



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:17 pm BST

PDB ID : 1N8W  
Title : Biochemical and Structural Studies of Malate Synthase from Mycobacterium tuberculosis  
Authors : Smith, C.V.; Huang, C.C.; Miczak, A.; Russell, D.G.; Sacchettini, J.C.; Honer zu Bentrup, K.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2002-11-21  
Resolution : 2.70 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](mailto: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.

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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 : 1.8.5 (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

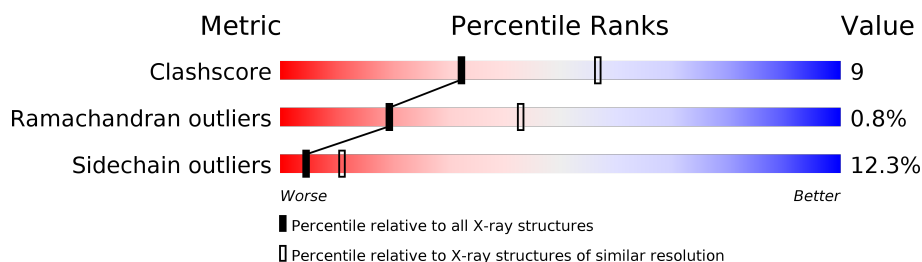
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	741	
1	B	741	

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
4	MLT	A	901	X	-	-	-
4	MLT	A	902	X	-	-	-
4	MLT	B	1902	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11696 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 Probable malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	718	Total	C	N	O	S	0	0	0
			5486	3448	964	1052	22			
1	B	715	Total	C	N	O	S	0	0	0
			5474	3441	964	1047	22			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

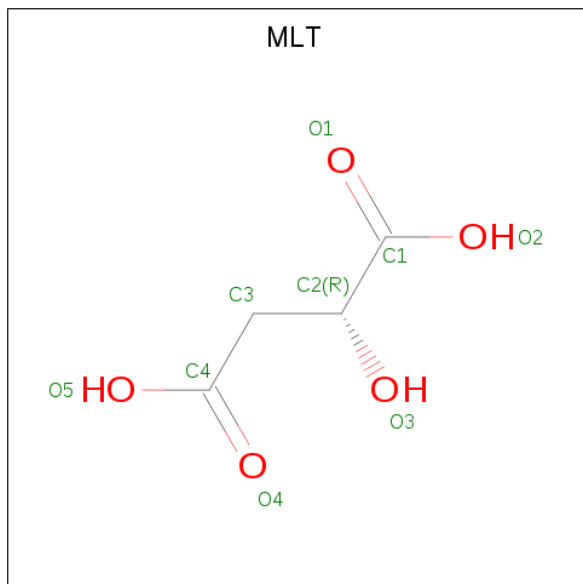
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is D-MALATE (three-letter code: MLT) (formula:  $C_4H_6O_5$ ).



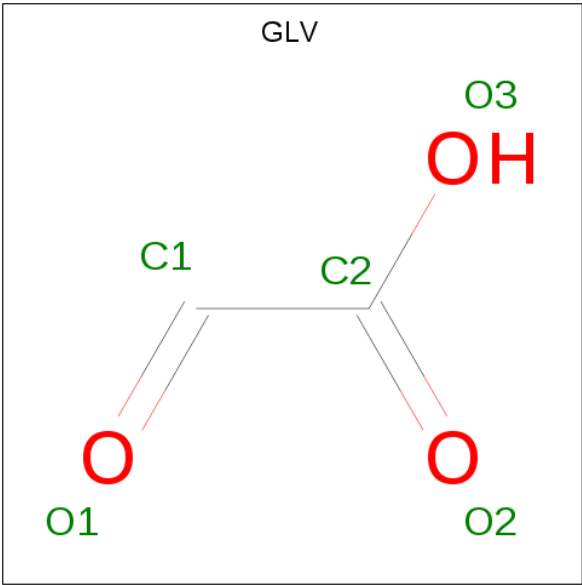
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	4	5		
4	A	1	Total	C	O	0	0
			9	4	5		
4	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 5 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 6 is GLYOXYLIC ACID (three-letter code: GLV) (formula: C<sub>2</sub>H<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			5	2	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	348	Total 348	O 348	0	0
7	B	291	Total 291	O 291	0	0

### 3 Residue-property plots

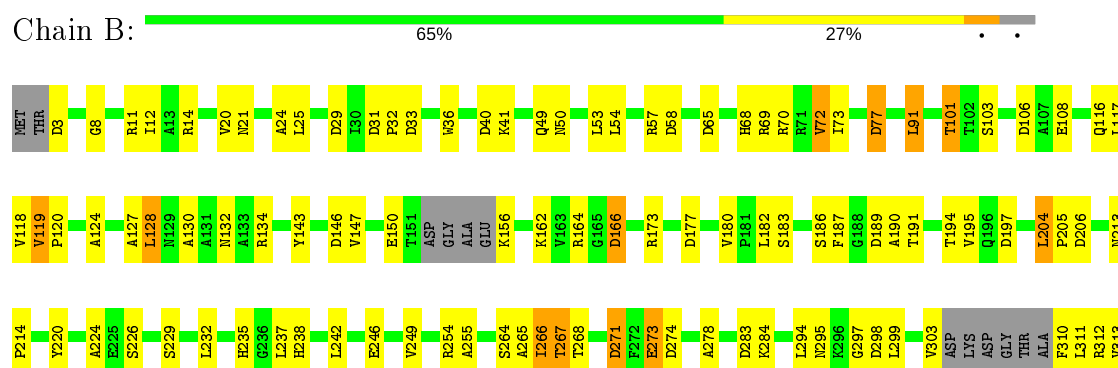
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Probable malate synthase G



#### • Molecule 1: Probable malate synthase G



I314	I315	R316	D317	R318	Q327	F328	T329	R333	S334	I335	M336	R339	N340	V341	L344	M345	T346	N347	D348	V351	D352	T353	D354	E357	D364	A372	I373	H374	G375	L376	K377	A378	N382	I386	N387	S388	R389	I393	K397	A404	L412	V416	E417	D418
Q424	N425	K428	E434	E435	R436	T439	V440	K443	D451	F455	T456	N457	T458	D462	R463	H469	M472	V478	K484	R508	A509	Q510	K513	G514	M515	W516	E520	D524	P533	A537	S538	V542	P543	A547	L550	H556	Q557							
V558	D559	V560	Q565	R571	T574	I575	E576	Q577	F582	L583	A584	K585	E586	L587	A588	D592	R595	V598	D599	S604	G607	V610	R611	W612	W613	D614	V622	P623	D627	V628	D633	L637	L643	N646	I653	T654	D657	V658	R659					
R664	P667	L668	R671	Q672	V677	A683	P684	D687	D688	A691	I699	Q705	P706	N707	G708	Y709	T710	E720	R724	A725	A726	E727	LYS	PRO	ALA	PRO	SER	ASP	ARG	ALA	GLY	ASP	ASP	ALA	ALA	ARG								



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.98 Å   120.98 Å   232.79 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.36 – 2.70	Depositor
% Data completeness (in resolution range)	94.3 (29.36-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.190 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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: COA, MG, GLV, SO4, 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	0.42	0/5591	0.79	27/7606 (0.4%)
1	B	0.42	1/5578 (0.0%)	0.81	29/7586 (0.4%)
All	All	0.42	1/11169 (0.0%)	0.80	56/15192 (0.4%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	588	ALA	C-N	-6.08	1.20	1.34

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	589	TRP	O-C-N	-8.54	109.03	122.70
1	A	280	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	348	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A	298	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	206	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	633	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	433	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	58	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	462	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	65	ASP	CB-CG-OD2	6.41	124.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	592	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	298	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	177	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	364	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	166	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	354	ASP	CB-CG-OD2	6.11	123.79	118.30
1	A	97	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	418	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	687	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	688	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	614	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	189	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	189	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	354	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	418	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	589	TRP	CA-C-N	5.71	129.77	117.20
1	A	40	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	77	ASP	CB-CG-OD2	5.63	123.36	118.30
1	B	29	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	77	ASP	CB-CG-OD2	5.61	123.34	118.30
1	B	206	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	274	ASP	CB-CG-OD2	5.56	123.31	118.30
1	B	197	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	688	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	146	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	352	ASP	CB-CG-OD2	5.49	123.25	118.30
1	A	29	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	599	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	317	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	271	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	33	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	31	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	524	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	3	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	40	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	106	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	79	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	45	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	633	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	271	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	274	ASP	CB-CG-OD2	5.07	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	65	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	657	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	687	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	266	ILE	Peptide

## 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	5486	0	5433	80	0
1	B	5474	0	5425	112	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	18	0	7	3	0
4	B	9	0	4	0	0
5	A	48	0	32	4	0
6	B	5	0	1	0	0
7	A	348	0	0	11	0
7	B	291	0	0	11	0
All	All	11696	0	10902	193	0

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 9.

All (193) 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:B:571:ARG:HG2	1:B:571:ARG:HH11	1.22	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASP:HB3	7:A:1138:HOH:O	1.62	0.97
1:B:425:ASN:O	1:B:428:LYS:HE2	1.65	0.96
1:B:533:PRO:HB2	1:B:558:VAL:HG11	1.47	0.96
1:A:340:ASN:HD21	1:A:368:THR:HG21	1.31	0.93
1:B:101:THR:HG22	1:B:451:ASP:HB3	1.51	0.90
1:B:267:THR:HG21	1:B:510:GLN:HE22	1.37	0.89
1:A:415:ARG:HD3	7:A:1221:HOH:O	1.78	0.82
1:B:132:ASN:HD21	1:B:315:ASN:H	1.29	0.80
1:A:416:VAL:O	1:A:420:LEU:HG	1.84	0.77
1:B:439:THR:HG21	1:B:463:ARG:HE	1.49	0.77
1:B:91:LEU:HD11	1:B:575:ILE:HD13	1.67	0.77
1:B:515:MET:HE3	1:B:516:TRP:N	2.03	0.74
1:B:101:THR:HG22	1:B:451:ASP:CB	2.19	0.72
1:B:571:ARG:NH1	1:B:571:ARG:HG2	1.95	0.72
1:B:436:ARG:HA	1:B:439:THR:HG23	1.71	0.72
1:A:11:ARG:HD2	1:A:11:ARG:O	1.92	0.70
1:B:543:PRO:HD2	1:B:547:ALA:CB	2.22	0.70
1:A:694:ALA:HB2	1:A:717:ARG:HG2	1.74	0.69
1:B:204:LEU:HB3	1:B:205:PRO:HD2	1.74	0.69
1:A:204:LEU:HB3	1:A:205:PRO:HD2	1.75	0.68
1:A:425:ASN:O	1:A:428:LYS:NZ	2.24	0.68
1:A:640:SER:OG	7:A:1027:HOH:O	2.11	0.67
1:B:434:GLU:OE2	7:B:1140:HOH:O	2.12	0.66
1:B:515:MET:HE3	1:B:516:TRP:H	1.59	0.66
1:B:108:GLU:HB3	1:B:266:ILE:HG22	1.76	0.66
1:B:49:GLN:HG3	7:B:1229:HOH:O	1.97	0.65
1:B:317:ASP:HB3	1:B:329:THR:CG2	2.28	0.64
1:B:132:ASN:ND2	1:B:315:ASN:H	1.96	0.64
1:B:439:THR:HG21	1:B:463:ARG:NE	2.13	0.63
1:A:350:ILE:HG23	1:A:363:MET:SD	2.38	0.63
1:B:278:ALA:HA	1:B:283:ASP:HB3	1.79	0.63
1:B:533:PRO:HB2	1:B:558:VAL:CG1	2.27	0.61
1:B:436:ARG:HA	1:B:439:THR:CG2	2.30	0.61
1:B:599:ASP:OD1	1:B:664:ARG:NH1	2.34	0.61
1:A:10:LEU:HD22	1:A:350:ILE:HD11	1.83	0.60
1:B:472:MET:SD	1:B:646:ASN:HA	2.41	0.60
1:B:346:THR:HB	1:B:357:GLU:HB3	1.84	0.59
1:A:83:GLN:HG2	7:A:1123:HOH:O	2.03	0.59
1:B:116:GLN:HE21	1:B:267:THR:HB	1.67	0.59
1:A:126:PHE:CE2	5:A:903:COA:H2B	2.38	0.58
1:A:25:LEU:N	1:A:26:PRO:HD2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HB2	4:A:901:MLT:O1	2.04	0.57
1:A:475:GLY:HA2	1:A:650:HIS:CD2	2.40	0.57
1:B:11:ARG:HB2	1:B:351:VAL:HG12	1.86	0.57
1:B:377:LYS:HD2	1:B:378:ALA:H	1.69	0.57
1:B:297:GLY:HA2	1:B:314:LEU:HD23	1.88	0.56
1:A:95:PRO:HG2	1:A:443:LYS:HG2	1.88	0.56
1:B:128:LEU:HD22	1:B:314:LEU:HD13	1.87	0.56
1:B:106:ASP:HB3	1:B:108:GLU:OE1	2.06	0.56
1:B:119:VAL:HG22	1:B:120:PRO:HD2	1.87	0.55
1:B:478:VAL:HG12	1:B:584:ALA:HA	1.89	0.55
1:B:20:VAL:HA	1:B:24:ALA:HB3	1.89	0.55
1:B:637:LEU:HG	1:B:710:THR:HG21	1.88	0.55
1:A:605:ILE:HD13	1:A:699:ILE:HD11	1.88	0.54
1:A:339:ARG:HH12	4:A:901:MLT:H31	1.72	0.54
1:A:314:LEU:HB3	1:A:333:ARG:HD3	1.89	0.54
1:B:372:ALA:HB1	1:B:393:ILE:HG12	1.90	0.54
1:A:364:ASP:O	1:A:368:THR:HB	2.08	0.54
1:B:31:ASP:C	1:B:33:ASP:H	2.11	0.54
1:B:295:ASN:HD22	1:B:375:GLY:HA3	1.73	0.53
1:B:571:ARG:CG	1:B:571:ARG:HH11	2.06	0.53
1:B:610:VAL:HA	1:B:691:ALA:HB1	1.89	0.53
1:A:472:MET:O	1:A:650:HIS:HE1	1.90	0.53
1:B:134:ARG:HD3	1:B:333:ARG:O	2.09	0.53
1:A:608:TYR:CE1	1:A:633:ASP:HA	2.44	0.52
1:B:317:ASP:HB3	1:B:329:THR:HG23	1.91	0.52
1:A:180:VAL:HG21	1:A:232:LEU:HD13	1.91	0.52
1:A:429:ILE:HG22	1:A:452:ARG:HB3	1.91	0.52
1:B:377:LYS:HA	1:B:386:ILE:HD11	1.92	0.52
1:B:294:LEU:HG	1:B:299:LEU:HD22	1.92	0.52
1:B:101:THR:CG2	1:B:451:ASP:HB3	2.33	0.52
1:B:462:ASP:OD1	7:B:1140:HOH:O	2.19	0.52
1:A:292:LEU:HA	1:A:371:ILE:HG23	1.93	0.51
1:B:273:GLU:HG3	1:B:341:VAL:HA	1.92	0.51
1:B:237:LEU:HB2	1:B:556:HIS:CE1	2.46	0.51
1:A:161:ASN:OD1	1:A:163:VAL:N	2.44	0.50
1:A:291:TRP:CD1	1:A:371:ILE:HG21	2.47	0.50
1:B:127:ALA:HB1	1:B:294:LEU:HD11	1.93	0.50
1:B:130:ALA:HB1	1:B:268:THR:HG21	1.93	0.50
1:B:705:GLN:HG3	7:B:1202:HOH:O	2.12	0.50
1:A:129:ASN:ND2	1:A:312:ARG:HD3	2.26	0.50
1:B:12:ILE:HG12	1:B:36:TRP:CZ3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:VAL:HG11	1:B:232:LEU:HD22	1.94	0.49
1:B:455:PHE:CD1	1:B:455:PHE:C	2.86	0.49
1:A:641:SER:HB2	1:A:698:LEU:O	2.11	0.49
1:B:336:MET:HB2	1:B:387:ASN:OD1	2.13	0.49
1:A:22:ASN:O	1:A:26:PRO:HG3	2.13	0.49
1:B:143:TYR:O	1:B:164:ARG:NH2	2.44	0.49
1:B:688:ASP:OD2	1:B:688:ASP:N	2.46	0.49
1:A:12:ILE:HG23	1:A:16:LEU:HD23	1.94	0.48
1:A:291:TRP:CD1	1:A:371:ILE:CG2	2.96	0.48
1:B:664:ARG:O	1:B:667:PRO:HD2	2.13	0.48
1:B:469:HIS:CD2	1:B:707:ASN:HA	2.48	0.48
1:A:125:ARG:CZ	5:A:903:COA:O9A	2.61	0.48
1:B:404:ALA:HB3	7:B:1395:HOH:O	2.13	0.48
1:B:191:THR:O	1:B:255:ALA:HA	2.14	0.48
1:A:350:ILE:HG12	1:A:358:VAL:HG21	1.96	0.48
1:B:354:ASP:HB3	7:B:1386:HOH:O	2.13	0.48
1:B:576:GLU:HG2	7:B:1527:HOH:O	2.13	0.48
1:B:21:ASN:HD22	1:B:25:LEU:HD12	1.79	0.47
1:A:125:ARG:HD2	7:A:1543:HOH:O	2.14	0.47
1:B:586:GLU:HG3	1:B:588:ALA:HB3	1.96	0.47
1:B:424:GLN:O	1:B:425:ASN:HB2	2.15	0.47
1:A:543:PRO:HD2	1:A:547:ALA:CB	2.44	0.47
1:B:173:ARG:HD2	1:B:187:PHE:HB3	1.96	0.47
1:A:530:ILE:HG12	1:A:534:ARG:HD2	1.97	0.46
1:A:92:LEU:HB3	1:A:93:PRO:HD2	1.96	0.46
1:B:377:LYS:HD2	1:B:378:ALA:N	2.31	0.46
1:B:607:GLY:HA3	1:B:622:VAL:HG11	1.96	0.46
1:A:455:PHE:CD1	1:A:455:PHE:C	2.89	0.46
1:A:367:PHE:O	1:A:371:ILE:HD12	2.16	0.46
1:A:53:LEU:HD22	1:A:405:GLU:HG2	1.98	0.46
1:A:477:MET:HG2	1:A:646:ASN:OD1	2.16	0.45
1:B:271:ASP:OD2	1:B:339:ARG:NH2	2.42	0.45
1:B:623:PRO:HA	1:B:628:VAL:O	2.16	0.45
1:B:372:ALA:CB	1:B:393:ILE:HG12	2.45	0.45
1:A:180:VAL:HG12	1:A:216:GLN:NE2	2.31	0.45
1:B:264:SER:O	1:B:266:ILE:HG12	2.17	0.45
1:B:412:LEU:O	1:B:416:VAL:HG23	2.16	0.45
1:B:134:ARG:HA	1:B:265:ALA:O	2.15	0.45
1:A:595:ARG:NH2	7:A:1014:HOH:O	2.49	0.45
1:B:513:LYS:HD3	1:B:537:ALA:HB2	1.98	0.45
1:A:480:LYS:HD3	1:A:601:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ARG:HD3	7:A:1517:HOH:O	2.17	0.44
1:A:60:LEU:HD22	1:A:90:TYR:HB2	1.98	0.44
1:A:81:TYR:CE2	1:A:85:LEU:HD11	2.52	0.44
1:B:588:ALA:O	1:B:589:TRP:HB2	2.17	0.44
1:B:658:VAL:HG11	1:B:699:ILE:HG21	2.00	0.44
1:B:333:ARG:HH11	1:B:333:ARG:HG3	1.82	0.44
1:B:124:ALA:O	1:B:128:LEU:HB2	2.17	0.44
1:B:455:PHE:HD1	1:B:455:PHE:C	2.21	0.44
1:B:20:VAL:HG12	1:B:25:LEU:HG	1.99	0.44
1:B:147:VAL:HG21	1:B:550:LEU:HD13	1.99	0.44
1:A:516:TRP:CE2	1:A:525:MET:HB2	2.53	0.44
1:A:336:MET:H	1:A:387:ASN:HD21	1.64	0.44
1:B:68:HIS:O	1:B:72:VAL:HG22	2.18	0.43
1:A:541:TRP:HZ3	4:A:901:MLT:H32	1.82	0.43
1:A:311:LEU:HB2	1:B:313:VAL:HG11	2.00	0.43
1:A:161:ASN:OD1	1:A:161:ASN:C	2.57	0.43
1:B:57:ARG:NH1	1:B:709:TYR:HE1	2.16	0.43
1:B:213:ASN:HA	1:B:214:PRO:HD2	1.80	0.43
1:A:397:LYS:HG2	1:A:409:THR:HG21	1.99	0.43
1:A:47:THR:N	1:A:48:PRO:CD	2.81	0.43
1:B:190:ALA:O	1:B:255:ALA:HB2	2.18	0.43
1:A:11:ARG:C	1:A:11:ARG:HD2	2.38	0.43
1:A:463:ARG:HG3	1:A:488:TRP:HZ3	1.84	0.43
1:B:177:ASP:OD2	1:B:186:SER:HB2	2.18	0.43
1:A:607:GLY:HA2	1:A:669:VAL:HG11	2.00	0.43
1:A:590:ALA:HB1	1:A:591:PRO:HD2	2.01	0.42
1:B:574:THR:OG1	1:B:577:GLN:HG3	2.19	0.42
1:A:538:SER:HA	1:A:560:VAL:HG11	1.99	0.42
1:B:443:LYS:HD2	7:B:1279:HOH:O	2.18	0.42
1:A:216:GLN:NE2	1:A:234:ASN:HD22	2.18	0.42
1:A:440:VAL:HG11	1:A:579:LEU:HD21	2.01	0.42
1:B:386:ILE:HB	7:B:1630:HOH:O	2.18	0.42
1:B:515:MET:HE1	1:B:542:VAL:C	2.39	0.42
1:B:598:VAL:HG21	1:B:653:ILE:HG21	2.00	0.42
1:B:538:SER:HA	1:B:560:VAL:HG11	2.02	0.42
1:B:436:ARG:O	1:B:440:VAL:HG22	2.20	0.42
1:A:125:ARG:NH1	7:A:1391:HOH:O	2.51	0.42
5:A:903:COA:OAP	7:A:1343:HOH:O	2.22	0.42
1:B:515:MET:HE1	1:B:542:VAL:CA	2.50	0.42
1:A:16:LEU:HD21	1:A:367:PHE:CZ	2.55	0.42
1:B:49:GLN:O	1:B:53:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HB2	1:A:217:PHE:CD1	2.56	0.41
1:A:526:VAL:O	1:A:554:HIS:NE2	2.43	0.41
1:A:581:ILE:HG22	1:A:583:LEU:HG	2.03	0.41
1:B:119:VAL:HG22	1:B:120:PRO:CD	2.50	0.41
1:A:180:VAL:HG21	1:A:232:LEU:CD1	2.50	0.41
1:B:103:SER:O	1:B:428:LYS:NZ	2.54	0.41
1:B:508:ARG:HA	7:B:1433:HOH:O	2.20	0.41
1:B:344:LEU:HD22	1:B:709:TYR:CD1	2.56	0.41
1:A:415:ARG:NH1	1:A:415:ARG:HB3	2.34	0.41
1:B:195:VAL:HB	1:B:224:ALA:HB1	2.02	0.41
1:A:431:ILE:O	1:A:456:ILE:HA	2.20	0.41
1:B:374:HIS:HD2	1:B:382:ASN:HD22	1.69	0.41
1:A:278:ALA:HA	1:A:283:ASP:HB3	2.03	0.41
1:B:508:ARG:HG2	7:B:1433:HOH:O	2.21	0.41
1:B:683:ALA:HA	1:B:684:PRO:HA	1.81	0.41
1:A:598:VAL:HG21	1:A:653:ILE:HG21	2.03	0.41
1:B:478:VAL:HG13	1:B:582:PRO:O	2.21	0.41
1:A:50:ASN:HB3	1:A:359:PHE:CE1	2.56	0.41
1:A:488:TRP:HB3	1:A:580:THR:O	2.21	0.41
1:B:220:TYR:HB2	1:B:229:SER:O	2.20	0.41
1:B:232:LEU:O	1:B:238:HIS:HA	2.21	0.41
1:A:16:LEU:O	1:A:20:VAL:HG23	2.21	0.40
1:A:463:ARG:HG2	1:A:492:TYR:CE1	2.57	0.40
1:A:502:ALA:HB1	7:A:1534:HOH:O	2.21	0.40
1:B:543:PRO:HD2	1:B:547:ALA:HB1	1.98	0.40
1:A:175:PHE:CE2	1:A:262:LEU:HD21	2.56	0.40
1:A:110:THR:HB	1:A:507:GLY:O	2.20	0.40
5:A:903:COA:H131	7:A:1357:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 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	714/741 (96%)	667 (93%)	43 (6%)	4 (1%)	25	50
1	B	709/741 (96%)	656 (92%)	45 (6%)	8 (1%)	14	34
All	All	1423/1482 (96%)	1323 (93%)	88 (6%)	12 (1%)	19	43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	B	585	LYS
1	B	589	TRP
1	B	267	THR
1	B	726	ALA
1	A	725	ALA
1	B	32	PRO
1	B	484	LYS
1	B	235	HIS
1	B	8	GLY
1	A	8	GLY
1	A	75	PRO

### 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	577/594 (97%)	515 (89%)	62 (11%)	6	15
1	B	577/594 (97%)	497 (86%)	80 (14%)	3	8
All	All	1154/1188 (97%)	1012 (88%)	142 (12%)	4	11

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	11	ARG
1	A	14	ARG
1	A	15	VAL

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Mol	Chain	Res	Type
1	A	23	GLU
1	A	49	GLN
1	A	50	ASN
1	A	72	VAL
1	A	74	GLU
1	A	82	ARG
1	A	83	GLN
1	A	87	GLU
1	A	112	THR
1	A	134	ARG
1	A	155	GLU
1	A	156	LYS
1	A	174	LYS
1	A	194	THR
1	A	208	SER
1	A	229	SER
1	A	248	GLN
1	A	251	THR
1	A	286	LEU
1	A	316	ARG
1	A	327	GLN
1	A	348	ASP
1	A	350	ILE
1	A	353	THR
1	A	357	GLU
1	A	368	THR
1	A	370	LEU
1	A	381	VAL
1	A	386	ILE
1	A	389	ARG
1	A	455	PHE
1	A	457	ASN
1	A	471	SER
1	A	480	LYS
1	A	484	LYS
1	A	492	TYR
1	A	517	THR
1	A	520	GLU
1	A	527	GLU
1	A	557	GLN
1	A	571	ARG
1	A	575	ILE

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Mol	Chain	Res	Type
1	A	612	TRP
1	A	648	LEU
1	A	664	ARG
1	A	669	VAL
1	A	672	GLN
1	A	673	ASN
1	A	676	ASP
1	A	696	GLN
1	A	701	SER
1	A	704	GLN
1	A	705	GLN
1	A	711	GLU
1	A	717	ARG
1	A	720	GLU
1	A	724	ARG
1	A	727	GLU
1	B	14	ARG
1	B	41	LYS
1	B	50	ASN
1	B	54	LEU
1	B	69	ARG
1	B	70	ARG
1	B	72	VAL
1	B	73	ILE
1	B	77	ASP
1	B	91	LEU
1	B	101	THR
1	B	117	LEU
1	B	118	VAL
1	B	119	VAL
1	B	128	LEU
1	B	150	GLU
1	B	156	LYS
1	B	162	LYS
1	B	166	ASP
1	B	182	LEU
1	B	183	SER
1	B	194	THR
1	B	204	LEU
1	B	226	SER
1	B	242	LEU
1	B	246	GLU

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Mol	Chain	Res	Type
1	B	249	VAL
1	B	254	ARG
1	B	273	GLU
1	B	284	LYS
1	B	303	VAL
1	B	310	PHE
1	B	311	LEU
1	B	312	ARG
1	B	314	LEU
1	B	316	ARG
1	B	318	ARG
1	B	327	GLN
1	B	334	SER
1	B	336	MET
1	B	348	ASP
1	B	351	VAL
1	B	352	ASP
1	B	354	ASP
1	B	377	LYS
1	B	386	ILE
1	B	389	ARG
1	B	397	LYS
1	B	436	ARG
1	B	439	THR
1	B	455	PHE
1	B	457	ASN
1	B	458	THR
1	B	463	ARG
1	B	513	LYS
1	B	520	GLU
1	B	524	ASP
1	B	557	GLN
1	B	565	GLN
1	B	571	ARG
1	B	575	ILE
1	B	576	GLU
1	B	583	LEU
1	B	585	LYS
1	B	587	LEU
1	B	589	TRP
1	B	595	ARG
1	B	604	SER

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Mol	Chain	Res	Type
1	B	612	TRP
1	B	627	ASP
1	B	643	LEU
1	B	654	THR
1	B	659	ARG
1	B	668	LEU
1	B	671	ARG
1	B	672	GLN
1	B	677	VAL
1	B	688	ASP
1	B	720	GLU
1	B	724	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	129	ASN
1	A	196	GLN
1	A	213	ASN
1	A	234	ASN
1	A	248	GLN
1	A	290	ASN
1	A	340	ASN
1	A	382	ASN
1	A	387	ASN
1	A	457	ASN
1	A	642	GLN
1	A	650	HIS
1	A	707	ASN
1	B	21	ASN
1	B	49	GLN
1	B	63	GLN
1	B	116	GLN
1	B	132	ASN
1	B	216	GLN
1	B	290	ASN
1	B	295	ASN
1	B	327	GLN
1	B	340	ASN
1	B	374	HIS
1	B	457	ASN

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Mol	Chain	Res	Type
1	B	510	GLN
1	B	707	ASN
1	B	715	HIS

### 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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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
6	GLV	B	1901	2	1,4,4	6.26	1 (100%)	0,4,4	0.00	-
4	MLT	A	902	-	2,8,8	1.09	0	3,10,10	1.76	1 (33%)
4	MLT	B	1902	-	2,8,8	0.36	0	3,10,10	0.69	0
3	SO4	A	1802	-	4,4,4	0.13	0	6,6,6	0.13	0
4	MLT	A	901	2	2,8,8	0.44	0	3,10,10	1.31	0
3	SO4	B	1803	-	4,4,4	0.14	0	6,6,6	0.15	0
5	COA	A	903	-	41,50,50	1.77	4 (9%)	52,75,75	1.27	4 (7%)
3	SO4	A	1800	-	4,4,4	0.13	0	6,6,6	0.25	0

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
6	GLV	B	1901	2	-	0/0/2/2	-
4	MLT	A	901	2	1/1/3/3	2/2/8/8	-
4	MLT	A	902	-	1/1/3/3	2/2/8/8	-
4	MLT	B	1902	-	1/1/3/3	0/2/8/8	-
5	COA	A	903	-	-	19/44/64/64	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	903	COA	O9P-C9P	9.33	1.41	1.23
6	B	1901	GLV	O1-C1	6.26	1.43	1.21
5	A	903	COA	C2A-N3A	4.16	1.38	1.32
5	A	903	COA	C2A-N1A	2.80	1.39	1.33
5	A	903	COA	P3B-O3B	2.32	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	903	COA	N3A-C2A-N1A	-5.44	120.17	128.68
5	A	903	COA	P2A-O3A-P1A	-3.40	121.16	132.83
4	A	902	MLT	C3-C2-C1	-2.54	107.86	111.10
5	A	903	COA	C3B-C2B-C1B	2.54	105.51	99.89
5	A	903	COA	C4A-C5A-N7A	-2.09	107.22	109.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	902	MLT	C2
4	B	1902	MLT	C2
4	A	901	MLT	C2

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	MLT	O3-C2-C3-C4
4	A	901	MLT	C1-C2-C3-C4
4	A	901	MLT	O3-C2-C3-C4
5	A	903	COA	C4B-C5B-O5B-P1A

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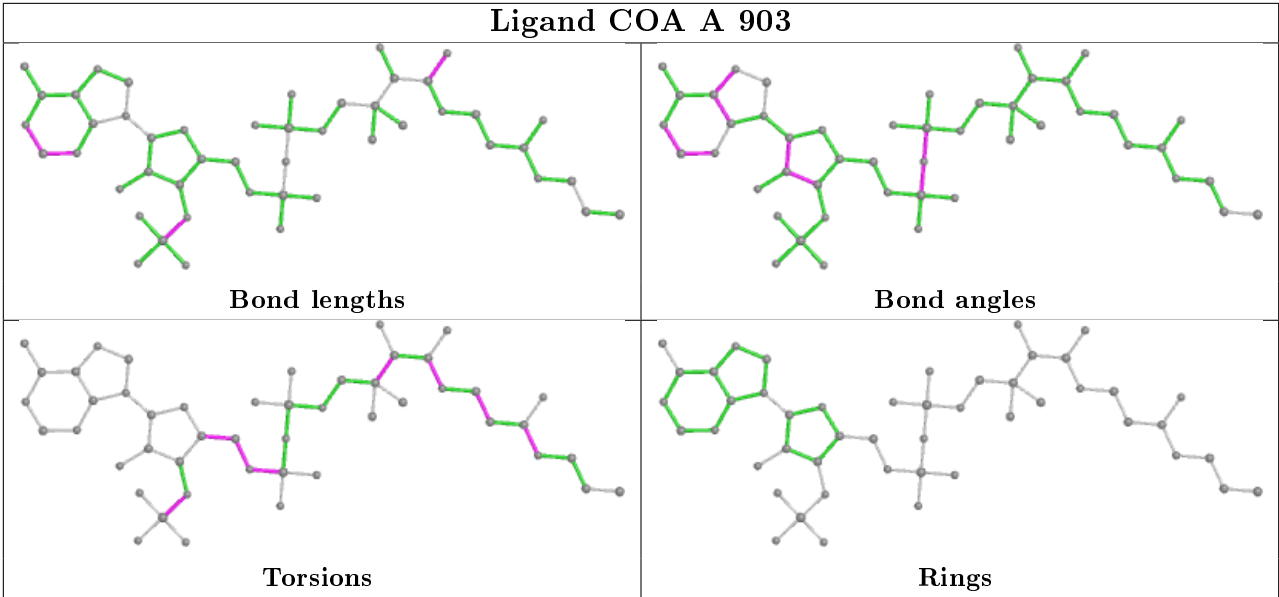
Mol	Chain	Res	Type	Atoms
5	A	903	COA	C5B-O5B-P1A-O1A
5	A	903	COA	C5B-O5B-P1A-O3A
5	A	903	COA	OAP-CAP-CBP-CCP
5	A	903	COA	C9P-CAP-CBP-CCP
5	A	903	COA	OAP-CAP-CBP-CDP
5	A	903	COA	C9P-CAP-CBP-CDP
5	A	903	COA	OAP-CAP-CBP-CEP
5	A	903	COA	C9P-CAP-CBP-CEP
5	A	903	COA	CAP-C9P-N8P-C7P
5	A	903	COA	O9P-C9P-N8P-C7P
5	A	903	COA	C5P-C6P-C7P-N8P
5	A	903	COA	C3B-C4B-C5B-O5B
5	A	903	COA	O4B-C4B-C5B-O5B
5	A	903	COA	C6P-C5P-N4P-C3P
5	A	903	COA	O5P-C5P-N4P-C3P
4	A	902	MLT	C1-C2-C3-C4
5	A	903	COA	C3B-O3B-P3B-O7A
5	A	903	COA	C3B-O3B-P3B-O8A
5	A	903	COA	C3B-O3B-P3B-O9A

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	MLT	3	0
5	A	903	COA	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	588:ALA	C	589:TRP	N	1.20

## 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.