



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:32 AM UTC

PDB ID : 8PRY / pdb_00008pry
Title : Crystal structure of Trypanosoma cruzi glycerol kinase
Authors : Lipinski, O.; Sonani, R.R.; Dubin, G.
Deposited on : 2023-07-12
Resolution : 2.07 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

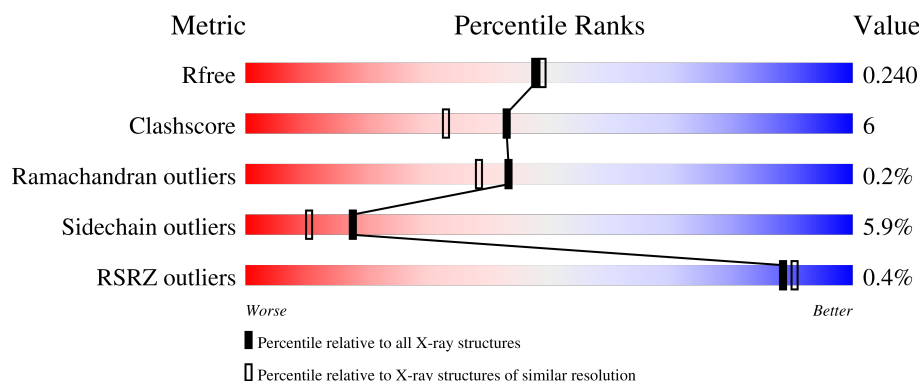
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	523	79% 17% ..
1	B	523	79% 16% ..
1	C	523	77% 16% ...
1	D	523	% 76% 16% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16378 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 glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3992	2538	694	732	28			
1	B	511	Total	C	N	O	S	0	0	0
			3984	2532	693	731	28			
1	C	512	Total	C	N	O	S	0	0	0
			3992	2538	694	732	28			
1	D	511	Total	C	N	O	S	0	0	0
			3983	2532	693	730	28			

There are 32 discrepancies between the modelled and reference sequences:

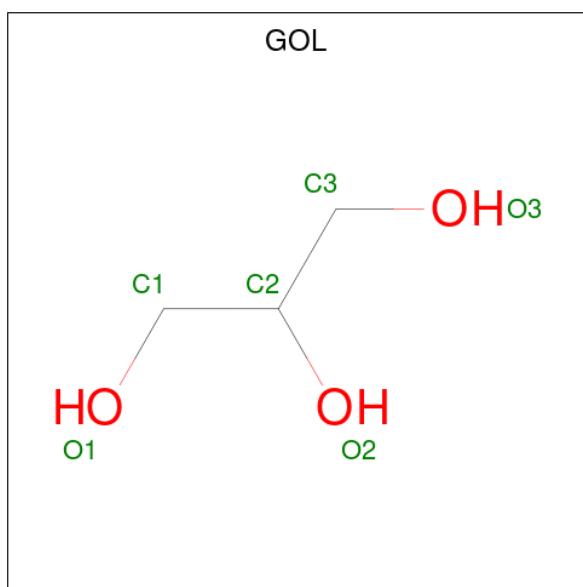
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP A0A2V2W444
A	-9	ALA	-	expression tag	UNP A0A2V2W444
A	-8	HIS	-	expression tag	UNP A0A2V2W444
A	-7	HIS	-	expression tag	UNP A0A2V2W444
A	-6	HIS	-	expression tag	UNP A0A2V2W444
A	-5	HIS	-	expression tag	UNP A0A2V2W444
A	-4	HIS	-	expression tag	UNP A0A2V2W444
A	-3	HIS	-	expression tag	UNP A0A2V2W444
B	-10	MET	-	initiating methionine	UNP A0A2V2W444
B	-9	ALA	-	expression tag	UNP A0A2V2W444
B	-8	HIS	-	expression tag	UNP A0A2V2W444
B	-7	HIS	-	expression tag	UNP A0A2V2W444
B	-6	HIS	-	expression tag	UNP A0A2V2W444
B	-5	HIS	-	expression tag	UNP A0A2V2W444
B	-4	HIS	-	expression tag	UNP A0A2V2W444
B	-3	HIS	-	expression tag	UNP A0A2V2W444
C	-10	MET	-	initiating methionine	UNP A0A2V2W444
C	-9	ALA	-	expression tag	UNP A0A2V2W444
C	-8	HIS	-	expression tag	UNP A0A2V2W444
C	-7	HIS	-	expression tag	UNP A0A2V2W444
C	-6	HIS	-	expression tag	UNP A0A2V2W444

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP A0A2V2W444
C	-4	HIS	-	expression tag	UNP A0A2V2W444
C	-3	HIS	-	expression tag	UNP A0A2V2W444
D	-10	MET	-	initiating methionine	UNP A0A2V2W444
D	-9	ALA	-	expression tag	UNP A0A2V2W444
D	-8	HIS	-	expression tag	UNP A0A2V2W444
D	-7	HIS	-	expression tag	UNP A0A2V2W444
D	-6	HIS	-	expression tag	UNP A0A2V2W444
D	-5	HIS	-	expression tag	UNP A0A2V2W444
D	-4	HIS	-	expression tag	UNP A0A2V2W444
D	-3	HIS	-	expression tag	UNP A0A2V2W444

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

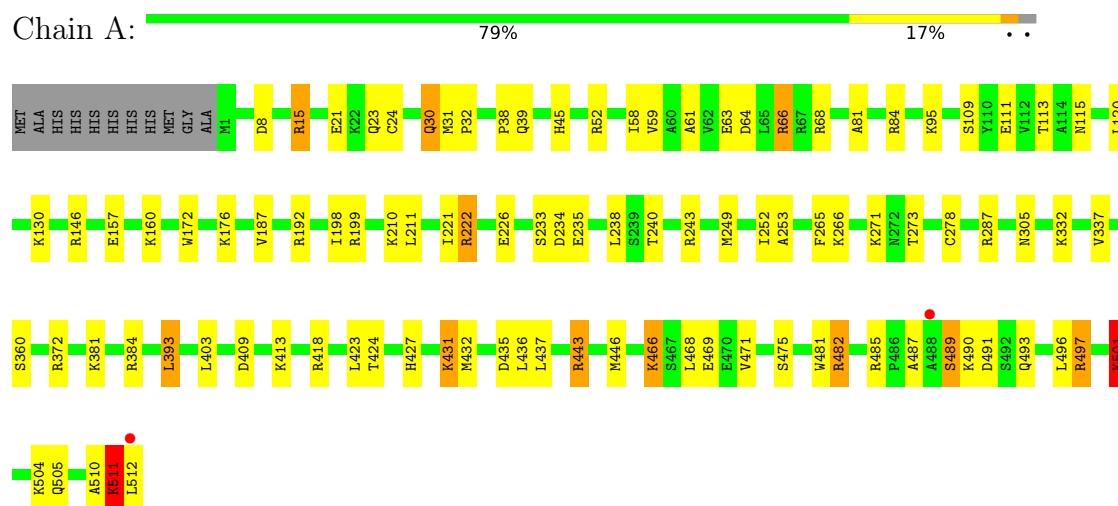
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total 112	O 112	0	0
3	B	156	Total 156	O 156	0	0
3	C	95	Total 95	O 95	0	0
3	D	40	Total 40	O 40	0	0

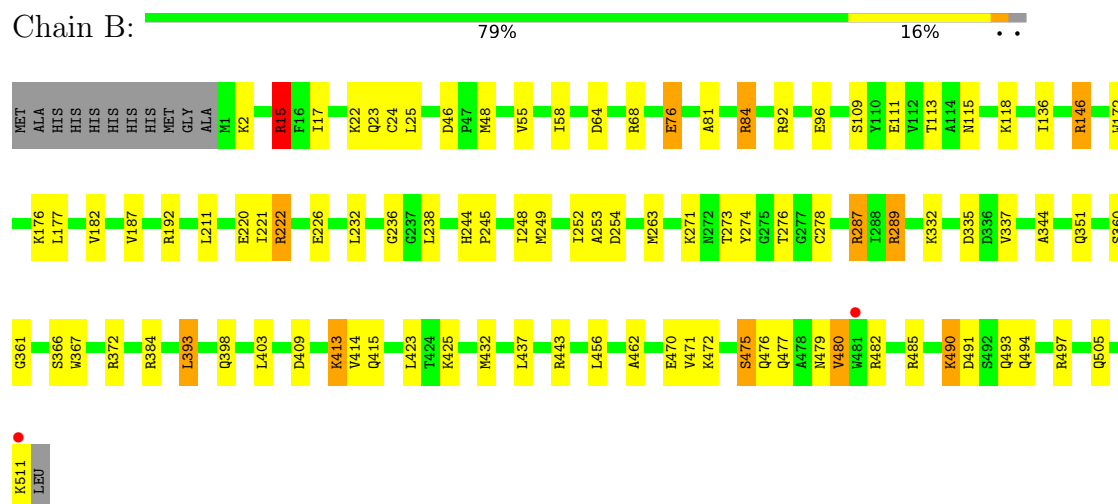
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: glycerol kinase

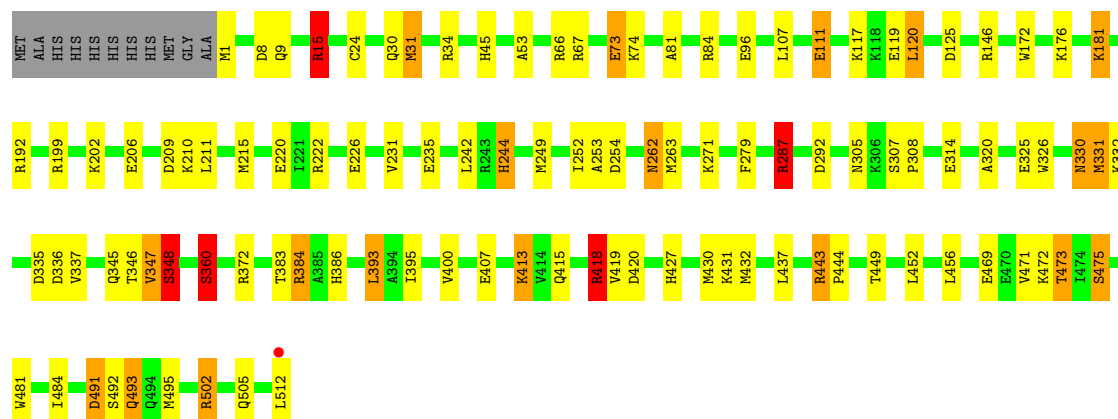


- Molecule 1: glycerol kinase

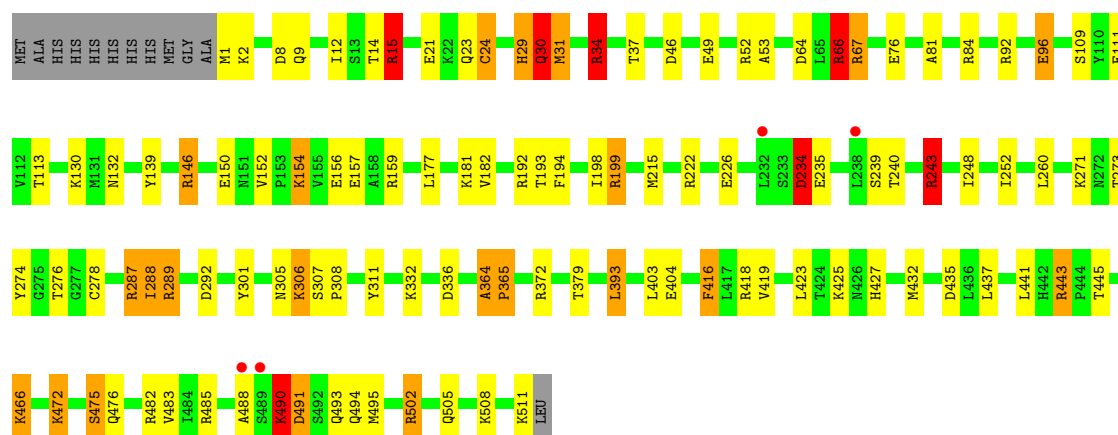
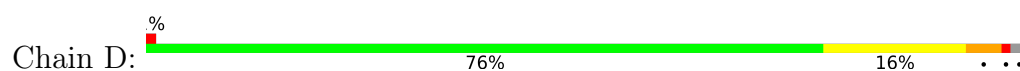


- Molecule 1: glycerol kinase





• Molecule 1: glycerol kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.78Å 89.32Å 97.16Å 117.35° 88.99° 93.68°	Depositor
Resolution (Å)	44.61 – 2.07 44.61 – 2.07	Depositor EDS
% Data completeness (in resolution range)	93.8 (44.61-2.07) 93.8 (44.61-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.07Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.176 , 0.238 0.184 , 0.240	Depositor DCC
R_{free} test set	5822 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,k+1	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16378	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSD

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	1.10	7/4064 (0.2%)	1.41	27/5496 (0.5%)
1	B	1.17	6/4056 (0.1%)	1.44	23/5485 (0.4%)
1	C	1.12	5/4064 (0.1%)	1.51	39/5496 (0.7%)
1	D	0.99	1/4055 (0.0%)	1.42	32/5483 (0.6%)
All	All	1.10	19/16239 (0.1%)	1.45	121/21960 (0.6%)

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	0	10
1	B	0	7
1	C	0	11
1	D	0	16
All	All	0	44

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	24	CSD	C-N	14.84	1.54	1.33
1	D	24	CSD	C-N	14.02	1.52	1.33
1	A	24	CSD	C-N	13.90	1.52	1.33
1	C	24	CSD	C-N	12.51	1.50	1.33
1	A	111	GLU	CD-OE2	7.41	1.39	1.25
1	C	45	HIS	CE1-NE2	6.85	1.39	1.32
1	C	244	HIS	CE1-NE2	6.70	1.39	1.32
1	B	470	GLU	CD-OE1	6.62	1.38	1.25
1	A	31	MET	CG-SD	-6.41	1.64	1.80
1	B	462	ALA	C-O	-6.23	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	HIS	CE1-NE2	6.08	1.38	1.32
1	B	136	ILE	C-O	-6.08	1.18	1.24
1	A	63	GLU	C-O	6.00	1.31	1.24
1	B	76	GLU	CD-OE1	5.53	1.35	1.25
1	C	314	GLU	CD-OE1	5.51	1.35	1.25
1	A	21	GLU	CD-OE2	-5.50	1.14	1.25
1	B	48	MET	CG-SD	5.25	1.93	1.80
1	C	360	SER	CA-CB	5.08	1.60	1.53
1	A	38	PRO	C-O	-5.07	1.17	1.24

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	ASP	CA-CB-CG	11.75	124.35	112.60
1	B	276	THR	CA-CB-OG1	-10.97	93.14	109.60
1	A	427	HIS	CA-CB-CG	-9.80	104.00	113.80
1	C	287	ARG	CG-CD-NE	9.35	132.57	112.00
1	C	330	ASN	N-CA-C	-8.12	97.83	110.42
1	A	497	ARG	CG-CD-NE	-7.84	94.76	112.00
1	C	292	ASP	CA-CB-CG	-7.80	104.80	112.60
1	D	491	ASP	CB-CA-C	-7.79	94.91	110.42
1	C	111	GLU	CB-CG-CD	7.75	125.78	112.60
1	A	265	PHE	CB-CA-C	-7.72	96.22	109.65
1	C	345	GLN	CB-CG-CD	-7.62	99.64	112.60
1	C	244	HIS	CA-CB-CG	7.51	121.31	113.80
1	B	372	ARG	NE-CZ-NH2	-7.48	112.47	119.20
1	C	8	ASP	CA-CB-CG	7.45	120.05	112.60
1	A	446	MET	CA-C-N	7.44	130.99	120.28
1	A	446	MET	C-N-CA	7.44	130.99	120.28
1	B	76	GLU	CB-CA-C	-7.32	98.64	110.79
1	C	491	ASP	CA-CB-CG	7.31	119.91	112.60
1	C	473	THR	CA-CB-OG1	-7.30	98.64	109.60
1	D	472	LYS	CB-CG-CD	7.17	127.78	111.30
1	B	222	ARG	CB-CG-CD	7.13	127.69	111.30
1	C	346	THR	CA-C-N	-7.09	116.02	122.97
1	C	346	THR	C-N-CA	-7.09	116.02	122.97
1	B	96	GLU	CB-CA-C	-7.06	97.44	109.51
1	A	66	ARG	CG-CD-NE	-7.04	96.50	112.00
1	A	332	LYS	CB-CA-C	-6.91	100.82	111.66
1	C	347	VAL	N-CA-CB	6.89	118.39	111.57
1	D	466	LYS	CB-CA-C	6.86	121.59	109.65
1	D	332	LYS	CB-CA-C	-6.79	101.89	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	332	LYS	CB-CA-C	-6.67	101.19	111.66
1	D	29	HIS	CB-CA-C	6.57	123.50	110.42
1	C	427	HIS	CA-CB-CG	6.56	120.36	113.80
1	C	491	ASP	CB-CA-C	-6.48	97.80	110.11
1	B	475	SER	O-C-N	-6.47	115.26	122.12
1	C	262	ASN	CB-CA-C	-6.46	98.39	110.01
1	C	15	ARG	CB-CA-C	6.39	123.74	109.56
1	A	409	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	240	THR	CA-CB-OG1	-6.30	100.15	109.60
1	B	361	GLY	CA-C-O	-6.16	117.65	122.52
1	D	111	GLU	CB-CG-CD	6.11	122.99	112.60
1	C	325	GLU	N-CA-CB	-6.11	100.84	109.94
1	D	156	GLU	CB-CA-C	6.09	120.89	110.79
1	D	139	TYR	CA-CB-CG	6.07	124.82	113.90
1	D	491	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	157	GLU	CB-CG-CD	6.00	122.80	112.60
1	C	348	SER	N-CA-CB	5.94	120.53	110.49
1	A	64	ASP	CB-CA-C	-5.94	100.93	110.79
1	B	335	ASP	CB-CA-C	-5.93	99.84	110.70
1	A	468	LEU	CA-C-N	-5.88	110.84	121.14
1	A	468	LEU	C-N-CA	-5.88	110.84	121.14
1	B	232	LEU	O-C-N	-5.87	115.38	122.48
1	D	34	ARG	O-C-N	5.82	130.09	122.93
1	B	254	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	39	GLN	CB-CA-C	-5.80	97.93	111.09
1	C	336	ASP	CB-CA-C	-5.79	97.92	109.79
1	C	449	THR	CA-CB-OG1	-5.77	100.95	109.60
1	D	34	ARG	CA-C-N	5.77	132.47	122.32
1	D	34	ARG	C-N-CA	5.77	132.47	122.32
1	B	471	VAL	N-CA-CB	5.76	120.50	110.65
1	D	49	GLU	CB-CG-CD	5.71	122.30	112.60
1	C	469	GLU	CB-CG-CD	5.69	122.28	112.60
1	C	287	ARG	CB-CG-CD	5.69	124.39	111.30
1	D	66	ARG	CG-CD-NE	-5.69	99.48	112.00
1	C	96	GLU	CB-CA-C	-5.66	99.83	109.51
1	B	505	GLN	CB-CG-CD	-5.63	103.02	112.60
1	A	485	ARG	CG-CD-NE	-5.62	99.63	112.00
1	D	96	GLU	N-CA-CB	5.62	119.79	110.63
1	C	254	ASP	CA-CB-CG	5.61	118.21	112.60
1	C	384	ARG	N-CA-CB	-5.56	101.72	110.06
1	C	502	ARG	CG-CD-NE	-5.56	99.77	112.00
1	C	15	ARG	CA-CB-CG	5.54	125.17	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ALA	CA-C-N	5.51	127.51	120.56
1	A	61	ALA	C-N-CA	5.51	127.51	120.56
1	D	292	ASP	CB-CA-C	5.49	120.00	110.94
1	C	209	ASP	CB-CA-C	-5.48	102.05	110.81
1	D	364	ALA	O-C-N	-5.47	116.43	121.30
1	A	413	LYS	CB-CA-C	5.47	119.05	110.19
1	C	415	GLN	CA-C-O	5.47	125.67	119.27
1	B	76	GLU	N-CA-CB	5.46	118.14	110.12
1	B	64	ASP	CB-CA-C	-5.44	101.77	110.79
1	A	482	ARG	NE-CZ-NH1	5.43	126.94	121.50
1	D	276	THR	CA-CB-OG1	-5.42	101.46	109.60
1	D	182	VAL	CA-CB-CG2	5.40	119.58	110.40
1	B	372	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	C	199	ARG	CD-NE-CZ	-5.39	116.86	124.40
1	B	384	ARG	CG-CD-NE	-5.36	100.20	112.00
1	B	332	LYS	CB-CA-C	-5.34	103.07	111.51
1	C	199	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	B	245	PRO	CB-CA-C	5.33	120.36	111.56
1	C	335	ASP	CA-C-O	-5.33	113.36	119.60
1	A	435	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	491	ASP	CA-CB-CG	5.30	117.90	112.60
1	D	132	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	244	HIS	CA-CB-CG	-5.27	108.53	113.80
1	A	501	LYS	CG-CD-CE	5.25	123.38	111.30
1	B	409	ASP	CA-CB-CG	5.24	117.84	112.60
1	D	8	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	491	ASP	N-CA-C	5.23	121.94	110.80
1	D	435	ASP	CA-CB-CG	5.22	117.82	112.60
1	D	427	HIS	CB-CA-C	5.18	119.66	110.85
1	C	73	GLU	CB-CG-CD	5.18	121.40	112.60
1	C	418	ARG	CB-CA-C	-5.16	101.02	109.53
1	C	443	ARG	NE-CZ-NH2	-5.15	114.56	119.20
1	D	243	ARG	CB-CG-CD	5.14	123.13	111.30
1	D	146	ARG	CB-CG-CD	-5.11	99.54	111.30
1	A	199	ARG	CG-CD-NE	5.11	123.24	112.00
1	A	481	TRP	CA-C-O	-5.10	114.90	120.36
1	D	502	ARG	CB-CA-C	5.10	119.26	110.79
1	D	427	HIS	CA-CB-CG	-5.08	108.72	113.80
1	D	404	GLU	CB-CG-CD	5.08	121.23	112.60
1	B	344	ALA	CA-C-N	5.07	127.08	120.28
1	B	344	ALA	C-N-CA	5.07	127.08	120.28
1	B	111	GLU	CB-CG-CD	5.06	121.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	MET	CG-SD-CE	-5.04	89.81	100.90
1	D	15	ARG	CB-CG-CD	5.04	122.89	111.30
1	C	360	SER	CB-CA-C	5.04	120.07	111.46
1	A	64	ASP	N-CA-CB	5.03	117.51	110.12
1	C	492	SER	N-CA-C	-5.01	106.43	112.54
1	A	95	LYS	CA-C-O	-5.00	114.36	120.12
1	A	8	ASP	CA-CB-CG	5.00	117.60	112.60
1	D	37	THR	CA-CB-CG2	5.00	119.00	110.50

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ARG	Sidechain
1	A	192	ARG	Sidechain
1	A	222	ARG	Sidechain
1	A	234	ASP	Peptide
1	A	287	ARG	Sidechain
1	A	372	ARG	Sidechain
1	A	384	ARG	Sidechain
1	A	418	ARG	Sidechain
1	A	443	ARG	Sidechain
1	A	489	SER	Peptide
1	B	146	ARG	Sidechain
1	B	15	ARG	Sidechain
1	B	192	ARG	Sidechain
1	B	287	ARG	Sidechain
1	B	289	ARG	Sidechain
1	B	497	ARG	Sidechain
1	B	84	ARG	Sidechain
1	C	15	ARG	Sidechain
1	C	192	ARG	Sidechain
1	C	287	ARG	Sidechain
1	C	34	ARG	Sidechain
1	C	372	ARG	Sidechain
1	C	384	ARG	Sidechain
1	C	418	ARG	Sidechain
1	C	443	ARG	Sidechain
1	C	502	ARG	Sidechain
1	C	66	ARG	Sidechain
1	C	67	ARG	Sidechain
1	D	15	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	150	GLU	Mainchain
1	D	159	ARG	Sidechain
1	D	192	ARG	Sidechain
1	D	199	ARG	Sidechain
1	D	287	ARG	Sidechain
1	D	289	ARG	Sidechain
1	D	34	ARG	Sidechain
1	D	364	ALA	Peptide,Mainchain
1	D	443	ARG	Sidechain
1	D	485	ARG	Sidechain
1	D	488	ALA	Peptide
1	D	490	LYS	Peptide
1	D	67	ARG	Sidechain
1	D	92	ARG	Sidechain

5.2 Too-close contacts

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	3992	0	4040	37	0
1	B	3984	0	4029	50	0
1	C	3992	0	4040	61	0
1	D	3983	0	4029	58	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	1	0
2	D	6	0	8	2	0
3	A	112	0	0	4	0
3	B	156	0	0	5	0
3	C	95	0	0	9	0
3	D	40	0	0	7	0
All	All	16378	0	16170	199	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 6.

All (199) 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:C:331:MET:N	3:C:701:HOH:O	1.70	1.13
1:A:52:ARG:NH1	3:A:701:HOH:O	1.86	1.07
1:D:493:GLN:NE2	3:D:702:HOH:O	1.90	1.04
1:D:24:CSD:OD2	3:D:701:HOH:O	1.84	0.96
1:C:119:GLU:HB2	1:C:120:LEU:HD13	1.47	0.93
1:A:30:GLN:NE2	3:A:702:HOH:O	2.03	0.89
1:B:68:ARG:NH1	3:B:701:HOH:O	2.02	0.88
1:A:23:GLN:HE22	1:A:475:SER:HB2	1.36	0.88
1:D:84:ARG:HH21	2:D:601:GOL:H12	1.39	0.87
1:D:29:HIS:O	1:D:30:GLN:HB3	1.76	0.84
1:D:66:ARG:HG3	1:D:66:ARG:NH1	1.94	0.82
1:A:493:GLN:O	1:A:497:ARG:HG3	1.80	0.81
1:A:436:LEU:HD23	1:A:493:GLN:OE1	1.81	0.79
1:A:115:ASN:HD22	1:A:146:ARG:HH22	1.31	0.79
1:A:482:ARG:HH11	1:A:482:ARG:HA	1.47	0.78
1:C:220:GLU:OE2	1:C:222:ARG:NH1	2.17	0.76
1:C:330:ASN:CA	3:C:701:HOH:O	2.33	0.76
1:B:92:ARG:HG3	1:B:92:ARG:NH1	2.00	0.75
1:D:306:LYS:H	1:D:306:LYS:HD2	1.51	0.73
1:D:222:ARG:HD2	1:D:226:GLU:OE2	1.89	0.73
1:C:326:TRP:O	1:C:330:ASN:O	2.07	0.72
1:D:152:VAL:HG12	1:D:154:LYS:HG3	1.72	0.72
1:C:74:LYS:CE	1:C:244:HIS:HB2	2.20	0.72
1:A:68:ARG:NH1	3:A:703:HOH:O	2.14	0.70
1:D:66:ARG:HG3	1:D:66:ARG:HH11	1.57	0.70
1:B:287:ARG:HH12	1:B:289:ARG:NE	1.89	0.69
1:C:330:ASN:HA	3:C:701:HOH:O	1.93	0.69
1:C:119:GLU:HB2	1:C:120:LEU:CD1	2.21	0.69
1:B:92:ARG:HG3	1:B:92:ARG:HH11	1.58	0.68
1:D:23:GLN:HE22	1:D:475:SER:HB2	1.59	0.67
1:D:287:ARG:HG2	1:D:289:ARG:HH11	1.60	0.66
1:C:74:LYS:HE2	1:C:244:HIS:HB2	1.77	0.65
1:C:305:ASN:ND2	1:C:305:ASN:H	1.95	0.65
1:D:416:PHE:CZ	1:D:418:ARG:NH1	2.64	0.65
1:A:233:SER:OG	1:A:235:GLU:HB2	1.98	0.63
1:B:287:ARG:NH1	1:B:289:ARG:NE	2.46	0.63
1:D:1:MET:N	3:D:704:HOH:O	2.32	0.63
1:C:262:ASN:OD1	3:C:703:HOH:O	2.16	0.63
1:D:235:GLU:CD	3:D:713:HOH:O	2.41	0.62
1:C:305:ASN:H	1:C:305:ASN:HD22	1.46	0.62
1:D:443:ARG:HG2	1:D:482:ARG:HH11	1.64	0.62
1:B:477:GLN:HE21	1:C:472:LYS:NZ	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ARG:HH12	1:B:482:ARG:NH1	1.97	0.62
1:B:15:ARG:CZ	1:B:15:ARG:HB2	2.30	0.61
1:C:220:GLU:CD	1:C:222:ARG:NH1	2.58	0.61
1:D:15:ARG:HG2	1:D:15:ARG:HH21	1.65	0.61
1:C:475:SER:HB2	3:C:756:HOH:O	2.01	0.61
1:B:403:LEU:HD11	1:B:414:VAL:HG21	1.84	0.60
1:C:107:LEU:HD21	1:C:360:SER:O	2.02	0.60
1:D:84:ARG:HH21	2:D:601:GOL:C1	2.13	0.59
1:C:320:ALA:HA	1:C:395:ILE:HG12	1.83	0.59
1:C:206:GLU:O	1:C:210:LYS:HG3	2.03	0.58
1:B:115:ASN:HD22	1:B:146:ARG:HH22	1.51	0.58
1:D:491:ASP:HB3	1:D:494:GLN:HG2	1.86	0.58
1:A:120:LEU:HD22	1:A:210:LYS:HG2	1.86	0.58
1:C:1:MET:N	3:C:704:HOH:O	2.36	0.58
1:C:419:VAL:O	1:C:444:PRO:HD2	2.05	0.56
1:C:263:MET:HE3	1:C:475:SER:CB	2.35	0.56
1:B:477:GLN:NE2	1:C:472:LYS:NZ	2.53	0.56
1:D:445:THR:HG22	1:D:482:ARG:NH2	2.20	0.56
1:D:2:LYS:HB3	1:D:76:GLU:HG3	1.88	0.56
1:D:52:ARG:HG2	3:D:713:HOH:O	2.06	0.56
1:D:234:ASP:HB3	1:D:239:SER:HB2	1.88	0.55
1:C:347:VAL:O	1:C:348:SER:CB	2.52	0.55
1:C:393:LEU:HD13	1:C:432:MET:SD	2.47	0.55
1:C:73:GLU:HG3	1:C:74:LYS:HG3	1.89	0.55
1:D:34:ARG:HH12	1:D:46:ASP:HB3	1.73	0.54
1:D:403:LEU:HD23	1:D:437:LEU:HD22	1.89	0.54
1:C:383:THR:H	1:C:386:HIS:HD2	1.55	0.54
1:C:279:PHE:CZ	2:C:601:GOL:H32	2.43	0.53
1:A:23:GLN:NE2	1:A:475:SER:HB2	2.17	0.53
1:C:407:GLU:OE1	1:C:413:LYS:HE2	2.09	0.53
1:C:263:MET:HE3	1:C:475:SER:HB3	1.90	0.53
1:D:505:GLN:NE2	1:D:508:LYS:HE2	2.23	0.53
1:B:23:GLN:NE2	1:B:475:SER:HB3	2.24	0.53
1:B:22:LYS:HD3	1:C:481:TRP:O	2.09	0.52
1:B:177:LEU:HD13	1:B:248:ILE:HD13	1.89	0.52
1:D:419:VAL:HG11	1:D:441:LEU:HD13	1.91	0.52
1:B:480:VAL:HG11	1:C:473:THR:HG23	1.91	0.52
1:B:403:LEU:HD23	1:B:437:LEU:HD22	1.91	0.52
1:A:115:ASN:ND2	1:A:146:ARG:HH22	2.05	0.52
1:B:393:LEU:HD13	1:B:432:MET:SD	2.51	0.51
1:B:398:GLN:NE2	3:B:703:HOH:O	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:MET:HG2	1:C:53:ALA:HB1	1.91	0.51
1:A:510:ALA:O	1:A:511:LYS:O	2.28	0.51
1:B:23:GLN:HE22	1:B:475:SER:HB3	1.75	0.51
1:C:117:LYS:HD2	1:C:125:ASP:OD1	2.10	0.51
1:D:288:ILE:HG12	1:D:311:TYR:CZ	2.46	0.51
1:D:490:LYS:HD2	1:D:491:ASP:OD1	2.11	0.51
1:D:416:PHE:C	1:D:416:PHE:CD1	2.87	0.51
1:B:477:GLN:NE2	1:C:472:LYS:HZ2	2.09	0.51
1:D:307:SER:HB3	1:D:308:PRO:HD2	1.92	0.51
1:B:58:ILE:HG21	1:B:238:LEU:HD11	1.93	0.50
1:C:418:ARG:HH11	1:C:418:ARG:HG3	1.76	0.50
1:B:92:ARG:HH11	1:B:92:ARG:CG	2.23	0.50
1:B:477:GLN:HE21	1:C:472:LYS:HZ1	1.58	0.50
1:C:307:SER:HB3	1:C:308:PRO:HD2	1.94	0.50
1:D:274:TYR:HB3	1:D:423:LEU:HB3	1.92	0.50
1:D:64:ASP:HA	1:D:67:ARG:NH2	2.26	0.49
1:D:289:ARG:NE	3:D:703:HOH:O	2.21	0.49
1:C:119:GLU:CB	1:C:120:LEU:HD13	2.33	0.49
1:C:119:GLU:CB	1:C:120:LEU:CD1	2.89	0.49
1:B:220:GLU:OE1	1:B:222:ARG:HD3	2.12	0.48
1:B:480:VAL:HG21	1:C:473:THR:HA	1.95	0.48
1:C:81:ALA:HA	1:C:252:ILE:O	2.14	0.48
1:D:1:MET:SD	1:D:21:GLU:HG2	2.53	0.48
1:D:12:ILE:O	1:D:12:ILE:HG22	2.13	0.48
1:A:403:LEU:HD23	1:A:437:LEU:HD22	1.96	0.48
1:B:366:SER:O	1:B:367:TRP:C	2.56	0.48
1:A:109:SER:O	1:A:113:THR:HG23	2.13	0.47
1:B:109:SER:O	1:B:113:THR:HG23	2.14	0.47
1:A:501:LYS:HE2	1:A:504:LYS:CE	2.45	0.47
1:B:475:SER:O	1:B:476:GLN:C	2.56	0.47
1:A:469:GLU:OE1	1:A:469:GLU:N	2.47	0.47
1:D:14:THR:O	1:D:30:GLN:HA	2.15	0.47
1:A:66:ARG:HH22	1:A:243:ARG:HG3	1.79	0.47
1:A:424:THR:HB	1:A:443:ARG:HD3	1.95	0.47
1:C:271:LYS:HD2	1:C:271:LYS:C	2.40	0.47
1:B:274:TYR:HB3	1:B:423:LEU:HB3	1.95	0.47
1:D:52:ARG:CG	3:D:713:HOH:O	2.61	0.47
1:C:172:TRP:CH2	1:C:176:LYS:HD3	2.50	0.46
1:C:262:ASN:ND2	1:C:420:ASP:OD2	2.42	0.46
1:B:172:TRP:CH2	1:B:176:LYS:HD3	2.51	0.46
1:B:177:LEU:HD13	1:B:248:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:MET:HB3	1:C:484:ILE:HD13	1.97	0.46
1:A:271:LYS:HD2	1:A:271:LYS:C	2.40	0.46
1:C:119:GLU:C	1:C:120:LEU:HD12	2.41	0.45
1:D:288:ILE:HG12	1:D:311:TYR:CE2	2.51	0.45
1:C:347:VAL:O	1:C:348:SER:HB3	2.15	0.45
1:C:493:GLN:HB2	3:C:719:HOH:O	2.16	0.45
1:A:172:TRP:CH2	1:A:176:LYS:HD3	2.51	0.45
1:D:416:PHE:CD1	1:D:416:PHE:N	2.84	0.45
1:B:413:LYS:O	1:B:415:GLN:NE2	2.49	0.45
1:A:52:ARG:NH2	3:A:712:HOH:O	2.49	0.45
1:B:263:MET:HE1	1:B:456:LEU:HD11	1.97	0.45
1:C:231:VAL:HG11	1:C:242:LEU:HD12	1.99	0.45
1:A:273:THR:O	1:A:278:CYS:HA	2.17	0.45
1:D:109:SER:O	1:D:113:THR:HG23	2.17	0.44
1:D:81:ALA:HA	1:D:252:ILE:O	2.18	0.44
1:A:403:LEU:HD23	1:A:437:LEU:CD2	2.48	0.44
1:A:431:LYS:HE2	1:A:487:ALA:HB3	1.99	0.44
1:B:187:VAL:HG13	1:B:222:ARG:O	2.16	0.44
1:A:187:VAL:HG12	1:A:221:ILE:CG2	2.47	0.44
1:D:152:VAL:CG1	1:D:154:LYS:HG3	2.46	0.44
1:B:273:THR:O	1:B:278:CYS:HA	2.18	0.44
1:B:485:ARG:HG2	1:B:485:ARG:HH11	1.83	0.44
1:A:84:ARG:CD	1:A:253:ALA:HB1	2.48	0.43
1:C:181:LYS:HA	1:C:181:LYS:HD3	1.65	0.43
1:C:452:LEU:O	1:C:456:LEU:HG	2.17	0.43
1:D:416:PHE:CE1	1:D:418:ARG:NH1	2.86	0.43
1:C:493:GLN:CB	3:C:719:HOH:O	2.66	0.43
1:B:81:ALA:HA	1:B:252:ILE:O	2.18	0.43
1:D:29:HIS:O	1:D:30:GLN:CB	2.56	0.43
1:B:68:ARG:HD2	3:B:701:HOH:O	2.17	0.43
1:C:400:VAL:HG22	1:C:437:LEU:HD23	2.00	0.43
1:B:226:GLU:O	1:B:249:MET:HA	2.19	0.43
1:D:31:MET:HE2	1:D:53:ALA:HB2	2.00	0.43
1:A:511:LYS:HB3	1:A:511:LYS:HE2	1.70	0.43
1:B:46:ASP:OD1	1:B:46:ASP:C	2.62	0.43
1:D:146:ARG:HA	1:D:146:ARG:HD2	1.76	0.43
1:C:226:GLU:O	1:C:249:MET:HA	2.19	0.43
1:D:177:LEU:HD13	1:D:248:ILE:CD1	2.49	0.43
1:A:81:ALA:HA	1:A:252:ILE:O	2.18	0.43
1:B:25:LEU:C	1:B:25:LEU:HD23	2.43	0.43
1:C:84:ARG:CD	1:C:253:ALA:HB1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ASN:ND2	1:C:305:ASN:N	2.66	0.43
1:A:466:LYS:HD3	1:A:466:LYS:HA	1.75	0.42
1:D:287:ARG:HG2	1:D:289:ARG:NH1	2.32	0.42
1:B:17:ILE:HG23	1:B:25:LEU:HG	2.01	0.42
1:C:31:MET:HE2	1:C:53:ALA:HA	2.01	0.42
1:A:226:GLU:O	1:A:249:MET:HA	2.19	0.42
1:B:479:ASN:HB2	3:B:847:HOH:O	2.19	0.42
1:D:393:LEU:HD13	1:D:432:MET:HE2	2.00	0.42
1:B:55:VAL:HG11	1:B:236:GLY:HA3	2.01	0.42
1:B:271:LYS:HD2	1:B:271:LYS:C	2.44	0.42
1:C:495:MET:HE2	1:C:495:MET:HB3	1.97	0.42
1:D:198:ILE:HA	1:D:198:ILE:HD12	1.87	0.42
1:A:501:LYS:HE3	1:A:504:LYS:NZ	2.35	0.42
1:B:2:LYS:HD3	1:B:76:GLU:HG3	2.01	0.42
1:C:287:ARG:HG2	3:C:761:HOH:O	2.19	0.42
1:B:84:ARG:CD	1:B:253:ALA:HB1	2.50	0.41
1:B:187:VAL:HG12	1:B:221:ILE:CG2	2.50	0.41
1:A:501:LYS:CE	1:A:504:LYS:NZ	2.83	0.41
1:A:436:LEU:HA	1:A:493:GLN:OE1	2.20	0.41
1:B:287:ARG:NH1	1:B:287:ARG:HG2	2.36	0.41
1:D:372:ARG:HA	1:D:372:ARG:HD3	1.88	0.41
1:A:187:VAL:HG13	1:A:222:ARG:O	2.21	0.41
1:D:193:THR:O	1:D:194:PHE:CB	2.68	0.41
1:D:260:LEU:HD11	1:D:301:TYR:CD2	2.56	0.41
1:D:273:THR:O	1:D:278:CYS:HA	2.21	0.41
1:D:416:PHE:HD1	1:D:416:PHE:O	2.03	0.41
1:D:505:GLN:HE21	1:D:508:LYS:HE2	1.86	0.41
1:A:58:ILE:HG21	1:A:238:LEU:HD11	2.03	0.41
1:A:393:LEU:HD13	1:A:432:MET:SD	2.61	0.41
1:B:398:GLN:CD	3:B:703:HOH:O	2.64	0.40
1:C:120:LEU:CD1	1:C:120:LEU:N	2.84	0.40
1:D:96:GLU:HA	1:D:96:GLU:OE1	2.22	0.40
1:D:240:THR:O	1:D:243:ARG:HG2	2.21	0.40
1:C:418:ARG:HG3	1:C:418:ARG:NH1	2.37	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	509/523 (97%)	492 (97%)	16 (3%)	1 (0%)	43	38
1	B	508/523 (97%)	489 (96%)	18 (4%)	1 (0%)	43	38
1	C	509/523 (97%)	489 (96%)	19 (4%)	1 (0%)	43	38
1	D	508/523 (97%)	487 (96%)	19 (4%)	2 (0%)	30	23
All	All	2034/2092 (97%)	1957 (96%)	72 (4%)	5 (0%)	43	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	LYS
1	B	490	LYS
1	D	30	GLN
1	C	348	SER
1	D	365	PRO

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	424/432 (98%)	399 (94%)	25 (6%)	18	10
1	B	423/432 (98%)	406 (96%)	17 (4%)	28	22
1	C	424/432 (98%)	399 (94%)	25 (6%)	18	10
1	D	423/432 (98%)	390 (92%)	33 (8%)	11	5
All	All	1694/1728 (98%)	1594 (94%)	100 (6%)	18	10

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	30	GLN
1	A	32	PRO
1	A	59	VAL
1	A	130	LYS
1	A	160	LYS
1	A	198	ILE
1	A	211	LEU
1	A	266	LYS
1	A	305	ASN
1	A	337	VAL
1	A	360	SER
1	A	381	LYS
1	A	393	LEU
1	A	423	LEU
1	A	431	LYS
1	A	466	LYS
1	A	471	VAL
1	A	489	SER
1	A	490	LYS
1	A	496	LEU
1	A	501	LYS
1	A	505	GLN
1	A	511	LYS
1	A	512	LEU
1	B	15	ARG
1	B	118	LYS
1	B	182	VAL
1	B	211	LEU
1	B	337	VAL
1	B	351	GLN
1	B	360	SER
1	B	393	LEU
1	B	413	LYS
1	B	425	LYS
1	B	472	LYS
1	B	480	VAL
1	B	490	LYS
1	B	491	ASP
1	B	493	GLN
1	B	494	GLN
1	B	511	LYS

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Mol	Chain	Res	Type
1	C	9	GLN
1	C	15	ARG
1	C	30	GLN
1	C	31	MET
1	C	111	GLU
1	C	120	LEU
1	C	146	ARG
1	C	181	LYS
1	C	202	LYS
1	C	211	LEU
1	C	215	MET
1	C	235	GLU
1	C	287	ARG
1	C	337	VAL
1	C	348	SER
1	C	360	SER
1	C	393	LEU
1	C	413	LYS
1	C	431	LYS
1	C	471	VAL
1	C	475	SER
1	C	491	ASP
1	C	493	GLN
1	C	505	GLN
1	C	512	LEU
1	D	9	GLN
1	D	15	ARG
1	D	30	GLN
1	D	31	MET
1	D	34	ARG
1	D	66	ARG
1	D	130	LYS
1	D	154	LYS
1	D	157	GLU
1	D	181	LYS
1	D	199	ARG
1	D	215	MET
1	D	234	ASP
1	D	243	ARG
1	D	271	LYS
1	D	288	ILE
1	D	305	ASN

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Mol	Chain	Res	Type
1	D	306	LYS
1	D	336	ASP
1	D	365	PRO
1	D	379	THR
1	D	393	LEU
1	D	416	PHE
1	D	425	LYS
1	D	466	LYS
1	D	472	LYS
1	D	475	SER
1	D	476	GLN
1	D	483	VAL
1	D	490	LYS
1	D	495	MET
1	D	502	ARG
1	D	511	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	115	ASN
1	A	244	HIS
1	A	262	ASN
1	A	505	GLN
1	A	506	GLN
1	B	23	GLN
1	B	115	ASN
1	B	351	GLN
1	B	476	GLN
1	B	477	GLN
1	B	493	GLN
1	C	305	ASN
1	C	330	ASN
1	C	386	HIS
1	C	494	GLN
1	D	23	GLN
1	D	262	ASN
1	D	479	ASN
1	D	505	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSD	D	24	1	3,6,8	0.74	0	1,6,10	0.73	0
1	CSD	A	24	1	3,6,8	0.82	0	1,6,10	0.19	0
1	CSD	C	24	1	3,6,8	0.62	0	1,6,10	0.44	0
1	CSD	B	24	1	3,6,8	1.08	0	1,6,10	0.76	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
1	CSD	D	24	1	-	0/1/5/8	-
1	CSD	A	24	1	-	0/1/5/8	-
1	CSD	C	24	1	-	0/1/5/8	-
1	CSD	B	24	1	-	0/1/5/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	24	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	GOL	A	601	-	5,5,5	0.31	0	5,5,5	0.77	0
2	GOL	B	601	-	5,5,5	0.39	0	5,5,5	1.64	1 (20%)
2	GOL	D	601	-	5,5,5	0.41	0	5,5,5	0.75	0
2	GOL	C	601	-	5,5,5	0.52	0	5,5,5	1.63	1 (20%)

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	GOL	A	601	-	-	0/4/4/4	-
2	GOL	B	601	-	-	4/4/4/4	-
2	GOL	D	601	-	-	2/4/4/4	-
2	GOL	C	601	-	-	3/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GOL	O2-C2-C1	2.67	120.25	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	GOL	O1-C1-C2	2.58	121.98	110.38

There are no chirality outliers.

All (9) torsion outliers are listed below:

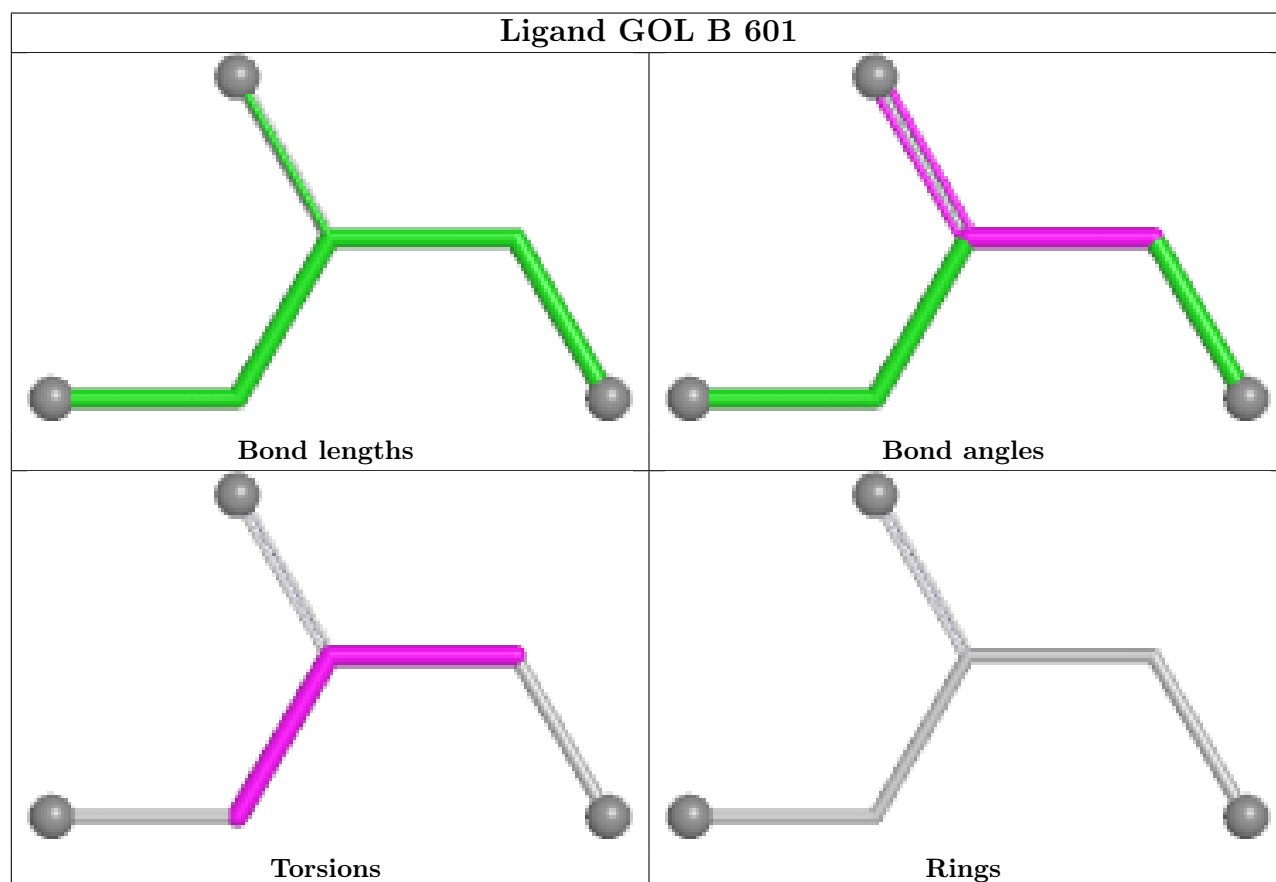
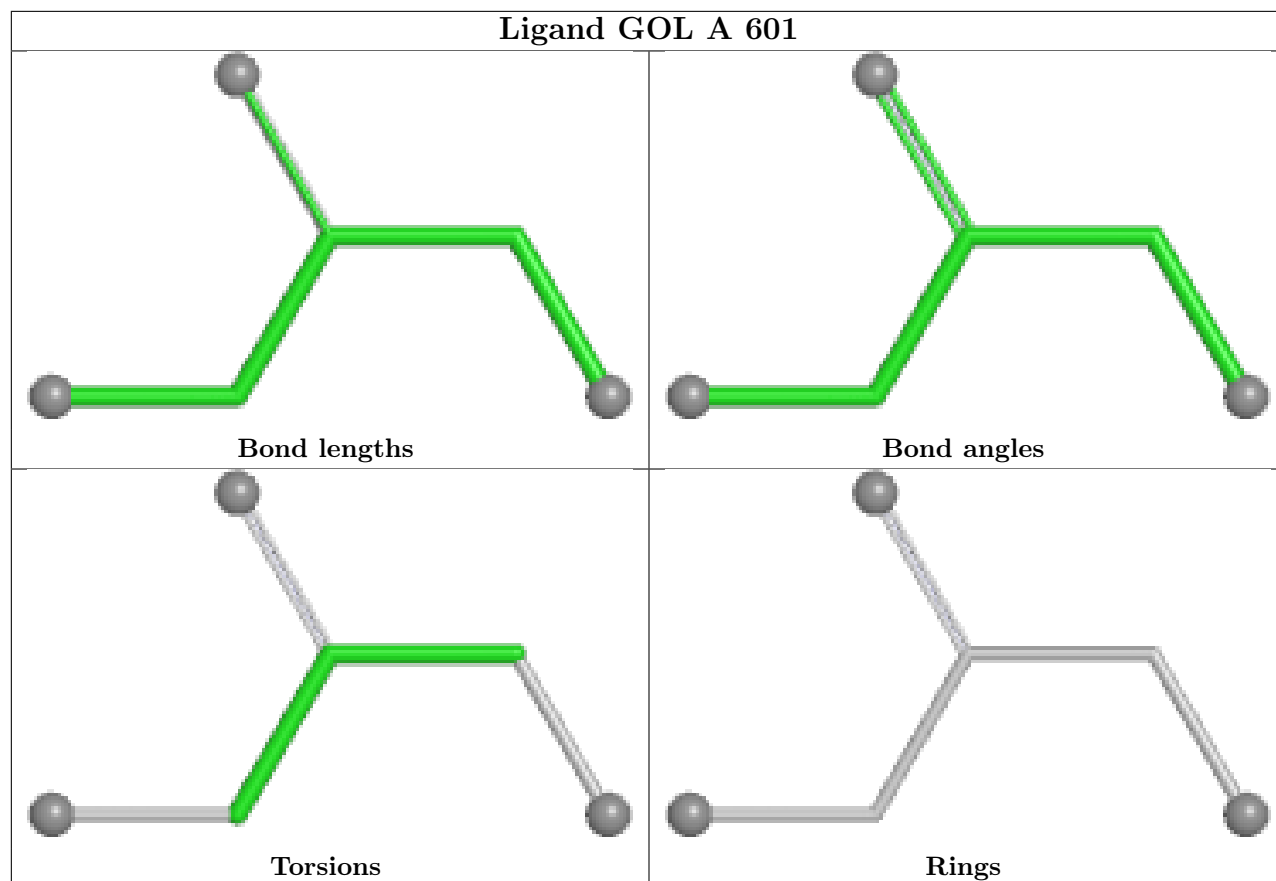
Mol	Chain	Res	Type	Atoms
2	B	601	GOL	O1-C1-C2-C3
2	B	601	GOL	C1-C2-C3-O3
2	D	601	GOL	O1-C1-C2-O2
2	D	601	GOL	O1-C1-C2-C3
2	C	601	GOL	C1-C2-C3-O3
2	B	601	GOL	O1-C1-C2-O2
2	B	601	GOL	O2-C2-C3-O3
2	C	601	GOL	O1-C1-C2-O2
2	C	601	GOL	O2-C2-C3-O3

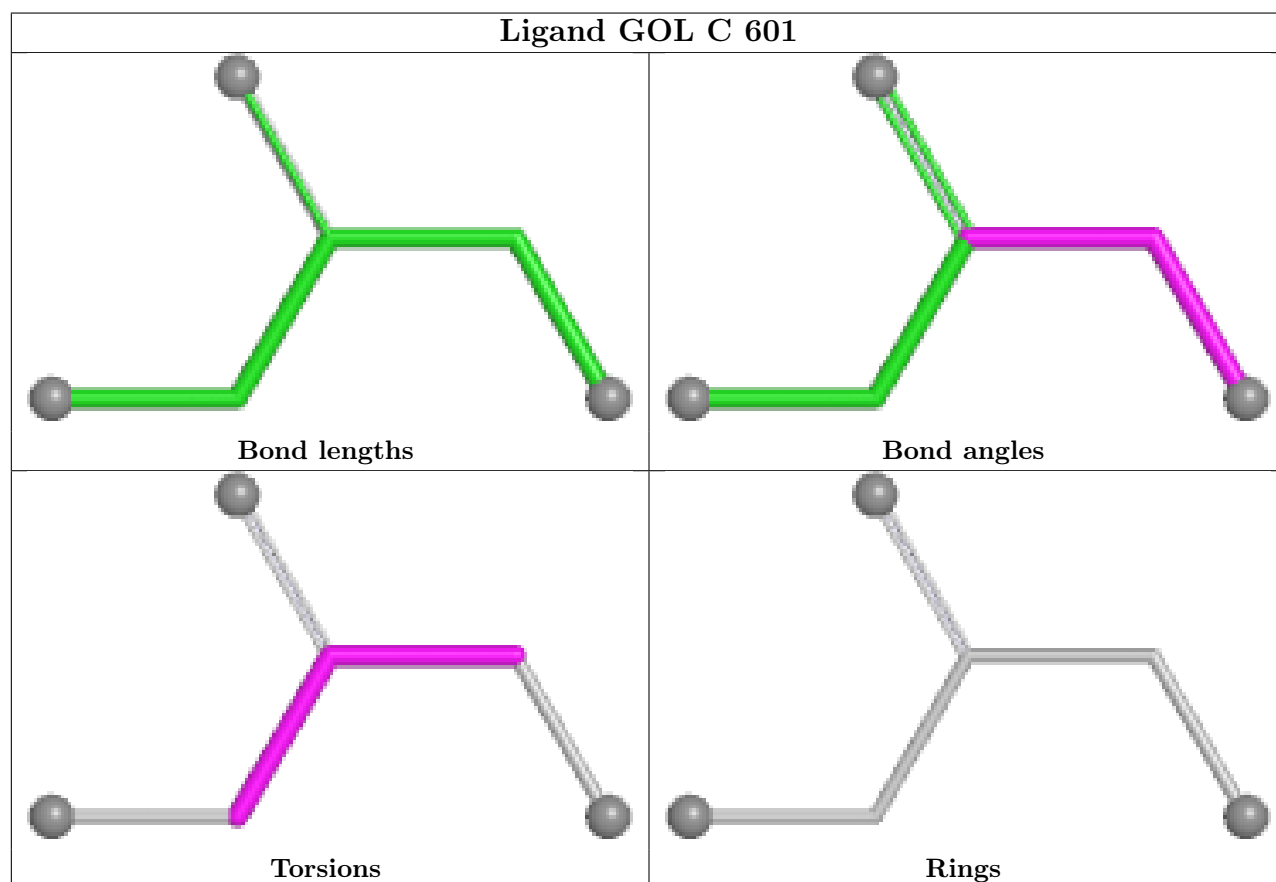
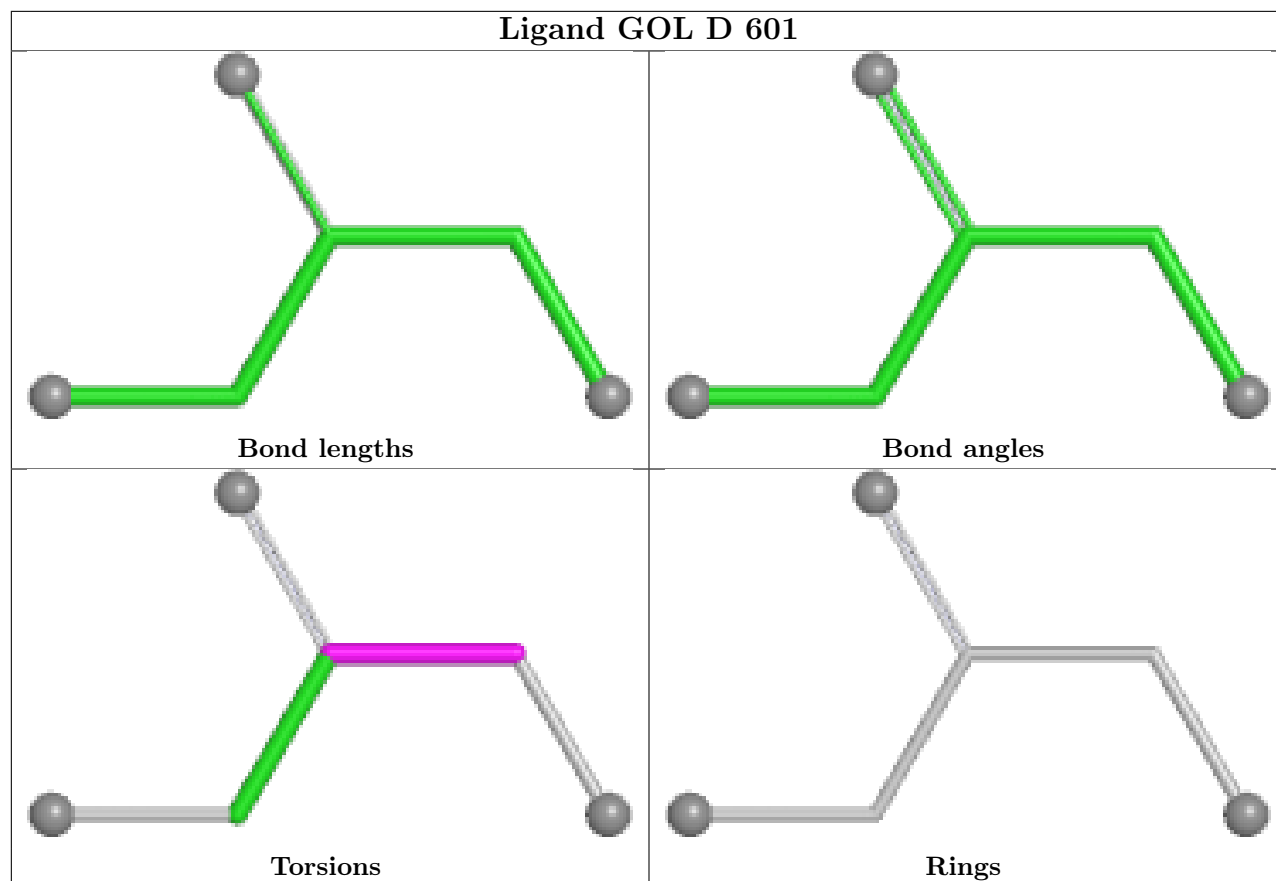
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	GOL	2	0
2	C	601	GOL	1	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	511/523 (97%)	-0.40	2 (0%) 88 90	26, 41, 62, 123	0
1	B	510/523 (97%)	-0.52	2 (0%) 88 90	26, 37, 58, 92	0
1	C	511/523 (97%)	-0.38	1 (0%) 91 93	29, 41, 67, 105	0
1	D	510/523 (97%)	0.01	4 (0%) 82 84	34, 52, 81, 114	0
All	All	2042/2092 (97%)	-0.32	9 (0%) 88 90	26, 43, 71, 123	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	LEU	3.8
1	D	488	ALA	3.7
1	A	488	ALA	3.4
1	C	512	LEU	3.1
1	B	511	LYS	2.5
1	D	489	SER	2.2
1	D	232	LEU	2.2
1	D	238	LEU	2.0
1	B	481	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	C	24	7/9	0.89	0.09	36,38,50,62	0
1	CSD	B	24	7/9	0.95	0.06	29,36,43,53	0
1	CSD	A	24	7/9	0.96	0.07	36,41,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSD	D	24	7/9	0.96	0.06	44,53,60,61	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

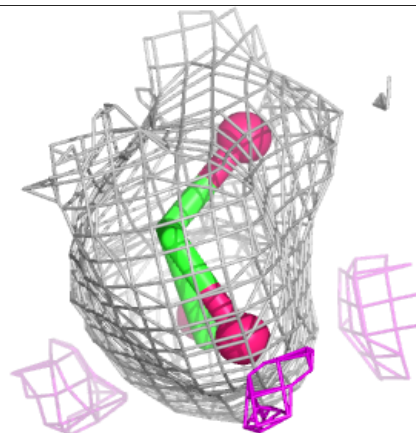
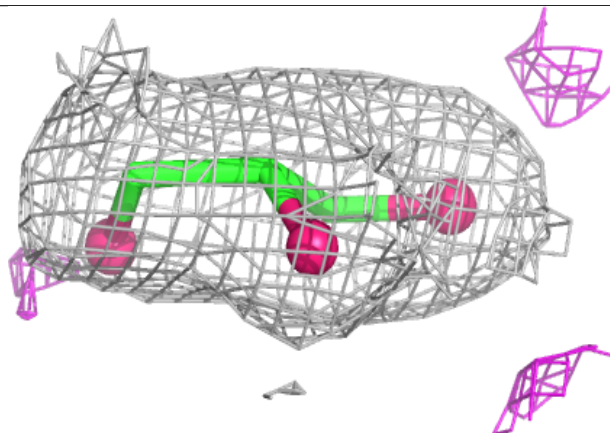
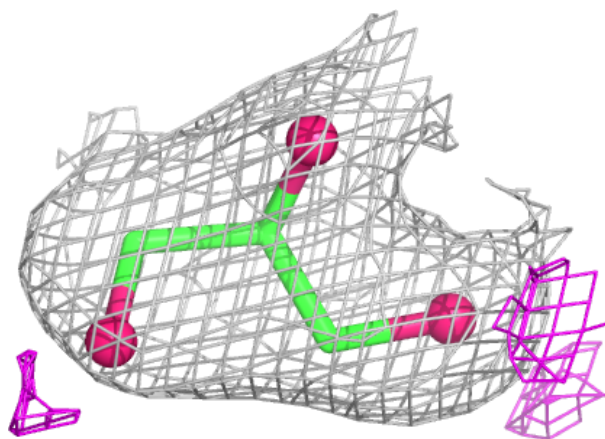
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	D	601	6/6	0.90	0.10	35,39,41,43	0
2	GOL	B	601	6/6	0.96	0.06	25,30,33,36	0
2	GOL	C	601	6/6	0.97	0.06	27,35,37,39	0
2	GOL	A	601	6/6	0.98	0.05	26,27,28,29	0

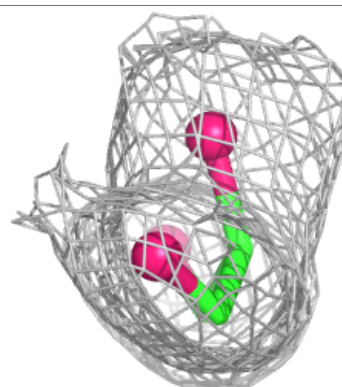
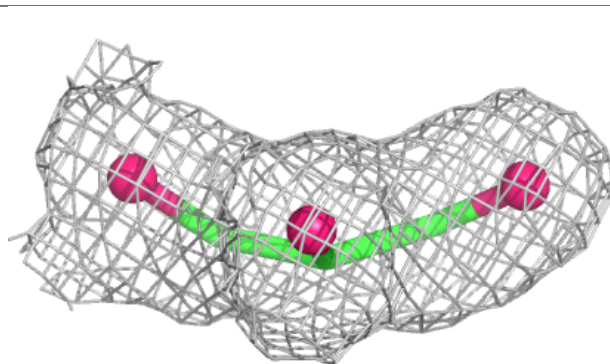
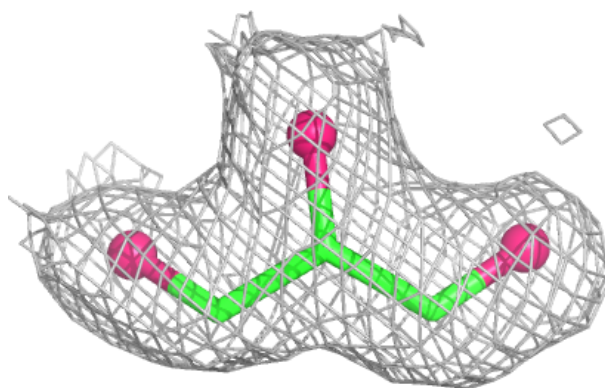
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GOL D 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

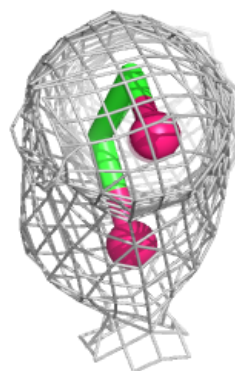
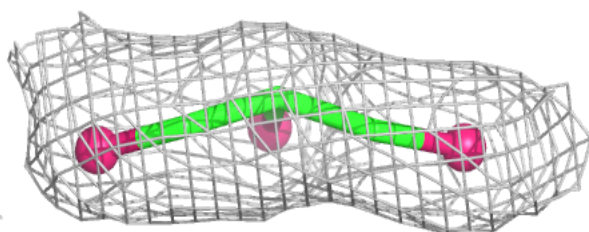
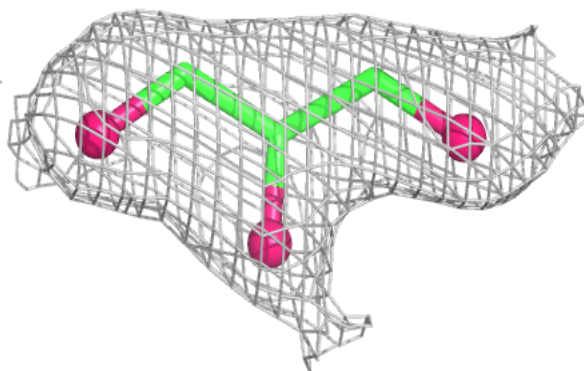
**Electron density around GOL B 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

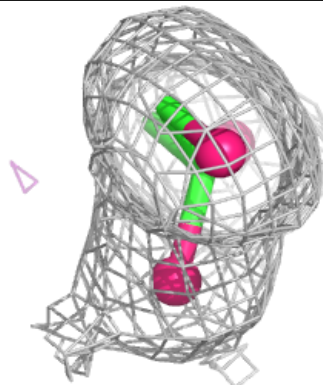
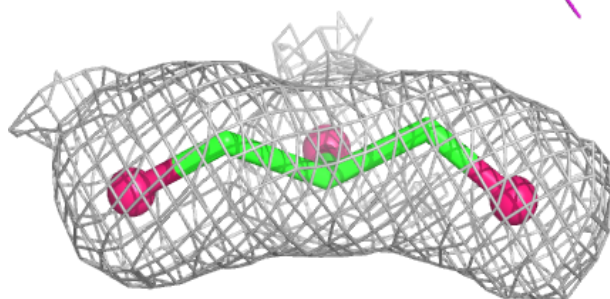
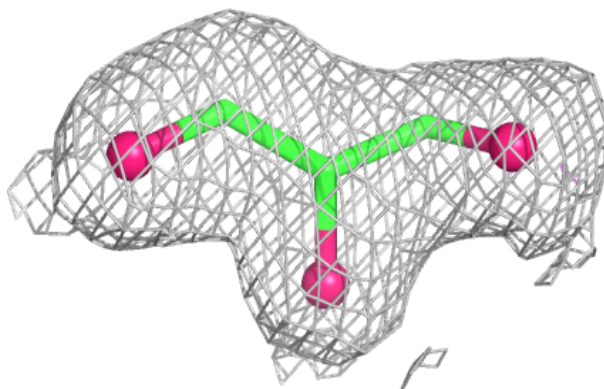


Electron density around GOL C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GOL A 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.