



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:00 AM UTC

PDB ID : 3CSC / pdb_00003csc
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 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

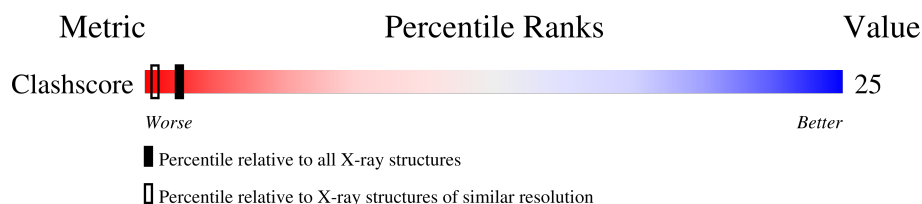
1 Overall quality at a glance

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	190562	8410 (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 of 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	56% 36% 7% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LMR	A	702	-	X	-	-

2 Entry composition [i](#)

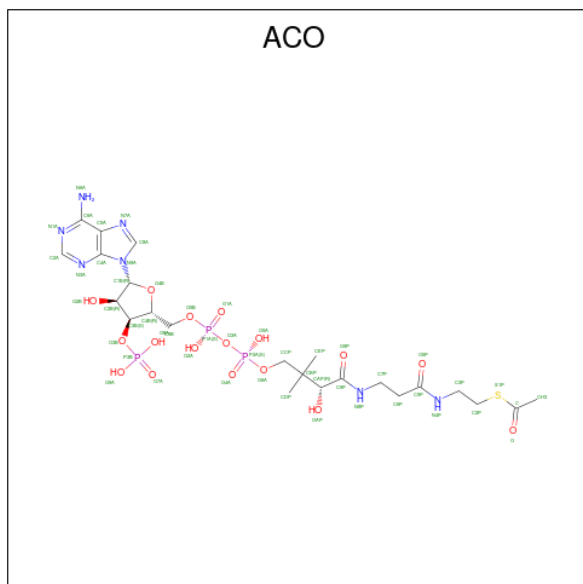
There are 4 unique types of molecules in this entry. The entry contains 3467 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

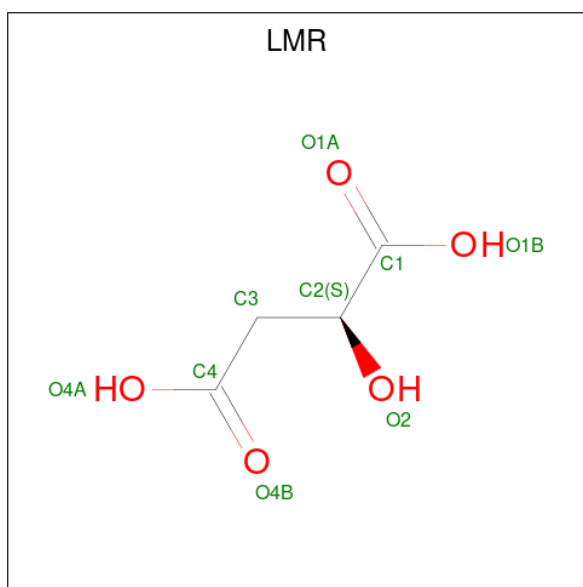
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3306	2115	571	603	17	0	0	0

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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-hydroxybutanedioic acid (CCD ID: LMR) (formula: C₄H₆O₅).



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

- Molecule 4 is water.

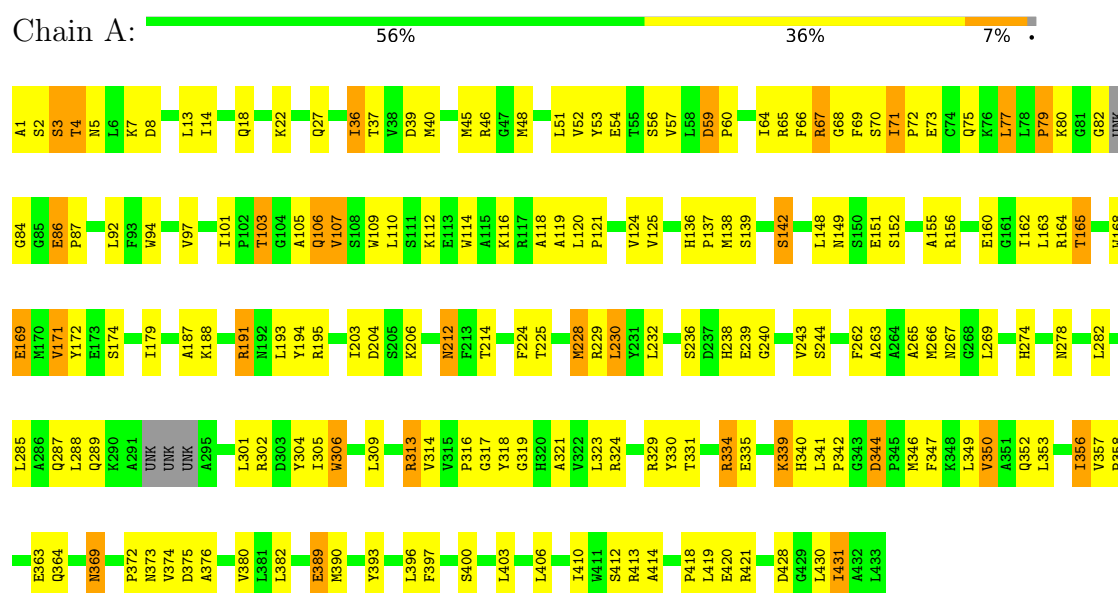
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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



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, α , β , γ	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 ²)	22.0	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: 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	1.65	27/3386 (0.8%)	1.75	74/4598 (1.6%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	ILE	CA-CB	-15.65	1.46	1.54
1	A	2	SER	C-N	7.40	1.39	1.33
1	A	278	ASN	CA-CB	6.71	1.64	1.53
1	A	309	LEU	N-CA	-6.55	1.38	1.46
1	A	103	THR	CB-OG1	6.51	1.54	1.43
1	A	306	TRP	C-N	-6.45	1.25	1.34
1	A	54	GLU	CA-C	-6.33	1.44	1.52
1	A	397	PHE	N-CA	6.29	1.53	1.46
1	A	165	THR	CB-OG1	6.26	1.53	1.43
1	A	39	ASP	N-CA	-6.21	1.38	1.46
1	A	369	ASN	C-O	-6.14	1.20	1.25
1	A	263	ALA	CA-C	6.05	1.60	1.52
1	A	239	GLU	CD-OE2	5.93	1.36	1.25
1	A	13	LEU	CA-C	5.88	1.60	1.52
1	A	107	VAL	N-CA	-5.80	1.39	1.46
1	A	54	GLU	CD-OE2	5.80	1.36	1.25
1	A	27	GLN	N-CA	-5.74	1.38	1.46
1	A	412	SER	C-O	5.68	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	VAL	CA-C	-5.55	1.46	1.52
1	A	36	ILE	N-CA	-5.35	1.40	1.46
1	A	57	VAL	CA-C	-5.29	1.46	1.52
1	A	142	SER	CA-C	5.18	1.59	1.52
1	A	56	SER	CA-C	-5.09	1.46	1.52
1	A	8	ASP	CG-OD2	5.05	1.34	1.25
1	A	171	VAL	N-CA	-5.04	1.40	1.46
1	A	396	LEU	CA-C	-5.03	1.46	1.52
1	A	119	ALA	CA-C	-5.01	1.46	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	LYS	N-CA-CB	8.83	122.81	109.91
1	A	289	GLN	CB-CG-CD	-8.77	97.70	112.60
1	A	278	ASN	CA-CB-CG	-8.60	104.00	112.60
1	A	66	PHE	O-C-N	-8.45	112.14	122.11
1	A	54	GLU	CB-CG-CD	-7.72	99.48	112.60
1	A	86	GLU	CB-CA-C	7.52	119.69	108.86
1	A	350	VAL	N-CA-CB	7.38	120.58	110.54
1	A	174	SER	CB-CA-C	7.34	123.02	110.84
1	A	289	GLN	CB-CA-C	-7.14	96.20	110.42
1	A	344	ASP	CA-C-N	7.07	126.90	119.05
1	A	344	ASP	C-N-CA	7.07	126.90	119.05
1	A	106	GLN	N-CA-CB	6.95	120.44	110.16
1	A	66	PHE	CA-C-N	-6.78	108.60	121.54
1	A	66	PHE	C-N-CA	-6.78	108.60	121.54
1	A	389	GLU	CA-C-N	6.69	129.24	120.28
1	A	389	GLU	C-N-CA	6.69	129.24	120.28
1	A	54	GLU	N-CA-C	6.65	122.49	113.97
1	A	22	LYS	N-CA-C	6.33	117.87	110.97
1	A	86	GLU	N-CA-CB	6.33	117.69	110.03
1	A	228	MET	CG-SD-CE	-6.29	87.05	100.90
1	A	86	GLU	N-CA-C	6.28	118.95	110.29
1	A	334	ARG	CD-NE-CZ	-6.27	115.62	124.40
1	A	431	ILE	N-CA-CB	6.17	118.94	110.54
1	A	1	ALA	N-CA-CB	6.15	119.63	110.40
1	A	431	ILE	CA-CB-CG1	6.14	120.84	110.40
1	A	59	ASP	CA-C-N	6.12	126.58	119.47
1	A	59	ASP	C-N-CA	6.12	126.58	119.47
1	A	1	ALA	CB-CA-C	6.11	119.67	110.50
1	A	403	LEU	N-CA-CB	6.04	118.95	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLY	N-CA-C	-5.99	98.99	113.18
1	A	51	LEU	CA-C-N	-5.95	115.39	123.12
1	A	51	LEU	C-N-CA	-5.95	115.39	123.12
1	A	77	LEU	N-CA-C	5.94	120.60	113.23
1	A	79	PRO	N-CA-CB	5.85	108.78	103.34
1	A	67	ARG	CB-CA-C	-5.84	98.79	110.42
1	A	412	SER	O-C-N	5.83	128.16	122.09
1	A	418	PRO	CB-CA-C	-5.79	102.00	111.56
1	A	106	GLN	CB-CG-CD	-5.78	102.78	112.60
1	A	212	ASN	N-CA-CB	5.70	119.11	110.28
1	A	4	THR	N-CA-C	5.63	118.41	109.96
1	A	66	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	244	SER	CB-CA-C	5.60	119.59	110.96
1	A	344	ASP	O-C-N	5.56	126.84	121.28
1	A	239	GLU	CB-CA-C	5.54	121.45	110.42
1	A	321	ALA	CA-C-N	-5.54	116.96	122.77
1	A	321	ALA	C-N-CA	-5.54	116.96	122.77
1	A	420	GLU	CA-C-N	-5.52	116.03	122.00
1	A	420	GLU	C-N-CA	-5.52	116.03	122.00
1	A	339	LYS	N-CA-CB	5.49	118.38	110.20
1	A	106	GLN	CB-CA-C	-5.45	101.59	110.85
1	A	289	GLN	CG-CD-NE2	-5.44	108.23	116.40
1	A	22	LYS	CB-CA-C	5.43	119.32	110.96
1	A	340	HIS	N-CA-C	5.41	120.90	113.97
1	A	313	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	A	66	PHE	CB-CA-C	5.32	119.84	111.39
1	A	191	ARG	N-CA-CB	-5.31	102.37	110.07
1	A	313	ARG	CA-C-N	-5.26	115.02	122.34
1	A	313	ARG	C-N-CA	-5.26	115.02	122.34
1	A	230	LEU	CB-CA-C	-5.26	102.58	110.90
1	A	67	ARG	N-CA-C	-5.26	99.59	110.80
1	A	382	LEU	CA-C-N	5.25	127.63	120.54
1	A	382	LEU	C-N-CA	5.25	127.63	120.54
1	A	306	TRP	CA-C-O	5.22	125.97	119.97
1	A	243	VAL	N-CA-C	5.21	115.83	110.36
1	A	313	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	A	350	VAL	CB-CA-C	5.19	119.15	112.14
1	A	52	VAL	N-CA-CB	5.19	118.00	111.46
1	A	356	ILE	N-CA-C	5.14	116.31	111.48
1	A	105	ALA	CA-C-N	-5.09	113.06	120.29
1	A	105	ALA	C-N-CA	-5.09	113.06	120.29
1	A	3	SER	N-CA-C	5.07	118.03	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLU	CG-CD-OE2	-5.07	106.74	118.40
1	A	169	GLU	N-CA-C	5.07	116.80	111.28
1	A	71	ILE	O-C-N	5.04	123.65	120.42

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 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	164	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	169	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 25.

All (169) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:282:LEU:HD23	1:A:390:MET:HE2	1.67	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: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:80:LYS:N	1:A:80:LYS:HD2	2.09	0.66
1:A:124:VAL:HG21	1:A:148:LEU:HD23	1.78	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:5:ASN:HD22	1:A:5:ASN:C	2.07	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
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:349:LEU:O	1:A:353:LEU:HD22	2.02	0.58
1:A:428:ASP:O	1:A:431:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:92:LEU:HD23	1:A:236:SER:OG	2.05	0.56
1:A:317:GLY:O	1:A:376:ALA:HB2	2.04	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:319:GLY:HA2	1:A:369:ASN:O	2.05	0.55
1:A:323:LEU:O	1:A:324:ARG:NH1	2.40	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:306:TRP:HZ2	1:A:363:GLU:CD	2.14	0.55
1:A:106:GLN:HE21	1:A:106:GLN:HA	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
1:A:82:GLY:C	1:A:84:GLY:HA2	2.33	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: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: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:64:ILE:HG13	1:A:65:ARG:N	2.24	0.51
1:A:67:ARG:HB2	1:A:69:PHE:CE1	2.45	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
1:A:287:GLN:CA	1:A:287:GLN:NE2	2.72	0.50
1:A:288:LEU:CD1	1:A:304:TYR:CG	2.95	0.50
2:A:700:ACO:H21	2:A:700:ACO:H131	1.93	0.50
1:A:419:LEU:CD2	1:A:421:ARG:HB2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:CD1	1:A:163:LEU:C	2.87	0.48
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
2:A:700:ACO:N7A	2:A:700:ACO:OAP	2.45	0.48
1:A:266:MET:HA	1:A:266:MET:HE2	1.96	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:HE3	1:A:206:LYS:HB2	1.39	0.46
1:A:341:LEU:N	1:A:342:PRO:HD3	2.29	0.46
2:A:700:ACO:HH32	3:A:702:LMR:O2	2.15	0.46
1:A:266:MET:HE1	1:A:269:LEU:HD22	1.97	0.46
1:A:431:ILE:HD12	1:A:431:ILE:HG21	1.51	0.46
1:A:53:TYR:CD2	1:A:240:GLY:HA3	2.51	0.46
1:A:331:THR:O	1:A:334:ARG:HB3	2.16	0.46
1:A:323:LEU:C	1:A:324:ARG:HD3	2.41	0.45
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:HH11	1:A:334:ARG:HD2	1.40	0.45
1:A:163:LEU:CD1	1:A:164:ARG:N	2.80	0.45
1:A:92:LEU:CD2	1:A:236:SER:OG	2.64	0.45
1:A:350:VAL:HG13	1:A:380:VAL:HG21	1.96	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
1:A:171:VAL:HG21	1:A:413:ARG:HG3	2.00	0.43
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HA	1:A:121:PRO:HD2	1.88	0.43
1:A:410:ILE:HD13	1:A:410:ILE:HG21	1.70	0.43
1:A:40:MET:HE2	1:A:46:ARG:O	2.19	0.43
1:A:118:ALA:CB	1:A:203:ILE:HD12	2.48	0.43
1:A:163:LEU:HD12	1:A:163:LEU:C	2.43	0.43
1:A:86:GLU:CG	1:A:87:PRO:CD	2.95	0.43
1:A:136:HIS:CG	1:A:137:PRO:HD2	2.53	0.43
1:A:344:ASP:O	1:A:347:PHE:HB3	2.19	0.43
1:A:228:MET:HE2	1:A:232:LEU:HD11	2.00	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:228:MET:HE3	1:A:232:LEU:HG	2.01	0.42
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.81	0.42
1:A:347:PHE:O	1:A:347:PHE:CD2	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:86:GLU:CG	1:A:87:PRO:HD2	2.50	0.42
1:A:136:HIS:HA	1:A:137:PRO:HD3	1.88	0.42
1:A:238:HIS:ND1	3:A:702:LMR:H2	2.34	0.42
1:A:67:ARG:HB2	1:A:69:PHE:HD1	1.81	0.42
1:A:45:MET:HE2	1:A:48:MET:SD	2.60	0.41
1:A:214:THR:CG2	1:A:228:MET:HG2	2.51	0.41
1:A:36:ILE:HD13	1:A:36:ILE:HG21	1.82	0.41
1:A:305:ILE:CD1	1:A:357:VAL:HG22	2.48	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:172:TYR:CD2	1:A:172:TYR:C	2.99	0.41
1:A:324:ARG:HD3	1:A:324:ARG:HA	1.59	0.41
1:A:94:TRP:CE3	1:A:110:LEU:HD21	2.56	0.41
1:A:110:LEU:HD23	1:A:110:LEU:N	2.35	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:149:ASN:C	1:A:151:GLU:N	2.80	0.40
1:A:285:LEU:HD11	1:A:350:VAL:HG12	2.03	0.40
1:A:390:MET:HE2	1:A:390:MET:HB3	1.76	0.40
1:A:335:GLU:HG3	1:A:339:LYS:CE	2.50	0.40
1:A:149:ASN:C	1:A:151:GLU:H	2.29	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:SER:O	1:A:313:ARG:NH2[1_554]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides 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	LMR	A	702	-	8,8,8	2.21	4 (50%)	10,10,10	1.84	5 (50%)
2	ACO	A	700	-	51,53,53	2.20	13 (25%)	73,79,79	1.46	10 (13%)

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	LMR	A	702	-	-	2/8/8/8	-
2	ACO	A	700	-	-	7/51/67/67	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	ACO	O9P-C9P	6.77	1.36	1.23
2	A	700	ACO	P1A-O3A	-5.72	1.53	1.59
2	A	700	ACO	CH3-C	-5.40	1.28	1.50
2	A	700	ACO	P2A-O3A	4.74	1.64	1.59
2	A	700	ACO	P3B-O3B	4.69	1.67	1.59
3	A	702	LMR	O4B-C4	3.93	1.34	1.22
3	A	702	LMR	C2-C1	-3.02	1.48	1.52
2	A	700	ACO	O5P-C5P	3.01	1.29	1.23
2	A	700	ACO	P3B-O7A	2.97	1.59	1.50
2	A	700	ACO	C3P-N4P	2.87	1.52	1.46
2	A	700	ACO	C5A-C6A	2.65	1.48	1.41
2	A	700	ACO	C2A-N1A	2.57	1.38	1.33
3	A	702	LMR	O2-C2	2.55	1.48	1.42
2	A	700	ACO	O4B-C4B	2.27	1.50	1.45
2	A	700	ACO	C8A-N7A	2.24	1.36	1.31
2	A	700	ACO	OAP-CAP	2.07	1.46	1.42
3	A	702	LMR	C3-C2	-2.05	1.48	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ACO	P3B-O3B-C3B	-4.72	110.82	123.43
2	A	700	ACO	CEP-CBP-CCP	-4.17	101.34	108.22
2	A	700	ACO	CDP-CBP-CCP	3.60	114.17	108.22
2	A	700	ACO	C2P-C3P-N4P	-3.17	105.80	112.41
2	A	700	ACO	O-C-S1P	-3.03	110.41	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	ACO	O5A-P2A-O3A	2.89	115.08	107.27
2	A	700	ACO	CEP-CBP-CAP	2.83	113.60	108.77
2	A	700	ACO	C2B-C3B-C4B	-2.57	98.74	103.24
2	A	700	ACO	C6P-C7P-N8P	-2.55	106.56	112.00
2	A	700	ACO	O4B-C1B-C2B	-2.51	101.25	106.62
3	A	702	LMR	O4A-C4-C3	2.45	121.63	114.00
3	A	702	LMR	O2-C2-C3	2.36	115.65	109.96
3	A	702	LMR	O4B-C4-C3	-2.31	115.74	122.84
3	A	702	LMR	O1A-C1-C2	-2.18	118.25	122.60
3	A	702	LMR	C2-C3-C4	-2.15	106.46	112.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	ACO	S1P-C2P-C3P-N4P
2	A	700	ACO	C3P-C2P-S1P-C
2	A	700	ACO	O-C-S1P-C2P
2	A	700	ACO	CH3-C-S1P-C2P
3	A	702	LMR	C1-C2-C3-C4
3	A	702	LMR	O2-C2-C3-C4
2	A	700	ACO	CEP-CBP-CCP-O6A
2	A	700	ACO	C5B-O5B-P1A-O1A
2	A	700	ACO	CDP-CBP-CCP-O6A

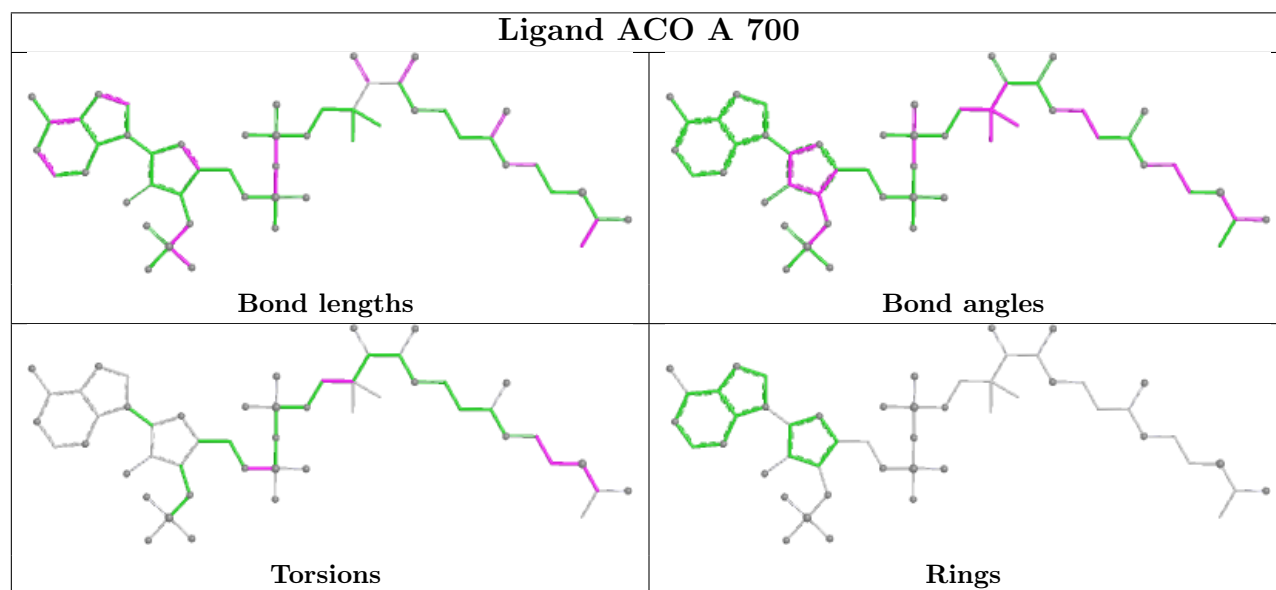
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	LMR	3	0
2	A	700	ACO	8	0

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 than 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.