



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:49 PM UTC

PDB ID : 5SUL / pdb_00005sul
Title : Inhibited state structure of yGsy2p
Authors : Mahalingan, K.K.; Hurley, T.D.
Deposited on : 2016-08-03
Resolution : 3.30 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

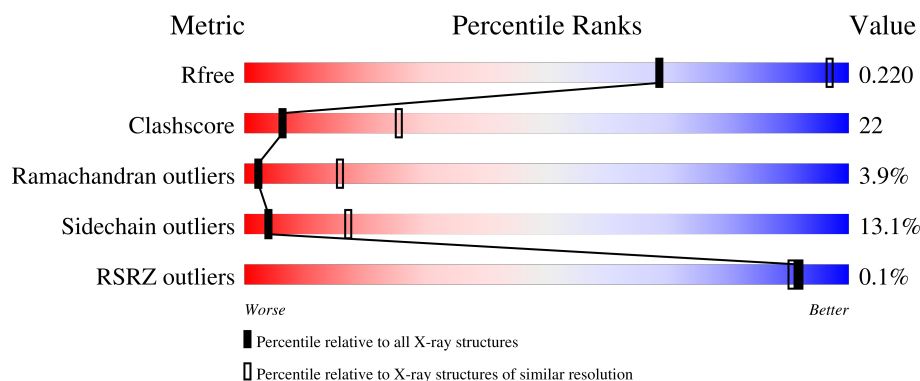
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	725	
1	B	725	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9615 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 Glycogen [starch] synthase isoform 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4849	3087	838	905	19			
1	B	606	Total	C	N	O	S	0	0	0
			4720	3016	806	880	18			

There are 46 discrepancies between the modelled and reference sequences:

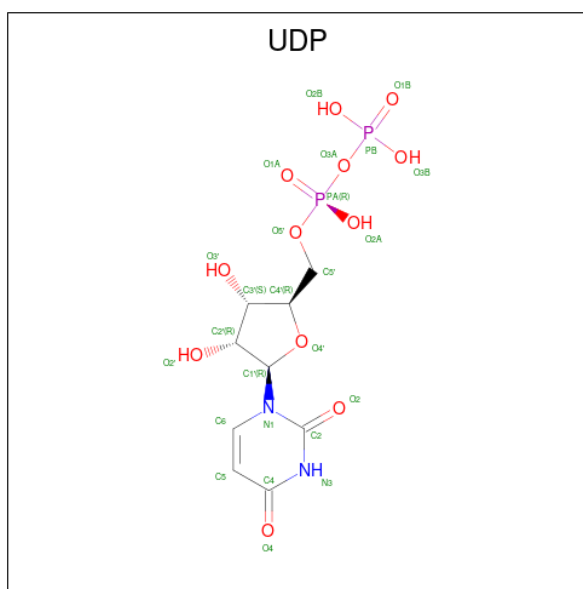
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	535	SER	ALA	conflict	UNP P27472
A	589	ALA	ARG	conflict	UNP P27472
A	592	ALA	ARG	conflict	UNP P27472
B	-19	MET	-	initiating methionine	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472

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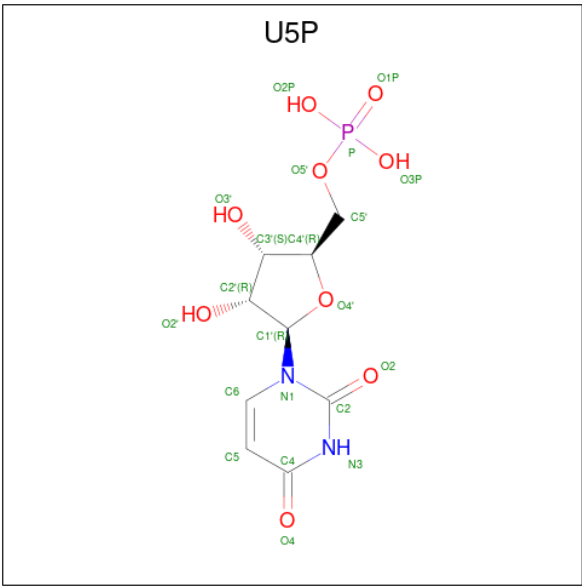
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	535	SER	ALA	conflict	UNP P27472
B	589	ALA	ARG	conflict	UNP P27472
B	592	ALA	ARG	conflict	UNP P27472

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: C₉H₁₃N₂O₉P).



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

GLU	R615	G522	K447	E374	Y297	L213	L125	K51
VAL			V448	V375	R298		V126	A52
ASN	Y618	T528	D449	A377	G299	F225		T53
ASN	F619	N529	D450	L378			P129	Y54
ALA	D620	V530	A451		H302	I227	S130	I60
ASP	D621	S531	N452	T381	F307	Y228	P131	L61
ASP	F622	G532	N453	V382	D308	H229	E132	D62
TYR	R623		L454		L309	Y231	N133	W63
PHE		R537		T386			F135	K64
SER			K458	T387	T312	A237		K65
LEU		I541		S388	L313	A238	L142	P66
GLY		E542	V462	I389	Y314	H239	L143	E67
VAL		T543	O463				G144	
VAL		N544	L464	R392	I317	D242		S70
ASN			F465			V243	V147	D71
ASN		Y549		D395	Y321	F244		R74
ASP		G550	S469		E322	T245	F150	P75
ASP		I551	D470	I398	Y323	T246		V76
ASP			R471	R399	K324		E153	Q77
ASP		V554	K473	Y400	N325	Q249	V154	A78
ALA		D555		P401	K326	I250	L157	A79
ASP		R556	F476	HIS	G327		D158	L80
GLY		R557	H477	ASN	D328	F253		Q81
GLY		F558	P478	GLY	D329	E254	H161	T82
TYR		K559	E479	LEU	N330	A255	A162	M83
ALA		A560	F480	THR		E256	I163	
ASP			L481	THR	E333	H257		H88
ASP		E563	L484	GLU	A334	L258	H168	V89
SER		S564		LEU	L335			F90
		V565	V484	PRO	A336	R261	V174	Y91
			I487	THR	R337	K262	A175	Y92
		L568	L488	ASP	L338		L176	G93
		V569	G489	LEU		G285	P177	W95
		M572	L490	GLY	L342	I266		I96
			D491	E415	K343	L267	R180	
		R581	Y492	L416	V344	P268	K181	
		Q582			S345		K182	
			R497	S419	G346	N272	R183	A100
		R587	G498	V423	K349	V273	I184	P101
		N588	C499	M424	T350	I274	K102	K103
		A589	H500	L425	V351	K275	V186	V103
		T590		K426	V352	F276	V187	I104
		E591	V503	R427			T188	L106
		A592	F504	R428		ALA	F106	
		L593	P505	I429	T355	PHE	D107	
		S594	S506	L430	N357	HIS	L108	D109
		D595	Y507		P358	GLU	T192	S110
		L596			A359	PHE	H193	V111
		L597	P510	R434		GLN	A194	R112
		D598		P435	N362	N284		G113
		W599	Y513	E436	S363	L285	G205	Y114
		K600	T514		F364		S206	S115
		R601	P515	P440		K289	F207	D121
		M602	A516	P441	L369	K290	D208	L122
			E517	T442	K370	E291	F209	W123
		R610	C518	V443	G371		Y210	C212
		Q611	T519	T444	Q372	N294	N211	
			V520	H445		D295		
		L614	M521	N446	A373	F296		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.45Å 122.45Å 279.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.04 – 3.30 46.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.04-3.30) 99.7 (46.04-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.158 , 0.223 0.155 , 0.220	Depositor DCC
R_{free} test set	1854 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	106.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.257 for -h,-k,l	Xtriage
Reported twinning fraction	0.681 for H, K, L 0.319 for -h,-k,l	Depositor
Outliers	0 of 37091 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9615	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, U5P

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	0.78	2/4964 (0.0%)	1.15	13/6752 (0.2%)
1	B	0.74	0/4836	1.16	12/6586 (0.2%)
All	All	0.76	2/9800 (0.0%)	1.15	25/13338 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLY	C-O	7.04	1.33	1.23
1	A	129	PRO	N-CA	5.20	1.53	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLY	CA-C-N	-13.69	101.14	122.08
1	A	205	GLY	C-N-CA	-13.69	101.14	122.08
1	B	477	HIS	CA-C-N	8.30	130.21	119.84
1	B	477	HIS	C-N-CA	8.30	130.21	119.84
1	A	206	SER	O-C-N	7.43	129.97	122.10
1	A	206	SER	N-CA-C	7.21	123.71	114.56
1	B	32	ALA	CA-C-N	-7.11	111.58	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	32	ALA	C-N-CA	-7.11	111.58	118.97
1	B	130	SER	CA-C-N	6.84	128.39	119.84
1	B	130	SER	C-N-CA	6.84	128.39	119.84
1	B	188	THR	N-CA-C	6.69	120.42	109.72
1	A	487	ILE	CB-CA-C	6.28	117.41	111.44
1	B	454	LEU	N-CA-C	5.69	117.48	111.28
1	B	416	LEU	N-CA-C	-5.67	106.03	113.17
1	A	434	ARG	CA-C-N	5.62	126.87	119.84
1	A	434	ARG	C-N-CA	5.62	126.87	119.84
1	A	509	GLU	CA-C-N	5.59	125.95	119.47
1	A	509	GLU	C-N-CA	5.59	125.95	119.47
1	A	265	GLY	N-CA-C	5.52	118.31	110.74
1	A	58	VAL	N-CA-C	5.44	115.73	108.11
1	B	114	TYR	N-CA-C	-5.40	104.65	113.19
1	A	228	TYR	N-CA-C	5.24	116.80	111.14
1	B	227	ILE	N-CA-C	5.16	117.07	112.17
1	A	543	THR	N-CA-C	5.12	121.70	110.80
1	B	265	GLY	N-CA-C	5.12	118.05	110.63

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	GLY	Peptide
1	B	484	ASN	Peptide

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	4849	0	4605	214	0
1	B	4720	0	4446	197	0
2	A	25	0	11	3	0
3	B	21	0	11	4	0
All	All	9615	0	9073	414	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 22.

All (414) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LEU:HD23	1:B:253:PHE:CE2	1.76	1.21
1:B:314:TYR:H	1:B:500:HIS:CD2	1.74	1.04
1:B:74:ARG:HE	1:B:77:GLN:NE2	1.56	1.04
1:B:213:LEU:HD23	1:B:253:PHE:HE2	0.87	0.99
1:B:213:LEU:CD2	1:B:253:PHE:HE2	1.77	0.97
1:A:207:PHE:O	1:A:209:PHE:N	2.01	0.94
1:B:16:GLU:HG2	1:B:25:TYR:HB2	1.49	0.92
1:B:74:ARG:HE	1:B:77:GLN:HE22	1.05	0.91
1:A:443:VAL:HG13	1:A:456:LEU:HD21	1.52	0.91
1:A:579:THR:H	1:A:582:GLN:HE21	1.19	0.91
1:B:314:TYR:N	1:B:500:HIS:HD2	1.70	0.89
1:A:123:TRP:CD2	1:A:129:PRO:HA	2.07	0.88
1:A:471:ARG:HE	1:A:471:ARG:HA	1.43	0.83
1:A:314:TYR:H	1:A:500:HIS:CD2	1.97	0.82
1:B:83:MET:O	1:B:88:VAL:HB	1.80	0.82
1:A:213:LEU:HA	1:A:216:VAL:HG23	1.62	0.81
1:A:208:ASP:HB3	1:A:211:ASN:HB2	1.61	0.81
1:A:579:THR:H	1:A:582:GLN:NE2	1.78	0.81
1:A:313:LEU:HA	1:A:500:HIS:CD2	2.16	0.80
1:B:74:ARG:NE	1:B:77:GLN:HE22	1.80	0.80
1:B:514:THR:OG1	1:B:515:PRO:HD3	1.83	0.78
1:A:174:VAL:O	1:A:177:PRO:HD2	1.83	0.77
1:B:528:THR:HG22	1:B:530:VAL:H	1.48	0.77
1:B:458:LYS:O	1:B:462:VAL:HG22	1.84	0.77
1:A:485:ASN:ND2	1:A:488:LEU:H	1.82	0.77
1:A:271:LEU:HD22	1:A:520:VAL:HG21	1.65	0.77
1:A:540:LEU:HD21	1:A:596:LEU:HD13	1.67	0.77
1:A:314:TYR:H	1:A:500:HIS:HD2	1.32	0.76
1:B:323:TYR:CE1	1:B:329:ASP:HB3	2.20	0.75
1:A:123:TRP:CE2	1:A:129:PRO:HA	2.21	0.75
1:A:443:VAL:CG1	1:A:456:LEU:HD21	2.16	0.75
1:B:34:ILE:HD12	1:B:600:LYS:HA	1.68	0.75
1:B:187:VAL:HG21	1:B:614:LEU:HD23	1.68	0.74
1:A:163:ILE:HB	1:A:186:VAL:HG12	1.69	0.74
1:B:522:GLY:HA3	1:B:591:GLU:HG3	1.69	0.74
1:B:163:ILE:HB	1:B:186:VAL:HG12	1.70	0.74
1:B:176:LEU:HD12	1:B:237:ALA:HB1	1.70	0.74
1:A:471:ARG:HA	1:A:471:ARG:NE	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:HG23	1:A:129:PRO:HD2	1.69	0.73
1:B:358:PRO:HA	1:B:478:PRO:O	1.90	0.72
1:A:374:GLU:OE1	1:A:374:GLU:HA	1.87	0.72
1:B:50:ASN:C	1:B:50:ASN:HD22	1.96	0.72
1:A:313:LEU:HA	1:A:500:HIS:HD2	1.54	0.71
1:B:3:ARG:NH2	1:B:158:ASP:O	2.23	0.71
1:B:66:PRO:O	1:B:74:ARG:NH2	2.23	0.71
1:B:323:TYR:HE1	1:B:329:ASP:HB3	1.56	0.70
1:B:434:ARG:HH21	1:B:440:PRO:HA	1.55	0.70
1:B:333:GLU:OE2	1:B:337:ARG:NH1	2.21	0.70
1:B:343:LYS:O	1:B:346:GLY:N	2.22	0.69
1:A:520:VAL:HA	1:A:594:SER:OG	1.92	0.69
1:A:549:TYR:O	1:A:590:THR:HG22	1.92	0.69
1:A:565:VAL:O	1:A:569:VAL:HG23	1.92	0.69
1:A:134:ASP:OD1	1:A:137:THR:HB	1.93	0.69
1:B:395:ASP:O	1:B:399:ARG:HB2	1.93	0.68
1:B:445:HIS:CD2	1:B:478:PRO:HD2	2.29	0.68
1:B:480:PHE:HD1	3:B:801:U5P:C4	2.07	0.68
1:A:399:ARG:HH11	1:A:399:ARG:HG2	1.58	0.67
1:A:458:LYS:HE3	1:A:461:GLN:OE1	1.95	0.67
1:B:109:ASP:HA	1:B:112:ARG:HD2	1.76	0.67
1:A:321:TYR:O	1:A:321:TYR:CD1	2.47	0.67
1:A:31:LYS:O	1:A:34:ILE:HG22	1.95	0.66
1:A:526:ILE:HG12	1:A:552:TYR:HB2	1.76	0.66
1:B:16:GLU:HG2	1:B:25:TYR:H	1.61	0.66
1:B:434:ARG:HH21	1:B:441:PRO:HD3	1.60	0.66
1:B:143:LEU:O	1:B:147:VAL:HG23	1.96	0.65
1:B:213:LEU:CD2	1:B:253:PHE:CE2	2.63	0.65
1:A:217:ASP:HB3	1:A:221:GLU:HG2	1.78	0.65
1:A:378:LEU:O	1:A:382:VAL:HG23	1.96	0.65
1:A:540:LEU:HD11	1:A:601:ARG:NH2	2.11	0.65
1:B:434:ARG:NH2	1:B:441:PRO:HD3	2.12	0.65
1:A:579:THR:N	1:A:582:GLN:HE21	1.90	0.64
1:A:344:VAL:C	1:A:346:GLY:H	2.06	0.64
1:A:213:LEU:HA	1:A:216:VAL:CG2	2.28	0.64
1:B:350:THR:OG1	1:B:471:ARG:NH1	2.31	0.63
1:B:14:ALA:HB2	1:B:168:HIS:HB2	1.81	0.63
1:B:74:ARG:N	1:B:75:PRO:HD2	2.13	0.63
1:A:29:LYS:HG3	1:A:97:ILE:HD13	1.81	0.63
1:B:121:ASP:O	1:B:124:SER:HB3	1.99	0.62
1:B:541:ILE:HD11	1:B:593:LEU:HD11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:O	1:A:126:VAL:HG23	1.99	0.62
1:B:8:HIS:HA	1:B:161:HIS:HB3	1.82	0.62
1:A:123:TRP:CE3	1:A:129:PRO:HB3	2.34	0.62
1:A:314:TYR:N	1:A:500:HIS:HD2	1.97	0.62
1:A:484:ASN:HD22	1:A:484:ASN:H	1.46	0.62
1:B:565:VAL:O	1:B:569:VAL:HG23	2.00	0.62
1:A:447:MET:HG3	1:A:456:LEU:HD11	1.82	0.61
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.82	0.61
1:A:267:LEU:HB3	1:A:606:TYR:CE2	2.36	0.61
1:B:541:ILE:CD1	1:B:593:LEU:HD11	2.31	0.61
1:A:488:LEU:HD11	1:A:490:LEU:HD12	1.82	0.61
1:A:485:ASN:HD22	1:A:488:LEU:H	1.49	0.60
1:B:112:ARG:HA	1:B:142:LEU:HD21	1.82	0.60
1:B:74:ARG:NE	1:B:77:GLN:NE2	2.38	0.60
1:A:61:LEU:HD12	1:A:93:GLY:HA2	1.82	0.60
1:A:8:HIS:HD2	1:A:164:VAL:HG23	1.64	0.60
1:A:31:LYS:HG2	1:A:35:THR:CG2	2.31	0.60
1:B:551:ILE:HD11	1:B:593:LEU:CD1	2.31	0.60
1:A:483:ALA:HB2	1:A:491:ASP:OD1	2.02	0.60
1:A:444:THR:OG1	1:A:445:HIS:HD2	1.85	0.59
1:B:321:TYR:HB2	1:B:358:PRO:O	2.01	0.59
1:A:3:ARG:NH1	1:A:185:ASP:OD2	2.32	0.59
1:A:188:THR:OG1	1:A:241:ALA:HA	2.03	0.59
1:A:458:LYS:CE	1:A:461:GLN:OE1	2.51	0.59
1:A:434:ARG:HD2	1:A:435:PRO:HD2	1.83	0.59
1:B:16:GLU:HG2	1:B:25:TYR:CB	2.27	0.59
1:A:308:ASP:OD2	1:A:310:ASP:HB2	2.03	0.58
1:B:144:GLY:HA3	1:B:174:VAL:HG12	1.85	0.58
1:A:31:LYS:HG2	1:A:35:THR:HG22	1.86	0.58
1:B:83:MET:HE3	1:B:88:VAL:HG11	1.85	0.58
1:A:234:GLU:OE2	1:A:259:LEU:HD21	2.05	0.57
1:B:231:TYR:C	1:B:231:TYR:CD2	2.82	0.57
1:A:512:GLY:O	1:A:515:PRO:HD2	2.04	0.57
1:B:560:ALA:HB3	1:B:563:GLU:H	1.68	0.57
1:A:551:ILE:HD11	1:A:593:LEU:HD13	1.86	0.57
1:A:3:ARG:NH2	1:A:158:ASP:O	2.38	0.57
1:A:458:LYS:HE2	1:A:462:VAL:HG13	1.86	0.57
1:A:456:LEU:O	1:A:460:ARG:HG3	2.04	0.57
1:B:357:MET:O	1:B:478:PRO:HA	2.05	0.57
1:A:79:ALA:O	1:A:83:MET:HG2	2.04	0.57
1:B:323:TYR:CD2	1:B:454:LEU:HB3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:O	1:B:450:ASP:N	2.37	0.57
1:B:520:VAL:HA	1:B:594:SER:OG	2.04	0.57
1:A:488:LEU:CD1	1:A:490:LEU:HD12	2.35	0.56
1:B:352:VAL:HG22	1:B:473:LYS:HB2	1.87	0.56
1:B:449:ASP:OD2	1:B:452:ASN:HB2	2.06	0.56
1:A:313:LEU:CA	1:A:500:HIS:HD2	2.18	0.56
1:A:581:ARG:HA	1:A:584:ILE:HD12	1.88	0.56
1:B:131:PRO:C	1:B:133:ASN:H	2.12	0.56
1:B:268:PRO:O	1:B:602:MET:HE3	2.05	0.56
1:B:480:PHE:CD1	3:B:801:U5P:C4	2.88	0.56
1:B:239:HIS:CE1	1:B:261:ARG:HB2	2.41	0.56
1:B:369:LEU:HD23	1:B:487:ILE:HD11	1.87	0.56
1:A:44:HIS:CD2	1:A:104:ILE:HD12	2.40	0.55
1:A:428:ARG:HA	1:A:428:ARG:NE	2.21	0.55
2:A:801:UDP:H5'2	2:A:801:UDP:O1B	2.05	0.55
1:B:362:ASN:HB2	1:B:446:ASN:HB2	1.89	0.55
1:B:321:TYR:CD2	1:B:359:ALA:HB2	2.41	0.55
1:A:126:VAL:HG12	1:A:127:GLY:N	2.21	0.55
1:A:179:CYS:SG	1:A:184:ILE:HD12	2.46	0.55
1:A:365:THR:HG23	1:A:368:ALA:CB	2.36	0.55
1:B:50:ASN:C	1:B:50:ASN:ND2	2.63	0.55
1:B:335:LEU:HD13	1:B:572:MET:HE1	1.87	0.55
1:A:14:ALA:HB2	1:A:168:HIS:HB2	1.89	0.55
1:A:449:ASP:OD2	1:A:452:ASN:HB2	2.07	0.55
1:B:542:GLU:O	1:B:544:ASN:N	2.39	0.55
1:B:499:CYS:O	1:B:587:ARG:NH2	2.40	0.55
1:B:274:ILE:C	1:B:276:PHE:H	2.15	0.55
1:A:485:ASN:HD22	1:A:487:ILE:H	1.54	0.55
1:A:514:THR:OG1	1:A:515:PRO:HD3	2.07	0.55
1:B:44:HIS:HD2	1:B:104:ILE:HD12	1.71	0.55
1:A:45:LEU:HB2	1:A:103:VAL:HG12	1.88	0.54
1:A:540:LEU:CD2	1:A:596:LEU:HD13	2.37	0.54
1:A:366:VAL:HG13	1:A:367:GLU:N	2.23	0.54
1:B:327:GLY:HA3	1:B:505:PRO:O	2.07	0.54
1:A:174:VAL:O	1:A:176:LEU:N	2.41	0.54
1:A:574:GLU:O	1:A:578:LYS:HG3	2.08	0.54
1:A:18:ALA:O	1:A:19:ASN:HB3	2.09	0.53
1:A:330:MET:HE3	1:A:565:VAL:HA	1.91	0.53
1:B:227:ILE:CG2	1:B:227:ILE:O	2.55	0.53
1:B:321:TYR:HD2	1:B:359:ALA:HB2	1.73	0.53
1:B:506:SER:O	1:B:528:THR:HG21	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:N	1:A:75:PRO:HD2	2.23	0.53
1:B:551:ILE:HD11	1:B:593:LEU:HD12	1.90	0.53
1:B:549:TYR:HA	1:B:589:ALA:HB1	1.91	0.53
1:B:276:PHE:CD1	1:B:520:VAL:HG11	2.43	0.53
1:A:551:ILE:CD1	1:A:593:LEU:HD13	2.39	0.53
1:A:634:ASN:HD22	1:A:637:ALA:HB2	1.74	0.53
1:B:70:SER:O	1:B:71:ASP:C	2.50	0.52
1:A:285:LEU:HD13	1:A:497:ARG:HD3	1.91	0.52
1:A:276:PHE:CE2	1:A:521:MET:HE2	2.44	0.52
1:B:372:GLN:HG3	1:B:487:ILE:HA	1.90	0.52
1:B:16:GLU:O	1:B:17:VAL:C	2.53	0.52
1:A:535:SER:OG	1:A:536:TYR:N	2.43	0.52
1:B:47:GLY:O	1:B:105:LEU:HA	2.10	0.52
1:B:205:GLY:O	1:B:207:PHE:N	2.43	0.51
1:B:16:GLU:CG	1:B:25:TYR:HB2	2.31	0.51
3:B:801:U5P:H2'	3:B:801:U5P:O2	2.10	0.51
1:A:90:PHE:HA	1:A:105:LEU:O	2.11	0.51
1:A:321:TYR:O	1:A:321:TYR:HD1	1.94	0.51
1:A:554:VAL:HA	1:A:567:GLN:NE2	2.25	0.51
1:A:205:GLY:CA	1:A:206:SER:OG	2.58	0.51
1:A:205:GLY:HA2	1:A:206:SER:OG	2.10	0.51
1:A:381:THR:O	1:A:385:VAL:HG23	2.11	0.51
1:B:209:PHE:O	1:B:211:ASN:N	2.43	0.51
1:A:511:TRP:HA	1:A:532:GLY:HA3	1.93	0.51
1:A:44:HIS:HD2	1:A:104:ILE:HD12	1.75	0.50
1:B:256:GLU:HB2	1:B:262:LYS:HA	1.92	0.50
1:B:107:ASP:HB3	1:B:110:SER:HB3	1.93	0.50
1:A:9:LEU:HD12	1:A:163:ILE:HG12	1.94	0.50
1:A:276:PHE:HE2	1:A:521:MET:HE2	1.76	0.50
1:A:488:LEU:C	1:A:488:LEU:HD12	2.37	0.50
1:B:191:THR:HA	1:B:245:THR:O	2.11	0.50
1:A:210:TYR:CD1	1:A:250:ILE:HD11	2.47	0.50
1:A:515:PRO:HB2	1:A:533:PHE:CD2	2.46	0.50
1:A:321:TYR:CD1	1:A:321:TYR:C	2.89	0.49
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.46	0.49
1:A:31:LYS:HE2	1:A:606:TYR:CE1	2.47	0.49
1:A:134:ASP:OD1	1:A:137:THR:CB	2.60	0.49
1:B:386:THR:HA	1:B:389:ILE:HD12	1.94	0.49
1:A:482:ASN:O	1:A:485:ASN:HB2	2.11	0.49
1:B:150:PHE:O	1:B:154:VAL:HG23	2.11	0.49
1:B:443:VAL:HG13	1:B:445:HIS:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:THR:HG22	1:A:246:THR:HG22	1.93	0.49
1:B:492:TYR:CD1	3:B:801:U5P:N3	2.81	0.49
1:B:135:PHE:H	1:B:135:PHE:HD2	1.59	0.49
1:B:599:TRP:C	1:B:601:ARG:H	2.20	0.49
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.95	0.49
1:A:488:LEU:HD11	1:A:490:LEU:CD1	2.43	0.49
1:B:302:HIS:CE1	1:B:434:ARG:HH11	2.30	0.49
1:A:128:ILE:CG2	1:A:129:PRO:HD2	2.38	0.48
1:A:463:GLN:HA	1:A:465:PHE:CE2	2.47	0.48
1:A:8:HIS:HB2	1:A:162:ALA:O	2.13	0.48
1:B:296:PHE:HB2	1:B:488:LEU:HD12	1.95	0.48
1:A:79:ALA:O	1:A:83:MET:CG	2.62	0.48
1:A:471:ARG:HE	1:A:471:ARG:CA	2.21	0.48
1:B:256:GLU:CD	1:B:262:LYS:HB2	2.38	0.48
1:B:516:ALA:O	1:B:520:VAL:HG23	2.13	0.48
1:B:67:GLU:H	1:B:67:GLU:CD	2.21	0.48
1:B:273:VAL:HG12	1:B:274:ILE:HG12	1.95	0.48
1:B:614:LEU:O	1:B:615:ARG:C	2.56	0.48
1:A:83:MET:O	1:A:88:VAL:HB	2.14	0.48
1:B:611:GLN:HE21	1:B:611:GLN:HA	1.79	0.48
1:A:447:MET:HG3	1:A:456:LEU:CD1	2.42	0.48
1:B:16:GLU:HG2	1:B:25:TYR:N	2.28	0.47
1:B:434:ARG:NH2	1:B:440:PRO:HA	2.24	0.47
1:A:321:TYR:HD1	1:A:321:TYR:C	2.22	0.47
1:A:526:ILE:HG21	1:A:568:LEU:CD1	2.44	0.47
1:B:314:TYR:N	1:B:500:HIS:CD2	2.59	0.47
1:B:349:LYS:O	1:B:471:ARG:HG3	2.14	0.47
1:A:132:GLU:HA	1:A:132:GLU:OE1	2.13	0.47
1:A:296:PHE:HA	1:A:372:GLN:OE1	2.14	0.47
1:B:63:TRP:H	1:B:63:TRP:CD1	2.33	0.47
1:A:63:TRP:H	1:A:63:TRP:CD1	2.30	0.47
1:A:174:VAL:C	1:A:176:LEU:H	2.22	0.47
1:A:207:PHE:C	1:A:209:PHE:N	2.71	0.47
1:B:250:ILE:HD12	1:B:250:ILE:HA	1.59	0.47
1:A:16:GLU:HG3	1:A:21:VAL:HB	1.95	0.47
1:A:119:LYS:O	1:A:123:TRP:CE3	2.68	0.47
1:A:209:PHE:C	1:A:211:ASN:H	2.22	0.47
1:B:302:HIS:CD2	1:B:371:GLY:HA2	2.49	0.47
1:B:63:TRP:CZ2	1:B:90:PHE:HZ	2.32	0.47
1:B:620:ASP:HB3	1:B:623:ARG:HH21	1.79	0.47
1:A:25:TYR:C	1:A:25:TYR:CD2	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:SER:HA	1:A:266:ILE:HD11	1.95	0.47
1:B:44:HIS:HD2	1:B:104:ILE:CD1	2.28	0.47
1:A:29:LYS:HG3	1:A:97:ILE:CD1	2.43	0.47
1:B:181:LYS:C	1:B:183:ARG:H	2.23	0.47
1:B:323:TYR:CD1	1:B:323:TYR:C	2.92	0.47
1:B:125:LEU:O	1:B:126:VAL:HG23	2.15	0.46
1:B:302:HIS:CE1	1:B:434:ARG:NH1	2.83	0.46
1:B:388:SER:HB3	1:B:392:ARG:NH1	2.30	0.46
1:A:419:SER:O	1:A:423:VAL:HG23	2.16	0.46
1:B:364:PHE:HB2	1:B:369:LEU:HD21	1.97	0.46
1:A:537:MET:HG2	1:A:551:ILE:HD13	1.98	0.46
1:B:537:MET:HE2	1:B:593:LEU:HD13	1.97	0.46
1:A:557:ARG:HD3	1:A:558:PHE:CE2	2.51	0.46
1:A:482:ASN:OD1	1:A:484:ASN:ND2	2.49	0.46
1:A:365:THR:HG23	1:A:368:ALA:HB2	1.98	0.46
1:A:219:ASP:O	1:A:221:GLU:N	2.48	0.46
1:A:513:TYR:HB2	2:A:801:UDP:O1A	2.16	0.46
1:A:97:ILE:O	1:A:98:GLU:C	2.58	0.45
1:A:420:SER:O	1:A:424:MET:HG2	2.16	0.45
1:A:143:LEU:O	1:A:147:VAL:HG23	2.17	0.45
1:A:319:GLY:O	1:A:320:ARG:C	2.60	0.45
1:B:192:THR:CG2	1:B:246:THR:HG22	2.46	0.45
1:A:16:GLU:HB3	1:A:25:TYR:HB2	1.99	0.45
1:B:32:ALA:O	1:B:33:PRO:C	2.56	0.45
1:B:63:TRP:CZ2	1:B:90:PHE:CZ	3.05	0.45
1:B:189:ILE:HD11	1:B:610:ARG:HA	1.99	0.45
1:B:92:TYR:OH	1:B:102:LYS:HD3	2.16	0.45
1:A:3:ARG:HD3	1:A:185:ASP:OD2	2.16	0.45
1:A:330:MET:HE2	1:A:568:LEU:HD22	1.99	0.45
1:B:317:ILE:HG13	1:B:503:VAL:O	2.16	0.45
1:A:366:VAL:CG1	1:A:367:GLU:N	2.79	0.45
1:B:274:ILE:C	1:B:276:PHE:N	2.75	0.45
1:A:217:ASP:CG	1:A:220:HIS:HB3	2.40	0.45
1:A:425:LEU:O	1:A:429:ILE:HG13	2.17	0.45
1:B:49:LEU:HD11	1:B:54:TYR:CG	2.52	0.45
1:B:50:ASN:O	1:B:52:ALA:N	2.49	0.45
1:B:484:ASN:N	1:B:484:ASN:HD22	2.13	0.45
1:A:221:GLU:O	1:A:225:PHE:HD2	1.99	0.45
1:A:484:ASN:HD22	1:A:484:ASN:N	2.14	0.45
1:A:551:ILE:CD1	1:A:593:LEU:CD1	2.95	0.45
1:B:299:GLY:HA2	1:B:375:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:O	1:A:19:ASN:N	2.50	0.44
1:A:542:GLU:CB	1:A:545:GLN:HE21	2.30	0.44
1:A:339:ASN:O	1:A:343:LYS:HG2	2.18	0.44
1:B:276:PHE:HD1	1:B:520:VAL:HG11	1.81	0.44
1:B:302:HIS:CD2	1:B:434:ARG:HH12	2.35	0.44
1:B:338:LEU:HG	1:B:342:LEU:HD12	1.98	0.44
1:B:471:ARG:CZ	1:B:471:ARG:HA	2.47	0.44
1:A:615:ARG:HE	1:A:632:ASP:HB3	1.82	0.44
1:B:211:ASN:O	1:B:213:LEU:N	2.49	0.44
1:B:12:GLU:O	1:B:45:LEU:HA	2.17	0.44
1:B:291:GLU:HA	1:B:294:ASN:HD22	1.83	0.44
1:B:481:LEU:HD22	1:B:488:LEU:HD23	1.99	0.44
1:B:253:PHE:O	1:B:254:GLU:C	2.57	0.44
1:B:307:PHE:CD1	1:B:350:THR:HG21	2.53	0.44
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.80	0.44
1:B:330:MET:HE2	1:B:568:LEU:HD22	1.99	0.44
1:B:463:GLN:HA	1:B:465:PHE:HE2	1.83	0.44
1:B:620:ASP:HB3	1:B:623:ARG:NH2	2.33	0.44
1:A:294:ASN:OD1	1:A:309:LEU:HD13	2.18	0.44
1:A:449:ASP:CG	1:A:452:ASN:HD22	2.26	0.44
1:A:526:ILE:HG21	1:A:568:LEU:HD12	2.00	0.44
1:A:31:LYS:O	1:A:32:ALA:C	2.61	0.44
1:A:248:SER:CB	1:A:532:GLY:HA2	2.48	0.44
1:B:16:GLU:OE2	1:B:24:ILE:HB	2.17	0.44
1:B:61:LEU:HB2	1:B:93:GLY:HA2	1.99	0.44
1:A:502:GLY:O	1:A:525:SER:HA	2.17	0.43
1:B:95:TRP:O	1:B:100:ALA:HA	2.18	0.43
1:A:17:VAL:O	1:A:18:ALA:C	2.60	0.43
1:A:64:LYS:HE2	1:A:84:GLU:OE2	2.18	0.43
1:A:357:MET:O	1:A:478:PRO:HA	2.18	0.43
1:A:557:ARG:HD3	1:A:558:PHE:CZ	2.53	0.43
2:A:801:UDP:O1B	2:A:801:UDP:C5'	2.65	0.43
1:B:225:PHE:N	1:B:225:PHE:CD2	2.87	0.43
1:B:549:TYR:HA	1:B:589:ALA:CB	2.48	0.43
1:A:458:LYS:HD3	1:A:458:LYS:C	2.44	0.43
1:B:112:ARG:C	1:B:114:TYR:H	2.26	0.43
1:B:112:ARG:O	1:B:115:SER:HB2	2.19	0.43
1:A:170:TRP:CH2	1:A:171:LEU:HD23	2.54	0.43
1:B:273:VAL:HB	1:B:598:ASP:OD1	2.19	0.43
1:B:378:LEU:O	1:B:382:VAL:HG23	2.18	0.43
1:B:444:THR:OG1	1:B:445:HIS:HD2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:GLU:O	1:B:377:ALA:HB3	2.19	0.43
1:B:449:ASP:OD1	1:B:452:ASN:ND2	2.46	0.43
1:A:216:VAL:CG1	1:A:221:GLU:HG3	2.49	0.43
1:A:330:MET:HG2	1:A:565:VAL:HG22	2.01	0.43
1:B:443:VAL:HG22	1:B:476:PHE:HD2	1.83	0.43
1:B:325:ASN:HA	1:B:507:TYR:HB3	2.01	0.43
1:B:443:VAL:CG1	1:B:445:HIS:H	2.31	0.43
1:A:207:PHE:O	1:A:208:ASP:C	2.59	0.42
1:A:399:ARG:HG2	1:A:399:ARG:NH1	2.28	0.42
1:A:12:GLU:HB3	1:A:45:LEU:HD23	2.00	0.42
1:A:36:VAL:O	1:A:36:VAL:HG12	2.17	0.42
1:A:170:TRP:HB3	1:A:234:GLU:HG3	2.01	0.42
1:A:293:ILE:O	1:A:294:ASN:C	2.62	0.42
1:B:285:LEU:HD13	1:B:497:ARG:HD2	2.01	0.42
1:A:269:ASN:HD22	1:A:511:TRP:CD1	2.38	0.42
1:A:289:LYS:NZ	1:A:494:GLU:HG2	2.34	0.42
1:A:290:LYS:HE2	1:A:314:TYR:CE2	2.54	0.42
1:A:545:GLN:O	1:A:549:TYR:CD2	2.72	0.42
1:B:65:LYS:HB2	1:B:65:LYS:HE3	1.75	0.42
1:B:618:TYR:HB3	1:B:621:GLN:HB2	2.01	0.42
1:A:8:HIS:CD2	1:A:164:VAL:HG23	2.50	0.42
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.35	0.42
1:B:79:ALA:O	1:B:83:MET:HG2	2.19	0.42
1:B:294:ASN:O	1:B:298:ARG:HG3	2.19	0.42
1:B:581:ARG:O	1:B:582:GLN:C	2.63	0.42
1:A:617:GLY:C	1:A:619:PRO:HD3	2.44	0.42
1:B:296:PHE:CB	1:B:488:LEU:HD12	2.50	0.42
1:B:443:VAL:CG2	1:B:476:PHE:HD2	2.32	0.42
1:B:514:THR:O	1:B:518:CYS:HB2	2.20	0.42
1:B:44:HIS:CD2	1:B:104:ILE:HD12	2.53	0.42
1:B:123:TRP:CH2	1:B:229:HIS:HB2	2.54	0.42
1:B:153:GLU:O	1:B:157:LEU:HD13	2.20	0.42
1:B:325:ASN:ND2	1:B:325:ASN:H	2.17	0.42
1:B:513:TYR:O	1:B:517:GLU:HG2	2.19	0.42
1:A:62:ASP:HB3	1:A:65:LYS:HD2	2.02	0.42
1:A:615:ARG:O	1:A:617:GLY:N	2.53	0.42
1:B:49:LEU:HD11	1:B:54:TYR:CD1	2.54	0.42
1:B:60:ILE:HG13	1:B:61:LEU:N	2.30	0.42
1:B:299:GLY:O	1:B:302:HIS:HD2	2.02	0.42
1:A:208:ASP:O	1:A:211:ASN:HB2	2.20	0.42
1:A:271:LEU:O	1:A:598:ASP:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:CD2	1:A:231:TYR:C	2.98	0.42
1:A:252:ALA:CB	1:A:263:PRO:HG2	2.50	0.42
1:A:344:VAL:C	1:A:346:GLY:N	2.73	0.42
1:B:510:PRO:O	1:B:532:GLY:HA3	2.20	0.42
1:B:618:TYR:O	1:B:621:GLN:HB2	2.20	0.42
1:A:73:MET:C	1:A:75:PRO:HD2	2.45	0.41
1:A:219:ASP:O	1:A:222:ALA:N	2.53	0.41
1:A:335:LEU:HD12	1:A:335:LEU:HA	1.93	0.41
1:A:483:ALA:HA	1:A:490:LEU:C	2.45	0.41
1:B:39:TYR:HB2	1:B:43:TYR:HB2	2.02	0.41
1:A:149:TRP:CD1	1:A:149:TRP:C	2.98	0.41
1:A:208:ASP:HB3	1:A:211:ASN:CB	2.39	0.41
1:B:231:TYR:C	1:B:231:TYR:HD2	2.27	0.41
1:B:426:LYS:O	1:B:430:LEU:HG	2.20	0.41
1:A:443:VAL:HG13	1:A:456:LEU:CD2	2.37	0.41
1:A:63:TRP:O	1:A:77:GLN:NE2	2.53	0.41
1:A:330:MET:HE2	1:A:330:MET:HB3	1.84	0.41
1:B:46:ILE:HG21	1:B:147:VAL:HG13	2.01	0.41
1:B:131:PRO:C	1:B:133:ASN:N	2.77	0.41
1:B:225:PHE:N	1:B:225:PHE:HD2	2.18	0.41
1:B:312:THR:HA	1:B:350:THR:O	2.20	0.41
1:B:488:LEU:O	1:B:490:LEU:N	2.53	0.41
1:A:47:GLY:O	1:A:105:LEU:HA	2.21	0.41
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.56	0.41
1:A:176:LEU:HB2	1:A:177:PRO:HD3	2.01	0.41
1:A:219:ASP:O	1:A:220:HIS:C	2.64	0.41
1:A:269:ASN:HD22	1:A:511:TRP:CG	2.38	0.41
1:A:316:PHE:CZ	1:A:496:VAL:HG13	2.55	0.41
1:A:636:ASP:O	1:A:637:ALA:C	2.64	0.41
1:B:29:LYS:HA	1:B:97:ILE:HD12	2.02	0.41
1:A:174:VAL:C	1:A:176:LEU:N	2.78	0.41
1:A:327:GLY:HA3	1:A:505:PRO:O	2.21	0.41
1:A:385:VAL:O	1:A:389:ILE:HG13	2.21	0.41
1:A:458:LYS:HD3	1:A:458:LYS:O	2.20	0.41
1:A:598:ASP:O	1:A:599:TRP:C	2.63	0.41
1:A:602:MET:H	1:A:602:MET:HG2	1.70	0.41
1:B:180:ARG:NH2	1:B:242:ASP:OD1	2.54	0.41
1:B:189:ILE:HG12	1:B:243:VAL:HB	2.03	0.41
1:B:193:HIS:O	1:B:194:ALA:HB2	2.20	0.41
1:B:325:ASN:O	1:B:507:TYR:N	2.34	0.41
1:B:593:LEU:HD23	1:B:593:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLY:HA3	1:B:174:VAL:CG1	2.50	0.41
1:A:154:VAL:HG12	1:A:163:ILE:HD13	2.03	0.40
1:A:252:ALA:HB1	1:A:263:PRO:HG2	2.03	0.40
1:A:336:ALA:HB2	1:A:462:VAL:HB	2.03	0.40
1:A:263:PRO:C	1:A:265:GLY:H	2.28	0.40
1:B:355:ILE:HB	1:B:476:PHE:HD1	1.87	0.40
1:A:503:VAL:HG12	1:A:505:PRO:HD3	2.04	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	613/725 (85%)	512 (84%)	79 (13%)	22 (4%)	2	17
1	B	600/725 (83%)	502 (84%)	73 (12%)	25 (4%)	2	14
All	All	1213/1450 (84%)	1014 (84%)	152 (12%)	47 (4%)	2	16

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	18	ALA
1	A	126	VAL
1	A	208	ASP
1	A	218	VAL
1	A	543	THR
1	A	616	ARG
1	B	131	PRO
1	B	194	ALA
1	B	206	SER
1	B	436	GLU

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Mol	Chain	Res	Type
1	B	543	THR
1	A	107	ASP
1	A	175	ALA
1	A	203	ALA
1	A	220	HIS
1	A	435	PRO
1	B	54	TYR
1	B	182	ARG
1	B	207	PHE
1	B	208	ASP
1	B	212	CYS
1	B	344	VAL
1	B	559	LYS
1	A	19	ASN
1	A	98	GLU
1	A	615	ARG
1	B	183	ARG
1	B	275	LYS
1	A	207	PHE
1	B	40	LYS
1	B	175	ALA
1	B	209	PHE
1	B	210	TYR
1	A	129	PRO
1	A	436	GLU
1	A	600	LYS
1	B	126	VAL
1	B	558	PHE
1	A	345	SER
1	B	132	GLU
1	B	489	GLY
1	A	21	VAL
1	B	129	PRO
1	B	435	PRO
1	B	448	VAL
1	A	346	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	502/623 (81%)	449 (89%)	53 (11%)	6	24
1	B	484/623 (78%)	408 (84%)	76 (16%)	2	12
All	All	986/1246 (79%)	857 (87%)	129 (13%)	4	17

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	ARG
1	A	35	THR
1	A	69	PHE
1	A	83	MET
1	A	86	ARG
1	A	104	ILE
1	A	125	LEU
1	A	184	ILE
1	A	187	VAL
1	A	192	THR
1	A	202	CYS
1	A	212	CYS
1	A	214	GLU
1	A	218	VAL
1	A	235	ARG
1	A	254	GLU
1	A	266	ILE
1	A	283	GLN
1	A	288	LEU
1	A	289	LYS
1	A	290	LYS
1	A	306	ASP
1	A	320	ARG
1	A	322	GLU
1	A	335	LEU
1	A	349	LYS
1	A	363	SER
1	A	379	GLU
1	A	395	ASP
1	A	399	ARG
1	A	419	SER
1	A	426	LYS

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Mol	Chain	Res	Type
1	A	434	ARG
1	A	448	VAL
1	A	454	LEU
1	A	458	LYS
1	A	479	GLU
1	A	484	ASN
1	A	485	ASN
1	A	487	ILE
1	A	488	LEU
1	A	504	PHE
1	A	513	TYR
1	A	544	ASN
1	A	554	VAL
1	A	556	ARG
1	A	594	SER
1	A	621	GLN
1	A	626	VAL
1	A	629	GLU
1	A	634	ASN
1	A	636	ASP
1	B	2	SER
1	B	3	ARG
1	B	6	GLN
1	B	12	GLU
1	B	15	THR
1	B	16	GLU
1	B	17	VAL
1	B	20	ARG
1	B	24	ILE
1	B	26	SER
1	B	31	LYS
1	B	38	GLN
1	B	40	LYS
1	B	50	ASN
1	B	60	ILE
1	B	61	LEU
1	B	65	LYS
1	B	67	GLU
1	B	74	ARG
1	B	81	GLN
1	B	88	VAL
1	B	104	ILE

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Mol	Chain	Res	Type
1	B	105	LEU
1	B	108	LEU
1	B	109	ASP
1	B	112	ARG
1	B	143	LEU
1	B	161	HIS
1	B	174	VAL
1	B	177	PRO
1	B	184	ILE
1	B	231	TYR
1	B	242	ASP
1	B	249	GLN
1	B	250	ILE
1	B	258	LEU
1	B	266	ILE
1	B	272	ASN
1	B	273	VAL
1	B	274	ILE
1	B	289	LYS
1	B	317	ILE
1	B	325	ASN
1	B	335	LEU
1	B	337	ARG
1	B	343	LYS
1	B	363	SER
1	B	369	LEU
1	B	370	LYS
1	B	376	ARG
1	B	381	THR
1	B	395	ASP
1	B	398	ILE
1	B	399	ARG
1	B	419	SER
1	B	423	VAL
1	B	425	LEU
1	B	428	ARG
1	B	443	VAL
1	B	458	LYS
1	B	469	SER
1	B	471	ARG
1	B	472	VAL
1	B	484	ASN

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Mol	Chain	Res	Type
1	B	487	ILE
1	B	518	CYS
1	B	530	VAL
1	B	537	MET
1	B	554	VAL
1	B	556	ARG
1	B	582	GLN
1	B	588	ASN
1	B	594	SER
1	B	596	LEU
1	B	620	ASP
1	B	621	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	56	ASN
1	A	81	GLN
1	A	138	ASN
1	A	156	HIS
1	A	249	GLN
1	A	257	HIS
1	A	269	ASN
1	A	283	GLN
1	A	445	HIS
1	A	452	ASN
1	A	484	ASN
1	A	485	ASN
1	A	500	HIS
1	A	544	ASN
1	A	545	GLN
1	A	567	GLN
1	A	582	GLN
1	A	634	ASN
1	B	6	GLN
1	B	7	ASN
1	B	44	HIS
1	B	50	ASN
1	B	77	GLN
1	B	89	HIS
1	B	257	HIS

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Mol	Chain	Res	Type
1	B	294	ASN
1	B	300	HIS
1	B	302	HIS
1	B	325	ASN
1	B	372	GLN
1	B	445	HIS
1	B	482	ASN
1	B	484	ASN
1	B	500	HIS
1	B	611	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	UDP	A	801	-	25,26,26	1.05	1 (4%)	38,40,40	1.78	6 (15%)
3	U5P	B	801	-	22,22,22	2.55	5 (22%)	32,33,33	1.82	7 (21%)

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	UDP	A	801	-	-	2/16/32/32	0/2/2/2
3	U5P	B	801	-	-	9/10/26/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	U5P	O2-C2	8.70	1.38	1.23
3	B	801	U5P	O4-C4	5.93	1.36	1.24
3	B	801	U5P	C2-N1	3.50	1.43	1.38
3	B	801	U5P	C6-C5	2.56	1.41	1.35
2	A	801	UDP	C6-C5	2.31	1.40	1.35
3	B	801	U5P	C4-N3	-2.19	1.34	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	UDP	C4-N3-C2	-5.58	119.68	126.61
3	B	801	U5P	C4-N3-C2	-4.68	120.81	126.61
2	A	801	UDP	N3-C2-N1	4.62	120.91	114.89
3	B	801	U5P	C5-C4-N3	4.43	121.00	114.80
2	A	801	UDP	C5-C4-N3	3.86	120.21	114.80
2	A	801	UDP	O2-C2-N1	-3.57	118.15	122.80
3	B	801	U5P	N3-C2-N1	3.44	119.37	114.89
2	A	801	UDP	O4-C4-C5	-2.51	120.83	125.16
3	B	801	U5P	C3'-C2'-C1'	2.35	105.90	101.46
3	B	801	U5P	O3P-P-O2P	2.23	116.18	107.80
2	A	801	UDP	C4'-O4'-C1'	-2.22	104.56	109.47
3	B	801	U5P	O4-C4-N3	-2.19	116.10	119.27
3	B	801	U5P	O2-C2-N3	-2.04	117.73	121.49

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	U5P	C5'-O5'-P-O1P
3	B	801	U5P	C5'-O5'-P-O2P
3	B	801	U5P	C5'-O5'-P-O3P

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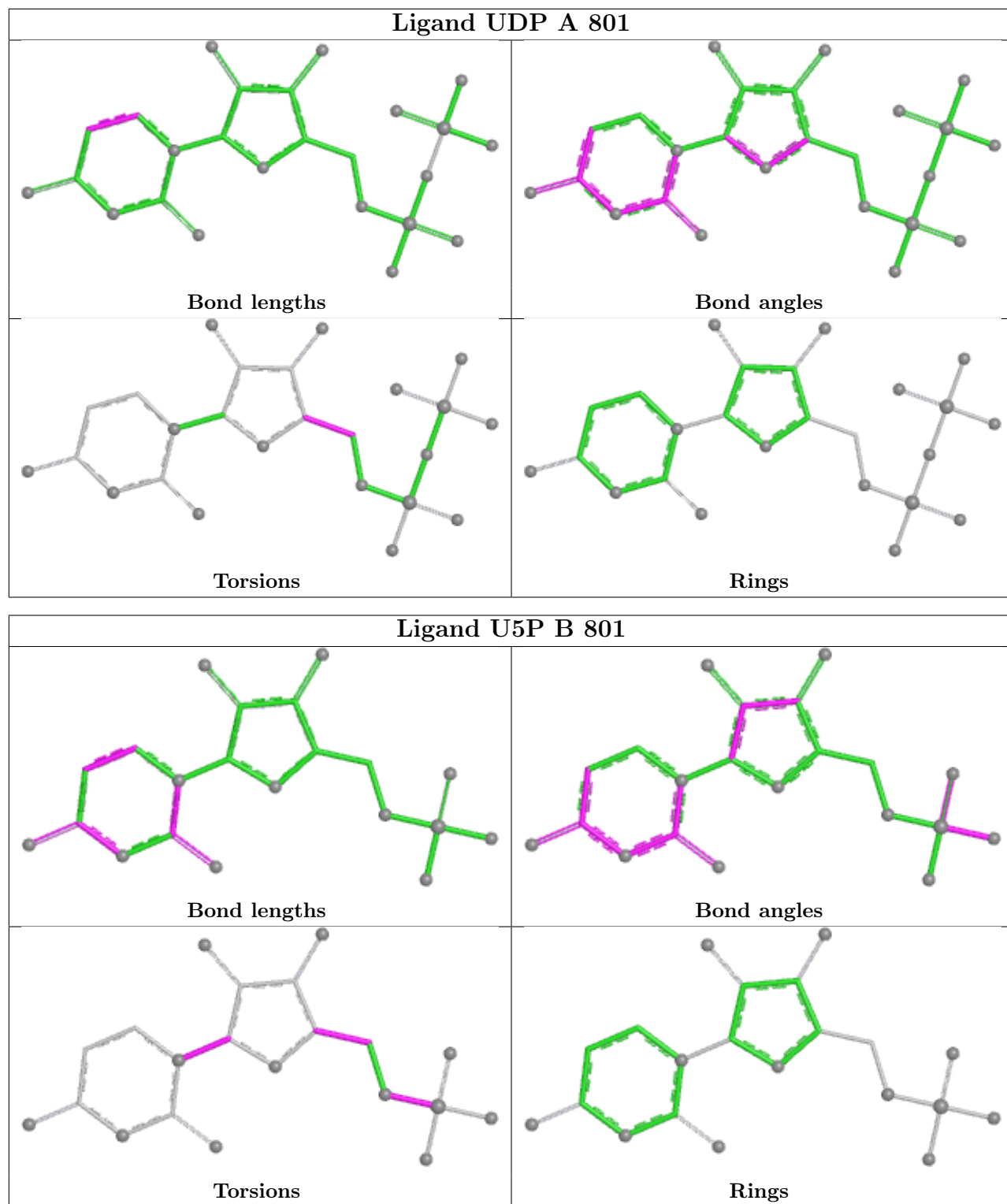
Mol	Chain	Res	Type	Atoms
2	A	801	UDP	C3'-C4'-C5'-O5'
2	A	801	UDP	O4'-C4'-C5'-O5'
3	B	801	U5P	O4'-C1'-N1-C6
3	B	801	U5P	O4'-C4'-C5'-O5'
3	B	801	U5P	C2'-C1'-N1-C6
3	B	801	U5P	C2'-C1'-N1-C2
3	B	801	U5P	O4'-C1'-N1-C2
3	B	801	U5P	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	UDP	3	0
3	B	801	U5P	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

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 [i](#)

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

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	619/725 (85%)	-1.36	0	100 100	71, 106, 145, 176	0
1	B	606/725 (83%)	-1.30	1 (0%)	91 86	73, 110, 154, 204	0
All	All	1225/1450 (84%)	-1.33	1 (0%)	92 90	71, 108, 150, 204	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	GLN	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

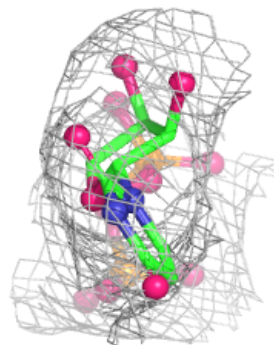
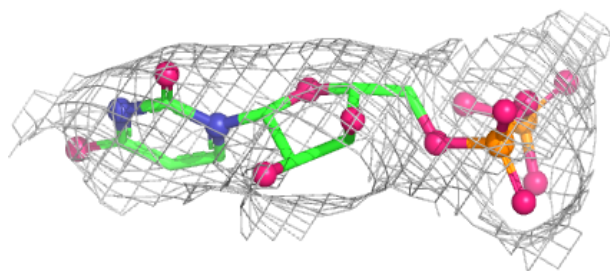
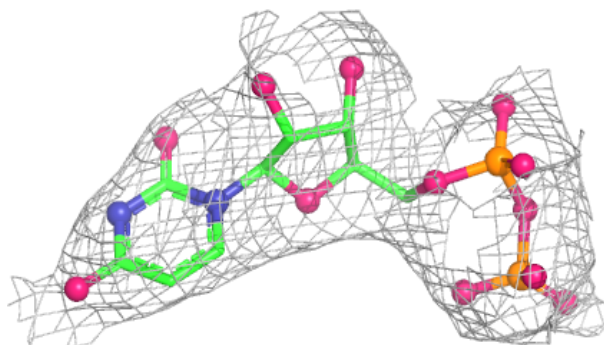
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UDP	A	801	25/25	0.99	0.03	92,121,165,169	0
3	U5P	B	801	21/21	0.99	0.04	88,108,120,130	0

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.

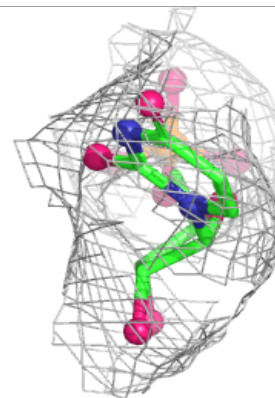
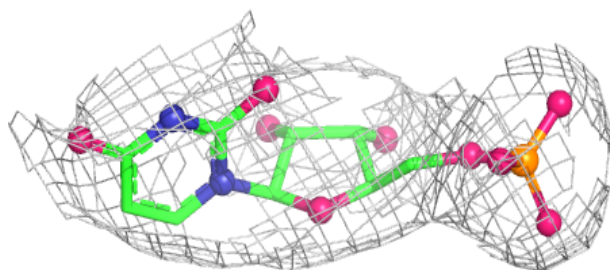
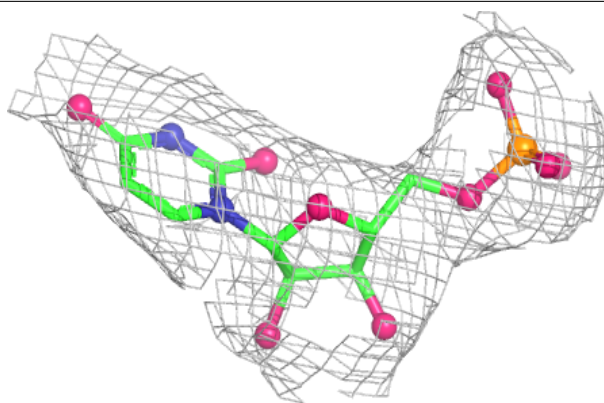
Electron density around UDP A 801:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.