Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 11:49 PM EDT

PDB ID	:	1CSC
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	:	1.70 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

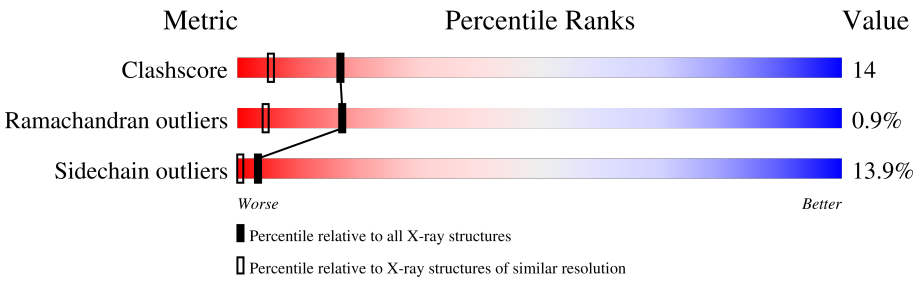
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	

2 Entry composition (i)

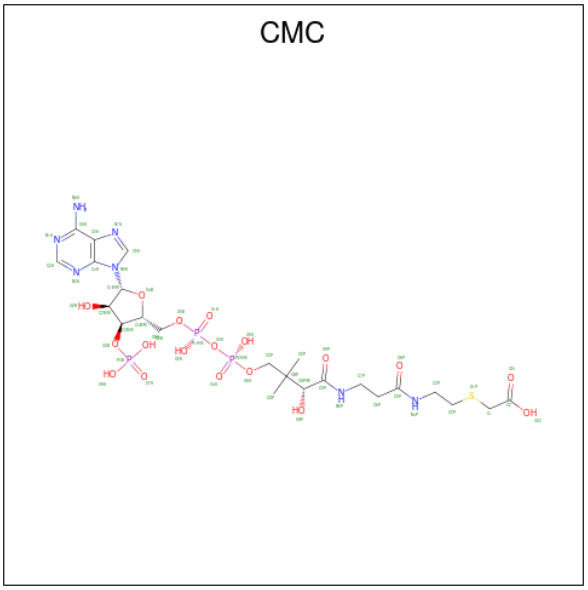
There are 4 unique types of molecules in this entry. The entry contains 3468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

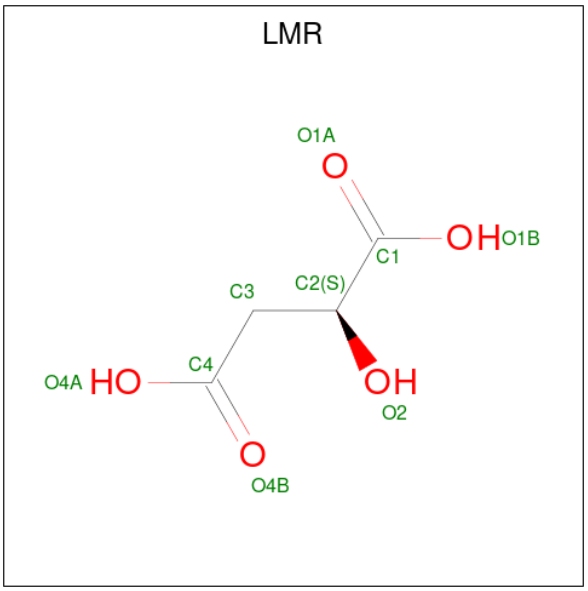
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3306	2115	571	603	17	0	0	0

- Molecule 2 is CARBOXYMETHYL COENZYME *A (three-letter code: CMC) (formula: $C_{23}H_{38}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	52	23	7	18	3	1	0	0

- Molecule 3 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: $C_4H_6O_5$).



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

- Molecule 4 is water.

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

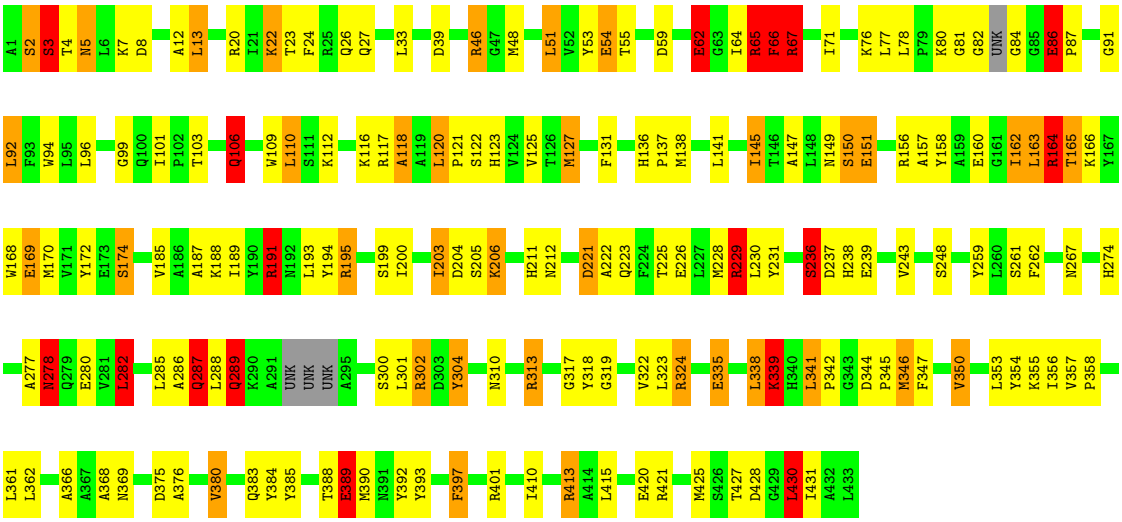
3 Residue-property plots (i)

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

Chain A: 57% 30% 8%



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 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.70)	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	3468	wwPDB-VP
Average B, all atoms ($Å^2$)	20.0	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, CMC

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	1.09	13/3386 (0.4%)	2.18	147/4598 (3.2%)

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	14

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	TYR	CE1-CZ	-7.99	1.28	1.38
1	A	392	TYR	CE2-CZ	7.37	1.48	1.38
1	A	280	GLU	CD-OE2	6.62	1.32	1.25
1	A	302	ARG	NE-CZ	-5.94	1.25	1.33
1	A	165	THR	CB-OG1	5.80	1.54	1.43
1	A	226	GLU	CD-OE2	5.75	1.31	1.25
1	A	62	GLU	CD-OE2	5.58	1.31	1.25
1	A	335	GLU	CD-OE2	5.44	1.31	1.25
1	A	151	GLU	CD-OE2	5.38	1.31	1.25
1	A	160	GLU	CD-OE1	-5.36	1.19	1.25
1	A	54	GLU	CG-CD	-5.16	1.44	1.51
1	A	304	TYR	CB-CG	-5.09	1.44	1.51
1	A	3	SER	CA-CB	-5.04	1.45	1.52

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH2	-24.12	108.24	120.30
1	A	229	ARG	NE-CZ-NH2	-23.35	108.63	120.30
1	A	191	ARG	NE-CZ-NH1	21.67	131.14	120.30
1	A	304	TYR	CB-CG-CD1	-19.13	109.52	121.00
1	A	228	MET	CG-SD-CE	-17.15	72.77	100.20
1	A	229	ARG	CD-NE-CZ	16.79	147.10	123.60
1	A	67	ARG	NE-CZ-NH1	16.60	128.60	120.30
1	A	313	ARG	NE-CZ-NH2	-13.37	113.61	120.30
1	A	117	ARG	NE-CZ-NH1	12.20	126.40	120.30
1	A	39	ASP	CB-CG-OD2	-12.11	107.40	118.30
1	A	127	MET	CG-SD-CE	-12.08	80.87	100.20
1	A	191	ARG	CD-NE-CZ	12.04	140.45	123.60
1	A	67	ARG	NE-CZ-NH2	-11.18	114.71	120.30
1	A	46	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	117	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	A	67	ARG	CD-NE-CZ	10.38	138.14	123.60
1	A	313	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	A	278	ASN	CB-CG-OD1	-10.00	101.60	121.60
1	A	302	ARG	CD-NE-CZ	-9.92	109.71	123.60
1	A	286	ALA	CB-CA-C	9.78	124.77	110.10
1	A	318	TYR	CB-CG-CD1	-9.76	115.14	121.00
1	A	66	PHE	CA-C-N	9.75	138.65	117.20
1	A	174	SER	CB-CA-C	9.73	128.59	110.10
1	A	195	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	A	33	LEU	CB-CG-CD1	-9.69	94.53	111.00
1	A	59	ASP	CB-CG-OD2	-9.57	109.69	118.30
1	A	380	VAL	CG1-CB-CG2	-9.53	95.65	110.90
1	A	221	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	A	67	ARG	CB-CA-C	-9.18	92.05	110.40
1	A	54	GLU	CG-CD-OE2	-8.96	100.38	118.30
1	A	390	MET	CA-CB-CG	-8.96	98.07	113.30
1	A	324	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	431	ILE	CG1-CB-CG2	-8.83	91.98	111.40
1	A	431	ILE	CA-CB-CG1	8.54	127.22	111.00
1	A	65	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	A	431	ILE	CA-CB-CG2	8.36	127.61	110.90
1	A	231	TYR	CB-CG-CD2	-8.34	115.99	121.00
1	A	13	LEU	CD1-CG-CD2	-8.27	85.68	110.50
1	A	51	LEU	CB-CA-C	-8.27	94.49	110.20
1	A	39	ASP	CB-CG-OD1	8.26	125.74	118.30
1	A	221	ASP	CB-CG-OD1	8.25	125.73	118.30
1	A	110	LEU	CA-CB-CG	-8.21	96.41	115.30
1	A	428	ASP	CB-CG-OD2	-8.01	111.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	48	MET	CG-SD-CE	-7.91	87.54	100.20
1	A	229	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	421	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	120	LEU	CB-CG-CD2	7.82	124.30	111.00
1	A	66	PHE	O-C-N	-7.75	110.31	122.70
1	A	430	LEU	CB-CG-CD1	-7.71	97.88	111.00
1	A	65	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	278	ASN	CA-CB-CG	-7.66	96.55	113.40
1	A	106	GLN	CA-CB-CG	7.62	130.16	113.40
1	A	287	GLN	N-CA-CB	-7.58	96.97	110.60
1	A	191	ARG	CG-CD-NE	-7.52	96.00	111.80
1	A	289	GLN	CB-CG-CD	-7.49	92.14	111.60
1	A	289	GLN	CB-CA-C	-7.45	95.50	110.40
1	A	389	GLU	CG-CD-OE2	-7.34	103.63	118.30
1	A	122	SER	N-CA-CB	-7.28	99.58	110.50
1	A	27	GLN	CG-CD-NE2	-7.28	99.23	116.70
1	A	8	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	A	200	ILE	C-N-CA	-7.25	107.08	122.30
1	A	229	ARG	CG-CD-NE	7.16	126.84	111.80
1	A	81	GLY	O-C-N	-7.03	111.24	123.20
1	A	401	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	392	TYR	CB-CG-CD2	7.01	125.21	121.00
1	A	3	SER	CB-CA-C	-6.98	96.84	110.10
1	A	81	GLY	C-N-CA	-6.97	107.66	122.30
1	A	304	TYR	CD1-CG-CD2	6.93	125.53	117.90
1	A	354	TYR	CB-CG-CD1	-6.92	116.84	121.00
1	A	54	GLU	CB-CG-CD	-6.88	95.64	114.20
1	A	339	LYS	N-CA-CB	6.85	122.93	110.60
1	A	118	ALA	CB-CA-C	-6.76	99.95	110.10
1	A	322	VAL	CA-CB-CG2	6.70	120.96	110.90
1	A	66	PHE	C-N-CA	-6.65	105.07	121.70
1	A	191	ARG	N-CA-CB	-6.58	98.75	110.60
1	A	427	THR	CA-CB-CG2	-6.56	103.21	112.40
1	A	59	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	117	ARG	CD-NE-CZ	6.53	132.74	123.60
1	A	67	ARG	CA-C-N	-6.46	103.28	116.20
1	A	388	THR	CA-CB-CG2	6.44	121.42	112.40
1	A	368	ALA	CB-CA-C	6.43	119.75	110.10
1	A	195	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	54	GLU	OE1-CD-OE2	6.36	130.93	123.30
1	A	33	LEU	CA-CB-CG	-6.34	100.72	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	2	SER	N-CA-CB	6.32	119.98	110.50
1	A	24	PHE	CB-CG-CD1	6.32	125.22	120.80
1	A	22	LYS	N-CA-CB	6.30	121.94	110.60
1	A	239	GLU	CB-CA-C	6.29	122.98	110.40
1	A	66	PHE	CB-CA-C	6.28	122.96	110.40
1	A	222	ALA	CB-CA-C	6.28	119.52	110.10
1	A	13	LEU	CA-CB-CG	6.25	129.68	115.30
1	A	165	THR	CA-CB-OG1	6.24	122.11	109.00
1	A	248	SER	N-CA-CB	6.23	119.85	110.50
1	A	3	SER	CA-CB-OG	-6.17	94.55	111.20
1	A	229	ARG	NH1-CZ-NH2	-6.15	112.63	119.40
1	A	339	LYS	CB-CA-C	-6.08	98.25	110.40
1	A	318	TYR	CB-CG-CD2	6.03	124.62	121.00
1	A	106	GLN	N-CA-CB	6.03	121.45	110.60
1	A	145	ILE	CB-CG1-CD1	-6.02	97.04	113.90
1	A	413	ARG	CG-CD-NE	6.01	124.42	111.80
1	A	46	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	27	GLN	CB-CG-CD	-5.96	96.09	111.60
1	A	431	ILE	N-CA-CB	5.96	124.52	110.80
1	A	397	PHE	CB-CG-CD2	-5.93	116.65	120.80
1	A	164	ARG	CG-CD-NE	5.91	124.21	111.80
1	A	304	TYR	CB-CG-CD2	5.88	124.53	121.00
1	A	286	ALA	O-C-N	-5.85	113.33	122.70
1	A	237	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	86	GLU	CA-CB-CG	-5.82	100.59	113.40
1	A	278	ASN	CA-C-N	-5.80	104.43	117.20
1	A	158	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	A	302	ARG	CB-CA-C	5.79	121.98	110.40
1	A	415	LEU	CB-CG-CD1	5.74	120.76	111.00
1	A	259	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	A	313	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	110	LEU	CB-CG-CD1	5.67	120.64	111.00
1	A	338	LEU	CB-CG-CD2	5.62	120.55	111.00
1	A	237	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	431	ILE	CB-CA-C	5.51	122.61	111.60
1	A	174	SER	O-C-N	-5.50	113.90	122.70
1	A	86	GLU	CG-CD-OE2	-5.46	107.37	118.30
1	A	304	TYR	CZ-CE2-CD2	-5.45	114.89	119.80
1	A	282	LEU	CA-CB-CG	-5.44	102.78	115.30
1	A	431	ILE	CB-CG1-CD1	-5.41	98.75	113.90
1	A	12	ALA	CB-CA-C	5.41	118.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	385	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	A	65	ARG	CD-NE-CZ	5.33	131.07	123.60
1	A	413	ARG	CB-CG-CD	5.31	125.41	111.60
1	A	222	ALA	N-CA-CB	-5.30	102.69	110.10
1	A	350	VAL	CG1-CB-CG2	5.30	119.37	110.90
1	A	53	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	366	ALA	CB-CA-C	5.24	117.95	110.10
1	A	236	SER	CA-CB-OG	-5.21	97.13	111.20
1	A	302	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	92	LEU	CA-CB-CG	-5.19	103.36	115.30
1	A	361	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	A	355	LYS	CA-CB-CG	-5.18	102.01	113.40
1	A	165	THR	OG1-CB-CG2	5.16	121.88	110.00
1	A	425	MET	CB-CG-SD	-5.16	96.92	112.40
1	A	304	TYR	CE1-CZ-OH	-5.13	106.26	120.10
1	A	156	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	388	THR	CA-CB-OG1	-5.06	98.37	109.00
1	A	166	LYS	N-CA-CB	-5.06	101.49	110.60
1	A	262	PHE	CB-CG-CD1	-5.02	117.29	120.80
1	A	285	LEU	CB-CG-CD2	5.01	119.52	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	431	ILE	CB

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	LYS	Mainchain
1	A	118	ALA	Mainchain
1	A	169	GLU	Sidechain
1	A	203	ILE	Mainchain
1	A	22	LYS	Mainchain
1	A	229	ARG	Sidechain
1	A	278	ASN	Sidechain
1	A	302	ARG	Sidechain
1	A	313	ARG	Sidechain
1	A	384	TYR	Sidechain
1	A	389	GLU	Sidechain,Mainchain
1	A	420	GLU	Sidechain
1	A	65	ARG	Mainchain

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	94	1
2	A	52	0	33	0	0
3	A	9	0	4	0	0
4	A	101	0	0	2	0
All	All	3468	0	3334	94	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 14.

All (94) 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:103:THR:H	1:A:106:GLN:HG2	1.10	1.14
1:A:346:MET:HG2	1:A:380:VAL:HG22	1.37	1.02
1:A:335:GLU:O	1:A:339:LYS:HE2	1.63	0.99
1:A:163:LEU:HD12	1:A:165:THR:H	1.32	0.94
1:A:136:HIS:HD2	1:A:138:MET:H	1.18	0.91
1:A:67:ARG:HA	4:A:548:HOH:O	1.70	0.90
1:A:103:THR:N	1:A:106:GLN:HG2	1.88	0.89
1:A:106:GLN:CA	1:A:106:GLN:HE21	1.83	0.86
1:A:125:VAL:HG13	1:A:188:LYS:HE2	1.63	0.81
1:A:109:TRP:CE3	1:A:110:LEU:HD23	2.17	0.80
1:A:86:GLU:HG3	1:A:87:PRO:HD2	1.66	0.76
1:A:86:GLU:CG	1:A:87:PRO:HD2	2.17	0.74
1:A:106:GLN:HE21	1:A:106:GLN:HA	1.53	0.73
1:A:301:LEU:HD23	1:A:356:ILE:CD1	2.20	0.70
1:A:136:HIS:CD2	1:A:138:MET:H	2.07	0.68
1:A:77:LEU:HD13	1:A:101:ILE:CD1	2.24	0.68
1:A:92:LEU:HD23	1:A:236:SER:OG	1.94	0.67
1:A:301:LEU:HD23	1:A:356:ILE:HD13	1.76	0.66
1:A:136:HIS:CD2	1:A:137:PRO:HD2	2.31	0.65
1:A:77:LEU:HD13	1:A:101:ILE:HD11	1.79	0.65
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.80	0.63
1:A:109:TRP:CZ3	1:A:110:LEU:HD23	2.35	0.62
1:A:168:TRP:CE2	1:A:169:GLU:HG2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:MET:HG2	1:A:380:VAL:CG2	2.24	0.58
1:A:282:LEU:HD22	1:A:393:TYR:HE2	1.69	0.57
1:A:86:GLU:HG2	1:A:230:LEU:HD13	1.86	0.57
1:A:163:LEU:HD13	1:A:164:ARG:N	2.19	0.56
1:A:109:TRP:CE3	1:A:110:LEU:CD2	2.89	0.56
1:A:109:TRP:HE3	1:A:110:LEU:HD23	1.68	0.56
1:A:77:LEU:HB3	1:A:101:ILE:HD13	1.88	0.56
1:A:289:GLN:HE21	1:A:289:GLN:CA	2.06	0.56
1:A:282:LEU:HD22	1:A:393:TYR:CE2	2.41	0.55
1:A:103:THR:H	1:A:106:GLN:CG	2.01	0.55
1:A:225:THR:O	1:A:229:ARG:HG3	2.07	0.55
1:A:5:ASN:HD22	1:A:7:LYS:H	1.53	0.55
1:A:94:TRP:HE3	1:A:110:LEU:HD11	1.73	0.54
1:A:323:LEU:O	1:A:324:ARG:HD3	2.07	0.54
1:A:287:GLN:HE21	1:A:287:GLN:N	2.06	0.53
1:A:5:ASN:ND2	1:A:7:LYS:H	2.06	0.53
1:A:194:TYR:CD2	1:A:389:GLU:HG3	2.43	0.52
1:A:150:SER:HB3	1:A:151:GLU:HG2	1.91	0.52
1:A:62:GLU:HG2	1:A:65:ARG:HH12	1.76	0.51
1:A:211:HIS:HD2	1:A:211:HIS:O	1.93	0.51
1:A:338:LEU:HD23	1:A:347:PHE:CE1	2.46	0.51
1:A:141:LEU:O	1:A:145:ILE:HD12	2.10	0.50
1:A:163:LEU:CD1	1:A:164:ARG:N	2.74	0.50
1:A:319:GLY:HA2	1:A:369:ASN:O	2.11	0.50
1:A:106:GLN:CA	1:A:106:GLN:NE2	2.62	0.50
1:A:109:TRP:HE3	1:A:110:LEU:CD2	2.24	0.50
1:A:3:SER:OG	1:A:4:THR:N	2.43	0.49
1:A:106:GLN:HA	1:A:106:GLN:NE2	2.25	0.49
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.94	0.49
1:A:86:GLU:HG3	1:A:87:PRO:CD	2.38	0.49
1:A:288:LEU:HD13	1:A:304:TYR:CD2	2.47	0.49
1:A:67:ARG:HD3	1:A:99:GLY:O	2.13	0.48
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.58	0.48
1:A:350:VAL:CG2	1:A:380:VAL:HG21	2.43	0.47
1:A:82:GLY:H	1:A:84:GLY:HA2	1.79	0.47
1:A:163:LEU:HD13	1:A:164:ARG:H	1.79	0.47
1:A:347:PHE:HA	1:A:380:VAL:HG11	1.96	0.47
1:A:243:VAL:HB	1:A:274:HIS:CD2	2.50	0.46
1:A:339:LYS:N	1:A:339:LYS:HD3	2.26	0.46
1:A:194:TYR:O	1:A:195:ARG:HD3	2.15	0.45
1:A:206:LYS:HB2	1:A:206:LYS:HE3	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLY:HA3	4:A:514:HOH:O	2.17	0.45
1:A:221:ASP:OD2	1:A:223:GLN:N	2.47	0.45
1:A:23:THR:HG22	1:A:23:THR:O	2.16	0.45
1:A:339:LYS:HD3	1:A:339:LYS:HA	1.65	0.45
1:A:204:ASP:H	1:A:212:ASN:ND2	2.16	0.44
1:A:341:LEU:N	1:A:342:PRO:HD3	2.31	0.44
1:A:78:LEU:O	1:A:80:LYS:HE3	2.18	0.44
1:A:346:MET:HB3	1:A:380:VAL:HG13	2.00	0.44
1:A:335:GLU:HG3	1:A:339:LYS:CE	2.47	0.44
1:A:64:ILE:HD13	1:A:238:HIS:CD2	2.53	0.44
1:A:66:PHE:O	1:A:67:ARG:O	2.36	0.43
1:A:157:ALA:O	1:A:162:ILE:HG12	2.18	0.43
1:A:288:LEU:HA	1:A:304:TYR:CZ	2.54	0.43
1:A:185:VAL:O	1:A:189:ILE:HG13	2.19	0.42
1:A:55:THR:HG22	1:A:96:LEU:O	2.20	0.42
1:A:335:GLU:HG3	1:A:339:LYS:HE3	2.00	0.42
1:A:211:HIS:O	1:A:211:HIS:CD2	2.72	0.42
1:A:310:ASN:HD22	1:A:310:ASN:HA	1.54	0.42
1:A:317:GLY:O	1:A:376:ALA:HB2	2.19	0.42
1:A:410:ILE:HG21	1:A:410:ILE:HD13	1.52	0.42
1:A:187:ALA:O	1:A:191:ARG:HB2	2.19	0.41
1:A:172:TYR:CD2	1:A:172:TYR:C	2.94	0.41
1:A:66:PHE:O	1:A:67:ARG:C	2.48	0.41
1:A:288:LEU:HD13	1:A:304:TYR:CG	2.56	0.41
1:A:344:ASP:OD2	1:A:345:PRO:HD2	2.20	0.41
1:A:92:LEU:HD12	1:A:92:LEU:HA	1.66	0.41
1:A:123:HIS:HE1	1:A:147:ALA:O	2.02	0.41
1:A:277:ALA:HB3	1:A:375:ASP:OD1	2.20	0.41
1:A:324:ARG:HD3	1:A:324:ARG:HA	1.71	0.41
1:A:120:LEU:HA	1:A:121:PRO:HD3	1.92	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]	2.05	0.15

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%)	409 (97%)	10 (2%)	4 (1%)	17 5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	PHE
1	A	67	ARG
1	A	236	SER
1	A	278	ASN

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 0

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

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	SER
1	A	5	ASN
1	A	13	LEU
1	A	20	ARG
1	A	26	GLN
1	A	46	ARG

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Mol	Chain	Res	Type
1	A	51	LEU
1	A	54	GLU
1	A	62	GLU
1	A	67	ARG
1	A	71	ILE
1	A	76	LYS
1	A	86	GLU
1	A	106	GLN
1	A	112	LYS
1	A	131	PHE
1	A	149	ASN
1	A	150	SER
1	A	162	ILE
1	A	163	LEU
1	A	164	ARG
1	A	170	MET
1	A	174	SER
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	229	ARG
1	A	236	SER
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	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	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
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	267	ASN
1	A	287	GLN
1	A	289	GLN
1	A	310	ASN
1	A	340	HIS
1	A	364	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
2	CMC	A	700	-	48,54,54	1.46	8 (16%)	62,80,80	1.71	14 (22%)
3	LMR	A	702	-	8,8,8	1.81	1 (12%)	10,10,10	2.15	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	CMC	A	700	-	-	4/48/68/68	0/3/3/3
3	LMR	A	702	-	-	1/8/8/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	CMC	P3B-O3B	4.42	1.67	1.59
3	A	702	LMR	O2-C2	4.24	1.52	1.42
2	A	700	CMC	O9P-C9P	3.58	1.30	1.23
2	A	700	CMC	P2A-O3A	3.39	1.63	1.59
2	A	700	CMC	P3B-O7A	2.69	1.58	1.50
2	A	700	CMC	P1A-O3A	-2.67	1.56	1.59
2	A	700	CMC	C3P-N4P	2.60	1.52	1.46
2	A	700	CMC	O5P-C5P	2.37	1.28	1.23
2	A	700	CMC	O4B-C1B	2.21	1.43	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	CMC	C2P-S1P-C1	5.85	111.36	101.72
3	A	702	LMR	O1A-C1-C2	-4.22	114.17	122.60
2	A	700	CMC	O6A-CCP-CBP	-3.78	104.46	110.55
2	A	700	CMC	O9A-P3B-O8A	3.35	120.37	107.80
3	A	702	LMR	O1B-C1-C2	3.12	119.35	112.74
2	A	700	CMC	O21-C2-C1	-3.08	114.52	122.85
2	A	700	CMC	C4A-C5A-N7A	2.89	112.39	109.34
2	A	700	CMC	O22-C2-C1	2.88	122.74	113.38
2	A	700	CMC	P3B-O3B-C3B	-2.64	116.38	123.43
2	A	700	CMC	C5B-C4B-C3B	2.61	123.07	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	700	CMC	CEP-CBP-CCP	-2.59	103.94	108.22
3	A	702	LMR	C3-C2-C1	2.37	116.34	110.53
2	A	700	CMC	CDP-CBP-CCP	2.24	111.92	108.22
2	A	700	CMC	O3B-P3B-O7A	-2.23	101.37	109.33
2	A	700	CMC	O5B-C5B-C4B	-2.13	101.74	108.99
2	A	700	CMC	O5A-P2A-O4A	2.12	122.31	112.44
3	A	702	LMR	C2-C3-C4	2.07	117.48	112.08
2	A	700	CMC	C2B-C3B-C4B	-2.02	99.70	103.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

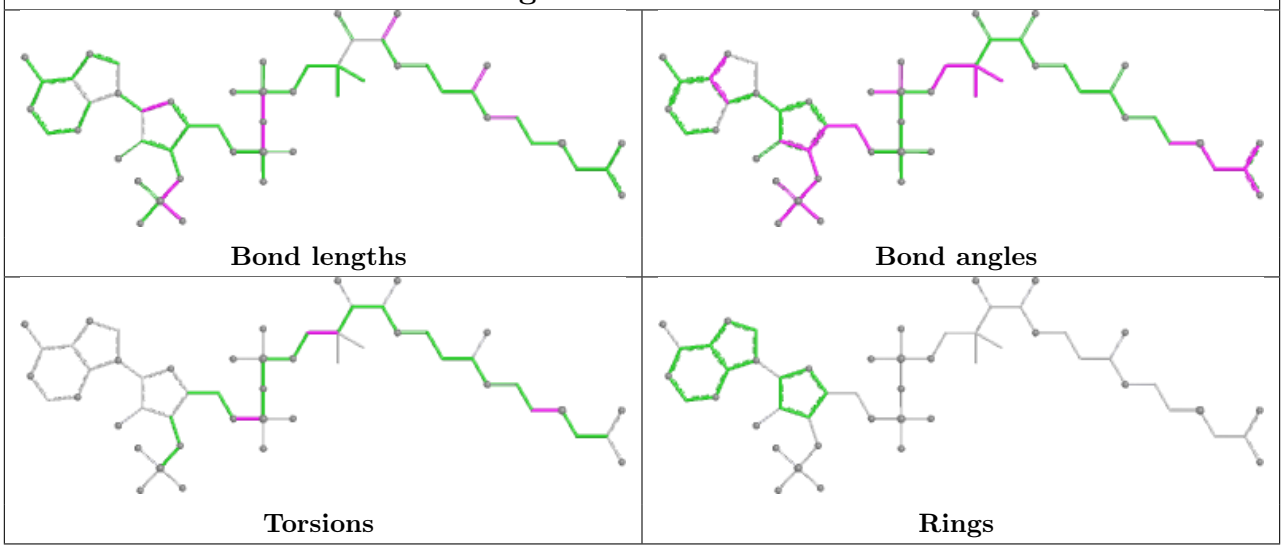
Mol	Chain	Res	Type	Atoms
2	A	700	CMC	C3P-C2P-S1P-C1
3	A	702	LMR	O1A-C1-C2-C3
2	A	700	CMC	CEP-CBP-CCP-O6A
2	A	700	CMC	C5B-O5B-P1A-O1A
2	A	700	CMC	CDP-CBP-CCP-O6A

There are no ring outliers.

No monomer is involved in short contacts.

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.

Ligand CMC A 700



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.