Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 11:41 am BST

PDB ID	:	6CTS
Title	:	PROPOSED MECHANISM FOR THE CONDENSATION REACTION OF CITRATE SYNTHASE. 1.9-ANGSTROMS STRUCTURE OF THE TERNARY COMPLEX WITH OXALOACETATE AND CARBOXYMETHYL COENZYME A
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Deposited on	:	1989-11-16
Resolution	:	2.50 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

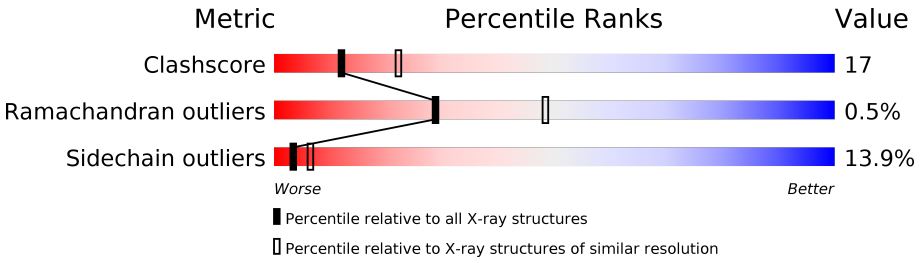
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	56% 34% 7%

2 Entry composition

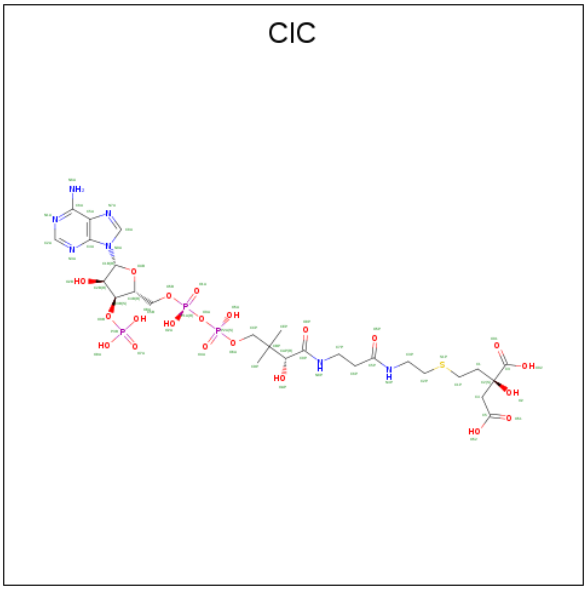
There are 3 unique types of molecules in this entry. The entry contains 3466 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CITRYL-THIOETHER-COENZYME *A (three-letter code: CIC) (formula: $C_{27}H_{44}N_7O_{21}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	59	27	7	21	3	1	0	0

- Molecule 3 is water.

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

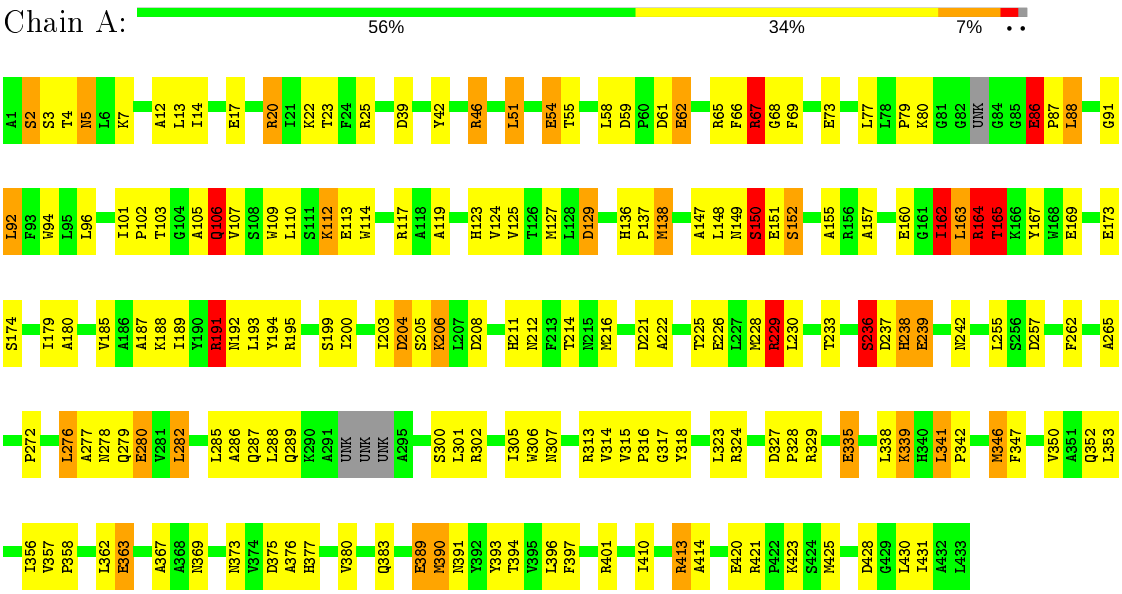
3 Residue-property plots (i)

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. 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. 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 (i)

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, α, β, γ	104.00Å 78.10Å 58.30Å 90.00° 78.90° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.110 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3466	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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: CIC

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	0.82	16/3386 (0.5%)	1.68	70/4598 (1.5%)

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	1	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	GLU	CD-OE2	6.47	1.32	1.25
1	A	335	GLU	CD-OE2	5.92	1.32	1.25
1	A	160	GLU	CD-OE2	5.91	1.32	1.25
1	A	173	GLU	CD-OE2	5.85	1.32	1.25
1	A	239	GLU	CD-OE2	5.67	1.31	1.25
1	A	169	GLU	CD-OE2	5.60	1.31	1.25
1	A	226	GLU	CD-OE2	5.50	1.31	1.25
1	A	86	GLU	CD-OE2	5.38	1.31	1.25
1	A	17	GLU	CD-OE2	5.29	1.31	1.25
1	A	113	GLU	CD-OE2	5.27	1.31	1.25
1	A	62	GLU	CD-OE2	5.24	1.31	1.25
1	A	280	GLU	CD-OE2	5.21	1.31	1.25
1	A	363	GLU	CD-OE2	5.08	1.31	1.25
1	A	420	GLU	CD-OE2	5.08	1.31	1.25
1	A	214	THR	CB-OG1	5.06	1.53	1.43
1	A	73	GLU	CD-OE2	5.02	1.31	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	ARG	NE-CZ-NH2	-19.59	110.50	120.30
1	A	229	ARG	NE-CZ-NH1	17.67	129.13	120.30
1	A	191	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	A	191	ARG	NE-CZ-NH2	-13.68	113.46	120.30
1	A	229	ARG	CD-NE-CZ	12.93	141.70	123.60
1	A	67	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	A	191	ARG	CD-NE-CZ	10.63	138.48	123.60
1	A	302	ARG	CD-NE-CZ	-9.33	110.53	123.60
1	A	313	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	313	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	65	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	65	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	51	LEU	CB-CA-C	-8.44	94.16	110.20
1	A	67	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	12	ALA	CB-CA-C	7.73	121.70	110.10
1	A	221	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	A	39	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	302	ARG	NE-CZ-NH1	-7.21	116.69	120.30
1	A	221	ASP	CB-CG-OD1	7.14	124.72	118.30
1	A	117	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	66	PHE	CB-CA-C	6.95	124.29	110.40
1	A	208	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	286	ALA	CB-CA-C	6.85	120.38	110.10
1	A	174	SER	CB-CA-C	6.83	123.07	110.10
1	A	46	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	318	TYR	CB-CG-CD1	-6.70	116.98	121.00
1	A	401	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	67	ARG	CA-C-N	-6.67	102.86	116.20
1	A	237	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	42	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	A	61	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	22	LYS	N-CA-CB	6.50	122.30	110.60
1	A	59	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	208	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	257	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	A	119	ALA	CB-CA-C	6.15	119.33	110.10
1	A	59	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	428	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	106	GLN	N-CA-CB	5.80	121.05	110.60
1	A	152	SER	N-CA-CB	5.80	119.20	110.50
1	A	237	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	165	THR	CA-CB-CG2	5.56	120.18	112.40
1	A	431	ILE	N-CA-CB	5.55	123.57	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	92	LEU	CA-CB-CG	-5.52	102.61	115.30
1	A	431	ILE	CA-CB-CG1	5.50	121.45	111.00
1	A	367	ALA	CB-CA-C	-5.47	101.90	110.10
1	A	25	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	54	GLU	CG-CD-OE2	-5.39	107.52	118.30
1	A	191	ARG	CG-CD-NE	-5.39	100.48	111.80
1	A	150	SER	CB-CA-C	-5.38	99.87	110.10
1	A	20	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	257	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	164	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	431	ILE	CG1-CB-CG2	-5.30	99.74	111.40
1	A	222	ALA	CB-CA-C	5.28	118.02	110.10
1	A	162	ILE	CB-CA-C	-5.26	101.08	111.60
1	A	300	SER	N-CA-CB	5.22	118.33	110.50
1	A	157	ALA	CB-CA-C	5.19	117.89	110.10
1	A	67	ARG	CD-NE-CZ	5.18	130.85	123.60
1	A	42	TYR	CB-CG-CD2	5.13	124.08	121.00
1	A	390	MET	CG-SD-CE	-5.12	92.00	100.20
1	A	68	GLY	N-CA-C	-5.12	100.31	113.10
1	A	2	SER	N-CA-C	5.09	124.74	111.00
1	A	112	LYS	N-CA-CB	5.09	119.76	110.60
1	A	431	ILE	CB-CA-C	5.07	121.74	111.60
1	A	180	ALA	N-CA-CB	-5.05	103.02	110.10
1	A	138	MET	CG-SD-CE	-5.03	92.15	100.20
1	A	106	GLN	CB-CA-C	-5.02	100.36	110.40
1	A	233	THR	CA-CB-CG2	-5.01	105.39	112.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	431	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	ARG	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	115	4
2	A	59	0	38	4	2
3	A	101	0	0	3	0
All	All	3466	0	3335	115	4

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 17.

All (115) 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:86:GLU:HG2	1:A:230:LEU:HB2	1.39	1.03
1:A:125:VAL:HG13	1:A:188:LYS:HE2	1.43	0.97
1:A:86:GLU:HG3	1:A:87:PRO:HD2	1.48	0.93
1:A:94:TRP:HB3	1:A:102:PRO:HG3	1.60	0.81
1:A:301:LEU:HD23	1:A:356:ILE:HD13	1.63	0.80
1:A:103:THR:H	1:A:106:GLN:HG2	1.48	0.78
1:A:14:ILE:HG12	1:A:414:ALA:HB1	1.66	0.75
1:A:67:ARG:HA	3:A:548:HOH:O	1.86	0.75
1:A:77:LEU:HB3	1:A:101:ILE:HD13	1.68	0.74
1:A:346:MET:HG2	1:A:380:VAL:HG22	1.69	0.74
1:A:305:ILE:HD13	1:A:357:VAL:HG22	1.71	0.72
1:A:92:LEU:HD23	1:A:236:SER:OG	1.89	0.71
1:A:352:GLN:O	1:A:356:ILE:HD12	1.90	0.71
1:A:194:TYR:CD2	1:A:389:GLU:HG3	2.26	0.71
1:A:136:HIS:HD2	1:A:138:MET:H	1.40	0.68
1:A:106:GLN:CA	1:A:106:GLN:HE21	2.06	0.68
1:A:77:LEU:HD13	1:A:101:ILE:CD1	2.24	0.67
1:A:301:LEU:O	1:A:305:ILE:HG13	1.94	0.67
1:A:136:HIS:CD2	1:A:137:PRO:HD2	2.30	0.67
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.77	0.66
1:A:86:GLU:CG	1:A:87:PRO:HD2	2.22	0.66
1:A:163:LEU:HD12	1:A:165:THR:H	1.62	0.65
1:A:228:MET:HE1	1:A:396:LEU:HD22	1.76	0.65
1:A:335:GLU:O	1:A:339:LYS:HE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:HG3	1:A:87:PRO:CD	2.26	0.60
1:A:327:ASP:OD2	1:A:329:ARG:HB2	2.01	0.60
1:A:88:LEU:HD12	1:A:229:ARG:HD2	1.82	0.59
1:A:301:LEU:HD23	1:A:356:ILE:CD1	2.31	0.59
1:A:77:LEU:HB3	1:A:101:ILE:CD1	2.33	0.58
1:A:282:LEU:HD22	1:A:393:TYR:HE2	1.67	0.58
1:A:185:VAL:O	1:A:189:ILE:HG13	2.05	0.56
1:A:136:HIS:CD2	1:A:138:MET:H	2.22	0.56
1:A:79:PRO:HG2	1:A:107:VAL:HG21	1.87	0.56
1:A:285:LEU:O	1:A:288:LEU:HB3	2.06	0.55
1:A:136:HIS:CG	1:A:137:PRO:HD2	2.41	0.55
1:A:77:LEU:HD13	1:A:101:ILE:HD11	1.87	0.55
1:A:204:ASP:H	1:A:212:ASN:HD21	1.54	0.54
1:A:341:LEU:N	1:A:342:PRO:HD3	2.22	0.54
1:A:163:LEU:HD12	1:A:164:ARG:N	2.23	0.54
1:A:277:ALA:HB3	1:A:375:ASP:OD1	2.08	0.54
1:A:279:GLN:HB2	1:A:390:MET:O	2.08	0.53
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.90	0.53
1:A:103:THR:N	1:A:106:GLN:HG2	2.20	0.53
1:A:338:LEU:HD23	1:A:347:PHE:CE1	2.44	0.53
1:A:323:LEU:O	1:A:324:ARG:NH1	2.42	0.53
1:A:317:GLY:O	1:A:376:ALA:HB2	2.09	0.52
1:A:187:ALA:O	1:A:191:ARG:HB2	2.11	0.51
1:A:106:GLN:HA	1:A:106:GLN:HE21	1.76	0.51
1:A:123:HIS:HE1	1:A:147:ALA:O	1.93	0.51
1:A:225:THR:O	1:A:229:ARG:HG2	2.11	0.51
1:A:262:PHE:O	1:A:265:ALA:HB3	2.11	0.51
1:A:413:ARG:HD2	3:A:588:HOH:O	2.11	0.50
1:A:194:TYR:O	1:A:195:ARG:HD3	2.11	0.50
1:A:67:ARG:HB2	1:A:69:PHE:CD1	2.47	0.50
1:A:162:ILE:HD12	1:A:167:TYR:CE1	2.47	0.49
1:A:338:LEU:HD23	1:A:347:PHE:HE1	1.77	0.49
1:A:282:LEU:HD22	1:A:393:TYR:CE2	2.47	0.49
1:A:163:LEU:CD1	1:A:164:ARG:N	2.76	0.49
1:A:306:TRP:HZ2	1:A:363:GLU:HG2	1.79	0.48
1:A:162:ILE:HD12	1:A:167:TYR:CD1	2.48	0.48
1:A:152:SER:HB3	1:A:155:ALA:HB3	1.96	0.48
1:A:77:LEU:HD13	1:A:101:ILE:HD12	1.95	0.47
1:A:106:GLN:NE2	1:A:106:GLN:CA	2.77	0.47
1:A:206:LYS:HB2	1:A:206:LYS:HE3	1.65	0.47
1:A:314:VAL:O	1:A:316:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:OD2	1:A:206:LYS:N	2.34	0.47
1:A:305:ILE:CD1	1:A:357:VAL:HG22	2.43	0.47
1:A:346:MET:HB3	1:A:380:VAL:HG13	1.97	0.46
1:A:129:ASP:OD2	1:A:188:LYS:NZ	2.29	0.46
1:A:162:ILE:CD1	1:A:167:TYR:CD1	2.99	0.46
1:A:272:PRO:HA	1:A:276:LEU:HB3	1.97	0.46
1:A:410:ILE:HG21	1:A:410:ILE:HD13	1.67	0.45
1:A:204:ASP:H	1:A:212:ASN:ND2	2.14	0.45
1:A:279:GLN:NE2	1:A:280:GLU:OE2	2.50	0.45
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.54	0.44
1:A:164:ARG:HG3	1:A:164:ARG:H	1.62	0.44
1:A:373:ASN:ND2	2:A:700:CIC:H31	2.32	0.44
1:A:347:PHE:HA	1:A:380:VAL:HG11	1.99	0.44
1:A:103:THR:OG1	1:A:105:ALA:HB3	2.17	0.44
1:A:327:ASP:HA	1:A:328:PRO:HD2	1.91	0.44
1:A:242:ASN:HB3	2:A:700:CIC:C5	2.47	0.44
1:A:150:SER:HB3	1:A:151:GLU:HG2	1.99	0.44
1:A:4:THR:HG22	1:A:5:ASN:N	2.32	0.44
1:A:278:ASN:HD22	1:A:394:THR:HA	1.82	0.44
1:A:350:VAL:CG2	1:A:380:VAL:HG21	2.47	0.44
1:A:324:ARG:HA	1:A:324:ARG:HD3	1.68	0.44
1:A:106:GLN:N	1:A:106:GLN:HE21	2.16	0.43
1:A:192:ASN:HA	1:A:192:ASN:HD22	1.47	0.43
1:A:339:LYS:HA	1:A:339:LYS:HD3	1.55	0.43
1:A:194:TYR:CG	1:A:389:GLU:HG3	2.54	0.43
1:A:3:SER:OG	1:A:4:THR:N	2.47	0.43
1:A:191:ARG:HD3	1:A:200:ILE:HG22	2.01	0.43
1:A:67:ARG:N	1:A:69:PHE:H	2.17	0.43
1:A:152:SER:HB3	1:A:155:ALA:CB	2.49	0.42
1:A:109:TRP:CZ3	1:A:110:LEU:HD23	2.54	0.42
1:A:124:VAL:HG21	1:A:148:LEU:HD23	2.00	0.42
1:A:5:ASN:HD22	1:A:7:LYS:H	1.68	0.42
1:A:77:LEU:CB	1:A:101:ILE:HD13	2.45	0.42
1:A:58:LEU:HD22	1:A:238:HIS:CE1	2.54	0.42
1:A:86:GLU:HG2	1:A:230:LEU:HD13	2.02	0.42
1:A:114:TRP:CZ2	1:A:179:ILE:HG21	2.55	0.42
1:A:124:VAL:HG21	1:A:148:LEU:CD2	2.50	0.41
1:A:194:TYR:CE2	1:A:389:GLU:HG3	2.54	0.41
1:A:191:ARG:HD3	1:A:216:MET:O	2.20	0.41
1:A:211:HIS:HD2	1:A:211:HIS:O	2.02	0.41
1:A:137:PRO:HG2	1:A:391:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLY:HA3	3:A:514:HOH:O	2.21	0.41
1:A:101:ILE:HA	1:A:102:PRO:HD3	1.86	0.41
1:A:324:ARG:HH11	1:A:369:ASN:HB2	1.85	0.41
1:A:315:VAL:O	2:A:700:CIC:N6A	2.51	0.41
1:A:341:LEU:N	1:A:342:PRO:CD	2.84	0.40
1:A:55:THR:HG22	1:A:96:LEU:O	2.22	0.40
1:A:110:LEU:HG	1:A:110:LEU:H	1.72	0.40
1:A:373:ASN:HD21	2:A:700:CIC:H31	1.86	0.40
1:A:377:HIS:O	1:A:377:HIS:ND1	2.53	0.40

All (4) 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]	1.97	0.23
1:A:58:LEU:O	1:A:423:LYS:NZ[2_555]	2.06	0.14
1:A:164:ARG:NH2	2:A:700:CIC:O8A[2_555]	2.10	0.10
1:A:421:ARG:NH2	2:A:700:CIC:O51[2_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	423/433 (98%)	402 (95%)	19 (4%)	2 (0%)	29 48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLU
1	A	236	SER

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	345/345 (100%)	297 (86%)	48 (14%)	3 6

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	5	ASN
1	A	13	LEU
1	A	20	ARG
1	A	23	THR
1	A	46	ARG
1	A	51	LEU
1	A	54	GLU
1	A	62	GLU
1	A	67	ARG
1	A	80	LYS
1	A	86	GLU
1	A	88	LEU
1	A	106	GLN
1	A	112	LYS
1	A	149	ASN
1	A	150	SER
1	A	162	ILE
1	A	163	LEU
1	A	164	ARG
1	A	165	THR
1	A	191	ARG
1	A	193	LEU
1	A	199	SER
1	A	203	ILE
1	A	204	ASP
1	A	205	SER
1	A	206	LYS
1	A	229	ARG
1	A	236	SER

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Mol	Chain	Res	Type
1	A	238	HIS
1	A	255	LEU
1	A	276	LEU
1	A	282	LEU
1	A	287	GLN
1	A	289	GLN
1	A	307	ASN
1	A	339	LYS
1	A	341	LEU
1	A	346	MET
1	A	353	LEU
1	A	362	LEU
1	A	383	GLN
1	A	389	GLU
1	A	397	PHE
1	A	413	ARG
1	A	425	MET
1	A	430	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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
1	A	310	ASN
1	A	340	HIS
1	A	364	GLN
1	A	383	GLN

5.3.3 RNA

There are no RNA molecules 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

1 ligand is 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	CIC	A	700	-	47,61,61	1.65	8 (17%)	57,91,91	2.13	11 (19%)

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	CIC	A	700	-	-	6/53/81/81	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	CIC	P3B-O3B	6.21	1.71	1.59
2	A	700	CIC	C4-C2	-4.23	1.48	1.54
2	A	700	CIC	O9P-C9P	3.79	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	CIC	P3B-O7A	2.83	1.59	1.50
2	A	700	CIC	O4B-C1B	2.58	1.44	1.41
2	A	700	CIC	C2B-C1B	-2.13	1.50	1.53
2	A	700	CIC	O4B-C4B	2.05	1.49	1.45
2	A	700	CIC	C2A-N1A	2.00	1.37	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	CIC	C2-C4-C5	8.09	127.94	114.98
2	A	700	CIC	C1-C2-C3	-6.74	99.65	111.52
2	A	700	CIC	O8A-P3B-O3B	-5.00	83.61	105.99
2	A	700	CIC	O4B-C1B-C2B	-4.80	99.91	106.93
2	A	700	CIC	C5A-C6A-N6A	3.43	125.56	120.35
2	A	700	CIC	C3P-N4P-C5P	-3.35	116.62	122.84
2	A	700	CIC	O3B-C3B-C4B	2.74	119.99	110.08
2	A	700	CIC	O3B-P3B-O7A	2.63	119.55	109.39
2	A	700	CIC	C5A-C6A-N1A	-2.55	114.57	120.35
2	A	700	CIC	CEP-CBP-CCP	-2.13	104.76	108.23
2	A	700	CIC	C2B-C3B-C4B	-2.05	99.59	103.22

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	CIC	C2-C1-C1P-S1P
2	A	700	CIC	C3B-O3B-P3B-O8A
2	A	700	CIC	CEP-CBP-CCP-O6A
2	A	700	CIC	CDP-CBP-CCP-O6A
2	A	700	CIC	C3P-C2P-S1P-C1P
2	A	700	CIC	C1-C1P-S1P-C2P

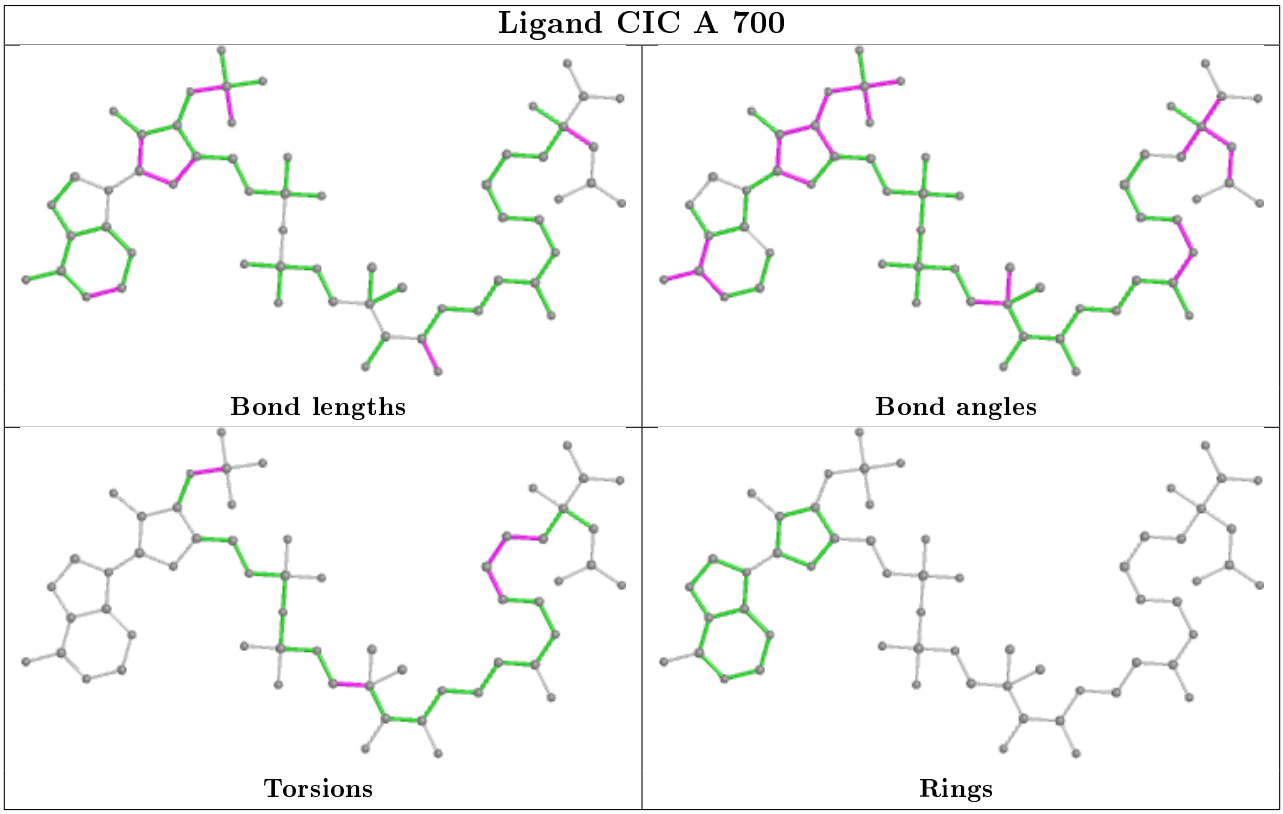
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	CIC	4	2

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.