



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:11 AM UTC

PDB ID : 4KQ2 / pdb_00004kq2
Title : Glucose1,2cyclic phosphate bound activated state of Yeast Glycogen Synthase
Authors : Chikwana, V.M.; Hurley, T.D.
Deposited on : 2013-05-14
Resolution : 2.95 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

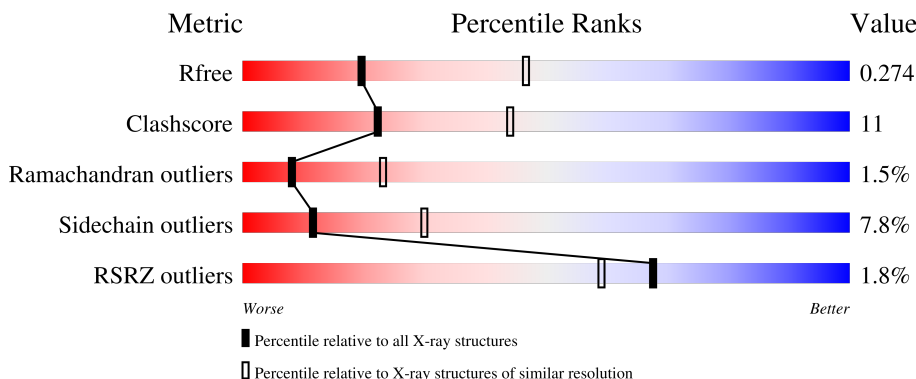
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	724	2% 65% 20% • 12%
1	B	724	% 65% 20% • 12%
1	C	724	2% 63% 22% • 12%
1	D	724	% 61% 24% • 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20806 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 Gsy2p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	B	638	Total	C	N	O	S	0	3	0
			5163	3298	900	946	19			
1	C	638	Total	C	N	O	S	0	1	0
			5154	3291	898	946	19			
1	D	636	Total	C	N	O	S	0	2	0
			5146	3284	897	946	19			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP E7NKU1
A	-17	GLY	-	expression tag	UNP E7NKU1
A	-16	SER	-	expression tag	UNP E7NKU1
A	-15	SER	-	expression tag	UNP E7NKU1
A	-14	HIS	-	expression tag	UNP E7NKU1
A	-13	HIS	-	expression tag	UNP E7NKU1
A	-12	HIS	-	expression tag	UNP E7NKU1
A	-11	HIS	-	expression tag	UNP E7NKU1
A	-10	HIS	-	expression tag	UNP E7NKU1
A	-9	HIS	-	expression tag	UNP E7NKU1
A	-8	SER	-	expression tag	UNP E7NKU1
A	-7	SER	-	expression tag	UNP E7NKU1
A	-6	GLY	-	expression tag	UNP E7NKU1
A	-5	LEU	-	expression tag	UNP E7NKU1
A	-4	VAL	-	expression tag	UNP E7NKU1
A	-3	PRO	-	expression tag	UNP E7NKU1
A	-2	ARG	-	expression tag	UNP E7NKU1
A	-1	GLY	-	expression tag	UNP E7NKU1
A	0	SER	-	expression tag	UNP E7NKU1
A	589	ALA	ARG	engineered mutation	UNP E7NKU1
A	592	ALA	ARG	engineered mutation	UNP E7NKU1

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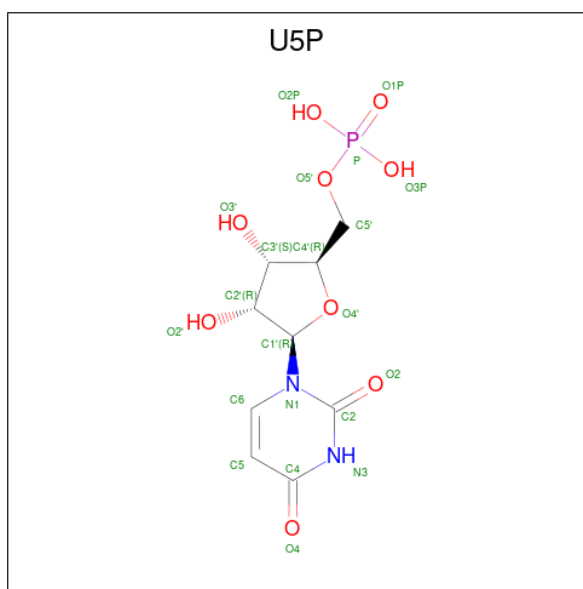
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP E7NKU1
B	-17	GLY	-	expression tag	UNP E7NKU1
B	-16	SER	-	expression tag	UNP E7NKU1
B	-15	SER	-	expression tag	UNP E7NKU1
B	-14	HIS	-	expression tag	UNP E7NKU1
B	-13	HIS	-	expression tag	UNP E7NKU1
B	-12	HIS	-	expression tag	UNP E7NKU1
B	-11	HIS	-	expression tag	UNP E7NKU1
B	-10	HIS	-	expression tag	UNP E7NKU1
B	-9	HIS	-	expression tag	UNP E7NKU1
B	-8	SER	-	expression tag	UNP E7NKU1
B	-7	SER	-	expression tag	UNP E7NKU1
B	-6	GLY	-	expression tag	UNP E7NKU1
B	-5	LEU	-	expression tag	UNP E7NKU1
B	-4	VAL	-	expression tag	UNP E7NKU1
B	-3	PRO	-	expression tag	UNP E7NKU1
B	-2	ARG	-	expression tag	UNP E7NKU1
B	-1	GLY	-	expression tag	UNP E7NKU1
B	0	SER	-	expression tag	UNP E7NKU1
B	589	ALA	ARG	engineered mutation	UNP E7NKU1
B	592	ALA	ARG	engineered mutation	UNP E7NKU1
C	-18	MET	-	initiating methionine	UNP E7NKU1
C	-17	GLY	-	expression tag	UNP E7NKU1
C	-16	SER	-	expression tag	UNP E7NKU1
C	-15	SER	-	expression tag	UNP E7NKU1
C	-14	HIS	-	expression tag	UNP E7NKU1
C	-13	HIS	-	expression tag	UNP E7NKU1
C	-12	HIS	-	expression tag	UNP E7NKU1
C	-11	HIS	-	expression tag	UNP E7NKU1
C	-10	HIS	-	expression tag	UNP E7NKU1
C	-9	HIS	-	expression tag	UNP E7NKU1
C	-8	SER	-	expression tag	UNP E7NKU1
C	-7	SER	-	expression tag	UNP E7NKU1
C	-6	GLY	-	expression tag	UNP E7NKU1
C	-5	LEU	-	expression tag	UNP E7NKU1
C	-4	VAL	-	expression tag	UNP E7NKU1
C	-3	PRO	-	expression tag	UNP E7NKU1
C	-2	ARG	-	expression tag	UNP E7NKU1
C	-1	GLY	-	expression tag	UNP E7NKU1
C	0	SER	-	expression tag	UNP E7NKU1
C	589	ALA	ARG	engineered mutation	UNP E7NKU1
C	592	ALA	ARG	engineered mutation	UNP E7NKU1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-18	MET	-	initiating methionine	UNP E7NKU1
D	-17	GLY	-	expression tag	UNP E7NKU1
D	-16	SER	-	expression tag	UNP E7NKU1
D	-15	SER	-	expression tag	UNP E7NKU1
D	-14	HIS	-	expression tag	UNP E7NKU1
D	-13	HIS	-	expression tag	UNP E7NKU1
D	-12	HIS	-	expression tag	UNP E7NKU1
D	-11	HIS	-	expression tag	UNP E7NKU1
D	-10	HIS	-	expression tag	UNP E7NKU1
D	-9	HIS	-	expression tag	UNP E7NKU1
D	-8	SER	-	expression tag	UNP E7NKU1
D	-7	SER	-	expression tag	UNP E7NKU1
D	-6	GLY	-	expression tag	UNP E7NKU1
D	-5	LEU	-	expression tag	UNP E7NKU1
D	-4	VAL	-	expression tag	UNP E7NKU1
D	-3	PRO	-	expression tag	UNP E7NKU1
D	-2	ARG	-	expression tag	UNP E7NKU1
D	-1	GLY	-	expression tag	UNP E7NKU1
D	0	SER	-	expression tag	UNP E7NKU1
D	589	ALA	ARG	engineered mutation	UNP E7NKU1
D	592	ALA	ARG	engineered mutation	UNP E7NKU1

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: $C_9H_{13}N_2O_9P$).



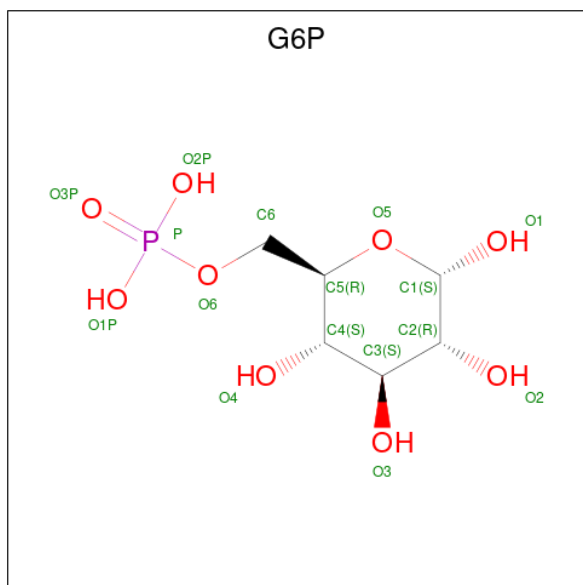
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

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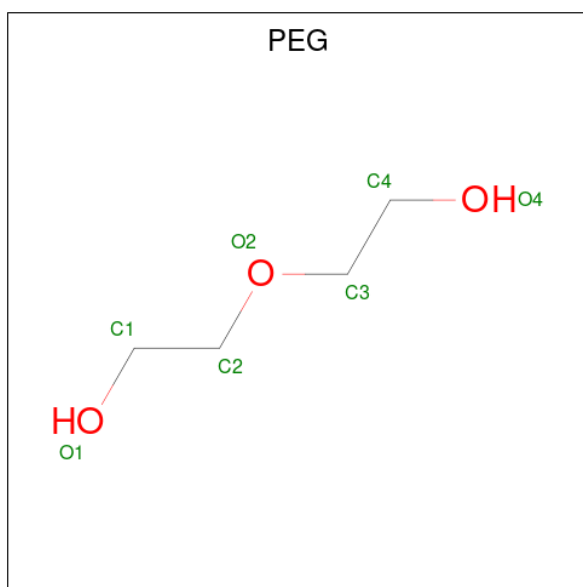
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

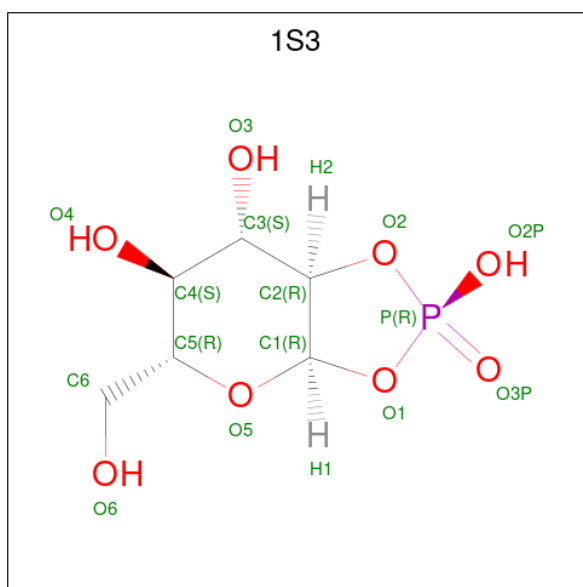


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is BARIUM ION (CCD ID: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ba	0	0
			2	2		
5	B	2	Total	Ba	0	0
			2	2		
5	C	1	Total	Ba	0	0
			1	1		
5	D	2	Total	Ba	0	0
			2	2		

- Molecule 6 is (2R,3aR,5R,6S,7S,7aR)-5-(hydroxymethyl)tetrahydro-3aH-[1,3,2]dioxaphospholo[4,5-b]pyran-2,6,7-triol 2-oxide (CCD ID: 1S3) (formula: C₆H₁₁O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	P	0	0
			15	6	8	1		

SER	G532	N446	F315	L213	Q77
PRO	F533	M447	F316	E214	H78
ASP	I541	D450	I317	D217	A79
LEU	Y552	L454	E322	V218	S85
ARG			K326	E221	G93
SER	R556	Q463			
ASN		L464	E333	R224	V103
SER	L568	F465	A334	I104	I103
THR		N466	L335	I227	L105
VAL	Y571	S467	A336	C232	V111
MET	M572		R337	I233	
THR		R471	L338		D121
PRO	T584	V472		V243	
GLY		R473			L125
ASP	R587	M474	K348		
LEU			K349	A252	
GLY	T590	P478	T350		I128
THR	E591			K260	P129
LEU		L481	I355		
GLN	S594	N482	V356	P263	I141
GLU	D595	A483		D264	
VAL	L596	N484	E367	G265	G144
ASN	L597	N485	A368		
ASN	D598	P486	L369	P268	F150
ALA	M599	A487	K370		
ASP	K600	L488	G371	L271	L157
ASP	R601		A373		D158
TYR	M602	D491	E374	I274	
PHE		Y492			A162
SER	V607	N493	L378	H280	I163
LEU		E494	E379	E281	
GLY	L612			F282	H166
VAL	A613	C499	I389	Q283	F167
ASN		H500	G390	N284	H168
PRO	F622	L501	K391	L285	
ALA		G502		H286	V174
ALA	N631	V503	N403	A287	A175
ASP		F504		L288	
ASP	M635	P505	L409	K289	L178
ASP	D636	S506			C179
ASP	A637	Y507	D412	I293	
ASP	L638			N294	R182
GLY	A639	F510	L416	D295	
PRO	GLY	M511	L417	F296	V186
TYR	GLY	G512		V297	V187
ALA	LYS	Y513	L425		T188
ASP	LYS	T514	K426	H302	I189
ASP	LEU		R427	G303	
SER	LYS	E517	R428	C304	L196
	VAL	C518	L429		
	ALA			F307	Y200
	ARG	V523	L430	D308	
PRO	PRO	F524	L432	L309	G205
LEU	SER	S525	R433	D310	SER
SER	VAL	T526	R434	N311	PHE
VAL	PRO	T527	P435	T312	D208
PRO	GLY	T528	H445	L313	
				Y314	C212

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	193.49Å 203.98Å 206.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 2.95 48.46 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.46-2.95) 99.7 (48.46-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.224 , 0.271 0.223 , 0.274	Depositor DCC
R_{free} test set	4240 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20806	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1S3, U5P, PEG, G6P, BA

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	0.47	0/5270	0.90	4/7141 (0.1%)
1	B	0.60	1/5298 (0.0%)	0.96	7/7180 (0.1%)
1	C	0.47	0/5279	0.86	2/7153 (0.0%)
1	D	0.57	3/5269 (0.1%)	0.93	3/7138 (0.0%)
All	All	0.53	4/21116 (0.0%)	0.91	16/28612 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	371	GLY	C-O	6.42	1.32	1.23
1	D	431	ALA	N-CA	5.40	1.53	1.46
1	B	296	PHE	CA-CB	5.35	1.61	1.53
1	D	485	ASN	CA-C	5.22	1.59	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	VAL	N-CA-C	-7.63	105.72	111.90
1	A	485	ASN	CA-C-N	7.21	126.92	119.56
1	A	485	ASN	C-N-CA	7.21	126.92	119.56
1	D	487	ILE	N-CA-C	7.20	118.00	111.81
1	B	517	GLU	N-CA-C	-6.26	104.37	111.07
1	C	509	GLU	CA-C-N	5.92	125.39	119.24
1	C	509	GLU	C-N-CA	5.92	125.39	119.24
1	D	502	GLY	N-CA-C	-5.77	104.70	112.14
1	B	493	ASP	N-CA-C	-5.46	105.33	111.28
1	B	440	PRO	CA-C-N	5.42	125.33	119.85
1	B	440	PRO	C-N-CA	5.42	125.33	119.85
1	A	491	ASP	N-CA-C	-5.28	102.67	110.48
1	B	576	VAL	CB-CA-C	-5.24	105.06	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	GLY	N-CA-C	5.24	117.66	110.69
1	A	543	THR	N-CA-C	5.21	116.96	111.28
1	D	485	ASN	N-CA-C	5.03	115.76	109.57

There are no chirality outliers.

There are no planarity outliers.

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	5145	0	5054	98	0
1	B	5163	0	5075	115	0
1	C	5154	0	5061	112	0
1	D	5146	0	5051	125	0
2	A	21	0	11	0	0
2	B	21	0	11	0	0
2	C	21	0	11	0	0
2	D	21	0	11	0	0
3	A	16	0	11	2	0
3	B	16	0	11	1	0
3	C	16	0	11	3	0
3	D	16	0	11	1	0
4	A	7	0	10	0	0
4	B	7	0	10	0	0
4	C	7	0	10	3	0
4	D	7	0	10	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	C	15	0	11	1	0
All	All	20806	0	20380	438	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 11.

All (438) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ALA:HB2	1:A:462:VAL:HG11	1.32	1.08
1:D:428:ARG:HH11	1:D:428:ARG:HG2	0.86	1.00
1:A:336:ALA:HB2	1:A:462:VAL:CG1	1.92	0.98
1:D:428:ARG:HH11	1:D:428:ARG:CG	1.78	0.96
1:D:428:ARG:HG2	1:D:428:ARG:NH1	1.65	0.95
1:B:471:ARG:HH11	1:B:471:ARG:HG2	1.30	0.93
1:A:283:GLN:HG2	1:D:280:HIS:CE1	2.07	0.90
1:C:336:ALA:HB2	1:C:462:VAL:HG11	1.54	0.88
1:C:391:LYS:HZ3	4:C:804:PEG:H22	1.40	0.85
1:A:336:ALA:CB	1:A:462:VAL:CG1	2.56	0.83
1:B:439:LEU:HD22	1:B:467:SER:HA	1.60	0.83
1:B:445[B]:HIS:ND1	1:B:478:PRO:HD2	1.93	0.83
1:B:445[A]:HIS:ND1	1:B:478:PRO:HD2	1.93	0.82
1:D:482:ASN:HD22	1:D:484:ASN:H	1.24	0.82
1:A:283:GLN:HG2	1:D:280:HIS:HE1	1.42	0.82
1:C:312:THR:HG22	1:C:350:THR:HB	1.59	0.81
1:A:323:TYR:OH	1:A:458:LYS:HG3	1.83	0.79
1:B:180:ARG:HG3	1:B:180:ARG:HH11	1.48	0.78
1:D:3:ARG:NH2	1:D:158:ASP:O	2.17	0.77
1:C:493:ASP:HB2	1:C:521:MET:HE1	1.66	0.76
1:C:330:MET:HG3	1:C:565:VAL:HG22	1.65	0.76
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.21	0.76
1:B:503:VAL:HG22	1:B:526:ILE:HD12	1.67	0.75
1:C:336:ALA:HB2	1:C:462:VAL:CG1	2.16	0.75
1:D:429:ILE:HA	1:D:432:LEU:HD12	1.67	0.75
1:D:74:ARG:N	1:D:75:PRO:HD2	2.01	0.74
1:D:482:ASN:ND2	1:D:484:ASN:H	1.86	0.72
1:A:299:GLY:HA2	1:A:375:VAL:HG21	1.69	0.72
1:A:369:LEU:HB3	1:C:369:LEU:HD22	1.72	0.72
1:A:501:LEU:HD21	1:A:526:ILE:HD12	1.71	0.71
1:A:177:PRO:HA	1:A:240:SER:OG	1.90	0.70
1:D:221:GLU:OE2	1:D:224:ARG:NH1	2.24	0.70
1:C:32:ALA:O	1:C:36:VAL:HG23	1.90	0.70
1:A:510:PRO:O	1:A:532:GLY:HA3	1.91	0.70
1:B:74:ARG:N	1:B:75:PRO:HD2	2.07	0.69
1:C:307:PHE:HD2	1:C:312:THR:HG21	1.56	0.69
1:D:471:ARG:HA	1:D:471:ARG:NE	2.06	0.69
1:B:367:GLU:O	1:B:369:LEU:N	2.24	0.69
1:D:471:ARG:HA	1:D:471:ARG:HE	1.59	0.68
1:C:163:ILE:HB	1:C:186:VAL:HG12	1.76	0.68
1:D:526:ILE:HG21	1:D:568:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:HIS:HD2	1:B:247:VAL:HG11	1.59	0.67
1:B:463:GLN:CG	1:B:465:PHE:HE2	2.07	0.67
1:D:309:LEU:C	1:D:311:ASN:H	2.03	0.67
1:D:481:LEU:O	1:D:482:ASN:HB2	1.94	0.67
1:B:514:THR:HB	1:B:515:PRO:CD	2.25	0.67
1:A:283:GLN:HG3	3:A:802:G6P:O1	1.95	0.66
1:D:511:TRP:HA	1:D:532:GLY:HA3	1.78	0.66
1:B:463:GLN:HG2	1:B:465:PHE:HE2	1.61	0.66
1:C:583:ARG:NH1	3:C:803:G6P:O1P	2.29	0.65
1:A:463:GLN:HG2	1:A:465:PHE:HE1	1.62	0.65
1:C:50:ASN:O	1:C:54:TYR:HB3	1.96	0.65
1:B:471:ARG:HG2	1:B:471:ARG:NH1	2.04	0.65
1:B:8:HIS:HB2	1:B:162:ALA:O	1.98	0.64
1:D:283:GLN:HG3	3:D:802:G6P:O1	1.97	0.64
1:D:485:ASN:OD1	1:D:488:LEU:N	2.26	0.64
1:C:527:THR:O	1:C:553:ILE:HA	1.98	0.64
1:B:370:LYS:O	1:B:371:GLY:C	2.39	0.64
1:B:180:ARG:HG3	1:B:180:ARG:NH1	2.05	0.63
1:C:217:ASP:HB3	1:C:220:HIS:HB2	1.78	0.63
1:D:463:GLN:HA	1:D:465:PHE:CE2	2.32	0.63
1:C:336:ALA:CB	1:C:462:VAL:CG1	2.76	0.63
1:B:180:ARG:HH11	1:B:180:ARG:CG	2.12	0.62
1:B:580:ARG:O	1:B:584:ILE:HG13	1.99	0.62
1:A:503:VAL:HG11	1:A:572:MET:HE3	1.82	0.62
1:A:580:ARG:HA	1:A:583:ARG:NH1	2.14	0.62
1:C:510:PRO:O	1:C:532:GLY:HA3	1.99	0.62
1:A:586:GLN:O	1:A:590:THR:HG22	2.00	0.62
1:B:482:ASN:O	1:B:484:ASN:N	2.30	0.61
1:C:307:PHE:CD2	1:C:312:THR:HG21	2.35	0.61
1:D:378:LEU:HA	1:D:428:ARG:HG3	1.81	0.61
1:C:16:GLU:HG2	1:C:22:GLY:H	1.65	0.61
1:A:357:MET:O	1:A:478:PRO:HA	1.99	0.61
1:B:6:GLN:HE21	1:B:625:LEU:HD23	1.66	0.61
1:C:458:LYS:O	1:C:462:VAL:HG23	2.01	0.60
1:A:144:GLY:HA3	1:A:174:VAL:HB	1.81	0.60
1:B:128:ILE:HG12	1:B:232:CYS:HB3	1.82	0.60
1:B:302:HIS:HD1	1:B:302:HIS:C	2.08	0.60
1:C:201:LEU:HB3	1:C:207:PHE:HE1	1.67	0.60
1:A:372:GLN:HE21	1:A:376:ARG:HH21	1.49	0.60
1:D:141:ILE:HA	1:D:174:VAL:HG11	1.84	0.60
1:A:264:ASP:OD1	1:A:616:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.01	0.59
1:A:587:ARG:HA	1:A:590:THR:HG23	1.84	0.59
1:B:482:ASN:C	1:B:484:ASN:H	2.10	0.59
1:B:330:MET:HE2	1:B:505:PRO:HB2	1.84	0.58
1:D:485:ASN:OD1	1:D:487:ILE:N	2.36	0.58
1:A:443:VAL:HG13	1:A:456:LEU:HD21	1.85	0.58
1:D:507:TYR:HB2	1:D:556:ARG:NH2	2.19	0.58
1:C:396:HIS:NE2	1:C:405:LEU:HD12	2.19	0.58
1:D:599:TRP:C	1:D:601:ARG:H	2.11	0.58
1:D:599:TRP:HA	1:D:599:TRP:CE3	2.38	0.58
1:C:61:LEU:HB2	1:C:93:GLY:HA2	1.85	0.58
1:B:213:LEU:HD21	1:B:253:PHE:CE1	2.39	0.58
1:C:322:GLU:HB3	1:C:325:ASN:HB2	1.86	0.57
1:D:335:LEU:HD22	1:D:472:VAL:HG11	1.87	0.57
1:A:283:GLN:NE2	1:A:588:ASN:OD1	2.38	0.57
1:A:336:ALA:CB	1:A:462:VAL:HG11	2.16	0.57
1:C:400:TYR:CD2	1:C:408:GLU:HA	2.39	0.57
1:A:339:ASN:O	1:A:343:LYS:HG3	2.04	0.57
1:D:14:ALA:HB2	1:D:168:HIS:HB2	1.87	0.57
1:C:264:ASP:O	1:C:634:ASN:HB2	2.03	0.57
1:B:110:SER:O	1:B:111:VAL:HG13	2.05	0.57
1:B:502:GLY:O	1:B:525:SER:HA	2.05	0.57
1:C:619:PRO:O	1:C:623:ARG:HB2	2.05	0.57
1:A:319:GLY:HA3	1:A:326:LYS:HE3	1.87	0.56
1:B:193:HIS:HD2	1:B:247:VAL:CG1	2.17	0.56
1:A:505:PRO:HA	1:A:528:THR:HG23	1.87	0.56
1:B:295:ASP:OD1	1:B:295:ASP:C	2.48	0.56
1:B:193:HIS:CD2	1:B:247:VAL:HG11	2.40	0.56
1:B:467:SER:O	1:B:470:ASP:HB2	2.05	0.56
1:C:238:ALA:O	1:C:261:ARG:NH1	2.37	0.56
1:D:307:PHE:H	1:D:307:PHE:HD1	1.53	0.56
1:B:367:GLU:O	1:B:368:ALA:C	2.48	0.56
1:C:445:HIS:ND1	1:C:478:PRO:HD2	2.21	0.56
1:D:349:LYS:O	1:D:471:ARG:HD3	2.06	0.56
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.88	0.56
1:C:4:ASP:OD2	1:C:7:ASN:HB3	2.06	0.55
1:A:336:ALA:CB	1:A:462:VAL:HG13	2.36	0.55
1:D:428:ARG:CG	1:D:428:ARG:NH1	2.49	0.55
1:B:395:ASP:O	1:B:398:ILE:HG22	2.07	0.55
1:C:391:LYS:NZ	4:C:804:PEG:H22	2.17	0.55
1:C:239:HIS:NE2	1:C:259:LEU:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:HIS:CE1	1:C:261:ARG:HB2	2.42	0.55
1:B:213:LEU:HD21	1:B:253:PHE:HE1	1.72	0.55
1:A:236:ALA:O	1:A:240:SER:HB2	2.07	0.55
1:B:357:MET:O	1:B:478:PRO:HA	2.06	0.55
1:D:503:VAL:O	1:D:505:PRO:HD3	2.07	0.54
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.37	0.54
1:D:374[B]:GLU:O	1:D:374[B]:GLU:CD	2.51	0.54
1:D:631:ASN:HB3	1:D:637:ALA:HB1	1.89	0.54
1:A:587:ARG:HA	1:A:590:THR:CG2	2.38	0.54
1:D:61:LEU:HB2	1:D:93:GLY:HA2	1.90	0.54
1:C:308:ASP:O	1:C:312:THR:HG23	2.08	0.54
1:C:443:VAL:HG22	1:C:445:HIS:H	1.73	0.54
1:D:314:TYR:O	1:D:315:PHE:HD1	1.91	0.54
1:A:327:GLY:HA3	1:A:505:PRO:O	2.08	0.53
1:C:264:ASP:CG	1:C:616:ARG:HH12	2.15	0.53
1:C:396:HIS:CD2	1:C:405:LEU:HD12	2.44	0.53
1:D:315:PHE:HE2	1:D:572:MET:HG2	1.74	0.53
1:D:283:GLN:HE21	1:D:584:ILE:HG23	1.72	0.53
1:C:225:PHE:O	1:C:227:ILE:HG12	2.08	0.53
1:D:333:GLU:OE2	1:D:337:ARG:NH1	2.39	0.53
1:C:560:ALA:C	1:C:562:ASP:H	2.15	0.53
4:C:804:PEG:H31	1:D:379:GLU:HG3	1.90	0.53
1:C:526:ILE:HG12	1:C:552:TYR:HB2	1.91	0.53
1:A:300:HIS:HD2	1:A:301:PHE:CE1	2.27	0.53
1:B:344:VAL:C	1:B:346:GLY:H	2.16	0.53
1:D:217:ASP:O	1:D:221:GLU:HG2	2.08	0.53
1:D:187:VAL:HG11	1:D:613:ALA:O	2.08	0.52
1:D:309:LEU:O	1:D:311:ASN:N	2.39	0.52
1:D:591:GLU:O	1:D:594:SER:HB3	2.09	0.52
1:A:264:ASP:CG	1:A:616:ARG:HH12	2.18	0.52
1:A:565:VAL:O	1:A:569:VAL:HG23	2.08	0.52
1:B:385:VAL:HG21	1:B:425:LEU:HD11	1.92	0.52
1:C:336:ALA:CB	1:C:462:VAL:HG13	2.38	0.52
1:D:74:ARG:N	1:D:75:PRO:CD	2.72	0.52
1:D:370:LYS:O	1:D:371:GLY:C	2.53	0.52
1:A:95:TRP:HB3	1:A:101:PRO:HD2	1.91	0.52
1:B:39:TYR:HB2	1:B:43:TYR:HB2	1.92	0.52
1:C:141:ILE:HA	1:C:174:VAL:HG11	1.92	0.52
1:B:607:VAL:HG23	1:B:610:ARG:HH21	1.75	0.52
1:B:80:LEU:HD22	1:B:90:PHE:CE2	2.45	0.51
1:A:141:ILE:HA	1:A:174:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LEU:HB3	1:C:207:PHE:CE1	2.44	0.51
1:D:482:ASN:HD22	1:D:484:ASN:N	2.01	0.51
1:A:366:VAL:O	1:A:370:LYS:HB2	2.11	0.51
1:B:456:LEU:O	1:B:458:LYS:N	2.43	0.51
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.45	0.51
1:D:282:PHE:CD2	1:D:591:GLU:HG3	2.46	0.51
1:B:31:LYS:HE2	1:B:606:TYR:CE2	2.45	0.51
1:C:283:GLN:HB3	3:C:803:G6P:O1	2.11	0.51
1:A:304:CYS:HB2	1:A:434:ARG:HD3	1.93	0.51
1:B:302:HIS:C	1:B:302:HIS:ND1	2.69	0.51
1:A:239:HIS:CE1	1:A:259:LEU:O	2.64	0.51
1:A:29:LYS:HG3	1:A:97:ILE:HD13	1.93	0.51
1:A:302:HIS:HB2	1:A:432:LEU:HD22	1.92	0.50
1:B:290:LYS:O	1:B:290:LYS:HG2	2.10	0.50
1:C:176:LEU:HB2	1:C:177:PRO:HD3	1.93	0.50
1:D:289:LYS:HE3	1:D:494:GLU:HG2	1.93	0.50
1:A:19:ASN:H	1:A:19:ASN:HD22	1.60	0.50
1:A:509:GLU:OE2	1:A:531:SER:HB2	2.11	0.50
1:B:513:TYR:CD1	1:B:513:TYR:N	2.79	0.50
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.46	0.50
1:D:63:TRP:H	1:D:63:TRP:CD1	2.29	0.50
1:B:286:HIS:HD2	1:B:587:ARG:NH2	2.10	0.50
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.94	0.50
1:B:94:ARG:HD3	1:B:100:ALA:HB1	1.94	0.49
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.93	0.49
1:D:282:PHE:CE2	1:D:591:GLU:HG3	2.47	0.49
1:B:315:PHE:CD2	1:B:351:VAL:HG11	2.46	0.49
1:C:512:GLY:O	1:C:515:PRO:HD2	2.12	0.49
1:B:193:HIS:CD2	1:B:247:VAL:CG1	2.96	0.49
1:D:302:HIS:O	1:D:434:ARG:HD2	2.12	0.49
1:D:19:ASN:HD22	1:D:19:ASN:N	2.11	0.49
1:C:16:GLU:HB3	1:C:25:TYR:HB2	1.95	0.49
1:A:128:ILE:HG12	1:A:232:CYS:HB3	1.93	0.49
1:A:283:GLN:CG	1:D:280:HIS:CE1	2.89	0.49
1:A:399:ARG:HD3	1:A:403:ASN:OD1	2.13	0.49
1:A:450:ASP:CG	1:A:460:ARG:HH22	2.20	0.49
1:B:17:VAL:C	1:B:19:ASN:H	2.21	0.49
1:C:128:ILE:HG12	1:C:232:CYS:HB3	1.95	0.49
1:D:309:LEU:HA	1:D:312:THR:OG1	2.12	0.49
1:B:513:TYR:H	1:B:513:TYR:HD1	1.61	0.49
1:D:178:LEU:O	1:D:182:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:HIS:O	1:D:287:ALA:C	2.55	0.49
1:A:314:TYR:CD1	1:A:354:PHE:HE2	2.31	0.49
1:D:315:PHE:CE2	1:D:572:MET:HG2	2.48	0.49
1:B:500:HIS:O	1:B:524:PRO:HD2	2.12	0.48
1:C:580:ARG:NE	3:C:803:G6P:O1P	2.40	0.48
1:D:513:TYR:CD1	1:D:513:TYR:N	2.81	0.48
1:D:596:LEU:HA	1:D:601:ARG:HD3	1.95	0.48
1:A:518:CYS:SG	1:A:523:VAL:HB	2.53	0.48
1:D:121:ASP:O	1:D:125:LEU:HB2	2.13	0.48
1:D:144:GLY:HA3	1:D:174:VAL:HB	1.95	0.48
1:A:403:ASN:N	1:A:403:ASN:ND2	2.60	0.48
1:D:31:LYS:O	1:D:34:ILE:HG22	2.14	0.48
1:D:587:ARG:HA	1:D:590:THR:HG22	1.95	0.48
1:A:61:LEU:HB2	1:A:93:GLY:HA2	1.95	0.48
1:A:628:GLU:HG3	1:A:630:LEU:HD23	1.95	0.48
1:C:65:LYS:HE2	1:C:67:GLU:HB3	1.96	0.48
1:D:612:LEU:HG	1:D:612:LEU:O	2.13	0.48
1:C:56:ASN:H	1:C:56:ASN:ND2	2.10	0.48
1:D:283:GLN:NE2	1:D:584:ILE:HG23	2.29	0.48
1:A:294:ASN:O	1:A:295:ASP:C	2.56	0.47
1:B:150:PHE:O	1:B:154:VAL:HG23	2.14	0.47
1:B:514:THR:HB	1:B:515:PRO:HD2	1.96	0.47
1:C:16:GLU:HG3	1:C:21:VAL:HB	1.96	0.47
1:D:309:LEU:C	1:D:311:ASN:N	2.70	0.47
1:A:440:PRO:O	1:A:441:PRO:O	2.32	0.47
1:B:11:PHE:HD1	1:B:46:ILE:HD11	1.79	0.47
1:D:374[A]:GLU:HG2	1:D:431:ALA:HB1	1.95	0.47
1:D:425:LEU:O	1:D:429:ILE:HG13	2.14	0.47
1:B:463:GLN:CG	1:B:465:PHE:CE2	2.94	0.47
1:B:306:ASP:OD2	1:B:468:PRO:HB3	2.15	0.47
1:D:39:TYR:HB2	1:D:43:TYR:HB2	1.95	0.47
1:D:268:PRO:HB2	1:D:602:MET:CE	2.45	0.47
1:B:82:THR:O	1:B:85:SER:HB2	2.15	0.47
1:C:74:ARG:N	1:C:75:PRO:HD2	2.29	0.47
1:C:145:TYR:O	1:C:149:TRP:HB2	2.15	0.47
1:C:374:GLU:HB3	1:C:432:LEU:HD23	1.97	0.47
1:D:12:GLU:HG3	1:D:166:HIS:HB3	1.97	0.47
1:D:510:PRO:O	1:D:532:GLY:HA3	2.15	0.47
1:C:306:ASP:HA	1:D:403:ASN:HD21	1.80	0.47
1:D:503:VAL:HG11	1:D:572:MET:HE3	1.97	0.47
1:D:513:TYR:O	1:D:517:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ALA:HB2	3:A:802:G6P:H2	1.97	0.47
1:C:336:ALA:HB1	1:C:462:VAL:HG13	1.96	0.46
1:C:458:LYS:HE2	1:C:462:VAL:CG2	2.44	0.46
1:C:28:LEU:HD22	1:C:45:LEU:HD21	1.98	0.46
1:C:184:ILE:HG22	1:C:185:ASP:H	1.81	0.46
1:C:580:ARG:O	1:C:581:ARG:C	2.59	0.46
1:D:79:ALA:HB2	1:D:157:LEU:HD12	1.98	0.46
1:A:409:LEU:HD12	1:B:426:LYS:HE3	1.97	0.46
1:B:385:VAL:O	1:B:387:THR:N	2.49	0.46
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.51	0.46
1:C:176:LEU:HD22	1:C:241:ALA:HB2	1.98	0.46
1:C:483:ALA:N	1:C:491:ASP:OD1	2.38	0.46
1:D:533:PHE:CD1	1:D:533:PHE:C	2.94	0.46
1:A:150:PHE:O	1:A:154:VAL:HG23	2.16	0.46
1:D:428:ARG:HA	1:D:428:ARG:HD3	1.57	0.46
1:A:60:ILE:HD12	1:A:60:ILE:H	1.81	0.46
1:B:286:HIS:CD2	1:B:587:ARG:CZ	2.99	0.46
1:B:39:TYR:HB3	1:B:42:HIS:HB2	1.98	0.45
1:C:170:TRP:HB3	1:C:234:GLU:HG3	1.96	0.45
1:C:307:PHE:HD2	1:C:312:THR:CG2	2.26	0.45
1:D:463:GLN:HA	1:D:465:PHE:HE2	1.79	0.45
1:D:501:LEU:HD21	1:D:526:ILE:CD1	2.46	0.45
1:D:528:THR:HG21	1:D:556:ARG:HG3	1.96	0.45
1:D:47:GLY:O	1:D:105:LEU:HA	2.17	0.45
1:D:471:ARG:HE	1:D:471:ARG:CA	2.29	0.45
1:D:227:ILE:O	1:D:227:ILE:HG22	2.16	0.45
1:A:195:THR:OG1	1:A:254:GLU:OE1	2.34	0.45
1:D:501:LEU:HD21	1:D:526:ILE:HD12	1.99	0.45
1:D:599:TRP:HA	1:D:599:TRP:HE3	1.79	0.45
1:A:213:LEU:O	1:A:216:VAL:HG22	2.17	0.45
1:A:471:ARG:NE	1:A:471:ARG:HA	2.30	0.45
1:B:11:PHE:CD1	1:B:46:ILE:HD11	2.51	0.45
1:C:320:ARG:NH2	1:C:322:GLU:OE1	2.49	0.45
1:B:210:TYR:CE1	1:B:250:ILE:HD11	2.51	0.45
1:B:305:PHE:HZ	1:B:309:LEU:HG	1.82	0.45
1:C:560:ALA:O	1:C:562:ASP:N	2.49	0.45
1:A:302:HIS:O	1:A:302:HIS:CG	2.70	0.45
1:B:267:LEU:HB3	1:B:606:TYR:CE1	2.51	0.45
1:C:330:MET:HE1	1:C:564:SER:HB3	1.98	0.45
1:C:400:TYR:CD1	1:C:400:TYR:C	2.95	0.45
1:D:523:VAL:HA	1:D:524:PRO:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLY:O	1:B:105:LEU:HA	2.17	0.45
1:B:410:PRO:HG2	1:B:416:LEU:HD21	1.99	0.45
1:C:17:VAL:HG13	1:C:45:LEU:HD22	1.99	0.45
1:C:417:LEU:HD22	1:C:422:LYS:HG3	1.99	0.45
1:D:41:ASP:OD2	1:D:73:MET:HG3	2.17	0.45
1:C:386:THR:HG21	1:D:390:GLY:CA	2.47	0.44
1:C:634:ASN:ND2	1:C:637:ALA:H	2.15	0.44
1:A:386:THR:HG21	1:B:390:GLY:CA	2.47	0.44
1:B:32:ALA:O	1:B:33:PRO:C	2.60	0.44
1:C:191:THR:HA	1:C:245:THR:O	2.17	0.44
1:D:482:ASN:ND2	1:D:484:ASN:HB2	2.32	0.44
1:B:491:ASP:OD1	1:D:427:ARG:NH2	2.33	0.44
1:C:65:LYS:HA	1:C:66:PRO:HD3	1.88	0.44
1:C:366:VAL:O	1:C:370:LYS:HB2	2.17	0.44
1:D:265:GLY:HA3	1:D:635:MET:HE2	1.99	0.44
1:B:482:ASN:C	1:B:484:ASN:N	2.74	0.44
1:A:25:TYR:CE2	1:A:95:TRP:HZ2	2.35	0.44
1:A:386:THR:HA	1:A:389:ILE:HD12	1.99	0.44
1:B:286:HIS:CD2	1:B:587:ARG:NH2	2.86	0.44
1:D:474:MET:HE3	1:D:474:MET:HB3	1.55	0.44
1:A:51:LYS:HA	1:A:54:TYR:CD1	2.53	0.44
1:A:176:LEU:HB2	1:A:177:PRO:HD3	1.99	0.44
1:A:447:MET:HB2	1:A:450:ASP:HB2	2.00	0.44
1:C:114:TYR:O	1:C:117:GLU:HG2	2.18	0.44
1:C:396:HIS:HE1	1:C:407:THR:O	2.01	0.44
1:A:322:GLU:HG2	1:A:325:ASN:HB2	1.99	0.44
1:D:144:GLY:O	1:D:175:ALA:HB2	2.17	0.44
1:D:434:ARG:HB2	1:D:435:PRO:HD2	2.00	0.44
1:B:385:VAL:O	1:B:386:THR:C	2.59	0.44
1:D:285:LEU:HD23	1:D:285:LEU:HA	1.78	0.44
1:B:340:TYR:O	1:B:341:ARG:C	2.59	0.44
1:C:518:CYS:SG	1:C:523:VAL:HB	2.58	0.43
1:A:527:THR:O	1:A:553:ILE:HA	2.18	0.43
1:A:386:THR:HG21	1:B:390:GLY:HA2	2.00	0.43
1:A:549:TYR:HD2	1:A:593:LEU:HG	1.82	0.43
1:B:80:LEU:HB3	1:B:90:PHE:CZ	2.53	0.43
1:C:511:TRP:HB3	6:C:801:1S3:O4	2.18	0.43
1:D:32:ALA:HB3	1:D:33:PRO:HD3	2.01	0.43
1:D:367:GLU:OE1	1:D:367:GLU:HA	2.18	0.43
1:A:410:PRO:HG2	1:A:416:LEU:HD21	1.99	0.43
1:B:114:TYR:N	1:B:114:TYR:CD1	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:HIS:CD2	1:B:371:GLY:HA2	2.53	0.43
1:D:599:TRP:C	1:D:601:ARG:N	2.76	0.43
1:B:283:GLN:O	1:B:286:HIS:HB3	2.19	0.43
1:C:494:GLU:O	1:C:495:PHE:C	2.61	0.43
1:D:293:ILE:O	1:D:297:VAL:HG23	2.19	0.43
1:D:317:ILE:HG22	1:D:355:ILE:HA	1.99	0.43
1:B:76:VAL:O	1:B:80:LEU:HG	2.18	0.43
1:C:372[A]:GLN:HE21	1:C:372[A]:GLN:HB3	1.67	0.43
1:D:447:MET:HE3	1:D:447:MET:HB3	1.97	0.43
1:A:634:ASN:HB2	1:A:637:ALA:H	1.84	0.43
1:B:256:GLU:O	1:B:260:LYS:HA	2.17	0.43
1:C:507:TYR:HB2	1:C:556:ARG:NH2	2.34	0.43
1:D:445:HIS:ND1	1:D:478:PRO:HD2	2.33	0.43
1:B:596:LEU:HA	1:B:601:ARG:HD3	2.00	0.42
1:C:17:VAL:HG21	1:C:47:GLY:HA3	2.01	0.42
1:D:338:LEU:HD22	1:D:572:MET:HB3	2.00	0.42
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.51	0.42
1:B:355:ILE:CD1	1:B:474:MET:HE1	2.49	0.42
1:D:189:ILE:HG23	1:D:243:VAL:HB	2.01	0.42
1:C:455:ILE:O	1:C:459:ILE:HG13	2.19	0.42
1:C:526:ILE:HG12	1:C:552:TYR:CB	2.49	0.42
1:C:580:ARG:O	1:C:584:ILE:HG13	2.19	0.42
1:D:294:ASN:O	1:D:295:ASP:C	2.62	0.42
1:A:467:SER:O	1:A:469:SER:N	2.53	0.42
1:B:459:ILE:CD1	1:B:474:MET:HE2	2.49	0.42
1:C:227:ILE:HG23	1:C:230:ARG:HD2	2.00	0.42
1:D:335:LEU:HD22	1:D:472:VAL:CG1	2.47	0.42
1:B:291:GLU:O	1:B:294:ASN:HB2	2.19	0.42
1:C:492:TYR:O	1:C:496:VAL:HG23	2.19	0.42
1:D:389:ILE:HG23	1:D:416:LEU:HD13	2.02	0.42
1:A:273:VAL:HG13	1:A:520:VAL:HG13	2.01	0.42
1:B:39:TYR:O	1:B:41:ASP:N	2.52	0.42
1:C:89:HIS:O	1:C:107:ASP:HB3	2.20	0.42
1:C:242:ASP:OD1	1:C:242:ASP:N	2.53	0.42
1:A:250:ILE:HD12	1:A:250:ILE:HA	1.80	0.42
1:B:290:LYS:NZ	3:B:802:G6P:O3P	2.50	0.42
1:B:514:THR:HB	1:B:515:PRO:HD3	2.00	0.42
1:C:174:VAL:HG22	1:C:233:ILE:HG21	2.01	0.42
1:C:289:LYS:HG3	1:C:494:GLU:HB3	2.01	0.42
1:C:396:HIS:HD2	1:C:415:GLU:OE2	2.02	0.42
1:C:549:TYR:HD2	1:C:593:LEU:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ALA:HB1	1:D:263:PRO:HG2	2.01	0.42
1:D:552:TYR:HB3	1:D:571:TYR:CD2	2.55	0.42
1:A:463:GLN:HA	1:A:465:PHE:CE1	2.55	0.42
1:C:195:THR:OG1	1:C:254:GLU:OE2	2.30	0.42
1:A:198:GLY:HA2	1:A:209:PHE:CE2	2.54	0.42
1:A:262:LYS:HA	1:A:263:PRO:HD3	1.88	0.42
1:B:119:LYS:HE2	1:B:132:GLU:OE2	2.20	0.42
1:B:296:PHE:HA	1:B:372[B]:GLN:NE2	2.35	0.42
1:B:456:LEU:C	1:B:458:LYS:N	2.77	0.42
1:D:75:PRO:CB	1:D:158:ASP:HB2	2.50	0.42
1:A:351:VAL:O	1:A:351:VAL:HG12	2.20	0.42
1:A:523:VAL:HA	1:A:524:PRO:HD3	1.93	0.42
1:C:417:LEU:HD23	1:C:421:ASP:HB2	2.01	0.42
1:B:61:LEU:HB2	1:B:93:GLY:HA2	2.01	0.41
1:B:599:TRP:HA	1:B:599:TRP:CE3	2.55	0.41
1:C:526:ILE:HG21	1:C:568:LEU:CD1	2.51	0.41
1:A:19:ASN:H	1:A:19:ASN:ND2	2.19	0.41
1:B:252:ALA:HA	1:B:263:PRO:HG2	2.02	0.41
1:B:400:TYR:CD2	1:B:401:PRO:HA	2.55	0.41
1:D:78:HIS:HB2	1:D:157:LEU:HD13	2.02	0.41
1:A:238:ALA:O	1:A:261:ARG:NH1	2.52	0.41
1:A:403:ASN:N	1:A:403:ASN:HD22	2.17	0.41
1:C:428:ARG:HA	1:C:428:ARG:HD3	1.70	0.41
1:A:247:VAL:O	1:A:268:PRO:HA	2.21	0.41
1:B:114:TYR:N	1:B:114:TYR:HD1	2.18	0.41
1:D:369:LEU:HD23	1:D:487:ILE:HG23	2.03	0.41
1:B:375:VAL:O	1:B:375:VAL:CG1	2.69	0.41
1:C:92:TYR:HD1	1:C:104:ILE:HG12	1.85	0.41
1:C:480:PHE:HD1	1:C:480:PHE:HA	1.80	0.41
1:A:115:SER:O	1:A:119:LYS:HG3	2.20	0.41
1:A:455:ILE:O	1:A:459:ILE:HG13	2.20	0.41
1:D:491:ASP:O	1:D:492:TYR:C	2.63	0.41
1:B:337:ARG:HH11	1:B:337:ARG:HD2	1.75	0.41
1:D:527:THR:OG1	1:D:528:THR:N	2.54	0.41
1:A:10:LEU:HD13	1:A:610:ARG:HD3	2.02	0.41
1:A:125:LEU:HD22	1:A:181:LYS:HG2	2.03	0.41
1:B:268:PRO:HB2	1:B:602:MET:HE1	2.03	0.41
1:B:483:ALA:HA	1:B:489:GLY:C	2.45	0.41
1:D:128:ILE:HA	1:D:129:PRO:HD2	1.98	0.41
1:D:174:VAL:HG22	1:D:233:ILE:HG21	2.03	0.41
1:A:30:SER:O	1:A:272:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:TYR:OH	1:B:458:LYS:HG2	2.20	0.41
1:B:367:GLU:C	1:B:369:LEU:N	2.78	0.41
1:B:483:ALA:HB2	1:B:491:ASP:N	2.36	0.41
1:C:269:ASN:HD22	1:C:511:TRP:CD1	2.38	0.41
1:D:196:LEU:O	1:D:200:TYR:HD2	2.04	0.41
1:A:357:MET:HA	1:A:358:PRO:HD3	1.93	0.40
1:B:74:ARG:N	1:B:75:PRO:CD	2.79	0.40
1:B:459:ILE:HD11	1:B:474:MET:HE2	2.02	0.40
1:B:471:ARG:NH1	1:B:471:ARG:CG	2.75	0.40
1:C:491:ASP:O	1:C:492:TYR:C	2.63	0.40
1:D:38:GLN:HB3	1:D:39:TYR:CD1	2.57	0.40
1:A:269:ASN:HB2	1:A:511:TRP:CD1	2.57	0.40
1:B:344:VAL:C	1:B:346:GLY:N	2.79	0.40
1:B:385:VAL:C	1:B:387:THR:N	2.79	0.40
1:B:439:LEU:HD22	1:B:467:SER:CA	2.40	0.40
1:C:74:ARG:NH1	1:C:77:GLN:OE1	2.54	0.40
1:C:425:LEU:HB3	1:D:409:LEU:HD21	2.04	0.40
1:C:560:ALA:C	1:C:562:ASP:N	2.79	0.40
1:A:491:ASP:O	1:A:492:TYR:C	2.65	0.40
1:A:606:TYR:HB3	1:A:610:ARG:NH2	2.37	0.40
1:B:137:THR:HG21	1:B:229:HIS:HD2	1.86	0.40
1:C:386:THR:HA	1:C:389:ILE:HD12	2.02	0.40
1:B:174:VAL:O	1:B:177:PRO:HD2	2.22	0.40
1:D:8:HIS:HB2	1:D:162:ALA:O	2.21	0.40
1:A:314:TYR:HD1	1:A:354:PHE:HE2	1.69	0.40
1:C:64:LYS:HG2	1:C:81:GLN:NE2	2.35	0.40
1:C:83:MET:HE1	1:C:149:TRP:HB3	2.04	0.40
1:C:289:LYS:O	1:C:292:LYS:HB2	2.21	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	636/724 (88%)	574 (90%)	53 (8%)	9 (1%)	9	24
1	B	639/724 (88%)	569 (89%)	59 (9%)	11 (2%)	7	20
1	C	637/724 (88%)	576 (90%)	52 (8%)	9 (1%)	9	24
1	D	634/724 (88%)	567 (89%)	57 (9%)	10 (2%)	7	21
All	All	2546/2896 (88%)	2286 (90%)	221 (9%)	39 (2%)	8	23

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	441	PRO
1	B	111	VAL
1	B	304	CYS
1	B	367	GLU
1	B	368	ALA
1	B	457	ASN
1	B	483	ALA
1	D	111	VAL
1	D	482	ASN
1	D	600	LYS
1	B	17	VAL
1	B	371	GLY
1	B	386	THR
1	C	6	GLN
1	C	17	VAL
1	D	310	ASP
1	D	311	ASN
1	D	601	ARG
1	A	419	SER
1	A	435	PRO
1	B	40	LYS
1	C	40	LYS
1	C	169	GLU
1	C	561	PRO
1	B	345	SER
1	C	115	SER
1	A	169	GLU
1	A	413	LEU
1	A	561	PRO
1	C	323	TYR
1	C	483	ALA
1	D	6	GLN

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Mol	Chain	Res	Type
1	D	499	CYS
1	C	75	PRO
1	A	273	VAL
1	D	512	GLY
1	A	33	PRO
1	D	371	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	551/622 (89%)	517 (94%)	34 (6%)	16	39
1	B	554/622 (89%)	511 (92%)	43 (8%)	11	30
1	C	552/622 (89%)	506 (92%)	46 (8%)	10	27
1	D	551/622 (89%)	502 (91%)	49 (9%)	9	24
All	All	2208/2488 (89%)	2036 (92%)	172 (8%)	11	30

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	35	THR
1	A	45	LEU
1	A	60	ILE
1	A	61	LEU
1	A	111	VAL
1	A	181	LYS
1	A	212	CYS
1	A	240	SER
1	A	250	ILE
1	A	272	ASN
1	A	283	GLN
1	A	304	CYS
1	A	310	ASP
1	A	317	ILE

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Mol	Chain	Res	Type
1	A	322	GLU
1	A	337	ARG
1	A	393	ILE
1	A	403	ASN
1	A	406	THR
1	A	420	SER
1	A	454	LEU
1	A	469	SER
1	A	471	ARG
1	A	479	GLU
1	A	485	ASN
1	A	521	MET
1	A	535	SER
1	A	541	ILE
1	A	553	ILE
1	A	556	ARG
1	A	581	ARG
1	A	590	THR
1	A	630	LEU
1	B	16	GLU
1	B	17	VAL
1	B	34	ILE
1	B	60	ILE
1	B	67	GLU
1	B	81	GLN
1	B	83	MET
1	B	97	ILE
1	B	111	VAL
1	B	114	TYR
1	B	126	VAL
1	B	136	GLU
1	B	151	LEU
1	B	180	ARG
1	B	181	LYS
1	B	192	THR
1	B	199	ARG
1	B	213	LEU
1	B	218	VAL
1	B	247	VAL
1	B	288	LEU
1	B	291	GLU
1	B	302	HIS

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Mol	Chain	Res	Type
1	B	337	ARG
1	B	370	LYS
1	B	376	ARG
1	B	381	THR
1	B	399	ARG
1	B	407	THR
1	B	423	VAL
1	B	458	LYS
1	B	469	SER
1	B	471	ARG
1	B	484	ASN
1	B	488	LEU
1	B	514	THR
1	B	518	CYS
1	B	525	SER
1	B	537	MET
1	B	556	ARG
1	B	570	ASP
1	B	601	ARG
1	B	607	VAL
1	C	9	LEU
1	C	15	THR
1	C	40	LYS
1	C	45	LEU
1	C	56	ASN
1	C	81	GLN
1	C	86	ARG
1	C	98	GLU
1	C	126	VAL
1	C	136	GLU
1	C	184	ILE
1	C	199	ARG
1	C	214	GLU
1	C	220	HIS
1	C	242	ASP
1	C	250	ILE
1	C	266	ILE
1	C	271	LEU
1	C	288	LEU
1	C	289	LYS
1	C	295	ASP
1	C	320	ARG

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Mol	Chain	Res	Type
1	C	366	VAL
1	C	369	LEU
1	C	370	LYS
1	C	376	ARG
1	C	387	THR
1	C	411	THR
1	C	412	ASP
1	C	417	LEU
1	C	419	SER
1	C	423	VAL
1	C	428	ARG
1	C	433	ARG
1	C	448	VAL
1	C	458	LYS
1	C	471	ARG
1	C	480	PHE
1	C	513	TYR
1	C	514	THR
1	C	537	MET
1	C	539	ASP
1	C	541	ILE
1	C	553	ILE
1	C	556	ARG
1	C	626	VAL
1	D	6	GLN
1	D	19	ASN
1	D	21	VAL
1	D	45	LEU
1	D	60	ILE
1	D	77	GLN
1	D	103	VAL
1	D	125	LEU
1	D	179	CYS
1	D	212	CYS
1	D	213	LEU
1	D	214	GLU
1	D	218	VAL
1	D	260	LYS
1	D	271	LEU
1	D	274	ILE
1	D	288	LEU
1	D	304	CYS

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Mol	Chain	Res	Type
1	D	322	GLU
1	D	326	LYS
1	D	337	ARG
1	D	348	LYS
1	D	350	THR
1	D	356	VAL
1	D	367	GLU
1	D	370	LYS
1	D	372[A]	GLN
1	D	372[B]	GLN
1	D	379	GLU
1	D	391	LYS
1	D	412	ASP
1	D	417	LEU
1	D	428	ARG
1	D	450	ASP
1	D	454	LEU
1	D	467	SER
1	D	474	MET
1	D	482	ASN
1	D	487	ILE
1	D	504	PHE
1	D	514	THR
1	D	518	CYS
1	D	533	PHE
1	D	541	ILE
1	D	556	ARG
1	D	591	GLU
1	D	597	LEU
1	D	599	TRP
1	D	607	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	38	GLN
1	A	133	ASN
1	A	277	GLN
1	A	300	HIS
1	A	372	GLN
1	A	461	GLN

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Mol	Chain	Res	Type
1	A	484	ASN
1	A	585	ASN
1	A	586	GLN
1	B	6	GLN
1	B	81	GLN
1	B	193	HIS
1	B	284	ASN
1	B	286	HIS
1	B	325	ASN
1	C	6	GLN
1	C	38	GLN
1	C	44	HIS
1	C	56	ASN
1	C	284	ASN
1	C	362	ASN
1	C	396	HIS
1	C	402	HIS
1	C	452	ASN
1	C	545	GLN
1	C	621	GLN
1	C	634	ASN
1	D	19	ASN
1	D	168	HIS
1	D	211	ASN
1	D	220	HIS
1	D	280	HIS
1	D	362	ASN
1	D	403	ASN
1	D	461	GLN
1	D	482	ASN
1	D	621	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	U5P	D	801	-	22,22,22	1.10	2 (9%)	32,33,33	1.77	5 (15%)
6	1S3	C	801	-	14,16,16	0.59	0	19,25,25	1.28	4 (21%)
3	G6P	D	802	-	16,16,16	0.48	0	23,24,24	0.98	2 (8%)
3	G6P	A	802	-	16,16,16	0.58	0	23,24,24	1.09	2 (8%)
4	PEG	D	803	-	6,6,6	0.42	0	5,5,5	0.41	0
3	G6P	C	803	-	16,16,16	0.57	0	23,24,24	0.81	0
3	G6P	B	802	-	16,16,16	0.46	0	23,24,24	1.08	1 (4%)
4	PEG	C	804	-	6,6,6	0.50	0	5,5,5	0.26	0
2	U5P	B	801	-	22,22,22	1.12	3 (13%)	32,33,33	1.89	5 (15%)
2	U5P	C	802	-	22,22,22	1.11	2 (9%)	32,33,33	1.80	7 (21%)
2	U5P	A	801	-	22,22,22	1.16	3 (13%)	32,33,33	1.78	7 (21%)
4	PEG	A	803	-	6,6,6	0.60	0	5,5,5	0.33	0
4	PEG	B	803	-	6,6,6	0.46	0	5,5,5	0.43	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
2	U5P	D	801	-	-	3/10/26/26	0/2/2/2
6	1S3	C	801	-	-	0/2/32/32	0/2/2/2
3	G6P	D	802	-	-	3/6/26/26	0/1/1/1
3	G6P	A	802	-	-	3/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	D	803	-	-	3/4/4/4	-
3	G6P	C	803	-	-	1/6/26/26	0/1/1/1
3	G6P	B	802	-	-	2/6/26/26	0/1/1/1
4	PEG	C	804	-	-	3/4/4/4	-
2	U5P	B	801	-	-	3/10/26/26	0/2/2/2
2	U5P	C	802	-	-	1/10/26/26	0/2/2/2
2	U5P	A	801	-	-	5/10/26/26	0/2/2/2
4	PEG	A	803	-	-	3/4/4/4	-
4	PEG	B	803	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	802	U5P	C2-N1	2.61	1.42	1.38
2	A	801	U5P	C4-N3	-2.58	1.34	1.38
2	B	801	U5P	C6-C5	2.35	1.40	1.35
2	B	801	U5P	C4-N3	-2.30	1.34	1.38
2	B	801	U5P	C2-N1	2.29	1.42	1.38
2	D	801	U5P	C6-C5	2.27	1.40	1.35
2	D	801	U5P	C4-N3	-2.24	1.34	1.38
2	A	801	U5P	C2-N3	-2.10	1.34	1.38
2	C	802	U5P	C2-N3	-2.03	1.34	1.38
2	A	801	U5P	C2-N1	2.03	1.41	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	U5P	N3-C2-N1	5.26	121.74	114.89
2	B	801	U5P	C4-N3-C2	-5.26	120.08	126.61
2	A	801	U5P	C4-N3-C2	-5.04	120.36	126.61
2	D	801	U5P	C4-N3-C2	-5.02	120.38	126.61
2	D	801	U5P	N3-C2-N1	4.84	121.19	114.89
2	C	802	U5P	C4-N3-C2	-4.57	120.94	126.61
2	A	801	U5P	N3-C2-N1	4.32	120.52	114.89
2	A	801	U5P	C5-C4-N3	4.12	120.57	114.80
2	C	802	U5P	N3-C2-N1	3.98	120.07	114.89
2	C	802	U5P	C5-C4-N3	3.92	120.29	114.80
2	B	801	U5P	C5-C4-N3	3.48	119.67	114.80
2	D	801	U5P	C5-C4-N3	3.41	119.57	114.80
2	C	802	U5P	O4-C4-C5	-3.19	119.66	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	U5P	O2-C2-N1	-2.92	118.99	122.80
3	A	802	G6P	O2P-P-O1P	2.90	118.66	107.80
2	A	801	U5P	O4-C4-C5	-2.84	120.27	125.16
2	B	801	U5P	O2-C2-N1	-2.81	119.14	122.80
3	B	802	G6P	C1-O5-C5	2.70	118.89	113.65
2	D	801	U5P	O4-C4-C5	-2.69	120.53	125.16
2	C	802	U5P	C3'-C2'-C1'	2.61	106.41	101.46
6	C	801	1S3	O5-C1-O1	2.59	113.93	109.33
2	B	801	U5P	O4-C4-C5	-2.45	120.94	125.16
2	A	801	U5P	C3'-C2'-C1'	2.28	105.77	101.46
3	D	802	G6P	O2P-P-O1P	2.22	116.14	107.80
3	A	802	G6P	O2P-P-O6	-2.22	100.89	106.67
6	C	801	1S3	P-O1-C1	-2.20	106.80	111.26
6	C	801	1S3	O2-P-O3P	-2.15	110.08	115.76
2	C	802	U5P	C2'-C1'-N1	-2.14	107.29	113.25
3	D	802	G6P	O5-C1-C2	-2.09	106.62	110.30
2	A	801	U5P	O2-C2-N1	-2.09	120.07	122.80
6	C	801	1S3	O1-P-O3P	-2.07	110.31	115.76
2	A	801	U5P	C2'-C3'-C4'	2.03	106.53	102.61
2	C	802	U5P	C1'-N1-C2	2.02	121.22	117.59

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	U5P	C5'-O5'-P-O2P
2	B	801	U5P	C5'-O5'-P-O3P
3	A	802	G6P	C6-O6-P-O3P
3	B	802	G6P	C4-C5-C6-O6
3	B	802	G6P	O5-C5-C6-O6
3	D	802	G6P	C6-O6-P-O2P
4	D	803	PEG	O1-C1-C2-O2
2	D	801	U5P	O4'-C4'-C5'-O5'
2	A	801	U5P	O4'-C4'-C5'-O5'
4	A	803	PEG	O1-C1-C2-O2
4	B	803	PEG	O2-C3-C4-O4
4	C	804	PEG	O2-C3-C4-O4
2	B	801	U5P	C5'-O5'-P-O1P
3	D	802	G6P	C6-O6-P-O3P
4	A	803	PEG	O2-C3-C4-O4
3	D	802	G6P	C6-O6-P-O1P
4	A	803	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	D	803	PEG	C1-C2-O2-C3
2	D	801	U5P	C3'-C4'-C5'-O5'
4	D	803	PEG	C4-C3-O2-C2
2	D	801	U5P	C4'-C5'-O5'-P
2	A	801	U5P	C3'-C4'-C5'-O5'
3	C	803	G6P	C4-C5-C6-O6
2	C	802	U5P	C4'-C5'-O5'-P
4	C	804	PEG	C4-C3-O2-C2
3	A	802	G6P	C6-O6-P-O1P
3	A	802	G6P	C6-O6-P-O2P
2	A	801	U5P	O4'-C1'-N1-C6
4	B	803	PEG	O1-C1-C2-O2
2	A	801	U5P	C2'-C1'-N1-C6
4	C	804	PEG	C1-C2-O2-C3
2	A	801	U5P	C4'-C5'-O5'-P

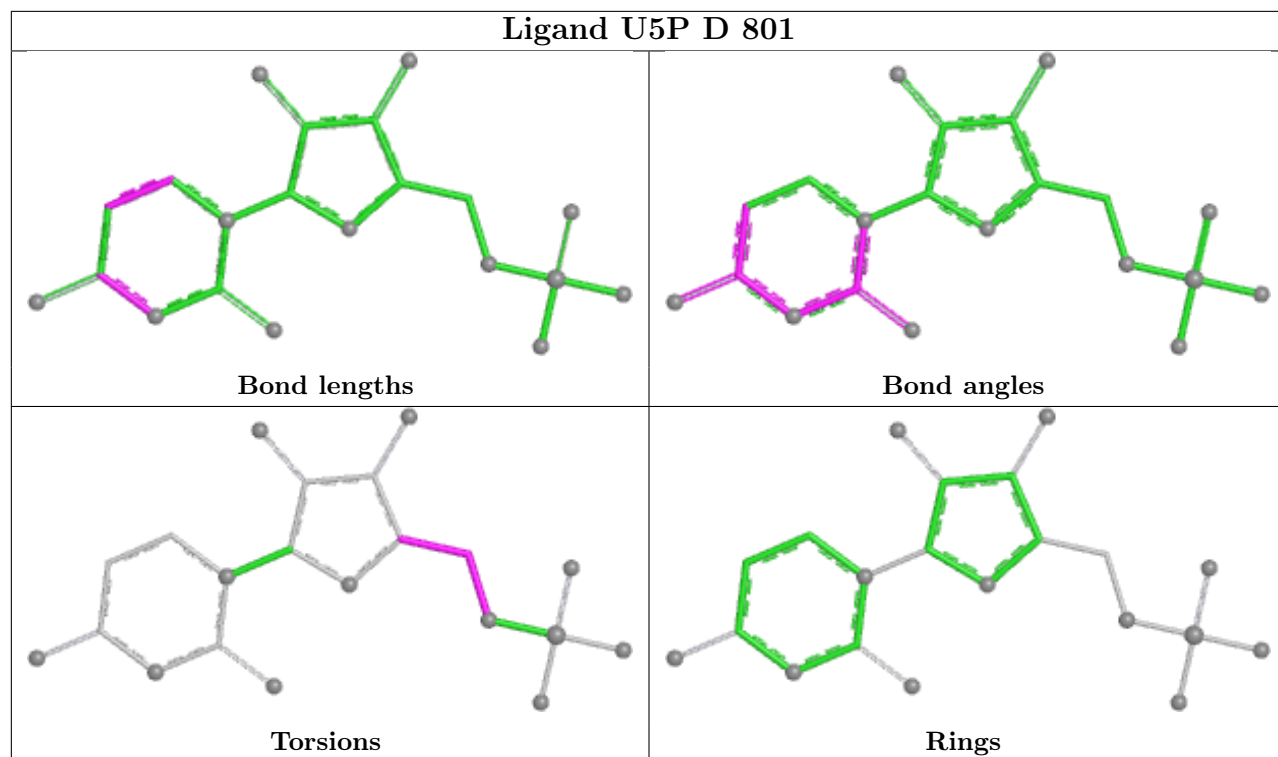
There are no ring outliers.

6 monomers are involved in 11 short contacts:

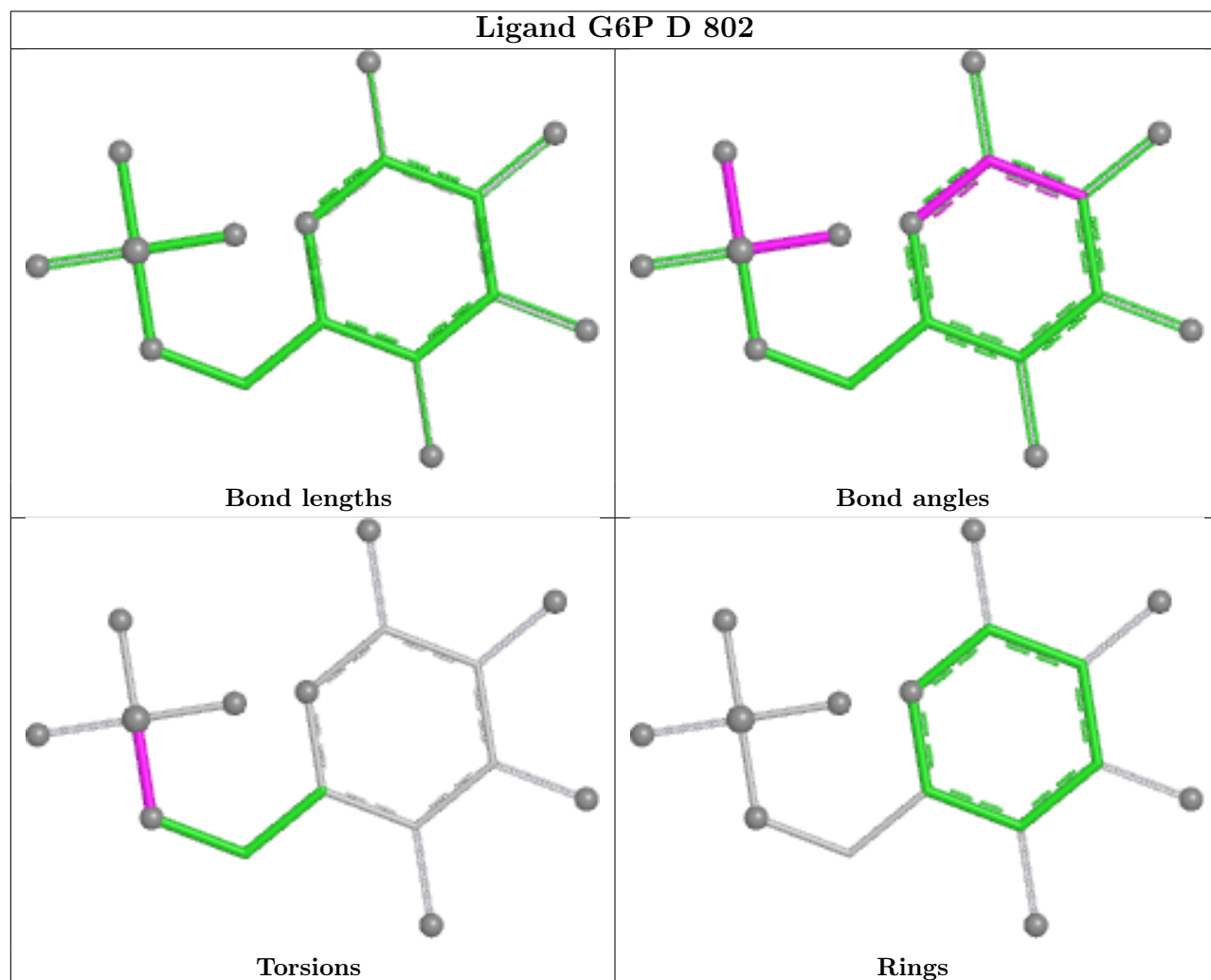
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	801	1S3	1	0
3	D	802	G6P	1	0
3	A	802	G6P	2	0
3	C	803	G6P	3	0
3	B	802	G6P	1	0
4	C	804	PEG	3	0

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.

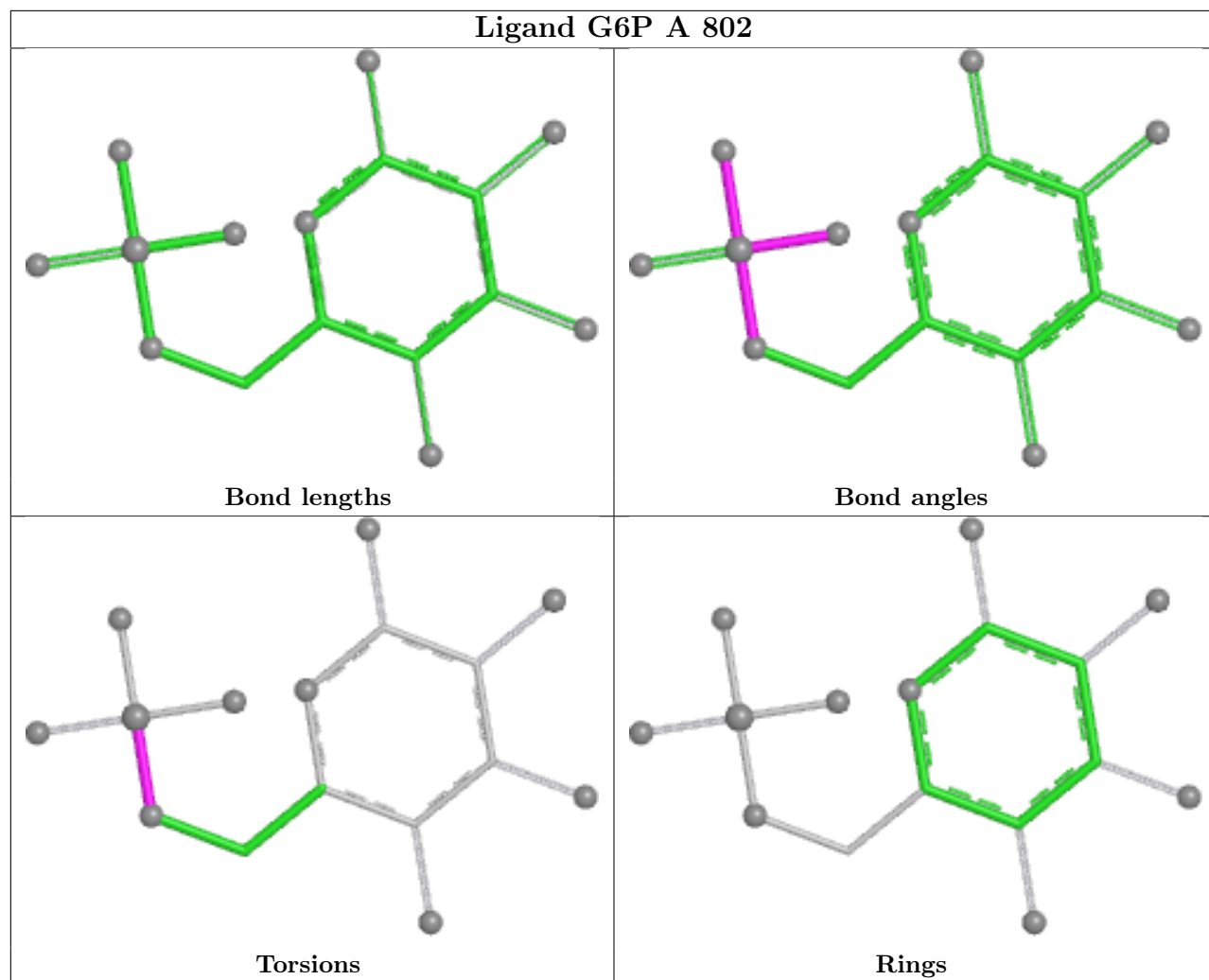
Ligand U5P D 801



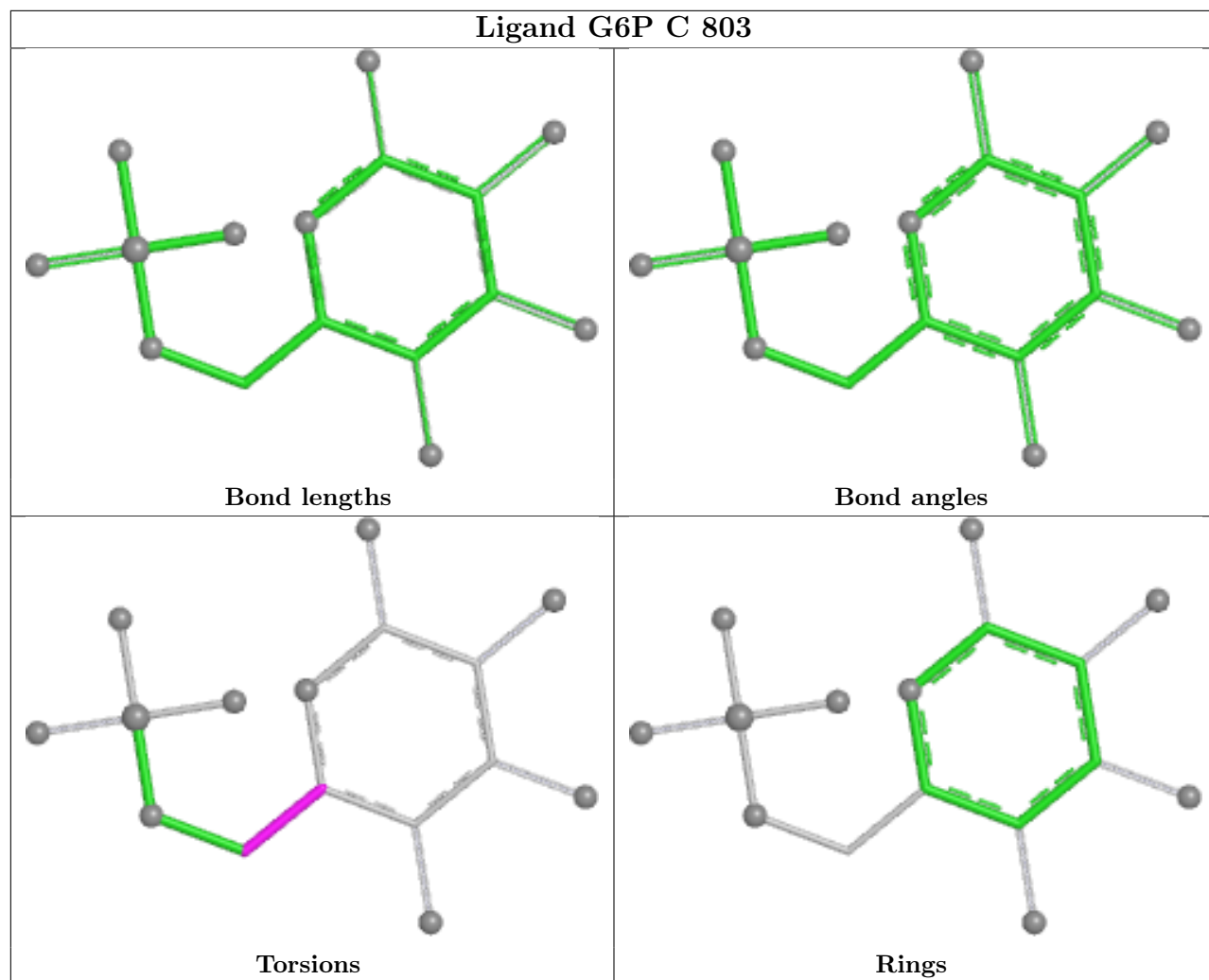
Ligand G6P D 802



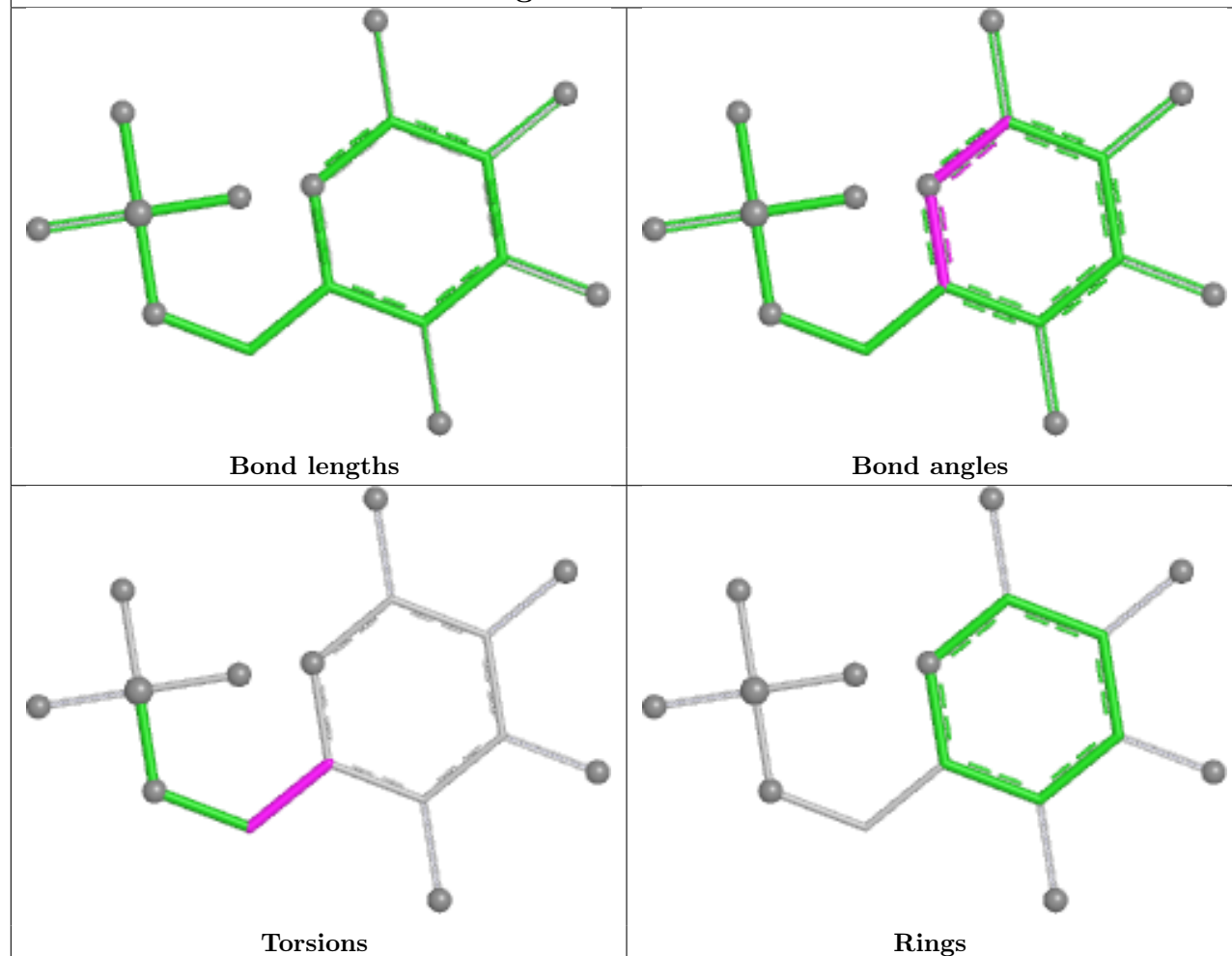
Ligand G6P A 802



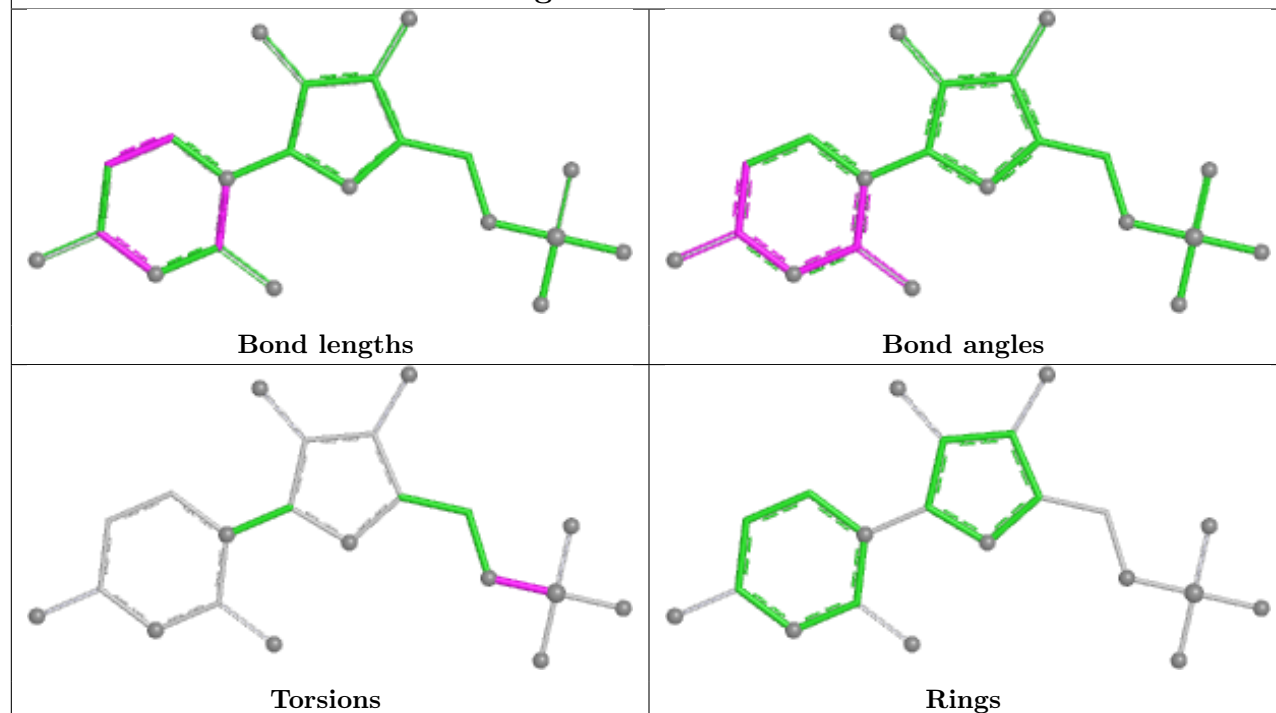
Ligand G6P C 803

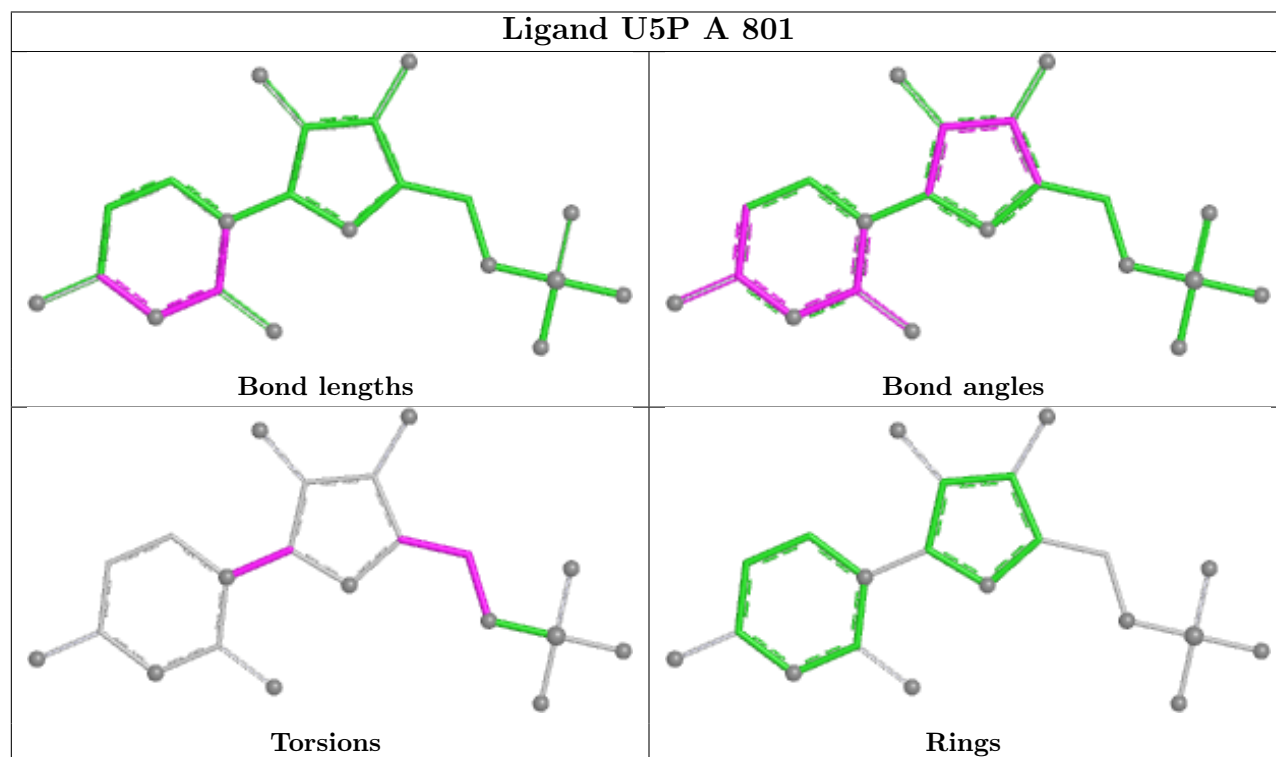
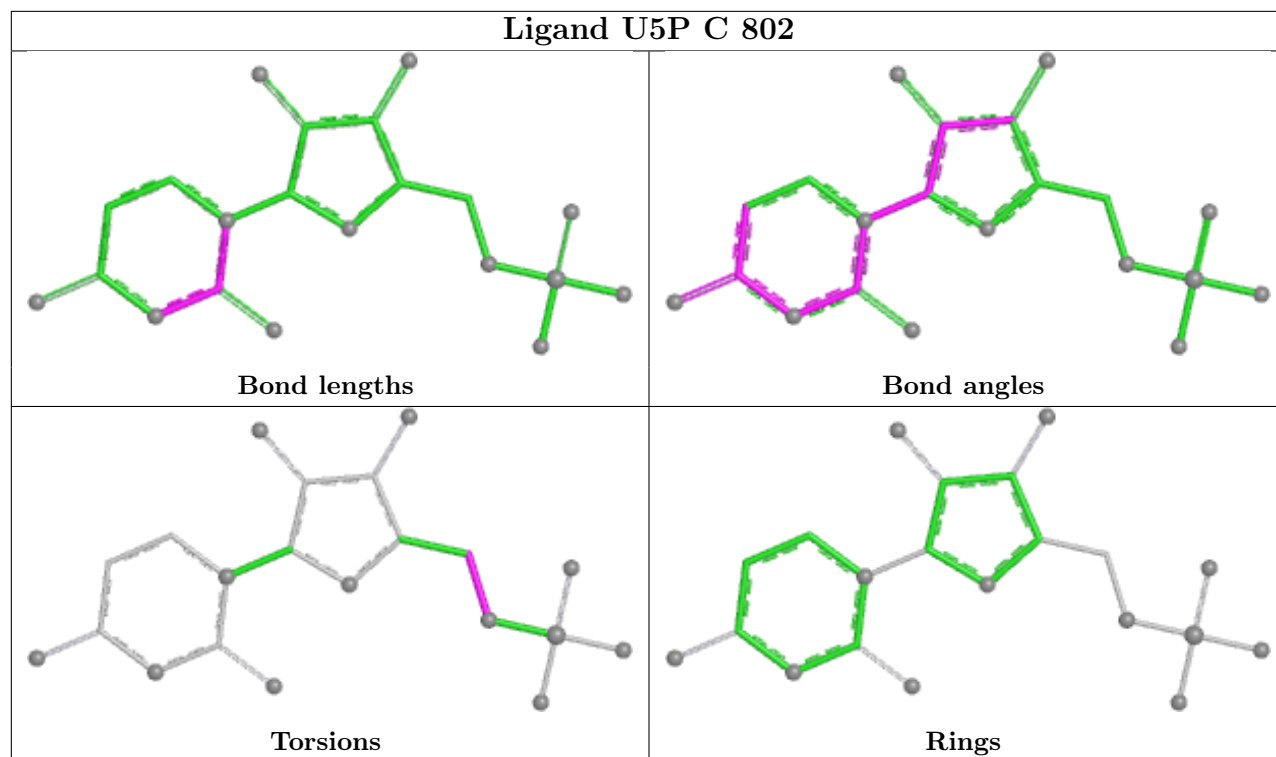


Ligand G6P B 802



Ligand U5P B 801





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	638/724 (88%)	0.06	15 (2%) 59 51	53, 103, 165, 226	0
1	B	638/724 (88%)	-0.10	6 (0%) 81 76	22, 86, 150, 198	3 (0%)
1	C	638/724 (88%)	0.27	18 (2%) 55 47	43, 108, 183, 247	1 (0%)
1	D	636/724 (87%)	0.03	7 (1%) 78 73	18, 104, 190, 223	2 (0%)
All	All	2550/2896 (88%)	0.07	46 (1%) 67 59	18, 101, 179, 247	6 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	PRO	3.4
1	C	173	GLY	3.3
1	A	305	PHE	3.3
1	D	205	GLY	3.2
1	C	279	PHE	3.2
1	D	638	LEU	3.1
1	C	18	ALA	3.1
1	D	622	PHE	2.9
1	C	505	PRO	2.9
1	C	507	TYR	2.8
1	C	76	VAL	2.8
1	A	18	ALA	2.8
1	A	508	TYR	2.8
1	A	129	PRO	2.8
1	C	103	VAL	2.7
1	C	24	ILE	2.6
1	D	125	LEU	2.5
1	A	507	TYR	2.5
1	A	321	TYR	2.5
1	B	630	LEU	2.5
1	C	154	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	197	LEU	2.4
1	A	274	ILE	2.3
1	C	585	ASN	2.3
1	C	172	ALA	2.3
1	B	85	SER	2.3
1	A	623	ARG	2.3
1	B	160	GLN	2.2
1	D	60	ILE	2.2
1	A	130	SER	2.2
1	C	155	ALA	2.2
1	B	513	TYR	2.1
1	A	593	LEU	2.1
1	C	141	ILE	2.1
1	C	177	PRO	2.1
1	B	205	GLY	2.1
1	B	632	ASP	2.1
1	D	85	SER	2.1
1	C	28	LEU	2.1
1	D	150	PHE	2.1
1	A	310	ASP	2.1
1	A	172	ALA	2.1
1	C	108	LEU	2.0
1	C	233	ILE	2.0
1	A	368	ALA	2.0
1	A	5	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

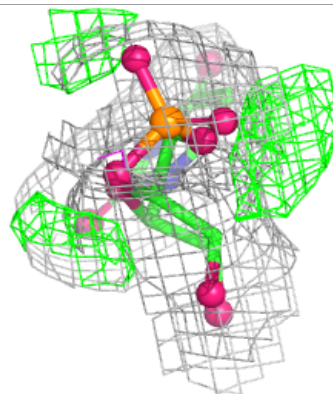
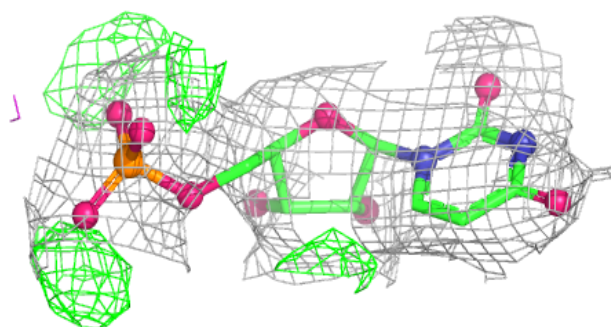
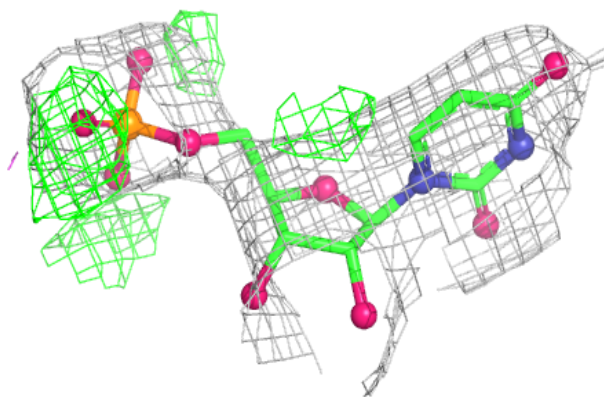
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	BA	B	805	1/1	0.81	0.08	245,245,245,245	0
2	U5P	C	802	21/21	0.83	0.13	95,123,162,163	0
6	1S3	C	801	15/15	0.84	0.11	107,130,156,156	0
4	PEG	D	803	7/7	0.89	0.19	90,90,95,96	0
4	PEG	B	803	7/7	0.90	0.16	98,103,115,115	0
5	BA	D	805	1/1	0.91	0.08	227,227,227,227	0
2	U5P	D	801	21/21	0.91	0.08	93,105,112,127	0
2	U5P	A	801	21/21	0.92	0.09	89,103,120,123	0
4	PEG	A	803	7/7	0.93	0.11	71,74,82,85	0
2	U5P	B	801	21/21	0.93	0.07	82,91,100,105	0
5	BA	D	804	1/1	0.94	0.09	159,159,159,159	0
5	BA	B	804	1/1	0.94	0.13	149,149,149,149	0
5	BA	A	805	1/1	0.94	0.04	212,212,212,212	0
3	G6P	A	802	16/16	0.95	0.08	80,92,98,102	0
3	G6P	C	803	16/16	0.96	0.06	66,77,83,84	0
3	G6P	D	802	16/16	0.97	0.07	55,67,75,78	0
4	PEG	C	804	7/7	0.97	0.10	88,89,96,96	0
3	G6P	B	802	16/16	0.97	0.07	56,74,80,80	0
5	BA	A	804	1/1	0.98	0.06	135,135,135,135	0
5	BA	C	805	1/1	0.99	0.07	145,145,145,145	0

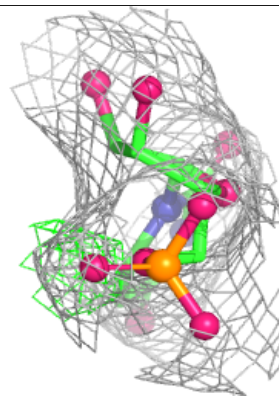
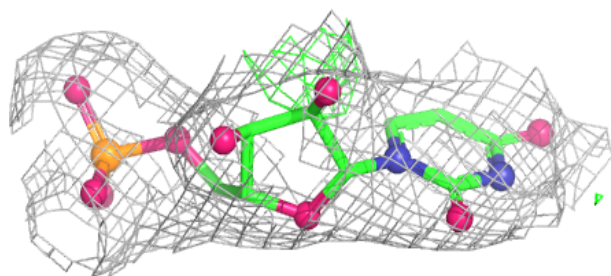
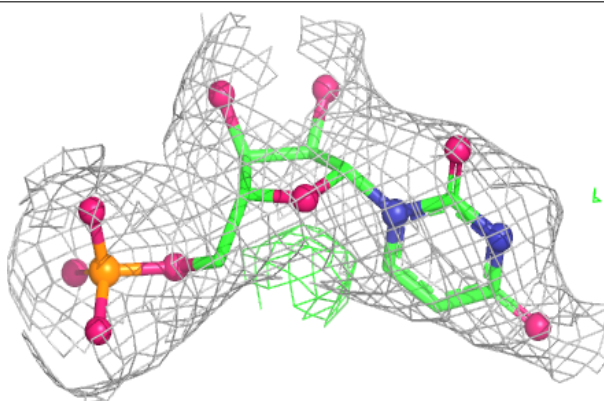
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U5P C 802:

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

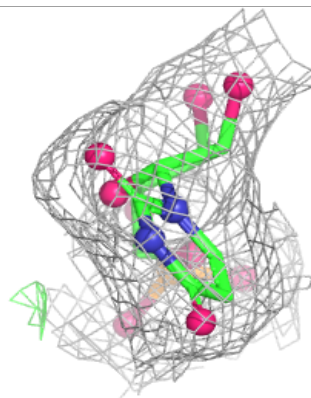
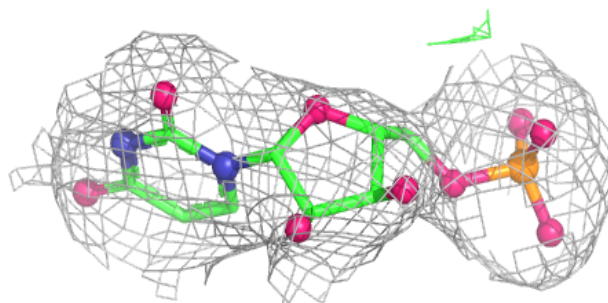
**Electron density around U5P D 801:**

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

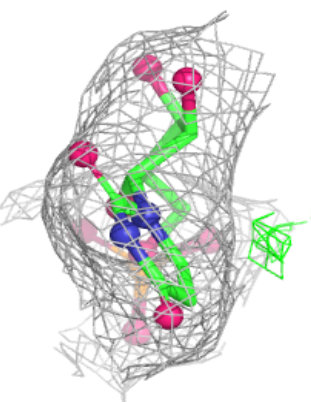
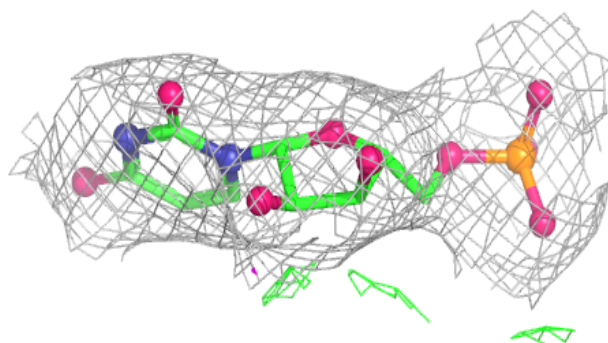
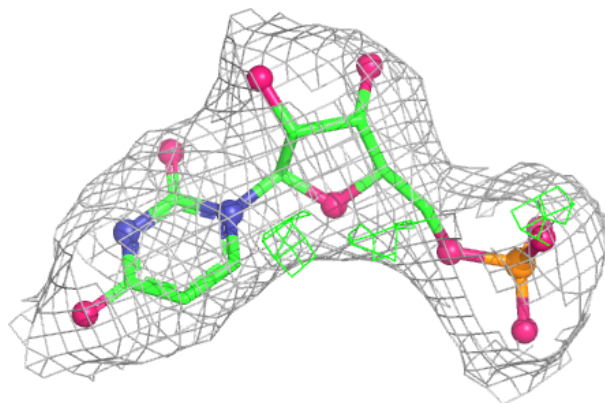


Electron density around U5P A 801:

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

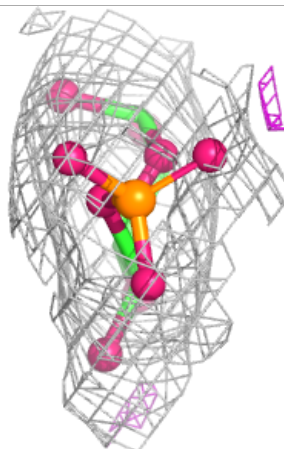
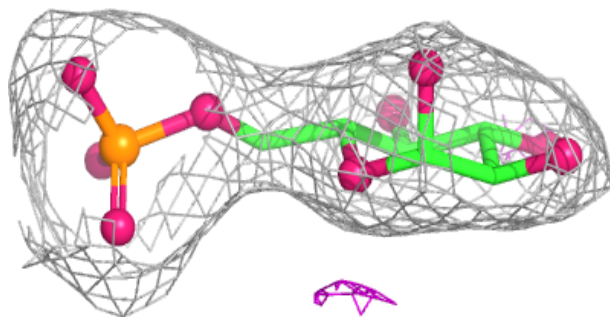
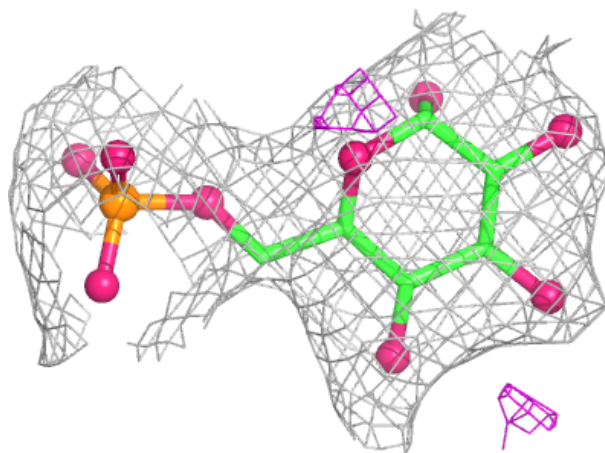
**Electron density around U5P B 801:**

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



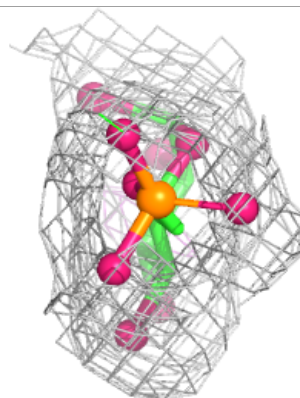
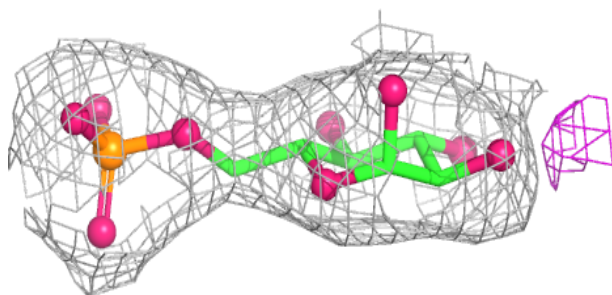
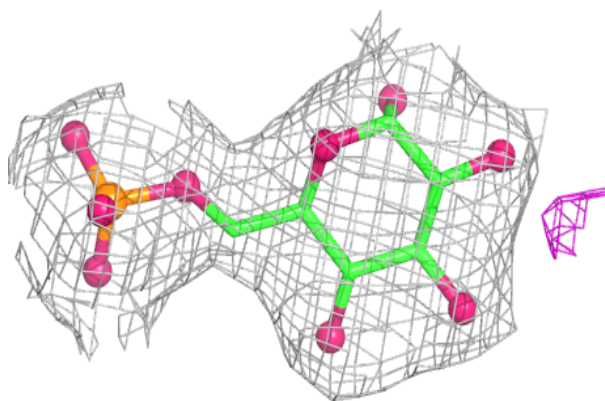
Electron density around G6P A 802:

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

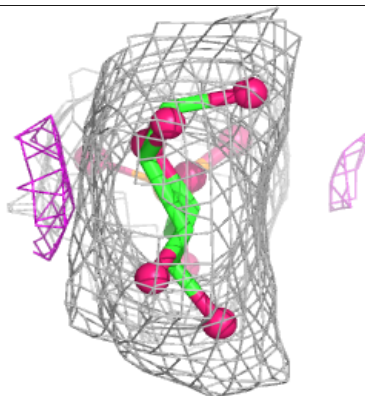
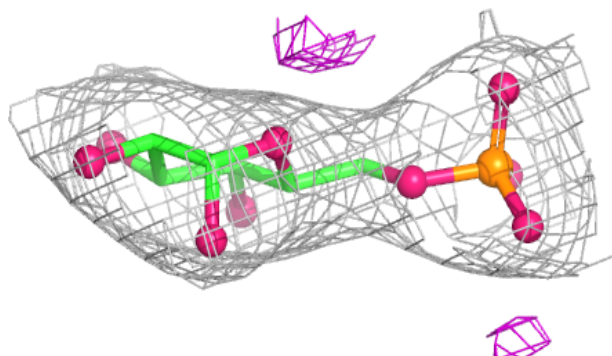
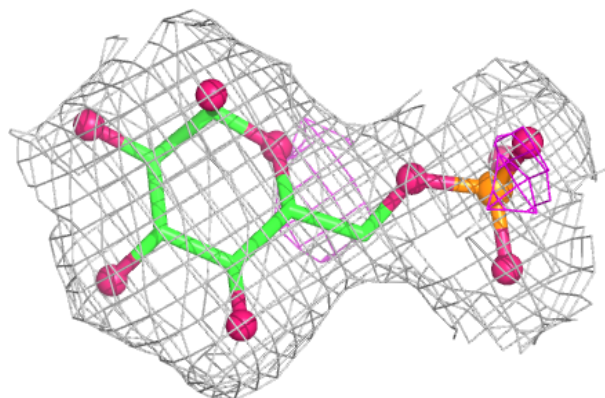


Electron density around G6P C 803:

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

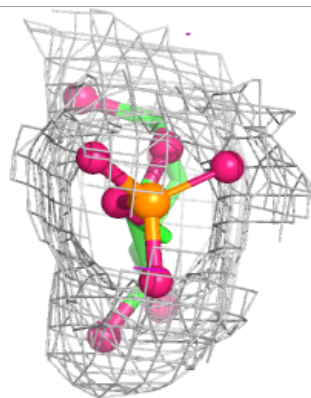
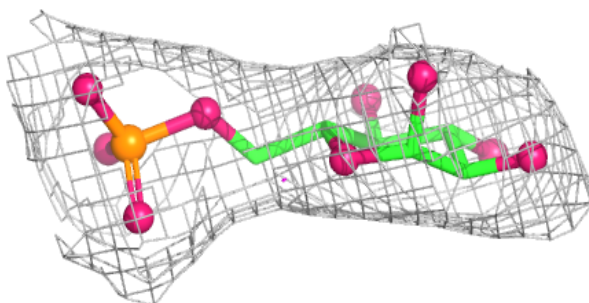
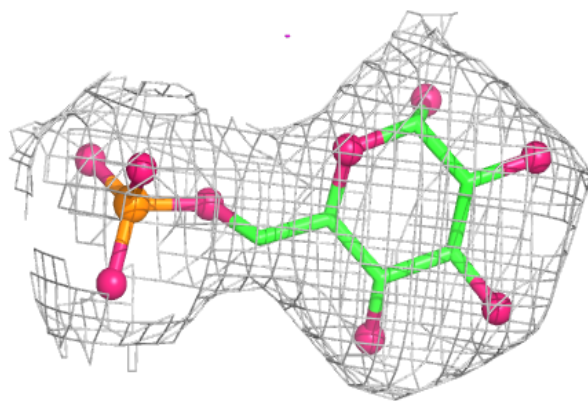
**Electron density around G6P D 802:**

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



Electron density around G6P B 802:

$2mF_o-DF_c$ (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.