



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2017 – 12:57 AM EST

PDB ID : 4CSC  
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 : unknown  
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) : rb-20030345

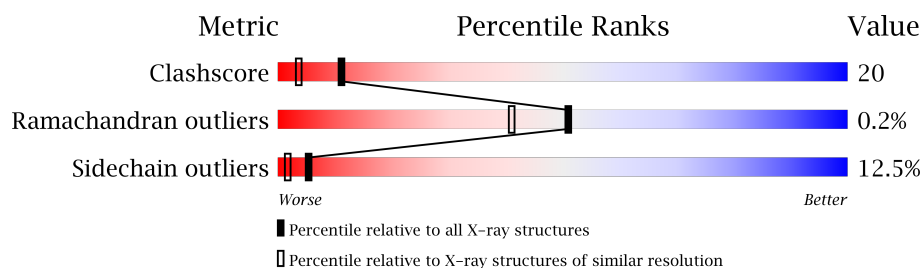
# 1 Overall quality at a glance

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	433	

## 2 Entry composition [i](#)

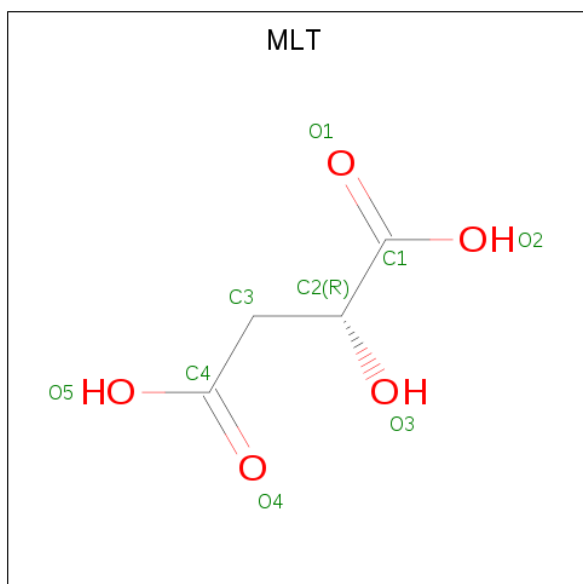
There are 4 unique types of molecules in this entry. The entry contains 3467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

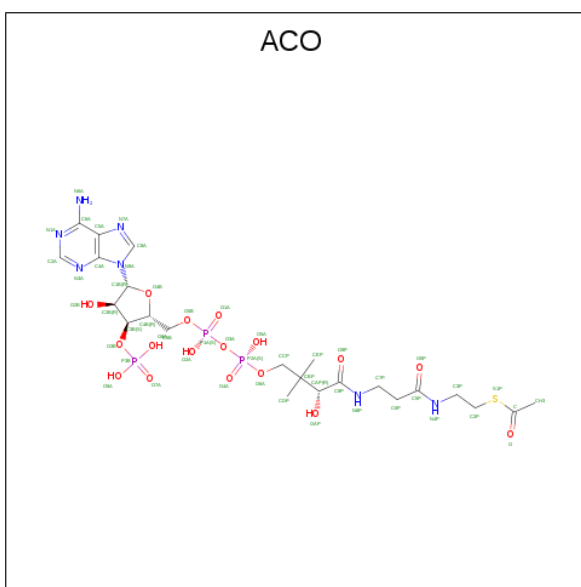
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3306	2115	571	603	17	0	0	0

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



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

- Molecule 3 is ACETYL COENZYME \*A (three-letter code: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).



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

- Molecule 4 is water.

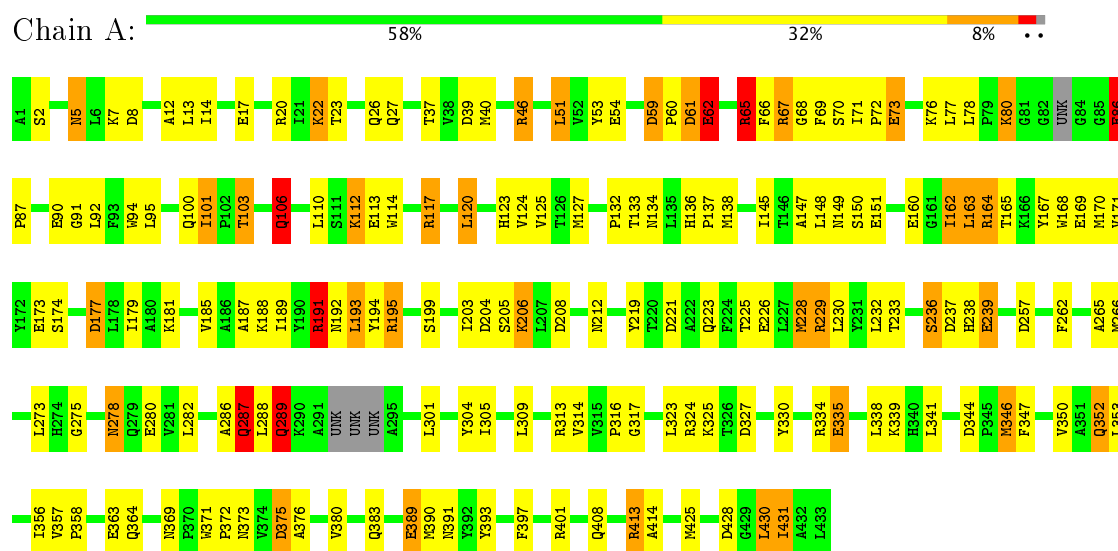
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	101	Total O 101 101	0	0

### 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.

Note EDS was not executed.

#### • 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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.00 Å   78.10 Å   58.30 Å 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, $R_{free}$	0.188 , (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> )	19.0	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: ACO, MLT

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	0.93	15/3386 (0.4%)	1.45	62/4598 (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	3	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	GLU	CD-OE2	7.76	1.34	1.25
1	A	239	GLU	CD-OE2	6.36	1.32	1.25
1	A	226	GLU	CD-OE2	6.17	1.32	1.25
1	A	173	GLU	CD-OE2	6.06	1.32	1.25
1	A	363	GLU	CD-OE2	5.86	1.32	1.25
1	A	280	GLU	CD-OE2	5.78	1.32	1.25
1	A	103	THR	CB-OG1	5.70	1.54	1.43
1	A	62	GLU	CD-OE2	5.51	1.31	1.25
1	A	113	GLU	CD-OE2	5.51	1.31	1.25
1	A	335	GLU	CD-OE2	5.48	1.31	1.25
1	A	151	GLU	CD-OE2	5.41	1.31	1.25
1	A	17	GLU	CD-OE2	5.40	1.31	1.25
1	A	86	GLU	CD-OE2	5.39	1.31	1.25
1	A	160	GLU	CD-OE2	5.25	1.31	1.25
1	A	73	GLU	CD-OE2	5.11	1.31	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	A	65	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	67	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	A	191	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	A	286	ALA	CB-CA-C	9.01	123.61	110.10
1	A	191	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	313	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	431	ILE	CA-CB-CG1	8.14	126.47	111.00
1	A	313	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	A	117	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	65	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	229	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	237	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	106	GLN	CB-CA-C	-6.99	96.42	110.40
1	A	51	LEU	CB-CA-C	-6.96	96.98	110.20
1	A	112	LYS	N-CA-CB	6.94	123.09	110.60
1	A	67	ARG	CA-C-N	-6.92	102.36	116.20
1	A	191	ARG	CD-NE-CZ	6.72	133.00	123.60
1	A	390	MET	CG-SD-CE	-6.58	89.67	100.20
1	A	257	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	401	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	413	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	65	ARG	N-CA-CB	6.39	122.10	110.60
1	A	59	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	195	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	208	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	39	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	59	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	2	SER	N-CA-CB	6.16	119.74	110.50
1	A	46	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	164	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	8	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	66	PHE	CB-CA-C	6.03	122.46	110.40
1	A	8	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	22	LYS	N-CA-CB	5.88	121.19	110.60
1	A	431	ILE	N-CA-CB	5.86	124.27	110.80
1	A	208	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	54	GLU	CB-CG-CD	-5.77	98.61	114.20
1	A	278	ASN	CA-CB-CG	-5.77	100.71	113.40
1	A	221	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	289	GLN	CB-CA-C	-5.71	98.98	110.40
1	A	289	GLN	CB-CG-CD	-5.69	96.81	111.60
1	A	12	ALA	CB-CA-C	5.69	118.63	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	191	ARG	N-CA-CB	-5.61	100.50	110.60
1	A	278	ASN	CB-CA-C	-5.55	99.29	110.40
1	A	174	SER	CB-CA-C	5.54	120.63	110.10
1	A	106	GLN	N-CA-CB	5.52	120.54	110.60
1	A	117	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	237	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	46	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	67	ARG	N-CA-C	-5.35	96.55	111.00
1	A	375	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	54	GLU	CG-CD-OE2	-5.27	107.75	118.30
1	A	191	ARG	CG-CD-NE	-5.27	100.73	111.80
1	A	61	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	344	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	221	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	177	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	219	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	A	228	MET	CG-SD-CE	-5.06	92.10	100.20
1	A	287	GLN	CB-CA-C	-5.03	100.34	110.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2	SER	CA
1	A	22	LYS	CA
1	A	431	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	GLN	Sidechain

## 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	3306	0	3297	130	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9	0	4	3	0
3	A	51	0	34	6	0
4	A	101	0	0	2	0
All	All	3467	0	3335	134	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 20.

All (134) 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:125:VAL:HG13	1:A:188:LYS:HE2	1.46	0.97
1:A:301:LEU:HD23	1:A:356:ILE:HD13	1.47	0.96
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.45	0.95
1:A:136:HIS:HD2	1:A:138:MET:H	1.10	0.92
1:A:103:THR:H	1:A:106:GLN:HG2	1.35	0.90
1:A:136:HIS:CD2	1:A:138:MET:H	1.92	0.86
1:A:163:LEU:HD12	1:A:165:THR:H	1.41	0.85
1:A:92:LEU:HD22	1:A:233:THR:HG23	1.59	0.84
2:A:702:MLT:H2	3:A:700:ACO:C	2.14	0.77
1:A:228:MET:HE3	1:A:232:LEU:HG	1.67	0.77
1:A:335:GLU:O	1:A:339:LYS:HG2	1.86	0.76
1:A:14:ILE:HG12	1:A:414:ALA:HB1	1.68	0.74
1:A:67:ARG:HA	4:A:548:HOH:O	1.87	0.74
1:A:301:LEU:HD23	1:A:356:ILE:CD1	2.17	0.74
1:A:305:ILE:HD13	1:A:357:VAL:HG22	1.68	0.74
1:A:86:GLU:CG	1:A:87:PRO:HD2	2.21	0.71
1:A:106:GLN:HA	1:A:106:GLN:HE21	1.56	0.70
1:A:103:THR:N	1:A:106:GLN:HG2	2.05	0.70
1:A:106:GLN:CA	1:A:106:GLN:HE21	2.05	0.70
1:A:136:HIS:CD2	1:A:137:PRO:HD2	2.28	0.69
1:A:86:GLU:HG3	1:A:87:PRO:HD2	1.72	0.69
1:A:287:GLN:HE21	1:A:287:GLN:N	1.91	0.69
1:A:282:LEU:HD22	1:A:393:TYR:HE2	1.58	0.68
1:A:185:VAL:O	1:A:189:ILE:HG13	1.92	0.68
1:A:225:THR:O	1:A:229:ARG:HG3	1.94	0.68
1:A:67:ARG:HB2	1:A:69:PHE:CD1	2.30	0.66
1:A:62:GLU:HG2	1:A:65:ARG:HH12	1.61	0.65
1:A:136:HIS:HD2	1:A:138:MET:N	1.91	0.64
1:A:324:ARG:HH11	1:A:369:ASN:HB2	1.63	0.63
1:A:335:GLU:O	1:A:339:LYS:HE2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ARG:O	1:A:338:LEU:HG	1.98	0.62
1:A:371:TRP:HB3	1:A:372:PRO:HD2	1.82	0.62
1:A:77:LEU:HD13	1:A:101:ILE:HD12	1.80	0.62
1:A:80:LYS:HD3	1:A:80:LYS:N	2.15	0.62
1:A:86:GLU:HG2	1:A:230:LEU:HD13	1.81	0.61
1:A:5:ASN:ND2	1:A:7:LYS:H	1.97	0.61
1:A:350:VAL:CG2	1:A:380:VAL:HG21	2.27	0.61
1:A:37:THR:OG1	1:A:40:MET:HG3	2.00	0.60
1:A:103:THR:H	1:A:106:GLN:CG	2.12	0.60
1:A:77:LEU:HD13	1:A:101:ILE:CD1	2.31	0.60
2:A:702:MLT:H2	3:A:700:ACO:CH3	2.31	0.60
1:A:67:ARG:HB2	1:A:69:PHE:CE1	2.37	0.60
1:A:5:ASN:HD22	1:A:7:LYS:H	1.48	0.59
1:A:282:LEU:HD22	1:A:393:TYR:CE2	2.38	0.58
1:A:338:LEU:HD23	1:A:347:PHE:CE1	2.38	0.58
1:A:287:GLN:H	1:A:287:GLN:HE21	1.51	0.57
1:A:163:LEU:HD12	1:A:164:ARG:N	2.19	0.57
2:A:702:MLT:H2	3:A:700:ACO:HH32	1.86	0.57
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.87	0.56
1:A:288:LEU:HD13	1:A:304:TYR:CG	2.41	0.56
1:A:233:THR:O	1:A:236:SER:HB2	2.08	0.54
1:A:194:TYR:CD2	1:A:389:GLU:HG3	2.43	0.53
1:A:346:MET:HG2	1:A:380:VAL:HG22	1.90	0.53
1:A:287:GLN:HB3	1:A:304:TYR:OH	2.08	0.53
1:A:91:GLY:HA3	4:A:514:HOH:O	2.08	0.53
1:A:71:ILE:HB	1:A:72:PRO:HD3	1.91	0.53
1:A:77:LEU:HB3	1:A:101:ILE:CD1	2.39	0.53
1:A:86:GLU:HG3	1:A:87:PRO:CD	2.39	0.52
1:A:194:TYR:O	1:A:195:ARG:HD3	2.09	0.52
1:A:65:ARG:HD3	1:A:68:GLY:O	2.09	0.52
1:A:375:ASP:OD1	3:A:700:ACO:HH33	2.09	0.51
1:A:78:LEU:O	1:A:80:LYS:HE3	2.09	0.51
1:A:204:ASP:H	1:A:212:ASN:HD21	1.57	0.51
1:A:136:HIS:CG	1:A:137:PRO:HD2	2.45	0.51
1:A:59:ASP:OD1	1:A:62:GLU:N	2.30	0.51
1:A:187:ALA:O	1:A:191:ARG:HB2	2.10	0.50
1:A:317:GLY:O	1:A:376:ALA:HB2	2.12	0.50
1:A:314:VAL:O	1:A:316:PRO:HD3	2.11	0.49
1:A:70:SER:HB2	1:A:72:PRO:HD2	1.93	0.49
1:A:114:TRP:CZ2	1:A:179:ILE:HG21	2.47	0.49
1:A:70:SER:OG	1:A:73:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HD3	1:A:177:ASP:OD2	2.13	0.49
1:A:137:PRO:HG2	1:A:391:ASN:O	2.13	0.49
1:A:132:PRO:HB2	1:A:134:ASN:OD1	2.13	0.48
1:A:90:GLU:O	1:A:110:LEU:HD13	2.13	0.48
1:A:262:PHE:O	1:A:265:ALA:HB3	2.14	0.48
1:A:59:ASP:HA	1:A:60:PRO:HD3	1.56	0.48
1:A:80:LYS:CD	1:A:80:LYS:N	2.76	0.48
1:A:369:ASN:OD1	1:A:371:TRP:HD1	1.96	0.48
1:A:163:LEU:CD1	1:A:164:ARG:N	2.77	0.48
1:A:162:ILE:HD12	1:A:167:TYR:CE1	2.49	0.47
1:A:177:ASP:O	1:A:181:LYS:HG3	2.14	0.47
1:A:301:LEU:HD22	1:A:352:GLN:OE1	2.15	0.47
1:A:347:PHE:HA	1:A:380:VAL:HG11	1.96	0.47
1:A:338:LEU:HD23	1:A:347:PHE:HE1	1.80	0.47
1:A:305:ILE:CD1	1:A:357:VAL:HG22	2.43	0.47
1:A:123:HIS:HE1	1:A:147:ALA:O	1.97	0.47
1:A:53:TYR:CE2	1:A:408:GLN:HG2	2.50	0.47
1:A:53:TYR:CD2	1:A:408:GLN:HG2	2.50	0.46
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.57	0.46
1:A:171:VAL:HG21	1:A:413:ARG:HG3	1.97	0.46
1:A:266:MET:CE	1:A:266:MET:HA	2.44	0.46
1:A:287:GLN:NE2	1:A:287:GLN:CA	2.78	0.46
1:A:94:TRP:HE3	1:A:110:LEU:HD21	1.80	0.46
1:A:273:LEU:HD23	1:A:273:LEU:HA	1.67	0.46
1:A:86:GLU:HG2	1:A:230:LEU:HB2	1.98	0.45
1:A:338:LEU:HD21	1:A:347:PHE:HZ	1.81	0.45
1:A:61:ASP:OD2	1:A:325:LYS:HE2	2.17	0.45
1:A:136:HIS:CD2	1:A:137:PRO:CD	2.99	0.44
1:A:330:TYR:CD2	1:A:372:PRO:HB2	2.53	0.44
1:A:323:LEU:O	1:A:324:ARG:NH1	2.51	0.44
1:A:133:THR:HA	1:A:193:LEU:HD11	1.99	0.44
1:A:124:VAL:HG21	1:A:148:LEU:HD23	1.99	0.44
1:A:67:ARG:H	1:A:69:PHE:H	1.66	0.44
1:A:338:LEU:CD2	1:A:347:PHE:CZ	3.01	0.44
1:A:352:GLN:O	1:A:356:ILE:HD12	2.17	0.44
1:A:163:LEU:HD12	1:A:165:THR:N	2.22	0.44
1:A:168:TRP:CZ2	1:A:169:GLU:HG2	2.53	0.43
1:A:373:ASN:ND2	3:A:700:ACO:H22	2.33	0.43
1:A:301:LEU:O	1:A:305:ILE:HG13	2.18	0.43
1:A:192:ASN:HD22	1:A:192:ASN:HA	1.51	0.43
1:A:120:LEU:HA	1:A:120:LEU:HD12	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASN:C	1:A:5:ASN:HD22	2.22	0.43
1:A:287:GLN:HE21	1:A:287:GLN:CA	2.32	0.43
1:A:431:ILE:HD12	1:A:431:ILE:HG21	1.31	0.43
1:A:338:LEU:HD21	1:A:347:PHE:CZ	2.53	0.43
1:A:162:ILE:CD1	1:A:167:TYR:CE1	3.02	0.42
1:A:327:ASP:O	1:A:330:TYR:HB3	2.18	0.42
1:A:177:ASP:HB3	1:A:181:LYS:HE2	2.01	0.42
1:A:95:LEU:HA	1:A:100:GLN:O	2.19	0.42
1:A:106:GLN:NE2	1:A:106:GLN:CA	2.80	0.42
1:A:339:LYS:HA	1:A:339:LYS:HD3	1.95	0.42
1:A:309:LEU:HD22	1:A:364:GLN:HE22	1.84	0.42
3:A:700:ACO:N7A	3:A:700:ACO:OAP	2.49	0.41
1:A:193:LEU:HA	1:A:193:LEU:HD12	1.85	0.41
1:A:428:ASP:O	1:A:431:ILE:HG22	2.21	0.41
1:A:162:ILE:HD12	1:A:167:TYR:HE1	1.86	0.40
1:A:324:ARG:HA	1:A:324:ARG:HD3	1.75	0.40
1:A:14:ILE:HD13	1:A:168:TRP:CE2	2.57	0.40
1:A:206:LYS:HB2	1:A:206:LYS:HE3	1.33	0.40
1:A:145:ILE:HD13	1:A:262:PHE:HD2	1.87	0.40
1:A:275:GLY:O	1:A:278:ASN:HB2	2.21	0.40
1:A:323:LEU:O	1:A:324:ARG:HD3	2.21	0.40
1:A:287:GLN:NE2	1:A:287:GLN:N	2.66	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)
1:A:127:MET:CE	1:A:127:MET:CE[2_555]	1.83	0.37

## 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	423/433 (98%)	402 (95%)	20 (5%)	1 (0%)	51 41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLU

### 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%)	302 (88%)	43 (12%)	5 2

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

Mol	Chain	Res	Type
1	A	5	ASN
1	A	13	LEU
1	A	20	ARG
1	A	22	LYS
1	A	23	THR
1	A	26	GLN
1	A	27	GLN
1	A	46	ARG
1	A	51	LEU
1	A	62	GLU
1	A	65	ARG
1	A	76	LYS
1	A	80	LYS
1	A	86	GLU
1	A	101	ILE
1	A	106	GLN
1	A	112	LYS
1	A	120	LEU
1	A	149	ASN
1	A	150	SER

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Mol	Chain	Res	Type
1	A	162	ILE
1	A	163	LEU
1	A	170	MET
1	A	191	ARG
1	A	193	LEU
1	A	199	SER
1	A	203	ILE
1	A	205	SER
1	A	206	LYS
1	A	223	GLN
1	A	236	SER
1	A	238	HIS
1	A	287	GLN
1	A	289	GLN
1	A	341	LEU
1	A	346	MET
1	A	352	GLN
1	A	353	LEU
1	A	383	GLN
1	A	389	GLU
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
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

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Mol	Chain	Res	Type
1	A	289	GLN
1	A	310	ASN
1	A	340	HIS
1	A	364	GLN
1	A	391	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](#)

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	$\# Z  > 2$
3	ACO	A	700	-	46,53,53	1.52	5 (10%)	53,79,79	1.41	7 (13%)
2	MLT	A	702	-	2,8,8	3.06	1 (50%)	4,10,10	2.75	2 (50%)

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	ACO	A	700	-	-	0/47/67/67	0/3/3/3
2	MLT	A	702	-	-	0/2/8/8	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	ACO	C2A-N1A	2.10	1.37	1.33
3	A	700	ACO	O4B-C1B	2.72	1.45	1.41
3	A	700	ACO	P3B-O7A	2.89	1.60	1.50
3	A	700	ACO	O9P-C9P	3.90	1.31	1.23
2	A	702	MLT	O3-C2	4.27	1.52	1.42
3	A	700	ACO	P3B-O3B	5.79	1.69	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	ACO	CEP-CBP-CCP	-4.62	101.58	108.37
3	A	700	ACO	N3A-C2A-N1A	-2.48	126.70	128.86
3	A	700	ACO	O-C-S1P	-2.48	110.39	122.65
3	A	700	ACO	C4B-O4B-C1B	-2.40	107.22	109.77
3	A	700	ACO	C5B-C4B-C3B	2.08	121.36	114.30
2	A	702	MLT	O3-C2-C3	2.30	113.70	108.65
3	A	700	ACO	CEP-CBP-CAP	2.53	113.21	108.82
3	A	700	ACO	CDP-CBP-CCP	2.92	112.66	108.37
2	A	702	MLT	C4-C3-C2	4.76	120.06	113.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	ACO	6	0
2	A	702	MLT	3	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.