



Full wwPDB X-ray Structure Validation Report i

Apr 4, 2022 – 02:08 PM EDT

PDB ID : 7MSN
Title : SunS glycosin S-glycosyltransferase
Authors : Garg, N.; Nair, S.K.
Deposited on : 2021-05-11
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

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

MolProbitiy : 4.02b-467
Xtriaige (Phenix) : 1.13
EDS : **FAILED**
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) : 2.27

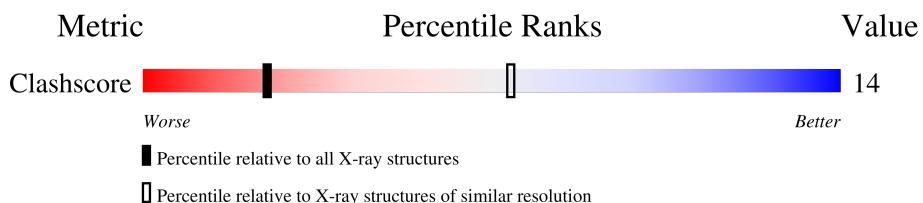
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain			
1	A	422	71%	27%	.	
1	B	422	70%	27%	..	

2 Entry composition [\(i\)](#)

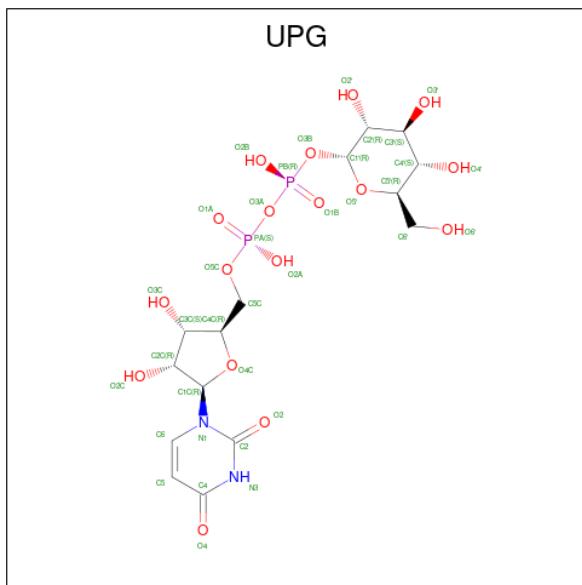
There are 2 unique types of molecules in this entry. The entry contains 6995 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SPbeta prophage-derived glycosyltransferase SunS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	417	3462	2218	570	659	15	0	0	0
1	B	416	3461	2217	569	660	15	0	0	0

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: C₁₅H₂₄N₂O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



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

3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

- Molecule 1: SPbeta prophage-derived glycosyltransferase SunS

Chain A: 71% 27%

Position	Mutation	Color
1	M1	Blue
2	S4	Green
3	D5	Green
4	I6	Green
5	V7	Yellow
6	E9	Green
7	L8	Yellow
8	I10	Yellow
9	G13	Yellow
10	I13	Yellow
11	N14	Yellow
12	H219	Yellow
13	N14	Yellow
14	D115	Yellow
15	F116	Yellow
16	P117	Yellow
17	S118	Yellow
18	TYR	Yellow
19	L19	Yellow
20	Y20	Yellow
21	A21	Yellow
22	I219	Yellow
23	N210	Yellow
24	F211	Yellow
25	P217	Yellow
26	Y218	Yellow
27	N220	Yellow
28	GLY	Yellow
29	R385	Yellow
30	ASN	Yellow
31	PRO	Yellow
32	S225	Yellow
33	R186	Yellow
34	L186	Yellow
35	K191	Yellow
36	P209	Yellow
37	N377	Yellow
38	N378	Yellow
39	F228	Yellow
40	L380	Yellow
41	I376	Yellow
42	V410	Yellow
43	L343	Yellow
44	V416	Yellow
45	R245	Yellow
46	K232	Yellow
47	I239	Yellow
48	P251	Yellow
49	E130	Yellow
50	W131	Yellow
51	I132	Yellow
52	Y126	Yellow
53	E125	Yellow
54	I127	Yellow
55	A127	Yellow
56	D42	Yellow
57	S43	Yellow
58	M39	Yellow
59	S40	Yellow
60	I41	Yellow
61	T57	Yellow
62	C58	Yellow
63	Y48	Yellow
64	S51	Yellow
65	T56	Yellow
66	E66	Yellow
67	V152	Yellow
68	L156	Yellow
69	E157	Yellow
70	K70	Yellow
71	K71	Yellow
72	C72	Yellow
73	L73	Yellow
74	Y63	Yellow
75	N64	Yellow
76	E65	Yellow
77	V76	Yellow
78	I169	Yellow
79	V165	Yellow
80	V308	Yellow
81	L312	Yellow
82	D315	Yellow
83	T173	Yellow
84	E170	Yellow
85	Y172	Yellow
86	E171	Yellow
87	G174	Yellow
88	H175	Yellow
89	L176	Yellow
90	Y177	Yellow
91	P322	Yellow
92	R323	Yellow
93	G324	Yellow
94	V325	Yellow
95	T319	Yellow
96	T319	Yellow
97	R181	Yellow
98	H182	Yellow
99	M183	Yellow
100	F184	Yellow
101	M339	Yellow
102	F330	Yellow
103	T94	Yellow
104	D93	Yellow
105	R181	Yellow
106	H182	Yellow
107	M183	Yellow
108	D96	Yellow
109	F184	Yellow
110	M339	Yellow

- Molecule 1: SPbeta prophage-derived glycosyltransferase SunS

4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.73Å 108.73Å 210.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 3.00	Depositor
% Data completeness (in resolution range)	98.8 (47.38-3.00)	Depositor
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	2.19 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R _{free}	0.204 , 0.280	Depositor
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.188	Xtriage
L-test for twinning ²	$< L > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6995	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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: UPG

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	0.53	0/3528	0.77	4/4760 (0.1%)
1	B	0.56	0/3527	0.82	6/4758 (0.1%)
All	All	0.54	0/7055	0.79	10/9518 (0.1%)

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	5

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	LEU	CB-CG-CD2	-7.31	98.57	111.00
1	B	294	LEU	CA-CB-CG	7.13	131.69	115.30
1	A	281	TYR	CB-CG-CD1	-6.84	116.89	121.00
1	B	281	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	A	281	TYR	CB-CG-CD2	5.45	124.27	121.00
1	B	323	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	354	LEU	CA-CB-CG	5.31	127.52	115.30
1	B	206	SER	CB-CA-C	-5.28	100.07	110.10
1	A	83	ILE	CG1-CB-CG2	-5.18	100.01	111.40
1	B	281	TYR	CB-CG-CD2	5.03	124.02	121.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	202	ASN	Peptide
1	B	205	HIS	Peptide
1	B	206	SER	Peptide
1	B	27	VAL	Peptide
1	B	62	VAL	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	3462	0	3450	100	0
1	B	3461	0	3452	101	0
2	A	36	0	21	2	0
2	B	36	0	21	5	0
All	All	6995	0	6944	190	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 14.

All (190) 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)
2:B:500:UPG:C4C	2:B:500:UPG:O4C	1.66	1.15
2:A:500:UPG:O4C	2:A:500:UPG:C4C	1.66	1.14
1:A:28:ASN:ND2	1:A:210:ASN:O	2.08	0.86
1:A:121:ASN:HA	1:A:191:LYS:HE2	1.67	0.77
1:A:165:VAL:HB	1:A:183:MET:HB3	1.68	0.76
1:B:323:ARG:HD3	1:B:323:ARG:H	1.52	0.75
1:B:195:LYS:HB3	1:B:239:LEU:HD12	1.70	0.74
1:A:323:ARG:HD3	1:A:323:ARG:H	1.53	0.73
1:A:114:ASN:HB3	1:A:239:LEU:HD21	1.70	0.72
1:A:57:THR:HG21	1:A:127:ALA:HB1	1.71	0.72
1:B:226:GLU:HG2	1:B:227:ASN:H	1.54	0.72
1:B:393:ILE:HG23	1:B:399:LYS:HE3	1.71	0.71
1:B:420:ILE:HG13	1:B:421:GLU:H	1.59	0.67
1:B:93:ASP:O	1:B:95:VAL:N	2.28	0.66
1:B:295:VAL:O	1:B:299:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:HB2	1:B:36:ILE:HD11	1.78	0.65
1:A:156:LEU:HD21	1:A:211:PHE:CD2	2.31	0.65
1:A:93:ASP:O	1:A:95:VAL:N	2.30	0.65
1:B:315:ASP:O	1:B:319:THR:HG23	1.97	0.64
1:A:410:LEU:HD12	1:B:410:LEU:HD12	1.79	0.64
1:A:149:ILE:H	1:A:149:ILE:HD12	1.63	0.63
1:A:295:VAL:O	1:A:299:THR:HG23	1.98	0.63
1:A:10:LEU:HD21	1:A:19:LEU:HD23	1.81	0.62
1:B:347:SER:HB2	1:B:376:LEU:HD22	1.80	0.62
1:B:383:TRP:HA	1:B:386:VAL:HG22	1.80	0.61
1:B:28:ASN:ND2	1:B:210:ASN:O	2.33	0.61
1:B:393:ILE:HD13	1:B:399:LYS:HG3	1.83	0.60
1:A:13:GLY:O	1:A:15:ALA:N	2.33	0.60
2:B:500:UPG:H5C2	2:B:500:UPG:H6	1.84	0.60
1:B:86:LEU:HD22	1:B:123:ILE:HG13	1.84	0.59
1:B:143:LYS:HD3	1:B:143:LYS:H	1.68	0.59
1:A:176:LEU:H	1:B:364:THR:HG21	1.68	0.58
1:A:359:TYR:CE2	1:B:323:ARG:HG2	2.38	0.58
1:B:36:ILE:HG21	1:B:159:PHE:HD1	1.69	0.58
2:A:500:UPG:O4C	2:A:500:UPG:C5C	2.50	0.58
1:A:93:ASP:HB2	1:A:96:ASP:OD1	2.04	0.57
1:A:176:LEU:H	1:B:364:THR:CG2	2.17	0.57
1:B:209:PHE:CE2	1:B:211:PHE:CD1	2.93	0.56
1:A:175:HIS:HA	1:B:364:THR:HG22	1.87	0.56
1:A:157:GLU:HG2	1:A:185:ARG:NH1	2.20	0.56
1:B:110:GLU:OE2	1:B:122:LYS:HE3	2.05	0.55
1:A:73:LEU:HA	1:A:76:VAL:HG22	1.89	0.55
1:A:39:MET:HB2	1:A:43:SER:OG	2.07	0.55
1:A:156:LEU:HD21	1:A:211:PHE:HD2	1.69	0.54
1:A:278:ILE:HD13	1:A:294:LEU:HD13	1.90	0.54
1:B:28:ASN:HD22	1:B:211:PHE:HA	1.71	0.54
1:B:202:ASN:O	1:B:206:SER:HB3	2.08	0.54
1:B:93:ASP:HB3	1:B:97:ILE:HG13	1.90	0.54
1:B:73:LEU:HA	1:B:76:VAL:HG12	1.90	0.54
1:A:379:GLN:CG	1:B:379:GLN:HG2	2.38	0.54
1:A:359:TYR:HE2	1:B:323:ARG:HG2	1.73	0.54
1:A:1:MET:HE1	1:A:38:VAL:HG21	1.90	0.53
1:A:173:THR:HA	1:B:395:ASN:HD21	1.73	0.53
1:A:179:ASP:OD1	1:A:181:ARG:NH1	2.42	0.53
1:B:55:THR:OG1	1:B:130:GLU:HG2	2.07	0.53
1:A:143:LYS:N	1:A:143:LYS:HD3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:A:38:VAL:HG21	2.39	0.52
1:A:323:ARG:H	1:A:323:ARG:CD	2.20	0.52
1:B:209:PHE:HE2	1:B:211:PHE:HD1	1.57	0.52
1:A:58:CYS:HB3	1:A:83:ILE:HG22	1.91	0.52
1:A:209:PHE:HE2	1:A:211:PHE:CD1	2.27	0.52
1:B:3:LEU:HG	1:B:29:ILE:HG23	1.92	0.52
1:B:219:HIS:CG	1:B:220:ASN:H	2.28	0.51
1:B:226:GLU:HG2	1:B:227:ASN:N	2.24	0.51
1:B:333:ALA:O	1:B:337:VAL:HG23	2.10	0.51
1:B:110:GLU:HG3	1:B:122:LYS:HG3	1.91	0.51
1:A:358:ARG:HH22	1:B:328:ASP:CG	2.14	0.51
1:B:209:PHE:CE2	1:B:211:PHE:CE1	2.99	0.51
1:B:143:LYS:HD3	1:B:143:LYS:N	2.27	0.50
1:B:56:ILE:HG13	1:B:131:TRP:HB2	1.92	0.50
1:A:88:SER:HB3	1:A:112:TRP:HB2	1.93	0.50
1:B:169:ILE:HG12	1:B:217:VAL:CG2	2.41	0.50
1:B:405:TYR:HA	1:B:408:ASN:ND2	2.27	0.50
1:A:228:ASN:ND2	1:A:232:LYS:HE2	2.27	0.50
1:B:23:LEU:HD12	1:B:26:LEU:HD22	1.94	0.49
1:A:219:HIS:CG	1:A:220:ASN:H	2.30	0.49
1:A:87:ASP:OD1	1:A:89:TYR:N	2.40	0.49
1:A:131:TRP:CE2	1:A:185:ARG:HG2	2.48	0.49
1:A:102:PHE:O	1:A:105:VAL:HG22	2.11	0.49
1:A:130:GLU:O	1:A:186:LEU:HB2	2.12	0.49
1:B:190:VAL:HG22	1:B:202:ASN:HB3	1.95	0.49
1:B:209:PHE:CE2	1:B:211:PHE:HD1	2.31	0.49
1:A:6:ILE:O	1:A:10:LEU:HD13	2.12	0.49
1:A:121:ASN:O	1:A:124:ILE:N	2.46	0.49
1:B:141:TYR:OH	1:B:149:ILE:HG12	2.12	0.49
1:A:169:ILE:HG12	1:A:217:VAL:HG13	1.94	0.49
1:A:385:ARG:HH11	1:A:385:ARG:HG3	1.77	0.49
1:B:10:LEU:HB3	1:B:20:TYR:HD1	1.78	0.48
1:B:310:LEU:O	1:B:314:LEU:HB2	2.13	0.48
1:B:323:ARG:H	1:B:323:ARG:CD	2.24	0.48
1:A:299:THR:HG22	1:A:330:PHE:HZ	1.77	0.48
1:A:84:ILE:HD13	1:A:126:TYR:HB2	1.96	0.48
1:A:124:ILE:HG23	1:A:186:LEU:CD2	2.43	0.48
1:B:373:LEU:HB3	1:B:389:ILE:HD13	1.95	0.48
1:B:3:LEU:HB2	1:B:36:ILE:CD1	2.43	0.48
1:B:229:ILE:HG13	1:B:230:LYS:N	2.28	0.48
1:A:379:GLN:HG2	1:B:379:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:HG21	1:A:181:ARG:HG2	1.95	0.48
1:A:343:LEU:HD22	1:A:376:LEU:HD22	1.96	0.48
1:B:57:THR:HG21	1:B:127:ALA:HB1	1.95	0.47
1:A:63:TYR:O	1:A:65:GLU:N	2.47	0.47
1:A:69:ILE:HG13	1:A:73:LEU:HD12	1.95	0.47
1:B:132:ILE:HB	1:B:186:LEU:HD11	1.96	0.47
1:A:339:MET:CE	1:B:342:LYS:HB3	2.45	0.47
1:A:19:LEU:HA	1:A:48:TYR:CD2	2.50	0.46
1:A:71:LYS:N	1:A:71:LYS:HD2	2.31	0.46
1:B:48:TYR:HD1	1:B:158:PHE:CD2	2.31	0.46
1:B:219:HIS:CG	1:B:220:ASN:N	2.84	0.46
1:A:10:LEU:HD23	1:A:20:TYR:HB2	1.98	0.46
1:B:209:PHE:HE2	1:B:211:PHE:CD1	2.30	0.46
1:A:308:VAL:O	1:A:312:LEU:HD13	2.16	0.46
1:A:121:ASN:HB2	1:A:191:LYS:HZ1	1.80	0.46
1:A:290:PHE:CE1	1:A:294:LEU:HD21	2.51	0.46
1:B:189:LYS:O	1:B:190:VAL:HB	2.16	0.46
1:A:171:GLU:OE2	1:A:177:TYR:HE1	1.98	0.45
1:B:141:TYR:OH	1:B:149:ILE:CG1	2.64	0.45
1:A:118:TYR:O	1:A:121:ASN:HB3	2.17	0.45
1:A:131:TRP:CZ2	1:A:185:ARG:HG2	2.52	0.45
1:A:96:ASP:HA	1:A:99:LYS:HD2	1.99	0.45
1:A:113:LYS:O	1:A:115:ASP:N	2.50	0.45
1:B:95:VAL:HG11	1:B:109:TYR:OH	2.17	0.45
1:A:416:VAL:HG23	1:B:387:LYS:HA	1.99	0.45
1:A:141:TYR:OH	1:A:149:ILE:CG1	2.65	0.45
1:B:233:THR:HG23	1:B:260:GLU:HG2	1.99	0.45
1:B:354:LEU:HD21	1:B:369:PHE:CG	2.52	0.45
1:A:80:PHE:O	1:A:81:ASN:HB2	2.17	0.44
1:A:105:VAL:HG23	1:A:105:VAL:O	2.16	0.44
1:A:171:GLU:HB3	1:A:173:THR:H	1.81	0.44
1:B:169:ILE:HG13	1:B:180:THR:HG21	1.98	0.44
1:B:189:LYS:HA	1:B:203:TYR:CD1	2.53	0.44
1:B:219:HIS:ND1	1:B:220:ASN:N	2.65	0.44
2:B:500:UPG:O4C	2:B:500:UPG:C5C	2.51	0.44
1:A:176:LEU:HB2	1:B:364:THR:HG21	1.99	0.44
1:B:414:GLU:HA	1:B:417:LEU:HB3	1.99	0.44
1:A:143:LYS:HD3	1:A:143:LYS:H	1.82	0.44
1:A:229:ILE:H	1:A:229:ILE:HD12	1.82	0.44
1:B:207:LEU:HD12	1:B:207:LEU:HA	1.86	0.44
1:B:63:TYR:O	1:B:65:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ILE:H	1:B:149:ILE:HD12	1.83	0.44
1:A:4:SER:O	1:A:8:LEU:HD23	2.18	0.44
1:B:314:LEU:HA	1:B:314:LEU:HD12	1.81	0.44
1:A:315:ASP:O	1:A:319:THR:HG23	2.18	0.43
1:A:377:ASN:HA	1:A:380:LEU:HB2	1.99	0.43
1:B:290:PHE:CE1	1:B:294:LEU:HD21	2.54	0.43
1:A:108:LYS:HG3	1:A:126:TYR:CD1	2.53	0.43
1:B:11:LYS:O	1:B:15:ALA:HB2	2.17	0.43
1:A:149:ILE:O	1:A:152:VAL:HB	2.17	0.43
1:A:156:LEU:HD21	1:A:211:PHE:CE2	2.53	0.43
1:A:19:LEU:HA	1:A:48:TYR:CE2	2.53	0.43
1:A:142:SER:OG	1:A:144:GLU:HG2	2.19	0.43
1:B:38:VAL:HG21	1:B:44:LEU:HD22	2.02	0.42
1:B:109:TYR:O	1:B:110:GLU:HG2	2.19	0.42
1:B:120:ARG:NH2	1:B:136:ASP:OD1	2.52	0.42
1:B:251:PRO:HG3	1:B:280:ASN:HB3	2.00	0.42
1:A:56:ILE:HD13	1:A:149:ILE:HG22	2.01	0.42
1:A:325:VAL:HG12	1:B:359:TYR:O	2.19	0.42
1:B:77:LYS:HA	1:B:83:ILE:CD1	2.50	0.42
1:A:28:ASN:HD22	1:A:211:PHE:HA	1.84	0.42
1:A:219:HIS:ND1	1:A:220:ASN:N	2.67	0.42
1:B:61:ILE:HG13	2:B:500:UPG:O4C	2.19	0.42
1:B:169:ILE:HG12	1:B:217:VAL:HG22	2.01	0.42
1:A:281:TYR:O	1:A:282:LYS:C	2.57	0.42
1:B:157:GLU:HG2	1:B:185:ARG:NH1	2.35	0.42
1:B:156:LEU:HD21	1:B:211:PHE:CD2	2.55	0.42
2:B:500:UPG:H5C2	2:B:500:UPG:C6	2.50	0.42
1:A:132:ILE:O	1:A:183:MET:HA	2.19	0.42
1:B:397:ASN:HA	1:B:400:LYS:HB3	2.01	0.42
1:A:48:TYR:O	1:A:51:SER:OG	2.19	0.42
1:B:203:TYR:C	1:B:205:HIS:H	2.22	0.42
1:B:393:ILE:HD11	1:B:399:LYS:N	2.35	0.42
1:A:116:PHE:O	1:A:120:ARG:HG2	2.21	0.41
1:A:403:LYS:HE2	1:B:421:GLU:O	2.20	0.41
1:A:83:ILE:HG21	1:A:83:ILE:HD13	1.79	0.41
1:B:143:LYS:HE2	1:B:143:LYS:HB2	1.96	0.41
1:B:320:GLU:HA	1:B:320:GLU:OE1	2.19	0.41
1:A:245:ARG:HB3	1:A:245:ARG:NH1	2.35	0.41
1:A:343:LEU:HD23	1:B:339:MET:SD	2.60	0.41
1:B:365:THR:OG1	1:B:367:ASP:HB2	2.21	0.41
1:A:164:VAL:CG2	1:A:181:ARG:HG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.92	0.41
1:A:403:LYS:HE2	1:B:421:GLU:C	2.41	0.41
1:B:76:VAL:HG23	1:B:80:PHE:HE2	1.86	0.40
1:B:251:PRO:HG3	1:B:280:ASN:CB	2.51	0.40
1:A:251:PRO:HB2	1:A:281:TYR:CD2	2.57	0.40
1:B:6:ILE:O	1:B:10:LEU:HD13	2.22	0.40
1:B:134:PHE:CE1	1:B:192:PHE:HE1	2.39	0.40
1:A:40:SER:OG	1:A:41:ILE:N	2.54	0.40
1:A:185:ARG:HE	1:A:185:ARG:HB3	1.72	0.40
1:A:322:PRO:HD2	1:A:323:ARG:HH21	1.87	0.40
1:B:86:LEU:HB2	1:B:123:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

5.3.2 Protein sidechains [\(i\)](#)

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

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

2 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

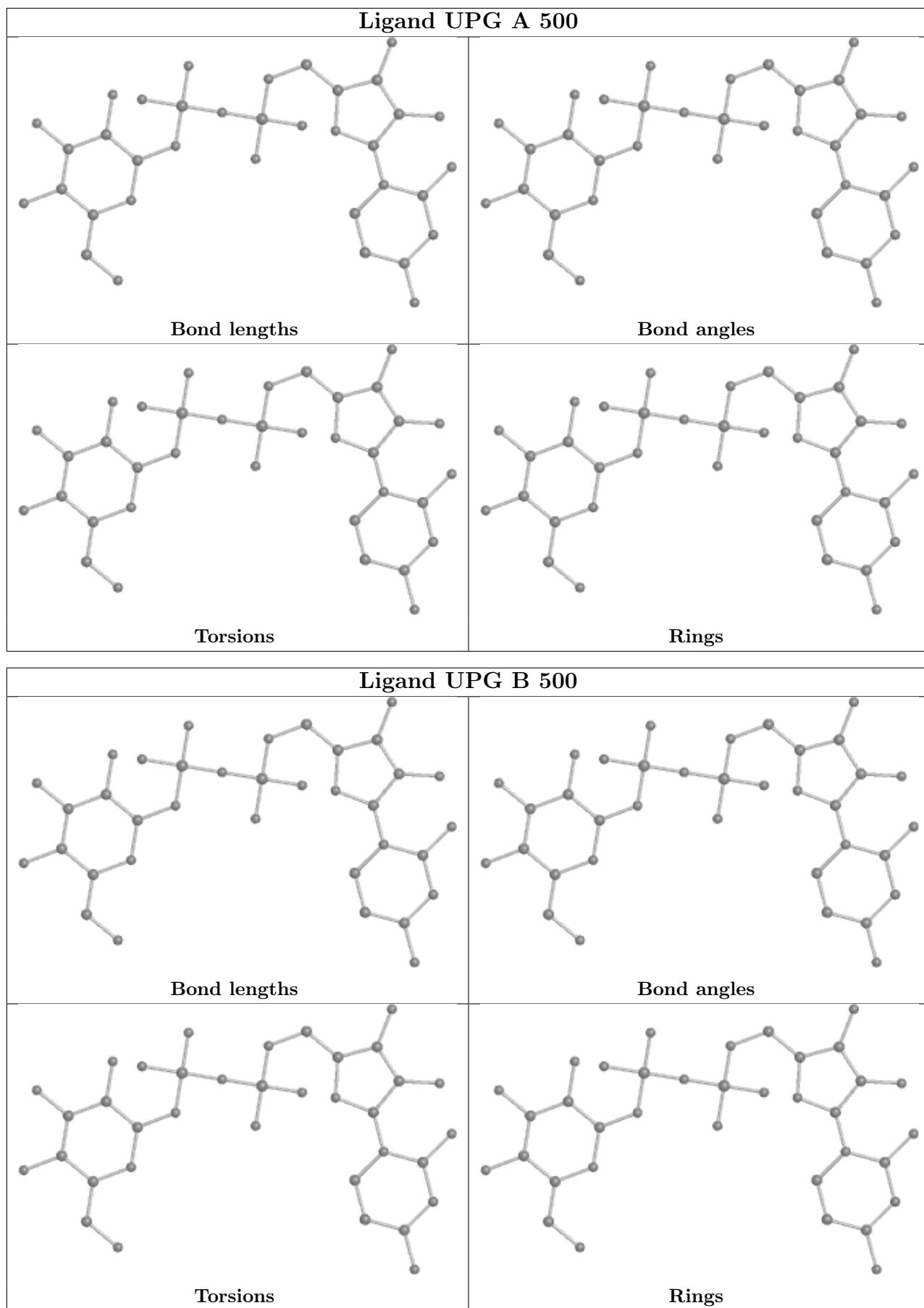
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [\(i\)](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

EDS failed to run properly - this section is therefore empty.