



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 09:14 AM EDT

PDB ID : 1GUP  
Title : STRUCTURE OF NUCLEOTIDYLTRANSFERASE COMPLEXED WITH  
UDP-GALACTOSE  
Authors : Thoden, J.B.; Rayment, I.; Holden, H.  
Deposited on : 1996-10-23  
Resolution : 1.80 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)  
Xtrriage (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) : 2.23.2

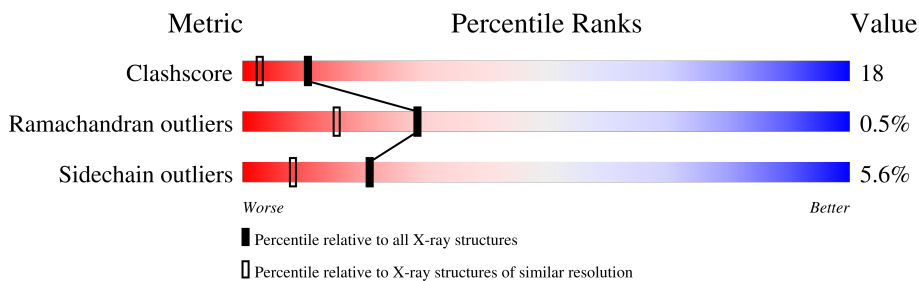
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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  $\geq 3$ , 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	348	
1	B	348	
1	C	348	
1	D	348	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12487 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.

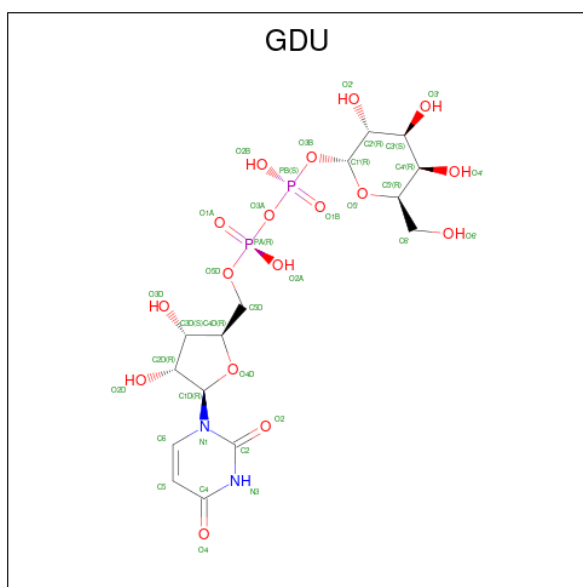
- Molecule 1 is a protein called GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2784	1763	492	516	13	0	0	0
1	B	344	2766	1753	489	511	13	0	0	0
1	C	344	2766	1753	489	511	13	0	0	0
1	D	344	2766	1753	489	511	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	GLY	HIS	engineered mutation	UNP P09148
B	166	GLY	HIS	engineered mutation	UNP P09148
C	166	GLY	HIS	engineered mutation	UNP P09148
D	166	GLY	HIS	engineered mutation	UNP P09148

- Molecule 2 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (three-letter code: GDU) (formula: C<sub>15</sub>H<sub>24</sub>N<sub>2</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
4	A	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Fe 1 1	0	0
4	C	1	Total Fe 1 1	0	0
4	D	1	Total Fe 1 1	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	371	Total O 371 371	0	0
6	B	330	Total O 330 330	0	0
6	C	291	Total O 291 291	0	0
6	D	257	Total O 257 257	0	0

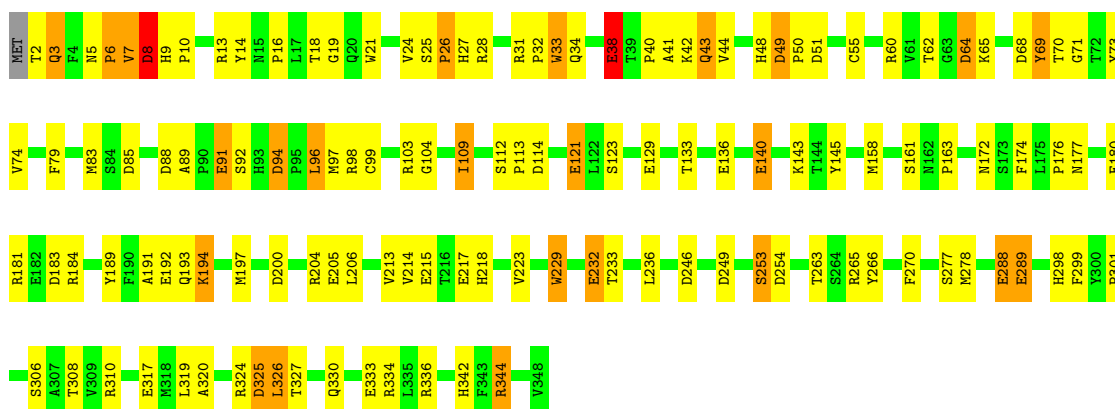
### 3 Residue-property plots

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. 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.

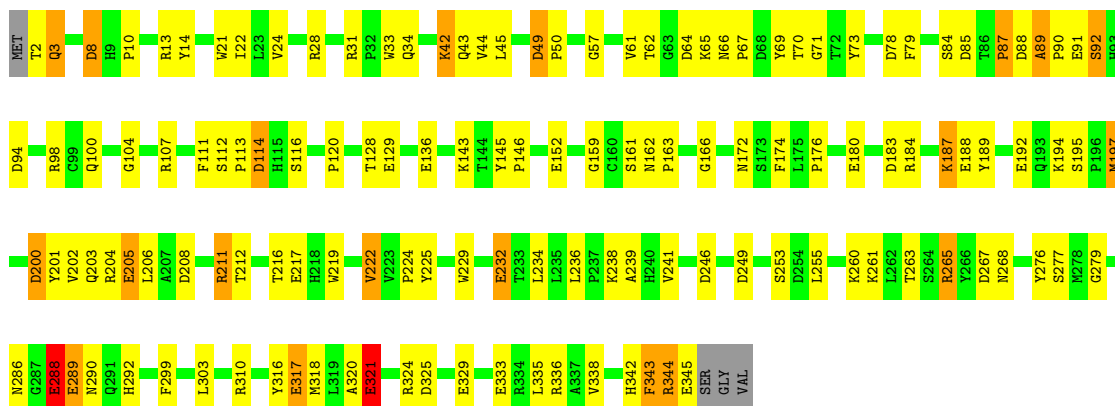
- Molecule 1: GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE

Chain A: 



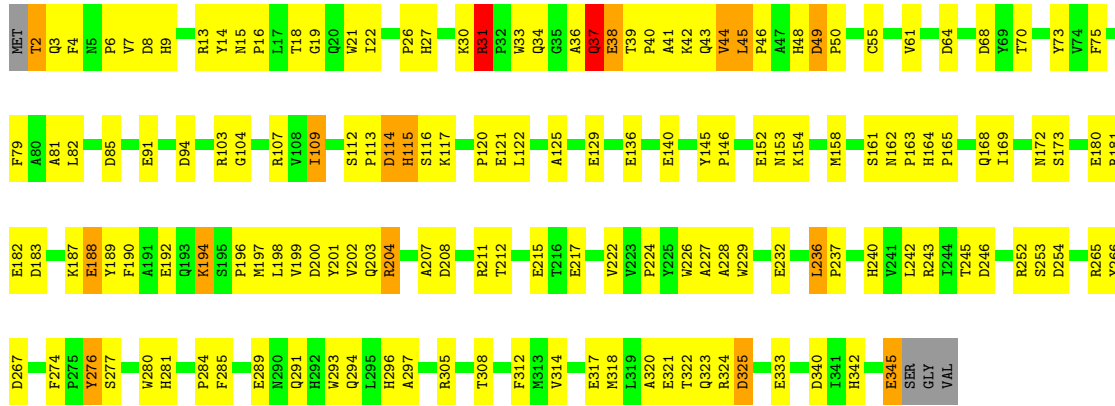
- Molecule 1: GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE

Chain B: 



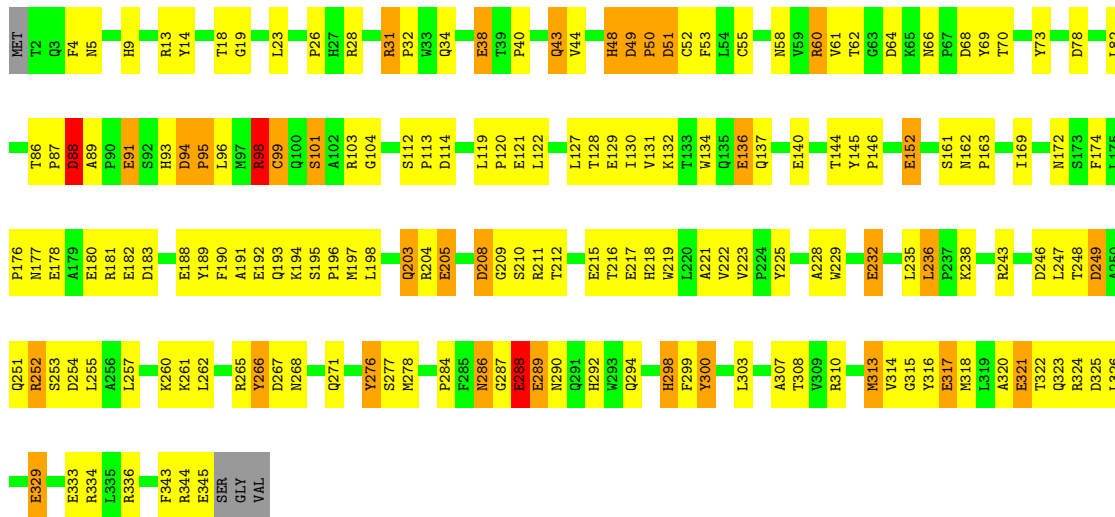
- Molecule 1: GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE

Chain C: 



● Molecule 1: GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE

Chain D: 49% 40% 9% ..



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.70Å 57.70Å 188.70Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12487	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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: FE, ZN, GDU, K

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	1.07	17/2869 (0.6%)	1.55	54/3912 (1.4%)
1	B	1.03	16/2851 (0.6%)	1.51	47/3889 (1.2%)
1	C	1.01	18/2851 (0.6%)	1.49	47/3889 (1.2%)
1	D	1.02	25/2851 (0.9%)	1.51	55/3889 (1.4%)
All	All	1.03	76/11422 (0.7%)	1.51	203/15579 (1.3%)

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	C	1	0

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	GLU	CD-OE1	10.54	1.37	1.25
1	A	129	GLU	CD-OE1	8.73	1.35	1.25
1	A	333	GLU	CD-OE2	8.53	1.35	1.25
1	C	182	GLU	CD-OE2	8.39	1.34	1.25
1	A	121	GLU	CD-OE2	8.35	1.34	1.25
1	A	217	GLU	CD-OE2	8.32	1.34	1.25
1	D	38	GLU	CD-OE1	7.99	1.34	1.25
1	D	345	GLU	CD-OE2	7.82	1.34	1.25
1	C	136	GLU	CD-OE2	7.64	1.34	1.25
1	C	289	GLU	CD-OE1	7.60	1.34	1.25
1	A	205	GLU	CD-OE2	7.57	1.33	1.25
1	D	178	GLU	CD-OE1	7.57	1.33	1.25
1	B	232	GLU	CD-OE1	7.40	1.33	1.25
1	D	329	GLU	CD-OE1	7.38	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	GLU	CD-OE2	7.29	1.33	1.25
1	C	91	GLU	CD-OE2	7.27	1.33	1.25
1	D	289	GLU	CD-OE2	7.11	1.33	1.25
1	B	289	GLU	CD-OE2	7.07	1.33	1.25
1	B	329	GLU	CD-OE1	6.88	1.33	1.25
1	A	91	GLU	CD-OE1	6.87	1.33	1.25
1	B	180	GLU	CD-OE1	6.82	1.33	1.25
1	D	205	GLU	CD-OE2	6.80	1.33	1.25
1	B	188	GLU	CD-OE2	6.76	1.33	1.25
1	D	192	GLU	CD-OE2	6.75	1.33	1.25
1	B	192	GLU	CD-OE2	6.75	1.33	1.25
1	B	333	GLU	CD-OE2	6.69	1.33	1.25
1	B	129	GLU	CD-OE2	6.65	1.32	1.25
1	A	192	GLU	CD-OE2	6.59	1.32	1.25
1	D	136	GLU	CD-OE1	6.56	1.32	1.25
1	D	321	GLU	CD-OE2	6.47	1.32	1.25
1	D	333	GLU	CD-OE2	6.47	1.32	1.25
1	B	317	GLU	CD-OE2	6.36	1.32	1.25
1	A	288	GLU	CD-OE1	6.36	1.32	1.25
1	C	333	GLU	CD-OE2	6.33	1.32	1.25
1	A	232	GLU	CD-OE1	6.29	1.32	1.25
1	A	140	GLU	CD-OE2	6.28	1.32	1.25
1	C	317	GLU	CD-OE2	6.17	1.32	1.25
1	B	288	GLU	CD-OE1	6.17	1.32	1.25
1	A	289	GLU	CD-OE2	6.15	1.32	1.25
1	D	91	GLU	CD-OE2	6.11	1.32	1.25
1	C	192	GLU	CD-OE2	6.05	1.32	1.25
1	B	217	GLU	CD-OE2	6.04	1.32	1.25
1	D	182	GLU	CD-OE2	6.04	1.32	1.25
1	A	38	GLU	CD-OE2	6.04	1.32	1.25
1	A	215	GLU	CD-OE1	6.02	1.32	1.25
1	D	321	GLU	CD-OE1	-6.00	1.19	1.25
1	C	345	GLU	CD-OE1	5.96	1.32	1.25
1	C	215	GLU	CD-OE1	5.96	1.32	1.25
1	C	121	GLU	CD-OE2	5.93	1.32	1.25
1	A	317	GLU	CD-OE2	5.89	1.32	1.25
1	D	317	GLU	CD-OE2	5.72	1.31	1.25
1	C	217	GLU	CD-OE2	5.71	1.31	1.25
1	C	38	GLU	CD-OE1	5.71	1.31	1.25
1	B	136	GLU	CD-OE2	5.70	1.31	1.25
1	D	140	GLU	CD-OE2	5.69	1.31	1.25
1	D	288	GLU	CD-OE1	5.68	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CD-OE1	5.65	1.31	1.25
1	D	232	GLU	CD-OE2	-5.64	1.19	1.25
1	B	152	GLU	CD-OE1	5.63	1.31	1.25
1	D	188	GLU	CD-OE2	5.50	1.31	1.25
1	A	136	GLU	CD-OE2	5.50	1.31	1.25
1	D	215	GLU	CD-OE1	5.49	1.31	1.25
1	D	28	ARG	CZ-NH1	5.47	1.40	1.33
1	B	205	GLU	CD-OE2	5.47	1.31	1.25
1	D	180	GLU	CD-OE1	5.37	1.31	1.25
1	C	188	GLU	CD-OE2	5.35	1.31	1.25
1	D	129	GLU	CD-OE1	5.34	1.31	1.25
1	A	121	GLU	CD-OE1	-5.27	1.19	1.25
1	C	129	GLU	CD-OE2	5.24	1.31	1.25
1	C	121	GLU	CD-OE1	-5.18	1.20	1.25
1	D	217	GLU	CD-OE2	5.16	1.31	1.25
1	B	321	GLU	CD-OE1	-5.16	1.20	1.25
1	C	140	GLU	CD-OE2	5.13	1.31	1.25
1	C	152	GLU	CD-OE1	5.04	1.31	1.25
1	D	152	GLU	CD-OE2	-5.02	1.20	1.25
1	D	121	GLU	CD-OE1	5.02	1.31	1.25

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	D	28	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	D	336	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	C	252	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	246	ASP	CB-CG-OD2	9.32	126.69	118.30
1	A	60	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	C	109	ILE	CB-CA-C	-8.99	93.61	111.60
1	C	114	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	B	249	ASP	CB-CG-OD1	-8.66	110.50	118.30
1	D	336	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	D	114	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	D	31	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	310	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	265	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	325	ASP	CB-CG-OD2	8.22	125.69	118.30
1	D	204	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	C	254	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	A	200	ASP	CB-CG-OD2	-8.09	111.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ASP	CB-CG-OD1	-8.08	111.03	118.30
1	A	246	ASP	CB-CG-OD1	-8.04	111.07	118.30
1	D	114	ASP	CB-CG-OD1	8.00	125.50	118.30
1	A	204	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	334	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	325	ASP	CB-CG-OD2	7.87	125.39	118.30
1	A	94	ASP	CB-CG-OD1	-7.86	111.23	118.30
1	C	224	PRO	N-CA-CB	7.78	112.64	103.30
1	C	340	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	28	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	A	277	SER	N-CA-CB	7.68	122.02	110.50
1	D	277	SER	N-CA-CB	7.65	121.98	110.50
1	B	336	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	A	96	LEU	N-CA-CB	7.54	125.48	110.40
1	D	64	ASP	CB-CG-OD1	-7.52	111.53	118.30
1	B	98	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	60	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	114	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	B	200	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	181	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	B	200	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	204	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	103	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	C	114	ASP	CB-CG-OD1	7.26	124.83	118.30
1	C	37	GLN	N-CA-CB	7.23	123.62	110.60
1	D	98	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	C	31	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	98	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	267	ASP	CB-CG-OD2	7.02	124.62	118.30
1	B	89	ALA	N-CA-CB	6.99	119.88	110.10
1	C	252	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	325	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	A	69	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	C	103	ARG	N-CA-CB	6.90	123.02	110.60
1	B	107	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	114	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	C	265	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	C	208	ASP	CB-CG-OD2	6.85	124.46	118.30
1	C	208	ASP	CB-CG-OD1	-6.85	112.14	118.30
1	B	318	MET	CG-SD-CE	-6.83	89.27	100.20
1	D	310	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	D	313	MET	CG-SD-CE	6.80	111.09	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	B	98	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	C	254	ASP	CB-CG-OD1	6.74	124.36	118.30
1	D	267	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	8	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	D	246	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	B	277	SER	N-CA-CB	6.62	120.44	110.50
1	A	49	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	321	GLU	N-CA-CB	-6.60	98.72	110.60
1	A	266	TYR	CB-CG-CD1	6.58	124.95	121.00
1	A	183	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	D	265	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	D	254	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	D	49	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	B	88	ASP	CB-CG-OD1	-6.56	112.40	118.30
1	B	249	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	85	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	336	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	64	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	183	ASP	CB-CG-OD1	-6.46	112.48	118.30
1	B	265	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	183	ASP	CB-CG-OD1	-6.46	112.49	118.30
1	D	78	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	C	277	SER	N-CA-CB	6.45	120.18	110.50
1	C	85	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	200	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	49	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	B	49	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	114	ASP	CB-CG-OD1	6.33	124.00	118.30
1	C	85	ASP	CB-CG-OD2	6.31	123.98	118.30
1	D	68	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	A	13	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	183	ASP	CB-CG-OD2	6.29	123.97	118.30
1	A	181	ARG	CD-NE-CZ	-6.29	114.80	123.60
1	B	94	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	C	107	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	8	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	78	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	C	94	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	8	ASP	CB-CG-OD1	6.22	123.89	118.30
1	D	68	ASP	CB-CG-OD2	6.21	123.88	118.30
1	D	325	ASP	CB-CG-OD2	6.19	123.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	28	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	C	64	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	D	289	GLU	N-CA-CB	6.11	121.60	110.60
1	C	289	GLU	N-CA-CB	6.09	121.56	110.60
1	B	28	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	183	ASP	CB-CG-OD2	6.08	123.78	118.30
1	D	94	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	344	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	D	208	ASP	CB-CG-OD2	6.04	123.73	118.30
1	D	99	CYS	CA-CB-SG	6.02	124.83	114.00
1	C	246	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	246	ASP	CB-CG-OD2	5.95	123.66	118.30
1	D	88	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	D	60	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	13	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	D	298	HIS	CB-CA-C	-5.85	98.70	110.40
1	C	115	HIS	N-CA-CB	-5.84	100.09	110.60
1	B	344	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	249	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	87	PRO	N-CA-CB	5.76	110.21	103.30
1	A	114	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	263	THR	CA-CB-CG2	-5.73	104.38	112.40
1	C	200	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	C	325	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	C	68	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	49	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	78	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	223	VAL	N-CA-C	-5.69	95.64	111.00
1	B	64	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	A	18	THR	CA-CB-CG2	-5.65	104.49	112.40
1	C	107	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	94	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	184	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	D	208	ASP	CB-CG-OD1	-5.56	113.29	118.30
1	C	13	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	344	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	40	PRO	N-CA-CB	5.53	109.94	103.30
1	B	84	SER	CB-CA-C	-5.53	99.60	110.10
1	D	267	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	B	208	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	223	VAL	N-CA-C	-5.48	96.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	B	299	PHE	N-CA-CB	5.46	120.42	110.60
1	B	85	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	B	324	ARG	N-CA-CB	5.43	120.38	110.60
1	D	13	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	13	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	D	249	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	85	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	C	325	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	267	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	C	229	TRP	CA-CB-CG	-5.36	103.53	113.70
1	D	48	HIS	N-CA-CB	5.35	120.22	110.60
1	C	211	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	73	TYR	N-CA-CB	5.33	120.20	110.60
1	A	233	THR	CA-CB-CG2	-5.33	104.94	112.40
1	A	51	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	B	246	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	158	MET	CG-SD-CE	5.29	108.67	100.20
1	D	334	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	184	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	64	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	62	THR	CA-CB-CG2	-5.29	105.00	112.40
1	C	305	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	88	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	49	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	334	ARG	CD-NE-CZ	5.25	130.95	123.60
1	D	300	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	D	88	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	103	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	286	ASN	CB-CA-C	5.18	120.76	110.40
1	D	196	PRO	N-CA-CB	5.17	109.51	103.30
1	B	222	VAL	CB-CA-C	-5.17	101.58	111.40
1	B	14	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	B	276	TYR	CB-CA-C	-5.14	100.12	110.40
1	A	103	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	310	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	88	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	246	ASP	CB-CG-OD1	-5.13	113.69	118.30
1	C	196	PRO	CA-N-CD	-5.13	104.32	111.50
1	B	224	PRO	N-CA-CB	5.12	109.45	103.30
1	C	44	VAL	CB-CA-C	5.12	121.13	111.40
1	C	49	ASP	CB-CG-OD2	-5.11	113.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	TYR	CB-CG-CD1	5.11	124.07	121.00
1	C	276	TYR	CB-CG-CD1	5.11	124.07	121.00
1	A	158	MET	N-CA-CB	5.11	119.79	110.60
1	A	229	TRP	CA-CB-CG	-5.11	104.00	113.70
1	C	340	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	336	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	183	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	51	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	51	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	68	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	252	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	85	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	69	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	A	191	ALA	CB-CA-C	-5.04	102.54	110.10
1	B	62	THR	N-CA-CB	-5.03	100.75	110.30
1	C	31	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	33	TRP	N-CA-CB	5.00	119.61	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	44	VAL	CA

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2784	0	2661	97	0
1	B	2766	0	2644	100	0
1	C	2766	0	2644	114	0
1	D	2766	0	2644	137	0
2	A	36	0	22	0	0
2	B	36	0	22	1	0
2	C	36	0	22	0	0
2	D	36	0	22	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	371	0	0	12	0
6	B	330	0	0	15	0
6	C	291	0	0	12	1
6	D	257	0	0	8	0
All	All	12487	0	10681	400	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 18.

All (400) 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:D:61:VAL:HG12	2:D:352:GDU:O4	1.62	1.00
1:D:98:ARG:HG2	1:D:98:ARG:HH11	1.33	0.91
1:C:9:HIS:HD2	1:D:87:PRO:HD2	1.41	0.86
1:B:42:LYS:H	1:B:42:LYS:HD2	1.40	0.85
1:C:33:TRP:CZ3	1:D:161:SER:HB3	2.11	0.85
1:C:154:LYS:HE2	1:C:274:PHE:O	1.79	0.83
1:C:7:VAL:HG13	6:C:797:HOH:O	1.80	0.81
1:A:43:GLN:HG3	1:A:43:GLN:O	1.79	0.81
1:A:253:SER:HB3	6:A:637:HOH:O	1.80	0.81
1:C:33:TRP:CE3	1:D:161:SER:HB3	2.17	0.79
1:D:52:CYS:HB3	1:D:55:CYS:HB2	1.66	0.78
1:D:43:GLN:HB3	1:D:344:ARG:HH12	1.49	0.78
1:B:203:GLN:HB2	6:B:644:HOH:O	1.85	0.77
1:D:236:LEU:HD12	1:D:236:LEU:N	1.98	0.76
1:A:3:GLN:HA	1:A:3:GLN:HE21	1.49	0.76
1:A:9:HIS:CE1	1:B:87:PRO:HG2	2.21	0.76
1:C:145:TYR:HB3	1:C:172:ASN:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASN:OD1	1:A:7:VAL:HG23	1.84	0.76
1:D:313:MET:HE2	6:D:1113:HOH:O	1.87	0.75
1:B:187:LYS:NZ	1:B:187:LYS:HB3	2.01	0.75
1:B:92:SER:HB2	6:B:638:HOH:O	1.86	0.75
1:D:14:TYR:CZ	1:D:19:GLY:HA2	2.22	0.74
1:A:5:ASN:ND2	1:A:8:ASP:OD2	2.19	0.74
1:B:89:ALA:HB1	1:B:90:PRO:HD2	1.69	0.74
1:C:164:HIS:CD2	1:C:165:PRO:HD2	2.22	0.74
1:C:38:GLU:HB2	1:C:308:THR:HA	1.71	0.72
1:A:194:LYS:HE3	6:A:702:HOH:O	1.89	0.72
1:A:121:GLU:OE1	1:A:344:ARG:NH1	2.23	0.72
1:B:70:THR:HG23	6:B:573:HOH:O	1.89	0.71
1:C:8:ASP:HA	1:C:27:HIS:NE2	2.06	0.71
1:A:9:HIS:ND1	1:B:87:PRO:HG2	2.07	0.70
1:B:42:LYS:HG2	1:B:45:LEU:HD21	1.74	0.70
1:B:216:THR:O	1:B:238:LYS:NZ	2.19	0.69
1:D:14:TYR:OH	1:D:19:GLY:HA2	1.92	0.69
1:D:236:LEU:HD12	1:D:236:LEU:H	1.56	0.69
1:B:42:LYS:HD2	1:B:42:LYS:N	2.01	0.69
1:C:26:PRO:O	6:C:871:HOH:O	2.11	0.68
1:C:125:ALA:O	6:C:893:HOH:O	2.11	0.68
1:A:32:PRO:HD3	1:B:79:PHE:CZ	2.29	0.68
1:B:42:LYS:HB2	6:B:613:HOH:O	1.94	0.67
1:C:4:PHE:CD2	1:D:89:ALA:HA	2.29	0.67
1:D:70:THR:HG23	6:D:1184:HOH:O	1.95	0.67
1:D:128:THR:O	1:D:132:LYS:HG3	1.95	0.66
1:A:99:CYS:SG	6:B:557:HOH:O	2.53	0.66
1:A:6:PRO:HB2	6:A:498:HOH:O	1.96	0.66
1:A:177:ASN:ND2	1:B:321:GLU:HB2	2.10	0.66
1:D:5:ASN:N	1:D:9:HIS:ND1	2.43	0.65
1:C:9:HIS:CD2	1:D:87:PRO:HD2	2.29	0.65
1:C:31:ARG:NE	2:D:352:GDU:O2B	2.28	0.65
1:C:243:ARG:NH2	1:C:284:PRO:O	2.26	0.64
1:C:345:GLU:OE1	6:C:1196:HOH:O	2.14	0.64
1:D:94:ASP:OD1	1:D:96:LEU:N	2.27	0.64
1:D:189:TYR:CZ	1:D:193:GLN:HG3	2.33	0.64
1:C:236:LEU:HB2	1:C:237:PRO:HD2	1.80	0.63
1:D:203:GLN:HA	1:D:203:GLN:OE1	1.98	0.63
1:A:218:HIS:HB2	1:A:254:ASP:OD2	1.98	0.63
1:A:344:ARG:NH2	6:A:572:HOH:O	2.30	0.63
1:B:2:THR:HG22	1:B:3:GLN:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:NH1	1:B:338:VAL:O	2.32	0.62
1:B:342:HIS:HE1	1:B:344:ARG:NH1	1.98	0.62
1:A:98:ARG:HG2	6:A:650:HOH:O	1.99	0.62
1:C:4:PHE:CE1	1:C:6:PRO:HD3	2.34	0.62
1:A:140:GLU:O	1:A:143:LYS:HB2	2.00	0.62
1:C:38:GLU:HB2	1:C:308:THR:C	2.20	0.62
1:C:189:TYR:CE1	1:C:197:MET:HA	2.35	0.62
1:D:43:GLN:HB3	1:D:344:ARG:NH1	2.14	0.61
1:A:94:ASP:O	1:A:98:ARG:HD3	2.00	0.61
1:C:38:GLU:HB2	1:C:308:THR:CA	2.30	0.61
1:D:43:GLN:CB	1:D:344:ARG:NH1	2.63	0.61
1:C:190:PHE:O	1:C:194:LYS:N	2.33	0.61
1:D:162:ASN:OD1	1:D:163:PRO:HD2	2.00	0.61
1:B:71:GLY:O	1:B:113:PRO:HD3	2.01	0.61
1:A:109:ILE:HD12	1:A:133:THR:HG21	1.82	0.60
1:C:48:HIS:CD2	1:C:55:CYS:HB3	2.35	0.60
1:D:119:LEU:HB2	1:D:120:PRO:HD3	1.83	0.60
1:A:65:LYS:HD3	6:A:600:HOH:O	2.01	0.60
1:B:10:PRO:HA	1:B:24:VAL:O	2.01	0.60
1:B:236:LEU:HD23	1:B:236:LEU:N	2.17	0.60
1:B:42:LYS:CD	1:B:45:LEU:HD21	2.32	0.60
1:B:146:PRO:HD2	1:B:172:ASN:O	2.01	0.59
1:C:45:LEU:HB3	1:C:116:SER:HB3	1.85	0.59
1:A:33:TRP:CZ3	1:B:161:SER:HB3	2.37	0.59
1:A:62:THR:OG1	1:A:64:ASP:OD2	2.12	0.59
1:D:104:GLY:HA2	1:D:145:TYR:CE2	2.38	0.59
1:A:161:SER:O	1:B:34:GLN:HB2	2.01	0.59
1:B:229:TRP:HB2	1:B:232:GLU:HB2	1.85	0.58
1:A:28:ARG:HG2	6:A:569:HOH:O	2.03	0.58
1:C:204:ARG:O	1:C:207:ALA:HB3	2.02	0.58
1:D:43:GLN:NE2	1:D:44:VAL:HG23	2.18	0.58
1:C:45:LEU:HB3	1:C:116:SER:CB	2.34	0.57
1:A:8:ASP:HB3	1:A:27:HIS:HE1	1.69	0.57
1:A:28:ARG:CB	1:A:325:ASP:OD1	2.51	0.57
1:D:49:ASP:O	1:D:51:ASP:N	2.37	0.57
1:B:219:TRP:CZ2	1:B:255:LEU:HB2	2.39	0.57
1:D:203:GLN:HG3	6:D:1205:HOH:O	2.04	0.57
1:B:42:LYS:CG	1:B:45:LEU:HD21	2.34	0.57
1:B:49:ASP:OD1	1:B:50:PRO:HD2	2.05	0.57
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.68	0.57
1:D:43:GLN:CB	1:D:344:ARG:HH12	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:HB3	1:B:225:TYR:CD2	2.40	0.57
1:D:257:LEU:O	1:D:261:LYS:HG3	2.05	0.56
1:B:89:ALA:HB1	1:B:90:PRO:CD	2.36	0.56
1:A:32:PRO:HG3	1:B:61:VAL:HG21	1.88	0.56
1:C:14:TYR:HB2	1:C:21:TRP:CH2	2.40	0.56
1:C:4:PHE:HE1	1:C:6:PRO:HG3	1.71	0.56
1:D:190:PHE:O	1:D:194:LYS:N	2.30	0.56
1:C:236:LEU:N	1:C:236:LEU:CD2	2.68	0.56
1:D:326:LEU:HD23	1:D:326:LEU:H	1.71	0.56
1:C:188:GLU:OE2	6:C:1176:HOH:O	2.18	0.55
1:C:280:TRP:CE3	1:C:297:ALA:HB2	2.41	0.55
1:B:343:PHE:CZ	1:B:344:ARG:NH1	2.74	0.55
1:C:9:HIS:HD2	1:D:87:PRO:CD	2.16	0.55
1:D:290:ASN:HA	1:D:292:HIS:CE1	2.41	0.55
1:C:236:LEU:HB2	1:C:237:PRO:CD	2.37	0.55
1:A:14:TYR:OH	1:A:19:GLY:HA2	2.06	0.55
1:A:104:GLY:HA2	1:A:145:TYR:CE1	2.42	0.55
1:B:104:GLY:HA2	1:B:145:TYR:CE1	2.41	0.55
1:A:189:TYR:CE1	1:A:197:MET:HA	2.42	0.55
1:C:201:TYR:HB2	1:D:96:LEU:HD13	1.89	0.55
1:D:94:ASP:OD2	1:D:95:PRO:HD2	2.06	0.55
1:A:14:TYR:CZ	1:A:19:GLY:HA2	2.42	0.54
1:A:28:ARG:HA	6:A:569:HOH:O	2.06	0.54
1:B:2:THR:CG2	1:B:3:GLN:N	2.70	0.54
1:C:114:ASP:OD1	1:C:116:SER:N	2.36	0.54
1:D:98:ARG:NH1	6:D:1172:HOH:O	2.26	0.54
1:D:248:THR:OG1	1:D:251:GLN:HG3	2.07	0.54
1:B:286:ASN:OD1	1:B:288:GLU:HB2	2.08	0.54
1:D:145:TYR:HB3	1:D:172:ASN:O	2.08	0.54
1:A:32:PRO:HD3	1:B:79:PHE:CE1	2.42	0.54
1:C:285:PHE:HB3	6:C:1133:HOH:O	2.06	0.54
1:C:26:PRO:HA	1:C:325:ASP:O	2.08	0.54
1:D:88:ASP:HA	1:D:101:SER:OG	2.06	0.54
1:A:41:ALA:HB3	6:A:605:HOH:O	2.08	0.53
1:A:74:VAL:HG22	1:A:109:ILE:HB	1.90	0.53
1:C:321:GLU:HA	6:D:763:HOH:O	2.09	0.53
1:C:104:GLY:HA2	1:C:145:TYR:CE1	2.44	0.53
1:C:323:GLN:NE2	1:C:325:ASP:OD1	2.32	0.53
1:D:212:THR:HA	1:D:222:VAL:HG12	1.90	0.53
1:D:278:MET:HA	1:D:298:HIS:O	2.08	0.53
1:C:321:GLU:HB2	1:D:177:ASN:ND2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:TRP:CE2	1:B:255:LEU:HB2	2.44	0.53
1:D:161:SER:OG	2:D:352:GDU:H5'2	2.09	0.53
1:C:198:LEU:O	1:C:202:VAL:HG23	2.08	0.53
1:D:88:ASP:OD1	1:D:88:ASP:N	2.41	0.53
1:C:9:HIS:CD2	1:D:87:PRO:CG	2.92	0.53
1:B:261:LYS:HE3	6:B:470:HOH:O	2.09	0.53
1:B:342:HIS:CE1	1:B:344:ARG:NH1	2.76	0.53
1:C:22:ILE:HD12	1:C:226:TRP:O	2.09	0.52
1:A:161:SER:HB3	1:B:33:TRP:CZ3	2.45	0.52
1:D:144:THR:HG22	1:D:145:TYR:CE1	2.44	0.52
1:C:38:GLU:N	1:C:308:THR:O	2.34	0.52
1:B:203:GLN:O	1:B:206:LEU:HB2	2.09	0.52
1:C:14:TYR:HB2	1:C:21:TRP:CZ3	2.45	0.52
1:D:38:GLU:HB2	1:D:308:THR:HA	1.92	0.52
1:D:249:ASP:OD1	1:D:252:ARG:NH2	2.42	0.52
1:A:7:VAL:O	1:A:26:PRO:HB3	2.09	0.52
1:C:4:PHE:CD1	1:C:4:PHE:C	2.83	0.52
1:C:31:ARG:HD2	2:D:352:GDU:H3D	1.92	0.52
1:C:34:GLN:HE22	1:D:162:ASN:ND2	2.07	0.52
1:B:61:VAL:HG11	1:B:79:PHE:CE1	2.44	0.52
1:D:86:THR:O	1:D:103:ARG:HD3	2.10	0.52
1:A:21:TRP:CH2	1:B:100:GLN:HG3	2.45	0.51
1:A:229:TRP:HB2	1:A:232:GLU:HB2	1.92	0.51
1:A:270:PHE:CE1	1:A:306:SER:HA	2.46	0.51
1:A:324:ARG:HH21	1:A:326:LEU:CD2	2.23	0.51
1:B:42:LYS:HD3	1:B:45:LEU:HD21	1.92	0.51
1:B:92:SER:CB	6:B:638:HOH:O	2.51	0.51
1:C:198:LEU:HB2	1:C:294:GLN:HB3	1.91	0.51
1:C:276:TYR:CD1	1:C:276:TYR:C	2.84	0.51
6:A:398:HOH:O	1:B:10:PRO:HG2	2.10	0.51
1:D:61:VAL:HG12	2:D:352:GDU:C4	2.40	0.51
1:D:120:PRO:O	1:D:260:LYS:NZ	2.43	0.51
1:D:344:ARG:NH2	6:D:1195:HOH:O	2.03	0.51
1:C:36:ALA:HB3	1:C:312:PHE:CZ	2.45	0.51
1:C:112:SER:HB2	1:C:113:PRO:HD2	1.92	0.51
1:D:137:GLN:HB3	1:D:169:ILE:CD1	2.40	0.51
1:D:144:THR:HG22	1:D:145:TYR:CD1	2.46	0.51
1:C:153:ASN:HD21	1:D:315:GLY:CA	2.23	0.51
1:C:204:ARG:NH2	1:D:94:ASP:OD1	2.43	0.51
2:D:352:GDU:O2B	2:D:352:GDU:H3D	2.10	0.51
1:B:65:LYS:NZ	6:B:683:HOH:O	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:HIS:NE2	1:C:55:CYS:HB3	2.25	0.51
1:C:190:PHE:CZ	1:C:291:GLN:HG3	2.46	0.51
1:D:314:VAL:HA	1:D:318:MET:HG3	1.91	0.51
1:C:9:HIS:CD2	1:D:87:PRO:CD	2.92	0.51
1:A:92:SER:OG	1:A:94:ASP:HB2	2.10	0.50
1:B:159:GLY:HA2	6:B:508:HOH:O	2.11	0.50
1:D:191:ALA:O	1:D:194:LYS:HE2	2.11	0.50
1:C:40:PRO:HG3	1:C:308:THR:HG22	1.93	0.50
1:C:48:HIS:HD2	6:C:1198:HOH:O	1.94	0.50
1:D:43:GLN:CD	1:D:44:VAL:HG23	2.32	0.50
1:B:143:LYS:NZ	6:B:483:HOH:O	2.45	0.50
1:C:154:LYS:CE	1:C:274:PHE:O	2.56	0.50
1:D:317:GLU:HA	1:D:321:GLU:O	2.10	0.50
1:A:38:GLU:HB2	1:A:308:THR:HA	1.94	0.49
1:A:172:ASN:ND2	1:A:176:PRO:HG3	2.27	0.49
1:C:342:HIS:HB2	6:C:1196:HOH:O	2.12	0.49
1:D:119:LEU:N	1:D:120:PRO:HD2	2.26	0.49
1:B:42:LYS:HG2	1:B:45:LEU:CD2	2.42	0.49
1:B:34:GLN:NE2	6:B:462:HOH:O	2.43	0.49
1:A:9:HIS:CE1	1:B:87:PRO:CG	2.94	0.49
1:A:10:PRO:HA	1:A:24:VAL:O	2.12	0.49
1:C:4:PHE:CD1	1:C:6:PRO:HD3	2.48	0.49
1:C:153:ASN:HD21	1:D:315:GLY:HA3	1.78	0.49
1:D:49:ASP:HB3	1:D:52:CYS:HB2	1.94	0.49
1:C:4:PHE:CE2	1:D:89:ALA:HA	2.47	0.49
1:C:9:HIS:CD2	1:D:87:PRO:HG2	2.48	0.49
1:A:342:HIS:ND1	1:A:344:ARG:HB2	2.28	0.48
1:D:43:GLN:NE2	1:D:44:VAL:CG2	2.76	0.48
1:A:34:GLN:HB2	1:B:161:SER:O	2.13	0.48
1:C:61:VAL:HG11	1:C:79:PHE:HE2	1.79	0.48
1:D:286:ASN:C	1:D:288:GLU:H	2.16	0.48
1:A:71:GLY:O	1:A:112:SER:HA	2.12	0.48
1:A:319:LEU:HD13	1:B:279:GLY:HA3	1.95	0.48
1:B:335:LEU:O	1:B:338:VAL:HG22	2.12	0.48
1:A:48:HIS:CE1	1:A:55:CYS:HB3	2.48	0.48
1:D:219:TRP:CZ2	1:D:255:LEU:HB2	2.49	0.48
1:A:28:ARG:HB2	1:A:325:ASP:OD1	2.14	0.48
1:C:125:ALA:HB1	6:C:893:HOH:O	2.13	0.48
1:D:144:THR:CG2	1:D:145:TYR:CE1	2.97	0.48
1:C:120:PRO:HB2	1:C:342:HIS:CD2	2.48	0.48
1:D:131:VAL:O	1:D:134:TRP:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:CG	1:B:31:ARG:HB3	2.48	0.47
1:C:314:VAL:HA	1:C:318:MET:HG3	1.95	0.47
1:C:2:THR:HB	1:D:87:PRO:HG3	1.96	0.47
1:C:164:HIS:CD2	1:C:165:PRO:CD	2.97	0.47
1:A:31:ARG:HA	1:B:79:PHE:CE2	2.49	0.47
1:A:2:THR:CG2	1:A:3:GLN:N	2.78	0.47
1:A:145:TYR:HB3	1:A:172:ASN:O	2.15	0.47
1:A:327:THR:HG23	1:A:330:GLN:NE2	2.29	0.47
1:B:317:GLU:HA	1:B:321:GLU:O	2.14	0.47
1:C:204:ARG:NH2	1:D:94:ASP:CG	2.68	0.47
1:D:23:LEU:O	1:D:323:GLN:HA	2.15	0.47
1:D:98:ARG:HH11	1:D:98:ARG:CG	2.17	0.47
1:D:216:THR:O	1:D:238:LYS:NZ	2.39	0.47
1:A:69:TYR:CD2	1:A:73:TYR:HB2	2.50	0.47
1:D:119:LEU:HA	1:D:122:LEU:HD12	1.97	0.47
1:D:198:LEU:HB2	1:D:294:GLN:HB3	1.96	0.47
1:A:324:ARG:HH21	1:A:326:LEU:HD23	1.79	0.47
1:D:49:ASP:C	1:D:51:ASP:H	2.19	0.47
1:D:286:ASN:O	1:D:288:GLU:N	2.48	0.47
1:C:31:ARG:HB2	2:D:352:GDU:O2D	2.14	0.46
1:D:205:GLU:OE1	1:D:211:ARG:NH2	2.40	0.46
1:B:22:ILE:HD12	1:B:22:ILE:N	2.30	0.46
1:B:128:THR:HB	6:B:579:HOH:O	2.15	0.46
1:C:281:HIS:HB2	1:C:296:HIS:CE1	2.50	0.46
1:C:33:TRP:CE3	1:D:161:SER:CB	2.95	0.46
1:C:46:PRO:O	1:C:115:HIS:HB3	2.16	0.46
1:C:73:TYR:CE2	1:C:75:PHE:CD1	3.03	0.46
1:C:240:HIS:NE2	1:C:293:TRP:O	2.46	0.46
1:D:268:ASN:OD1	1:D:343:PHE:HD1	1.98	0.46
1:B:236:LEU:HD23	1:B:236:LEU:H	1.80	0.46
1:A:5:ASN:O	1:A:8:ASP:N	2.38	0.46
1:B:111:PHE:CD2	1:B:166:GLY:HA2	2.50	0.46
1:C:4:PHE:CE1	1:C:6:PRO:CD	2.98	0.46
1:C:161:SER:O	1:D:34:GLN:HB2	2.16	0.46
1:D:145:TYR:HB3	1:D:146:PRO:HD2	1.98	0.46
1:C:187:LYS:HG2	6:C:1190:HOH:O	2.14	0.46
1:D:49:ASP:C	1:D:51:ASP:N	2.69	0.46
1:D:271:GLN:OE1	1:D:343:PHE:CG	2.69	0.46
1:D:316:TYR:O	1:D:320:ALA:HB3	2.16	0.46
1:B:114:ASP:OD1	1:B:116:SER:OG	2.25	0.46
1:C:320:ALA:HB1	1:D:176:PRO:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:CYS:HB3	1:D:55:CYS:CB	2.41	0.46
1:A:94:ASP:OD2	1:B:204:ARG:NH2	2.48	0.46
2:B:352:GDU:O2B	2:B:352:GDU:H3D	2.16	0.46
1:A:5:ASN:O	1:A:7:VAL:N	2.49	0.45
1:A:278:MET:HA	1:A:298:HIS:O	2.16	0.45
1:C:70:THR:HA	1:C:113:PRO:HG3	1.97	0.45
1:D:112:SER:HB2	1:D:113:PRO:HD2	1.97	0.45
1:D:211:ARG:HD3	1:D:329:GLU:OE2	2.16	0.45
1:A:109:ILE:HD12	1:A:133:THR:CG2	2.46	0.45
1:D:276:TYR:C	1:D:276:TYR:CD1	2.90	0.45
1:B:195:SER:OG	1:B:200:ASP:OD1	2.34	0.45
1:B:205:GLU:OE1	1:B:205:GLU:HA	2.16	0.45
1:C:199:VAL:O	1:C:203:GLN:HG2	2.16	0.45
1:D:98:ARG:NH1	1:D:98:ARG:CG	2.78	0.45
1:C:236:LEU:N	1:C:236:LEU:HD23	2.30	0.45
1:D:127:LEU:HD23	1:D:130:ILE:HD12	1.99	0.45
1:D:232:GLU:HG3	1:D:300:TYR:HD1	1.82	0.45
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.79	0.45
1:B:234:LEU:HG	1:B:236:LEU:HD22	1.99	0.45
1:C:280:TRP:CZ3	1:C:297:ALA:HB2	2.52	0.45
1:D:94:ASP:CG	1:D:95:PRO:HD2	2.37	0.45
1:D:211:ARG:HD2	1:D:225:TYR:HA	1.99	0.45
1:A:32:PRO:CD	1:B:79:PHE:CE1	3.00	0.45
1:D:98:ARG:HG2	1:D:98:ARG:NH1	2.09	0.45
1:C:15:ASN:O	1:C:19:GLY:N	2.46	0.44
1:D:44:VAL:O	1:D:44:VAL:HG12	2.17	0.44
1:B:174:PHE:CD1	1:B:174:PHE:N	2.85	0.44
1:D:326:LEU:HD23	1:D:326:LEU:N	2.31	0.44
1:A:96:LEU:HD13	1:B:201:TYR:HA	1.99	0.44
1:A:172:ASN:ND2	1:B:316:TYR:OH	2.50	0.44
1:C:267:ASP:OD2	1:C:342:HIS:NE2	2.29	0.44
1:B:286:ASN:CG	1:B:288:GLU:HB2	2.38	0.44
1:C:38:GLU:HB2	1:C:308:THR:O	2.18	0.44
1:C:114:ASP:OD1	1:C:114:ASP:C	2.55	0.44
1:C:228:ALA:HB1	1:C:322:THR:HG21	1.98	0.44
1:A:14:TYR:CE2	1:A:16:PRO:HA	2.52	0.44
1:A:40:PRO:HD3	1:A:308:THR:HG22	1.99	0.44
1:A:176:PRO:CB	1:B:320:ALA:HB1	2.48	0.44
1:C:212:THR:HA	1:C:222:VAL:HG12	1.99	0.44
1:A:69:TYR:CG	1:A:73:TYR:HB2	2.53	0.44
1:A:177:ASN:HD22	1:B:321:GLU:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:HIS:CE1	1:A:344:ARG:HB2	2.53	0.43
1:B:268:ASN:OD1	1:B:343:PHE:HD1	2.00	0.43
1:C:40:PRO:HD3	1:C:308:THR:HG22	1.99	0.43
1:C:281:HIS:CB	1:C:296:HIS:CE1	3.01	0.43
1:C:227:ALA:HB1	1:C:232:GLU:HB3	1.99	0.43
1:D:53:PHE:HD1	1:D:60:ARG:HA	1.83	0.43
1:D:82:LEU:CD1	1:D:172:ASN:HD22	2.31	0.43
1:A:3:GLN:HA	1:A:3:GLN:NE2	2.24	0.43
1:A:38:GLU:CB	1:A:308:THR:HA	2.49	0.43
1:A:140:GLU:HA	1:A:143:LYS:NZ	2.34	0.43
1:A:163:PRO:HG2	6:A:687:HOH:O	2.19	0.43
1:C:22:ILE:HD11	6:C:805:HOH:O	2.18	0.43
1:D:208:ASP:OD1	1:D:210:SER:OG	2.31	0.43
1:C:7:VAL:O	1:C:26:PRO:HB2	2.18	0.43
1:D:26:PRO:HD2	6:D:772:HOH:O	2.18	0.43
1:C:37:GLN:HG3	1:C:308:THR:HB	2.01	0.43
1:D:229:TRP:HB2	1:D:232:GLU:HB2	2.00	0.43
1:D:243:ARG:NH2	1:D:284:PRO:O	2.33	0.43
1:D:303:LEU:HD13	1:D:307:ALA:HA	1.99	0.43
1:A:49:ASP:OD1	1:A:50:PRO:HD2	2.19	0.43
1:D:119:LEU:N	1:D:120:PRO:CD	2.81	0.43
1:D:268:ASN:O	1:D:271:GLN:NE2	2.51	0.43
1:A:70:THR:HA	1:A:113:PRO:HG3	2.00	0.43
1:B:2:THR:CG2	1:B:3:GLN:H	2.29	0.43
1:A:25:SER:HA	1:A:26:PRO:HD2	1.71	0.43
1:B:290:ASN:HA	1:B:292:HIS:CE1	2.54	0.43
1:C:4:PHE:HB2	1:D:88:ASP:O	2.19	0.42
1:C:81:ALA:C	1:C:82:LEU:HG	2.38	0.42
1:A:320:ALA:HB1	1:B:176:PRO:CB	2.49	0.42
1:B:344:ARG:NH2	6:B:646:HOH:O	2.51	0.42
1:D:53:PHE:O	1:D:66:ASN:ND2	2.47	0.42
1:A:89:ALA:O	1:A:91:GLU:HG3	2.19	0.42
1:C:324:ARG:HH11	1:C:324:ARG:HD2	1.62	0.42
1:B:57:GLY:HA2	1:B:66:ASN:O	2.20	0.42
1:B:342:HIS:O	1:B:344:ARG:N	2.53	0.42
1:D:316:TYR:CD1	1:D:316:TYR:C	2.93	0.42
1:B:212:THR:HA	1:B:222:VAL:HG12	2.01	0.42
1:B:239:ALA:O	1:B:241:VAL:HG23	2.19	0.42
1:D:324:ARG:NE	1:D:326:LEU:O	2.44	0.42
1:A:104:GLY:HA2	1:A:145:TYR:CZ	2.54	0.42
1:A:189:TYR:CZ	1:A:193:GLN:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:TRP:C	1:B:22:ILE:HD12	2.40	0.42
1:D:169:ILE:HG21	1:D:169:ILE:HD13	1.80	0.42
1:D:209:GLY:HA2	6:D:867:HOH:O	2.19	0.42
1:D:221:ALA:HB2	1:D:235:LEU:HD13	2.02	0.42
1:B:43:GLN:OE1	1:B:344:ARG:HD3	2.19	0.42
1:C:117:LYS:HD3	1:C:122:LEU:HD23	2.02	0.42
1:D:48:HIS:HE1	1:D:50:PRO:HA	1.84	0.42
1:D:218:HIS:HB2	1:D:219:TRP:CD1	2.55	0.42
1:A:289:GLU:HG3	6:A:496:HOH:O	2.20	0.41
1:C:41:ALA:HA	6:C:1075:HOH:O	2.19	0.41
1:D:55:CYS:HB2	1:D:58:ASN:ND2	2.35	0.41
1:D:247:LEU:HA	1:D:251:GLN:OE1	2.19	0.41
1:A:99:CYS:HB3	1:B:225:TYR:OH	2.19	0.41
1:B:120:PRO:HB3	1:B:263:THR:OG1	2.20	0.41
1:D:18:THR:HA	1:D:181:ARG:HD2	2.02	0.41
1:D:174:PHE:CD1	1:D:174:PHE:N	2.88	0.41
1:B:120:PRO:O	1:B:260:LYS:NZ	2.54	0.41
1:B:288:GLU:HG3	6:B:612:HOH:O	2.20	0.41
1:C:4:PHE:CE2	1:D:89:ALA:HB2	2.55	0.41
1:C:168:GLN:C	1:C:169:ILE:HG13	2.41	0.41
1:A:94:ASP:CG	1:B:204:ARG:HH12	2.24	0.41
1:D:146:PRO:HD2	1:D:172:ASN:O	2.21	0.41
1:D:232:GLU:HG3	1:D:299:PHE:O	2.20	0.41
1:D:286:ASN:C	1:D:288:GLU:N	2.74	0.41
1:B:69:TYR:CG	1:B:73:TYR:HB2	2.55	0.41
1:C:31:ARG:HG2	1:C:31:ARG:NH1	2.32	0.41
1:C:112:SER:CB	1:C:113:PRO:HD2	2.50	0.41
1:D:228:ALA:HB1	1:D:322:THR:HG21	2.03	0.41
1:A:97:MET:HB3	1:B:225:TYR:CE2	2.56	0.41
1:B:162:ASN:HA	1:B:163:PRO:HD3	1.85	0.41
1:B:236:LEU:N	1:B:236:LEU:CD2	2.83	0.41
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.79	0.41
1:C:146:PRO:HD2	1:C:173:SER:HA	2.03	0.41
1:D:152:GLU:HB3	1:D:278:MET:HG3	2.02	0.41
1:A:2:THR:HG22	1:A:3:GLN:N	2.35	0.41
1:B:211:ARG:HH11	1:B:211:ARG:HD3	1.69	0.41
1:C:45:LEU:HB3	1:C:116:SER:HB2	2.03	0.41
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.77	0.41
1:D:257:LEU:HD11	1:D:261:LYS:HE2	2.02	0.41
1:A:28:ARG:HB3	1:A:325:ASP:OD1	2.20	0.40
1:A:213:VAL:HG12	1:A:214:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:CD1	1:A:174:PHE:N	2.88	0.40
1:A:324:ARG:NH2	1:A:326:LEU:HD21	2.36	0.40
1:C:18:THR:HB	1:C:181:ARG:CZ	2.52	0.40
1:C:162:ASN:OD1	1:C:163:PRO:HD2	2.22	0.40
1:D:31:ARG:HB2	1:D:32:PRO:HD2	2.03	0.40
1:D:137:GLN:HB3	1:D:169:ILE:HD13	2.01	0.40
1:C:49:ASP:HA	1:C:50:PRO:HD2	1.85	0.40
1:A:299:PHE:O	1:A:301:PRO:HD3	2.21	0.40
1:B:189:TYR:CG	1:B:197:MET:HB2	2.56	0.40
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.71	0.40
1:D:189:TYR:CE1	1:D:197:MET:HA	2.56	0.40
1:A:319:LEU:CD1	1:B:279:GLY:HA3	2.51	0.40
1:B:67:PRO:HA	6:B:683:HOH:O	2.21	0.40
1:D:4:PHE:HA	1:D:9:HIS:ND1	2.36	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)
6:C:1190:HOH:O	6:C:1239:HOH:O[2_657]	1.72	0.48

## 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	345/348 (99%)	325 (94%)	18 (5%)	2 (1%)	25 12
1	B	342/348 (98%)	325 (95%)	16 (5%)	1 (0%)	41 27
1	C	342/348 (98%)	321 (94%)	19 (6%)	2 (1%)	25 12
1	D	342/348 (98%)	324 (95%)	16 (5%)	2 (1%)	25 12
All	All	1371/1392 (98%)	1295 (94%)	69 (5%)	7 (0%)	29 15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	GLN
1	C	44	VAL
1	A	26	PRO
1	B	343	PHE
1	D	50	PRO
1	D	287	GLY
1	A	6	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	297/298 (100%)	282 (95%)	15 (5%)	24	10
1	B	295/298 (99%)	279 (95%)	16 (5%)	22	9
1	C	295/298 (99%)	278 (94%)	17 (6%)	20	7
1	D	295/298 (99%)	277 (94%)	18 (6%)	18	7
All	All	1182/1192 (99%)	1116 (94%)	66 (6%)	21	8

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	VAL
1	A	8	ASP
1	A	38	GLU
1	A	42	LYS
1	A	43	GLN
1	A	44	VAL
1	A	83	MET
1	A	109	ILE
1	A	123	SER
1	A	194	LYS
1	A	236	LEU
1	A	253	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	288	GLU
1	A	326	LEU
1	B	3	GLN
1	B	8	ASP
1	B	42	LYS
1	B	44	VAL
1	B	91	GLU
1	B	92	SER
1	B	112	SER
1	B	187	LYS
1	B	194	LYS
1	B	197	MET
1	B	202	VAL
1	B	211	ARG
1	B	253	SER
1	B	288	GLU
1	B	289	GLU
1	B	321	GLU
1	C	2	THR
1	C	3	GLN
1	C	16	PRO
1	C	30	LYS
1	C	31	ARG
1	C	37	GLN
1	C	39	THR
1	C	42	LYS
1	C	45	LEU
1	C	109	ILE
1	C	194	LYS
1	C	204	ARG
1	C	236	LEU
1	C	242	LEU
1	C	245	THR
1	C	253	SER
1	C	266	TYR
1	D	43	GLN
1	D	88	ASP
1	D	91	GLU
1	D	93	HIS
1	D	95	PRO
1	D	98	ARG
1	D	99	CYS

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Mol	Chain	Res	Type
1	D	101	SER
1	D	136	GLU
1	D	195	SER
1	D	203	GLN
1	D	236	LEU
1	D	253	SER
1	D	262	LEU
1	D	266	TYR
1	D	276	TYR
1	D	288	GLU
1	D	289	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	27	HIS
1	A	34	GLN
1	A	37	GLN
1	A	100	GLN
1	A	172	ASN
1	A	193	GLN
1	A	330	GLN
1	B	34	GLN
1	B	37	GLN
1	B	291	GLN
1	C	20	GLN
1	C	34	GLN
1	C	48	HIS
1	C	100	GLN
1	C	153	ASN
1	D	34	GLN
1	D	37	GLN
1	D	43	GLN
1	D	48	HIS
1	D	100	GLN
1	D	291	GLN

### 5.3.3 RNA

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](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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
2	GDU	D	352	-	31,38,38	1.19	3 (9%)	41,58,58	1.45	6 (14%)
2	GDU	B	352	-	31,38,38	1.25	3 (9%)	41,58,58	1.30	4 (9%)
2	GDU	C	352	-	31,38,38	1.39	3 (9%)	41,58,58	1.33	5 (12%)
2	GDU	A	352	-	31,38,38	1.35	3 (9%)	41,58,58	1.32	3 (7%)

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	GDU	D	352	-	-	8/21/59/59	0/3/3/3
2	GDU	B	352	-	-	7/21/59/59	0/3/3/3
2	GDU	C	352	-	-	7/21/59/59	0/3/3/3
2	GDU	A	352	-	-	5/21/59/59	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	352	GDU	C4-N3	5.00	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	352	GDU	C4-N3	4.56	1.41	1.33
2	B	352	GDU	C4-N3	4.20	1.40	1.33
2	D	352	GDU	C4-N3	3.52	1.39	1.33
2	A	352	GDU	C6-N1	3.31	1.39	1.35
2	B	352	GDU	C6-C5	-3.07	1.31	1.38
2	D	352	GDU	C6-N1	3.03	1.39	1.35
2	C	352	GDU	C6-C5	-2.94	1.31	1.38
2	D	352	GDU	C6-C5	-2.77	1.32	1.38
2	C	352	GDU	C6-N1	2.58	1.39	1.35
2	B	352	GDU	C2D-C1D	-2.47	1.50	1.53
2	A	352	GDU	C6-C5	-2.24	1.33	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	352	GDU	C5-C4-N3	-4.72	112.92	123.31
2	D	352	GDU	C5-C4-N3	-4.54	113.33	123.31
2	B	352	GDU	C5-C4-N3	-4.12	114.25	123.31
2	A	352	GDU	C1'-O5'-C5'	3.67	120.90	113.69
2	C	352	GDU	C5-C4-N3	-3.30	116.05	123.31
2	C	352	GDU	O5'-C1'-O3B	-3.05	107.38	111.36
2	D	352	GDU	O5'-C5'-C4'	2.70	114.60	109.69
2	B	352	GDU	O4'-C4'-C5'	2.66	115.89	109.30
2	D	352	GDU	O3A-PB-O3B	2.58	107.69	102.48
2	B	352	GDU	O4D-C4D-C3D	2.53	110.11	105.11
2	C	352	GDU	O5D-PA-O1A	2.40	118.45	109.07
2	D	352	GDU	O3'-C3'-C2'	-2.36	104.89	110.35
2	D	352	GDU	O4D-C1D-C2D	-2.25	103.63	106.93
2	C	352	GDU	O4D-C4D-C3D	2.24	109.55	105.11
2	A	352	GDU	O4D-C4D-C3D	2.23	109.52	105.11
2	B	352	GDU	O5'-C5'-C4'	2.21	113.71	109.69
2	D	352	GDU	C4'-C3'-C2'	-2.13	107.10	110.82
2	C	352	GDU	C3'-C4'-C5'	-2.06	106.56	110.24

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	352	GDU	PB-O3A-PA-O5D
2	A	352	GDU	C1'-O3B-PB-O3A
2	B	352	GDU	C2D-C1D-N1-C6
2	B	352	GDU	O4D-C1D-N1-C6

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Mol	Chain	Res	Type	Atoms
2	B	352	GDU	PB-O3A-PA-O5D
2	B	352	GDU	C1'-O3B-PB-O3A
2	C	352	GDU	C5D-O5D-PA-O2A
2	C	352	GDU	C5D-O5D-PA-O3A
2	C	352	GDU	C1'-O3B-PB-O3A
2	D	352	GDU	C2D-C1D-N1-C6
2	D	352	GDU	O4D-C1D-N1-C6
2	D	352	GDU	C1'-O3B-PB-O3A
2	A	352	GDU	O4D-C4D-C5D-O5D
2	B	352	GDU	O4D-C4D-C5D-O5D
2	D	352	GDU	C3D-C4D-C5D-O5D
2	D	352	GDU	O4D-C4D-C5D-O5D
2	B	352	GDU	C3D-C4D-C5D-O5D
2	A	352	GDU	C3D-C4D-C5D-O5D
2	B	352	GDU	C2'-C1'-O3B-PB
2	C	352	GDU	C2'-C1'-O3B-PB
2	C	352	GDU	PB-O3A-PA-O1A
2	D	352	GDU	PB-O3A-PA-O1A
2	C	352	GDU	PB-O3A-PA-O5D
2	D	352	GDU	PB-O3A-PA-O5D
2	A	352	GDU	C2'-C1'-O3B-PB
2	D	352	GDU	C2'-C1'-O3B-PB
2	C	352	GDU	O4D-C4D-C5D-O5D

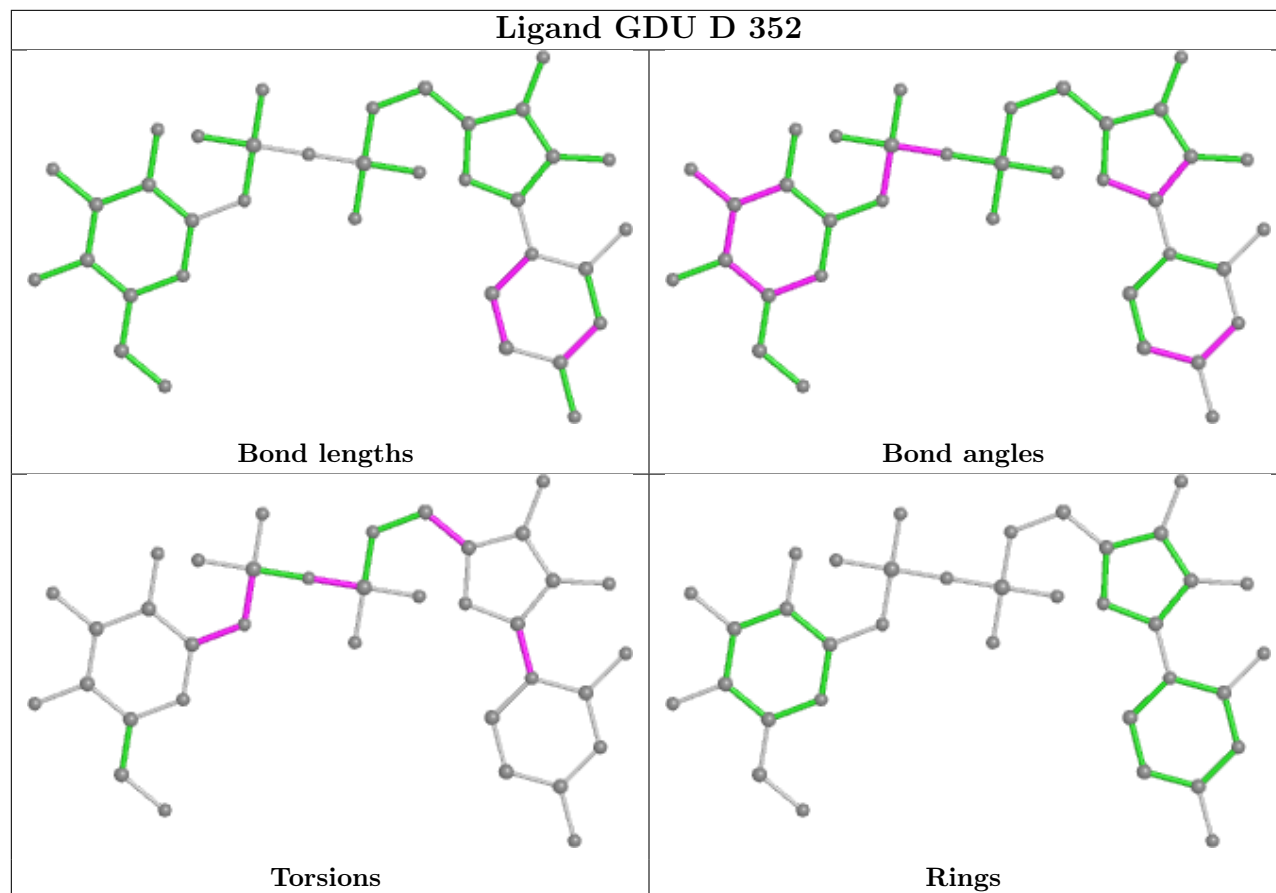
There are no ring outliers.

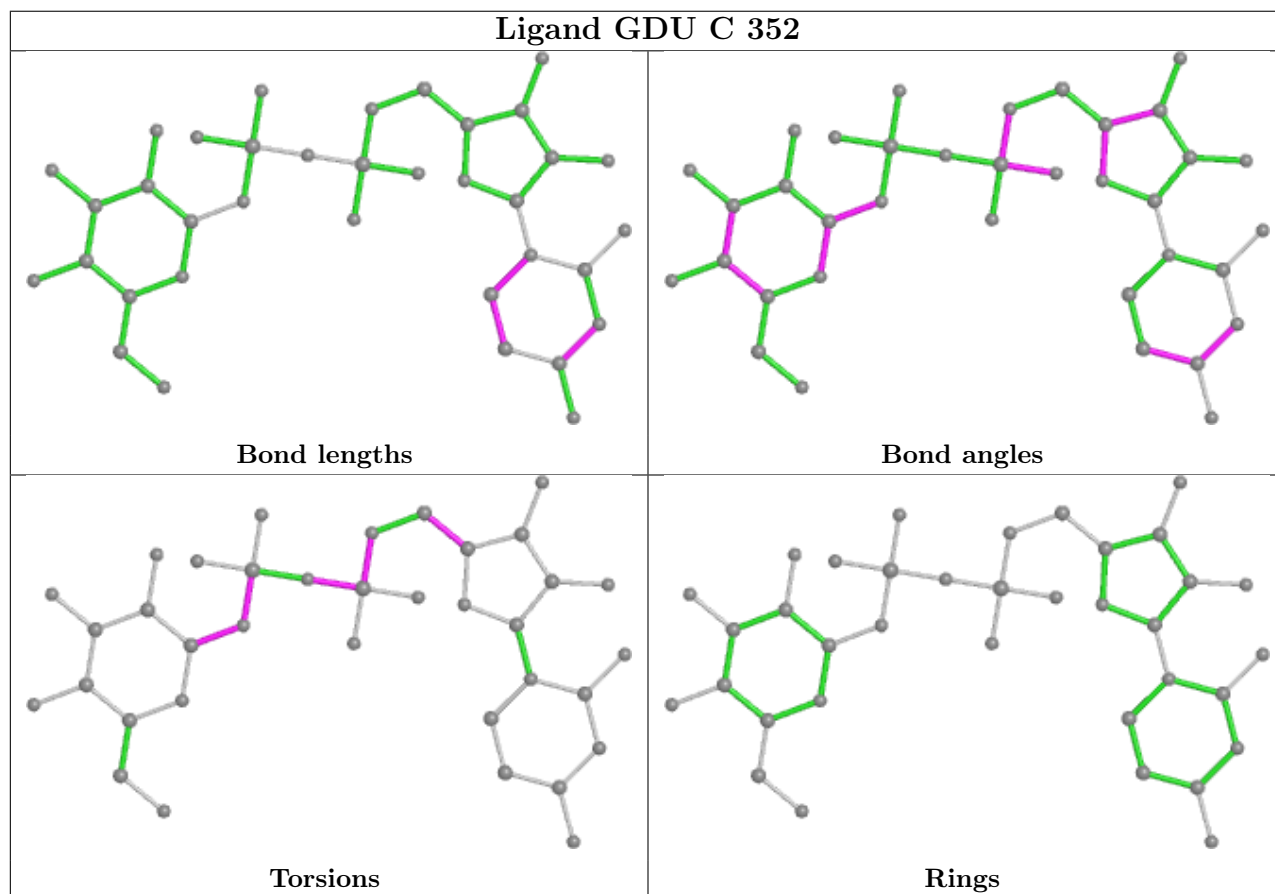
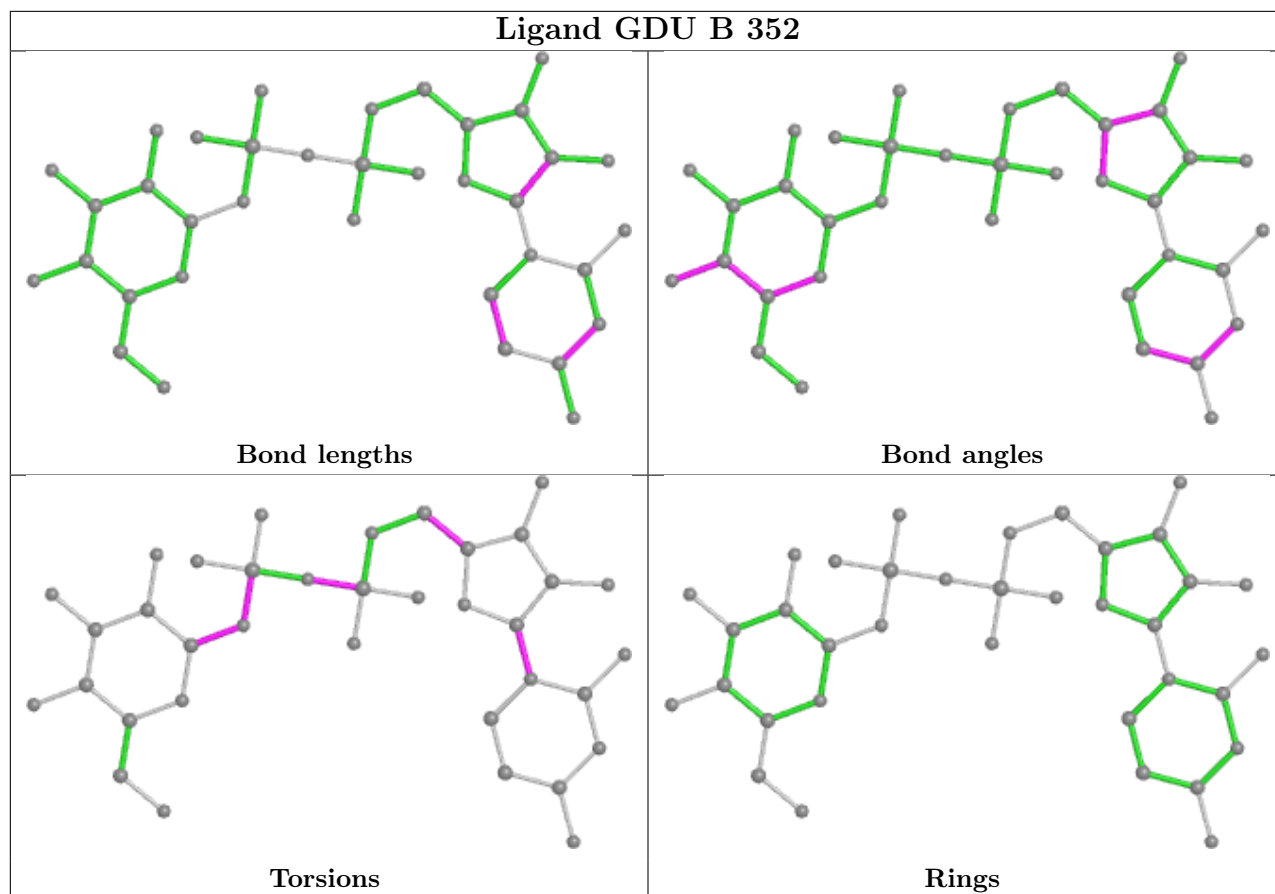
2 monomers are involved in 8 short contacts:

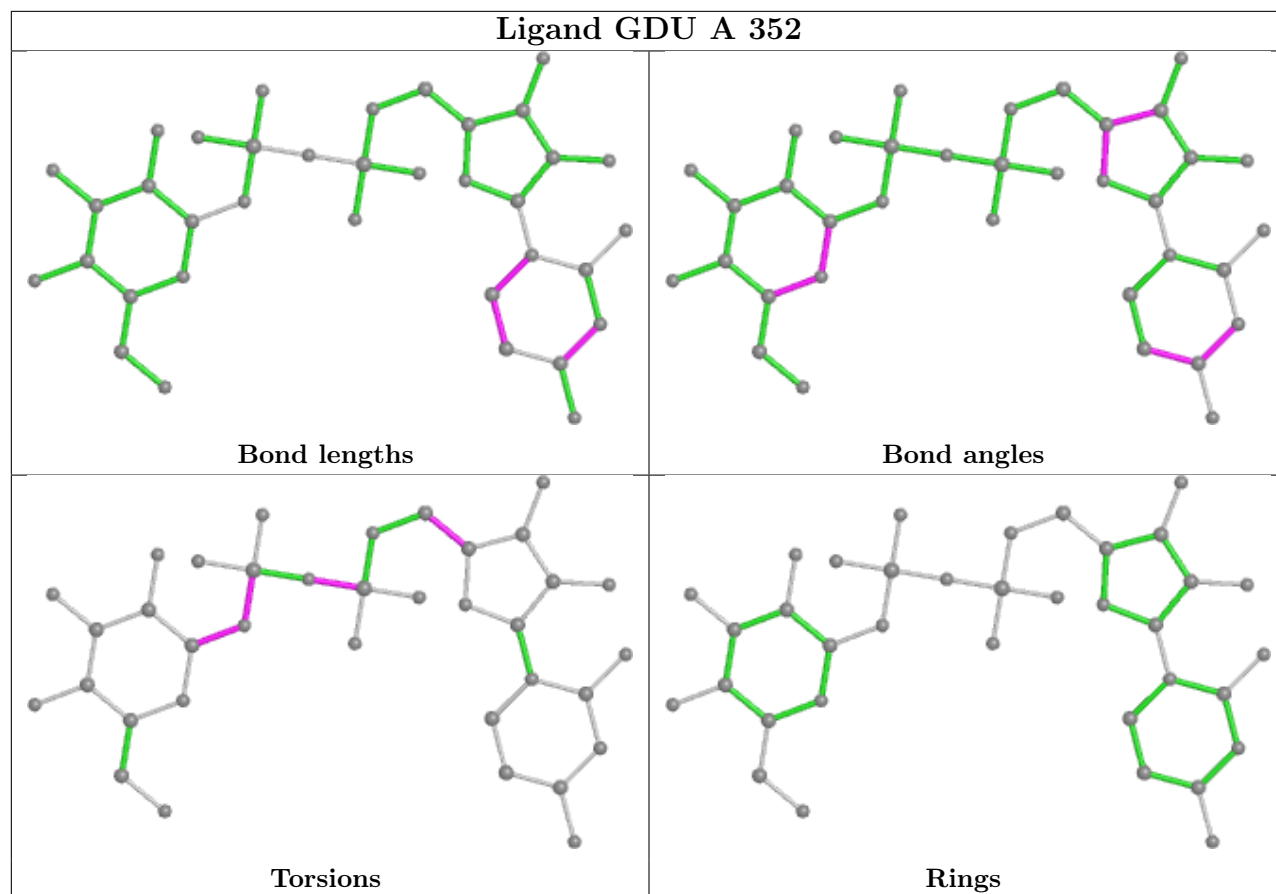
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	352	GDU	7	0
2	B	352	GDU	1	0

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

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.