ARG:HB2	2.42	0.49
1:A:82:GLY:C	1:A:84:GLY:HA2	2.33	0.49
1:A:77:LEU:CD1	1:A:101:ILE:CD1	2.90	0.49
1:A:224:PHE:HD2	4:A:581:HOH:O	1.94	0.49
1:A:282:LEU:HD23	1:A:390:MET:CE	2.41	0.49
1:A:288:LEU:HA	1:A:304:TYR:CZ	2.47	0.49
1:A:142:SER:OG	1:A:267:ASN:ND2	2.45	0.48
1:A:156:ARG:O	1:A:160:GLU:HG3	2.13	0.48
1:A:225:THR:O	1:A:229:ARG:HG3	2.13	0.48
1:A:204:ASP:HB3	1:A:212:ASN:HD21	1.79	0.47
1:A:329:ARG:HB3	1:A:374:VAL:HG23	1.96	0.47
1:A:163:LEU:HD12	1:A:165:THR:N	2.14	0.47
1:A:103:THR:H	1:A:106:GLN:CG	2.28	0.47
1:A:14:ILE:O	1:A:18:GLN:HG3	2.15	0.47
1:A:288:LEU:CD1	1:A:304:TYR:CD1	2.97	0.47
1:A:262:PHE:O	1:A:265:ALA:HB3	2.15	0.47
1:A:77:LEU:HB3	1:A:101:ILE:CD1	2.43	0.46
1:A:75:GLN:HE22	1:A:86:GLU:HG3	1.81	0.46
1:A:86:GLU:HG2	1:A:230:LEU:HG	1.97	0.46
1:A:206:LYS:HB2	1:A:206:LYS:HE3	1.39	0.46
2:A:700:ACO:HH32	3:A:702:LMR:O2	2.15	0.46
1:A:341:LEU:N	1:A:342:PRO:HD3	2.29	0.46
1:A:431:ILE:HG21	1:A:431:ILE:HD12	1.51	0.46
1:A:331:THR:O	1:A:334:ARG:HB3	2.16	0.46
1:A:53:TYR:CD2	1:A:240:GLY:HA3	2.51	0.46
1:A:114:TRP:CZ2	1:A:179:ILE:HG21	2.52	0.45
1:A:5:ASN:HD22	1:A:7:LYS:N	2.13	0.45
1:A:334:ARG:HD2	1:A:334:ARG:HH11	1.40	0.45
1:A:163:LEU:CD1	1:A:164:ARG:N	2.80	0.45
1:A:350:VAL:HG13	1:A:380:VAL:HG21	1.96	0.45
1:A:92:LEU:CD2	1:A:236:SER:OG	2.64	0.45
1:A:103:THR:O	1:A:107:VAL:HG23	2.17	0.45
1:A:70:SER:OG	1:A:73:GLU:HG3	2.16	0.44
1:A:364:GLN:HE21	1:A:364:GLN:HB3	1.49	0.44
1:A:194:TYR:CD1	1:A:389:GLU:HG2	2.52	0.44
1:A:314:VAL:O	1:A:316:PRO:HD3	2.17	0.44
1:A:59:ASP:OD2	1:A:60:PRO:HD2	2.17	0.44
1:A:194:TYR:O	1:A:195:ARG:HD3	2.17	0.44
1:A:330:TYR:CD2	1:A:372:PRO:HB2	2.52	0.44
1:A:64:ILE:HD13	1:A:238:HIS:HA	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:163:LEU:C	1:A:163:LEU:CD1	2.87	0.43
1:A:171:VAL:HG21	1:A:413:ARG:HG3	2.00	0.43
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.65	0.43
1:A:120:LEU:HA	1:A:121:PRO:HD2	1.88	0.43
1:A:410:ILE:HG21	1:A:410:ILE:HD13	1.70	0.43
1:A:118:ALA:CB	1:A:203:ILE:HD12	2.48	0.43
1:A:136:HIS:CG	1:A:137:PRO:HD2	2.53	0.43
1:A:86:GLU:CG	1:A:87:PRO:CD	2.95	0.43
1:A:344:ASP:O	1:A:347:PHE:HB3	2.19	0.43
1:A:334:ARG:HD2	4:A:604:HOH:O	2.19	0.43
1:A:136:HIS:CD2	1:A:137:PRO:CD	3.02	0.43
1:A:59:ASP:HA	1:A:60:PRO:HD3	1.78	0.42
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.81	0.42
1:A:347:PHE:CD2	1:A:347:PHE:O	2.72	0.42
1:A:341:LEU:N	1:A:342:PRO:CD	2.82	0.42
1:A:72:PRO:HD3	4:A:591:HOH:O	2.18	0.42
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.76	0.42
1:A:136:HIS:HA	1:A:137:PRO:HD3	1.88	0.42
1:A:86:GLU:CG	1:A:87:PRO:HD2	2.50	0.42
1:A:67:ARG:HB2	1:A:69:PHE:HD1	1.81	0.42
2:A:700:ACO:OAP	2:A:700:ACO:N7A	2.45	0.42
1:A:214:THR:CG2	1:A:228:MET:HG2	2.51	0.41
1:A:305:ILE:CD1	1:A:357:VAL:HG22	2.48	0.41
1:A:36:ILE:HG21	1:A:36:ILE:HD13	1.82	0.41
1:A:373:ASN:ND2	2:A:700:ACO:H22	2.35	0.41
1:A:318:TYR:CE1	1:A:357:VAL:CG1	3.03	0.41
1:A:324:ARG:HA	1:A:324:ARG:HD3	1.59	0.41
1:A:110:LEU:N	1:A:110:LEU:HD23	2.35	0.41
1:A:94:TRP:CE3	1:A:110:LEU:HD21	2.56	0.41
1:A:323:LEU:C	1:A:324:ARG:HD3	2.41	0.41
1:A:162:ILE:O	4:A:575:HOH:O	2.21	0.41
1:A:232:LEU:HA	1:A:400:SER:HB2	2.03	0.41
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.73	0.40
1:A:285:LEU:HD11	1:A:350:VAL:HG12	2.03	0.40
1:A:335:GLU:HG3	1:A:339:LYS:CE	2.50	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	Distance(Å)	Clash(Å)
1:A:3:SER:O	1:A:313:ARG:NH2[1_554]	2.19	0.01

## 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	423/433 (98%)	402 (95%)	19 (4%)	2 (0%)	38 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	236	SER

### 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	345/345 (100%)	296 (86%)	49 (14%)	5 1

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	5	ASN
1	A	10	LEU
1	A	13	LEU
1	A	17	GLU
1	A	20	ARG
1	A	22	LYS
1	A	23	THR
1	A	46	ARG
1	A	51	LEU
1	A	54	GLU
1	A	62	GLU

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Mol	Chain	Res	Type
1	A	80	LYS
1	A	86	GLU
1	A	106	GLN
1	A	116	LYS
1	A	149	ASN
1	A	162	ILE
1	A	163	LEU
1	A	170	MET
1	A	183	PRO
1	A	191	ARG
1	A	193	LEU
1	A	199	SER
1	A	205	SER
1	A	206	LYS
1	A	223	GLN
1	A	228	MET
1	A	230	LEU
1	A	255	LEU
1	A	261	SER
1	A	267	ASN
1	A	282	LEU
1	A	287	GLN
1	A	289	GLN
1	A	300	SER
1	A	313	ARG
1	A	328	PRO
1	A	341	LEU
1	A	346	MET
1	A	352	GLN
1	A	353	LEU
1	A	355	LYS
1	A	362	LEU
1	A	383	GLN
1	A	390	MET
1	A	397	PHE
1	A	425	MET
1	A	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN

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Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	106	GLN
1	A	123	HIS
1	A	136	HIS
1	A	140	GLN
1	A	149	ASN
1	A	192	ASN
1	A	211	HIS
1	A	212	ASN
1	A	215	ASN
1	A	223	GLN
1	A	267	ASN
1	A	287	GLN
1	A	289	GLN
1	A	310	ASN
1	A	340	HIS
1	A	364	GLN
1	A	391	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
2	ACO	A	700	-	53,53,53	1.93	14 (26%)	79,79,79	1.55	11 (13%)
3	LMR	A	702	-	8,8,8	2.09	4 (50%)	10,10,10	2.01	4 (40%)

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
2	ACO	A	700	-	-	1/51/67/67	0/1/3/3
3	LMR	A	702	-	-	0/8/8/8	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ACO	O9P-C9P	6.55	1.36	1.23
2	A	700	ACO	CH3-C	-5.88	1.28	1.50
2	A	700	ACO	P1A-O3A	-3.62	1.53	1.59
3	A	702	LMR	O4B-C4	3.56	1.34	1.22
2	A	700	ACO	O4B-C1B	2.87	1.45	1.41
3	A	702	LMR	C2-C1	-2.82	1.48	1.52
2	A	700	ACO	O5P-C5P	2.70	1.29	1.23
2	A	700	ACO	C3P-N4P	2.70	1.52	1.46
2	A	700	ACO	P2A-O3A	2.62	1.64	1.59
2	A	700	ACO	P3B-O3B	2.55	1.67	1.59
2	A	700	ACO	P3B-O7A	2.53	1.59	1.51
2	A	700	ACO	CBP-CAP	2.53	1.58	1.55
3	A	702	LMR	C3-C2	-2.41	1.48	1.52
3	A	702	LMR	O2-C2	2.41	1.48	1.42
2	A	700	ACO	C2A-N1A	2.33	1.38	1.33
2	A	700	ACO	O4B-C4B	2.14	1.50	1.45
2	A	700	ACO	OAP-CAP	2.04	1.46	1.42
2	A	700	ACO	C4A-N9A	2.02	1.40	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ACO	P3B-O3B-C3B	-5.29	110.82	121.96
2	A	700	ACO	CEP-CBP-CCP	-5.15	101.34	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	LMR	C3-C2-C1	3.98	115.16	109.88
2	A	700	ACO	CDP-CBP-CCP	3.76	114.17	108.76
2	A	700	ACO	O4B-C1B-C2B	-3.60	101.25	106.77
2	A	700	ACO	O-C-S1P	-3.23	110.41	122.06
2	A	700	ACO	C2P-C3P-N4P	-2.96	105.80	112.50
2	A	700	ACO	C4A-C5A-N7A	2.79	111.91	109.52
2	A	700	ACO	CEP-CBP-CAP	2.75	113.60	108.82
3	A	702	LMR	C2-C3-C4	-2.48	106.46	112.16
2	A	700	ACO	C6P-C7P-N8P	-2.46	106.56	111.87
3	A	702	LMR	O2-C2-C3	2.36	115.65	109.86
2	A	700	ACO	C2B-C3B-C4B	-2.27	98.74	103.16
3	A	702	LMR	O4A-C4-C3	2.15	121.63	114.20
2	A	700	ACO	O5A-P2A-O3A	2.09	115.08	105.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	ACO	CH3-C-S1P-C2P

There are no ring outliers.

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.