



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:26 pm BST

PDB ID : 5SUL
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

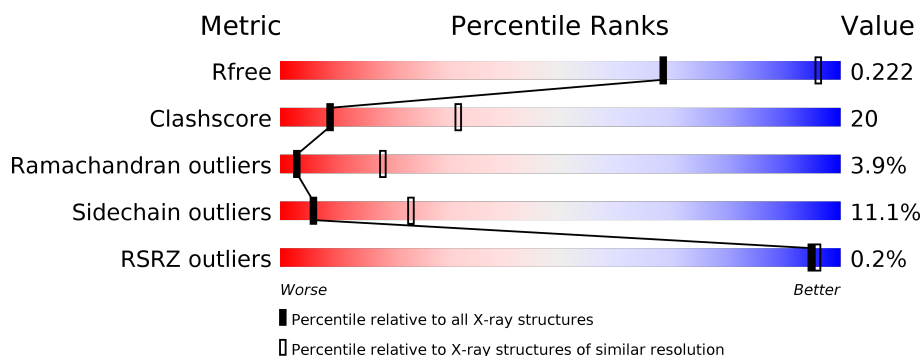
1 Overall quality at a glance ⓘ

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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:

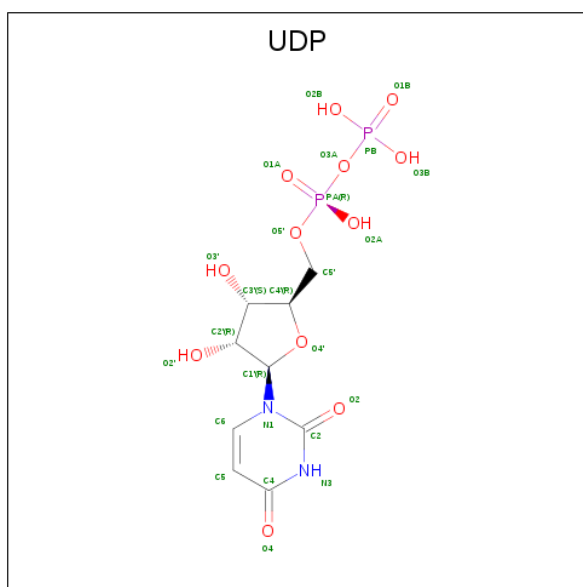
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression 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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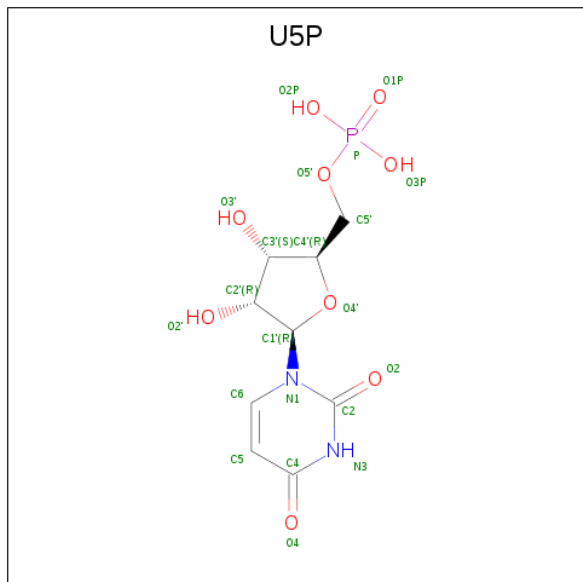
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	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 (three-letter code: 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 (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).

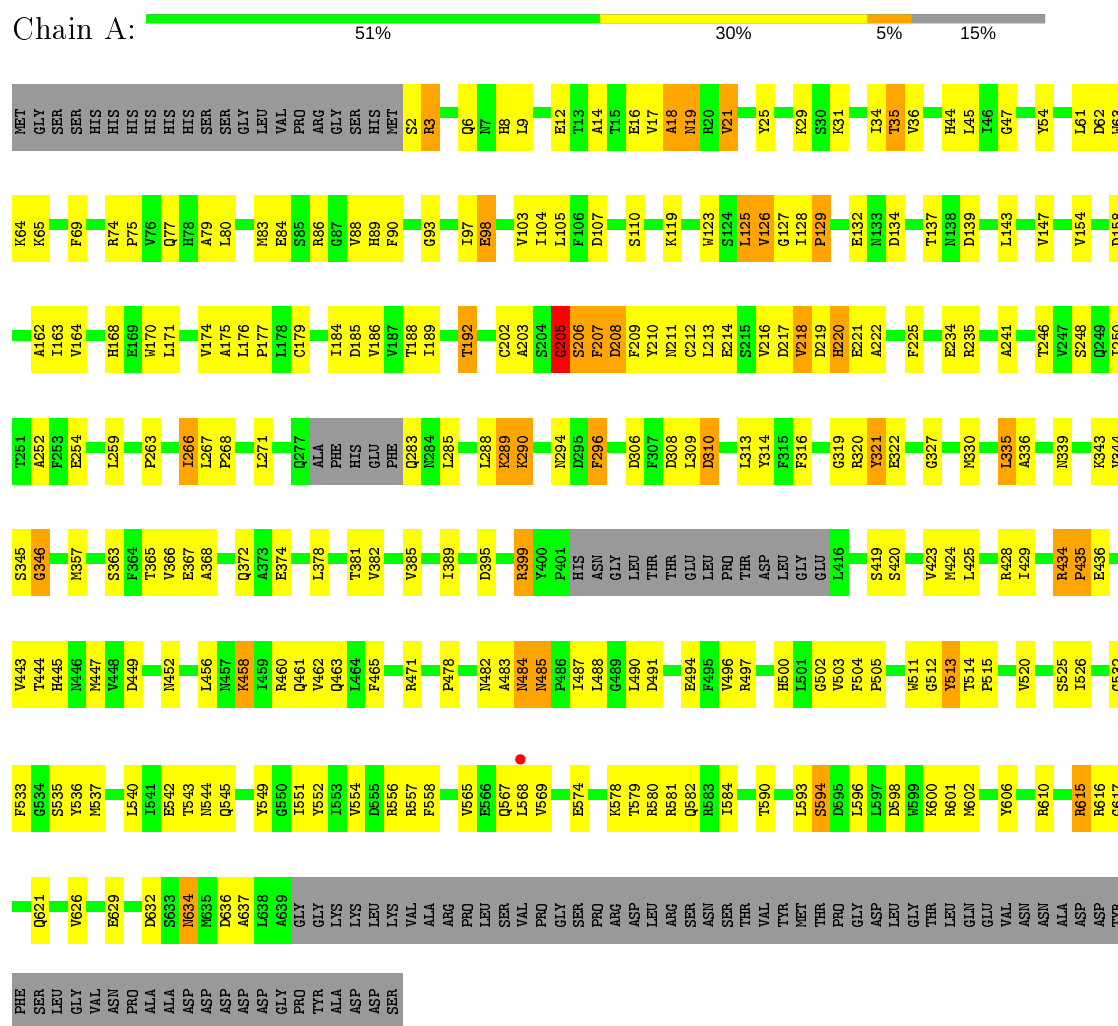


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	21	9	2	9	1	0	0

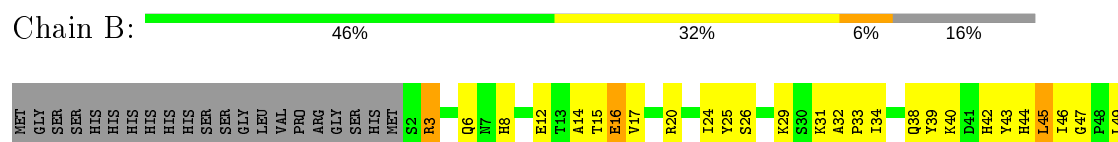
3 Residue-property plots

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

- Molecule 1: Glycogen [starch] synthase isoform 2



- Molecule 1: Glycogen [starch] synthase isoform 2



ASP	T543	L464	T387	G226	P129	N50
ASP	N544	F465	S388	I227	S130	A52
ASP	LEU		I389	I228	P131	T53
GLY	Y549	S469		E229	E132	Y54
PRO	G550	D470	R392	R230	N133	
GLY	I551	R471		Y231	D134	T60
LYS		K472	D395		F135	L61
LYS	R556	K473		A237		L61
ASP	R557		I398	A238		N63
LEU	R558	F476	R399	E239	L142	D62
LYS	K559	H477	Y400	E239	L143	X63
VAL	A560	P478	K324		G144	X64
ALA		F401	N325	D242		X65
ARG		E479	H15	V243		P66
ARG	E563	F480	ASN	F244	V147	E67
PRO	S564	L481	GLY	T245		
LEU	SER		A328	T246		S70
SER	V565		D329		F150	D71
VAL			LEU			
VAL	V569		THR		E153	R74
PRO			THR	Q249	V154	
GLY		I487	GLU	I250		P75
SER	Q582	L488	LEU		L157	V76
PRO		G489	PRO	F253	D158	Q77
ARG	R587	R490	THR	E254		H78
ALA	N588	D491	ASP	L255		A79
ALA	A589	Y492	LEU	E256	H161	
LEU			LEU	E257	A162	
ARG	T590	R497	GLY	L258	I163	X63
SER	E591	G498				
ASN	A592	C499	K343			
SER	L593	H500	S345	R261	H168	V68
THR	S594		G346	K262		H89
VAL	D595					F90
TYR	L596	V503	K349	V273	V174	V91
MET	L597	F504	T350	I274	A175	Y92
THR	D598	R427	V351	K275	L176	G93
PRO	N599	P505	R428	K276	R180	N94
GLY	K600	S506	I429	F276	K181	X95
GLY		Y507	L430	Q277	R182	L96
ASP	R601			ALA		I97
LEU		P510	R434	PHE	R183	
GLY	R610	W511	P435	H15	I184	
THR	Q611	G512	E436	GLU	D185	A100
LEU		Y513		PHE	V186	P101
GLN	L614	T514	P440	GLN	V187	K102
GLU	R615	P515	P441		T188	V103
VAL		A516	S363	L285	I189	I104
VAL	Y618	E517	V443		F190	L105
ASN	P619	C518	T444	K289	T191	F106
ALA	D620	T519	R445	K290	T192	D107
ASP	Q621	V520	N446	E291	H193	L108
ASP	F622	M521	N447		A194	D109
TYR	R623	G522	Q372	N294	S110	
PHE			V448			
SER			D449	D295	V111	G205
THR	V626	T528	A373	D295	S206	R112
LEU	GLY	N529	E374	F296	F207	
GLY	GLU	V530	V375	V297	D208	S115
VAL	GLU	S531	R376	R298	F209	
ASN	LEU	G532	A377	G299	Y210	D121
ASN	ASN		L378		M211	L122
ASP	ASP	M537	T381		C212	M123
ALA	ALA		V382	F307	L213	S124
ASP	ASN	I541	V462	X608		L125
ASP	ASN	E542	D462	I203		V126

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 0.158 , 0.222	Depositor DCC
R_{free} test set	1854 reflections (5.00%)	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 , 57.1	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 [i](#)

5.1 Standard geometry [i](#)

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	0.59	3/4964 (0.1%)	0.81	1/6752 (0.0%)
1	B	0.57	0/4836	0.79	1/6586 (0.0%)
All	All	0.58	3/9800 (0.0%)	0.80	2/13338 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLY	C-O	6.11	1.33	1.23
1	A	206	SER	CB-OG	5.92	1.50	1.42
1	A	206	SER	CA-CB	5.30	1.60	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLY	C-N-CA	-8.22	101.14	121.70
1	B	597	LEU	CA-CB-CG	5.44	127.81	115.30

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4849	0	4605	190	0
1	B	4720	0	4446	186	0
2	A	25	0	11	3	0
3	B	21	0	11	4	0
All	All	9615	0	9073	379	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 20.

All (379) 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:HA	1:A:471:ARG:HE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE	1:A:471:ARG:HA	2.03	0.73
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:HA	1:A:374:GLU:OE1	1.87	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:565:VAL:O	1:A:569:VAL:HG23	1.92	0.69
1:A:549:TYR:O	1:A:590:THR:HG22	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:B:50:ASN:C	1:B:50:ASN:HD22	1.96	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:TYR:CD1	1:A:321:TYR:O	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: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
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:H	1:A:484:ASN:HD22	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:A:344:VAL:C	1:A:346:GLY:H	2.06	0.59
1:B:321:TYR:HB2	1:B:358:PRO:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:234:GLU:OE2	1:A:259:LEU:HD21	2.05	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
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: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: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:A:485:ASN:HD22	1:A:487:ILE:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:227:ILE:O	1:B:227:ILE:CG2	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
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:231:TYR:C	1:B:231:TYR:CD2	2.82	0.53
1:A:285:LEU:HD13	1:A:497:ARG:HD3	1.91	0.52
1:B:372:GLN:HG3	1:B:487:ILE:HA	1.90	0.52
1:A:535:SER:OG	1:A:536:TYR:N	2.43	0.52
1:B:131:PRO:C	1:B:133:ASN:H	2.12	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:B:50:ASN:C	1:B:50:ASN:ND2	2.63	0.51
1:A:321:TYR:HD1	1:A:321:TYR:O	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:B:274:ILE:C	1:B:276:PHE:H	2.15	0.50
1:A:9:LEU:HD12	1:A:163:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:463:GLN:HA	1:B:465:PHE:CE2	2.46	0.49
1:A:134:ASP:OD1	1:A:137:THR:CB	2.60	0.49
1:A:31:LYS:HE2	1:A:606:TYR:CE1	2.47	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
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:HD2	1:B:135:PHE:H	1.59	0.49
1:A:488:LEU:HD11	1:A:490:LEU:CD1	2.43	0.49
1:A:189:ILE:HD11	1:A:610:ARG:HA	1.95	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:CA	1:A:471:ARG:HE	2.21	0.48
1:B:516:ALA:O	1:B:520:VAL:HG23	2.13	0.48
1:B:273:VAL:HG12	1:B:274:ILE:HG12	1.95	0.48
1:A:83:MET:O	1:A:88:VAL:HB	2.14	0.48
1:B:611:GLN:HA	1:B:611:GLN:HE21	1.79	0.48
1:B:70:SER:O	1:B:71:ASP:C	2.50	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:526:ILE:HG21	1:A:568:LEU:CD1	2.44	0.47
1:B:349:LYS:O	1:B:471:ARG:HG3	2.14	0.47
1:B:314:TYR:N	1:B:500:HIS:CD2	2.59	0.47
1:A:132:GLU:OE1	1:A:132:GLU:HA	2.13	0.47
1:A:296:PHE:HA	1:A:372:GLN:OE1	2.14	0.47
1:B:250:ILE:HA	1:B:250:ILE:HD12	1.59	0.47
1:A:119:LYS:O	1:A:123:TRP:CE3	2.68	0.47
1:A:16:GLU:HG3	1:A:21:VAL:HB	1.95	0.47
1:B:302:HIS:CD2	1:B:371:GLY:HA2	2.49	0.47
1:B:16:GLU:O	1:B:17:VAL:C	2.53	0.47
1:B:620:ASP:HB3	1:B:623:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:TRP:CZ2	1:B:90:PHE:HZ	2.32	0.47
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:A:366:VAL:CG1	1:A:367:GLU:N	2.79	0.46
1:B:125:LEU:O	1:B:126:VAL:HG23	2.15	0.46
1:B:388:SER:HB3	1:B:392:ARG:NH1	2.30	0.46
1:B:302:HIS:CE1	1:B:434:ARG:NH1	2.83	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: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: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: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:189:ILE:HD11	1:B:610:ARG:HA	1.99	0.45
1:B:63:TRP:CZ2	1:B:90:PHE:CZ	3.05	0.45
1:A:488:LEU:HD12	1:A:488:LEU:C	2.37	0.45
1:B:92:TYR:OH	1:B:102:LYS:HD3	2.16	0.45
1:A:321:TYR:C	1:A:321:TYR:CD1	2.89	0.45
1:A:3:ARG:HD3	1:A:185:ASP:OD2	2.16	0.45
1:B:317:ILE:HG13	1:B:503:VAL:O	2.16	0.45
1:A:425:LEU:O	1:A:429:ILE:HG13	2.17	0.45
1:B:484:ASN:HD22	1:B:484:ASN:N	2.13	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PHE:HD1	1:B:520:VAL:HG11	1.81	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:599:TRP:C	1:B:601:ARG:H	2.20	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: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:B:67:GLU:CD	1:B:67:GLU:H	2.21	0.44
1:A:294:ASN:OD1	1:A:309:LEU:HD13	2.18	0.44
1:A:526:ILE:HG21	1:A:568:LEU:HD12	2.00	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:256:GLU:CD	1:B:262:LYS:HB2	2.38	0.43
1:B:95:TRP:O	1:B:100:ALA:HA	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:C5'	2:A:801:UDP:O1B	2.65	0.43
1:A:64:LYS:HE2	1:A:84:GLU:OE2	2.18	0.43
1:B:225:PHE:CD2	1:B:225:PHE:N	2.87	0.43
1:B:549:TYR:HA	1:B:589:ALA:CB	2.48	0.43
1:B:614:LEU:O	1:B:615:ARG:C	2.56	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
1:A:36:VAL:HG12	1:A:36:VAL:O	2.17	0.43
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:321:TYR:C	1:A:321:TYR:HD1	2.22	0.43
1:A:330:MET:HG2	1:A:565:VAL:HG22	2.01	0.43
1:B:323:TYR:CD1	1:B:323:TYR:C	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:VAL:CG1	1:B:445:HIS:H	2.31	0.43
1:A:399:ARG:NH1	1:A:399:ARG:HG2	2.28	0.42
1:A:170:TRP:HB3	1:A:234:GLU:HG3	2.01	0.42
1:A:174:VAL:C	1:A:176:LEU:H	2.22	0.42
1:A:209:PHE:C	1:A:211:ASN:H	2.22	0.42
1:A:207:PHE:C	1:A:209:PHE:N	2.71	0.42
1:A:12:GLU:HB3	1:A:45:LEU:HD23	2.00	0.42
1:B:285:LEU:HD13	1:B:497:ARG:HD2	2.01	0.42
1:A:290:LYS:HE2	1:A:314:TYR:CE2	2.54	0.42
1:A:289:LYS:NZ	1:A:494:GLU:HG2	2.34	0.42
1:A:545:GLN:O	1:A:549:TYR:CD2	2.72	0.42
1:B:618:TYR:HB3	1:B:621:GLN:HB2	2.01	0.42
1:B:65:LYS:HE3	1:B:65:LYS:HB2	1.75	0.42
1:A:8:HIS:CD2	1:A:164:VAL:HG23	2.50	0.42
1:A:580:ARG:HB2	1:A:580:ARG:NH1	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:A:25:TYR:CD2	1:A:25:TYR:C	2.93	0.42
1:B:181:LYS:C	1:B:183:ARG:H	2.23	0.42
1:B:443:VAL:CG2	1:B:476:PHE:HD2	2.32	0.42
1:B:296:PHE:CB	1:B:488:LEU:HD12	2.50	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:153:GLU:O	1:B:157:LEU:HD13	2.20	0.42
1:B:123:TRP:CH2	1:B:229:HIS:HB2	2.54	0.42
1:B:253:PHE:O	1:B:254:GLU:C	2.57	0.42
1:B:325:ASN:H	1:B:325:ASN:ND2	2.17	0.42
1:B:513:TYR:O	1:B:517:GLU:HG2	2.19	0.42
1:A:615:ARG:O	1:A:617:GLY:N	2.53	0.42
1:A:62:ASP:HB3	1:A:65:LYS:HD2	2.02	0.42
1:B:299:GLY:O	1:B:302:HIS:HD2	2.02	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: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
1:A:252:ALA:CB	1:A:263:PRO:HG2	2.50	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:219:ASP:O	1:A:222:ALA:N	2.53	0.41
1:A:335:LEU:HA	1:A:335:LEU:HD12	1.93	0.41
1:B:39:TYR:HB2	1:B:43:TYR:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASP:HB3	1:A:211:ASN:CB	2.39	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:B:225:PHE:HD2	1:B:225:PHE:N	2.18	0.41
1:B:312:THR:HA	1:B:350:THR:O	2.20	0.41
1:B:46:ILE:HG21	1:B:147:VAL:HG13	2.01	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:176:LEU:HB2	1:A:177:PRO:HD3	2.01	0.41
1:A:316:PHE:CZ	1:A:496:VAL:HG13	2.55	0.41
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.56	0.41
1:B:29:LYS:HA	1:B:97:ILE:HD12	2.02	0.41
1:A:602:MET:HG2	1:A:602:MET:H	1.70	0.41
1:A:97:ILE:O	1:A:98:GLU:C	2.58	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
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: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:180:ARG:NH2	1:B:242:ASP:OD1	2.54	0.41
1:A:319:GLY:O	1:A:320:ARG:C	2.60	0.41
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:268:PRO:HB2	1:A:602:MET:HE1	2.03	0.40
1:A:217:ASP:CG	1:A:220:HIS:HB3	2.40	0.40
1:B:274:ILE:C	1:B:276:PHE:N	2.75	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

5.3.1 Protein backbone

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%)	3	20
1	B	600/725 (83%)	502 (84%)	73 (12%)	25 (4%)	3	17
All	All	1213/1450 (84%)	1014 (84%)	152 (12%)	47 (4%)	3	18

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
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

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Mol	Chain	Res	Type
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%)	457 (91%)	45 (9%)	9	32
1	B	484/623 (78%)	420 (87%)	64 (13%)	4	17
All	All	986/1246 (79%)	877 (89%)	109 (11%)	6	23

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER

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Mol	Chain	Res	Type
1	A	3	ARG
1	A	35	THR
1	A	54	TYR
1	A	69	PHE
1	A	86	ARG
1	A	89	HIS
1	A	110	SER
1	A	125	LEU
1	A	139	ASP
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	296	PHE
1	A	306	ASP
1	A	310	ASP
1	A	321	TYR
1	A	322	GLU
1	A	335	LEU
1	A	363	SER
1	A	395	ASP
1	A	399	ARG
1	A	434	ARG
1	A	458	LYS
1	A	484	ASN
1	A	485	ASN
1	A	504	PHE
1	A	513	TYR
1	A	544	ASN
1	A	556	ARG
1	A	594	SER
1	A	621	GLN
1	A	626	VAL
1	A	629	GLU

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Mol	Chain	Res	Type
1	A	634	ASN
1	A	636	ASP
1	B	3	ARG
1	B	6	GLN
1	B	15	THR
1	B	16	GLU
1	B	20	ARG
1	B	26	SER
1	B	31	LYS
1	B	38	GLN
1	B	42	HIS
1	B	45	LEU
1	B	50	ASN
1	B	54	TYR
1	B	60	ILE
1	B	61	LEU
1	B	67	GLU
1	B	74	ARG
1	B	105	LEU
1	B	108	LEU
1	B	109	ASP
1	B	112	ARG
1	B	161	HIS
1	B	184	ILE
1	B	225	PHE
1	B	231	TYR
1	B	242	ASP
1	B	249	GLN
1	B	250	ILE
1	B	258	LEU
1	B	273	VAL
1	B	274	ILE
1	B	289	LYS
1	B	321	TYR
1	B	325	ASN
1	B	326	LYS
1	B	335	LEU
1	B	337	ARG
1	B	363	SER
1	B	369	LEU
1	B	370	LYS
1	B	376	ARG

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Mol	Chain	Res	Type
1	B	381	THR
1	B	395	ASP
1	B	398	ILE
1	B	399	ARG
1	B	400	TYR
1	B	419	SER
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
1	B	497	ARG
1	B	513	TYR
1	B	518	CYS
1	B	537	MET
1	B	556	ARG
1	B	582	GLN
1	B	594	SER
1	B	596	LEU
1	B	620	ASP
1	B	621	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	HIS
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	445	HIS
1	A	484	ASN
1	A	485	ASN
1	A	500	HIS
1	A	545	GLN
1	A	567	GLN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
3	U5P	B	801	-	18,22,22	1.36	1 (5%)	21,33,33	1.40	2 (9%)
2	UDP	A	801	-	20,26,26	0.83	0	25,40,40	1.17	2 (8%)

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
3	U5P	B	801	-	-	6/8/26/26	0/2/2/2
2	UDP	A	801	-	-	2/14/32/32	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	U5P	O4-C4	4.58	1.36	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	UDP	PA-O3A-PB	-3.44	121.03	132.83
3	B	801	U5P	C3'-C2'-C1'	3.27	105.90	100.98
3	B	801	U5P	O3P-P-O2P	2.23	116.18	107.64
2	A	801	UDP	O4'-C1'-C2'	-2.05	103.94	106.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

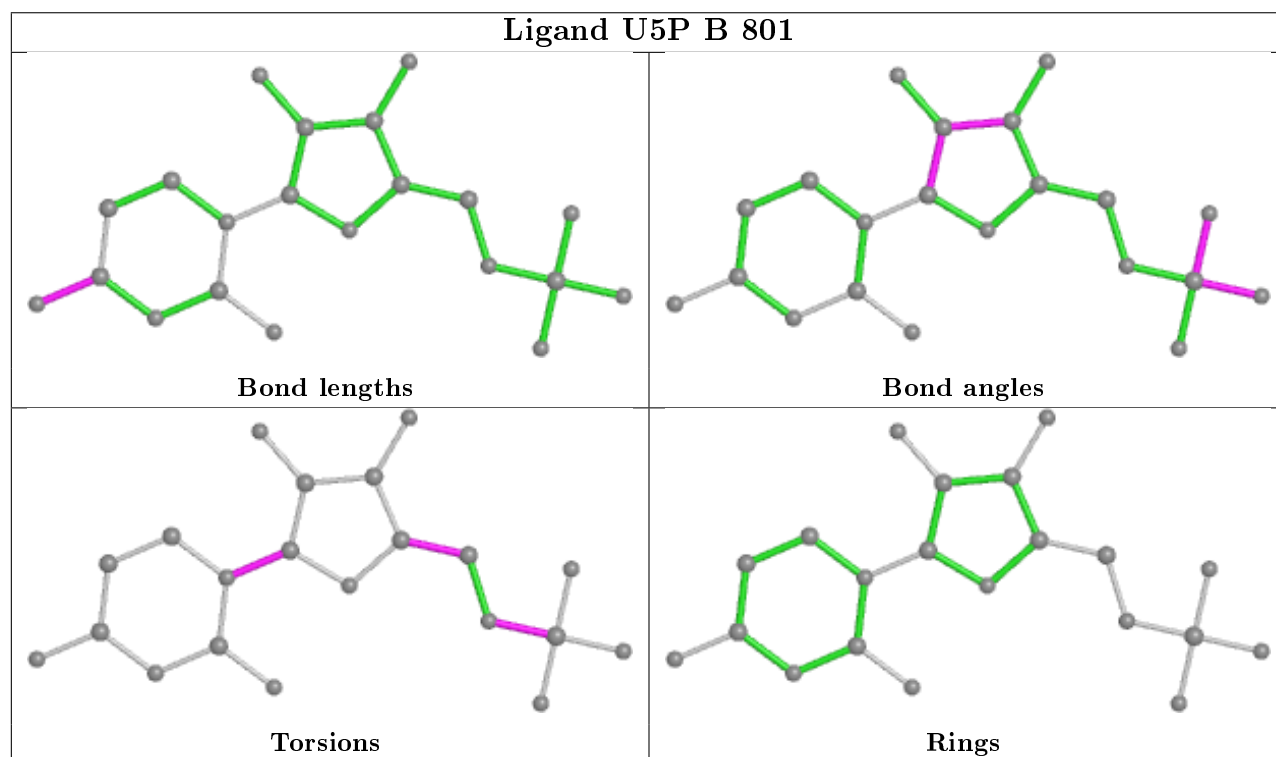
Mol	Chain	Res	Type	Atoms
3	B	801	U5P	C2'-C1'-N1-C6
3	B	801	U5P	C5'-O5'-P-O1P
3	B	801	U5P	C5'-O5'-P-O2P
3	B	801	U5P	C5'-O5'-P-O3P
2	A	801	UDP	C3'-C4'-C5'-O5'
2	A	801	UDP	O4'-C4'-C5'-O5'
3	B	801	U5P	O4'-C4'-C5'-O5'
3	B	801	U5P	C3'-C4'-C5'-O5'

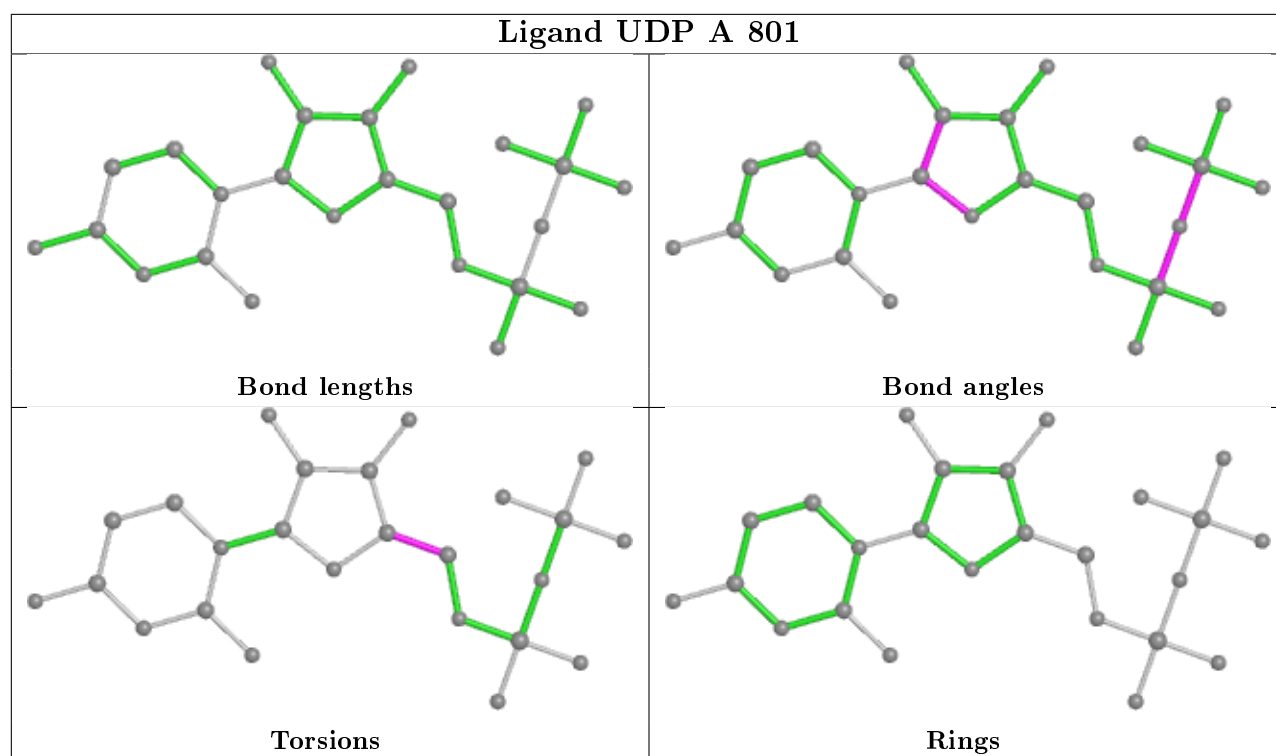
There are no ring outliers.

2 monomers are involved in 7 short contacts:

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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%)	-0.07	1 (0%) 95 96	71, 106, 145, 176	0
1	B	606/725 (83%)	-0.09	2 (0%) 94 94	73, 110, 154, 204	0
All	All	1225/1450 (84%)	-0.08	3 (0%) 95 96	71, 108, 150, 204	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	541	ILE	2.3
1	A	568	LEU	2.0
1	B	511	TRP	2.0

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](#)

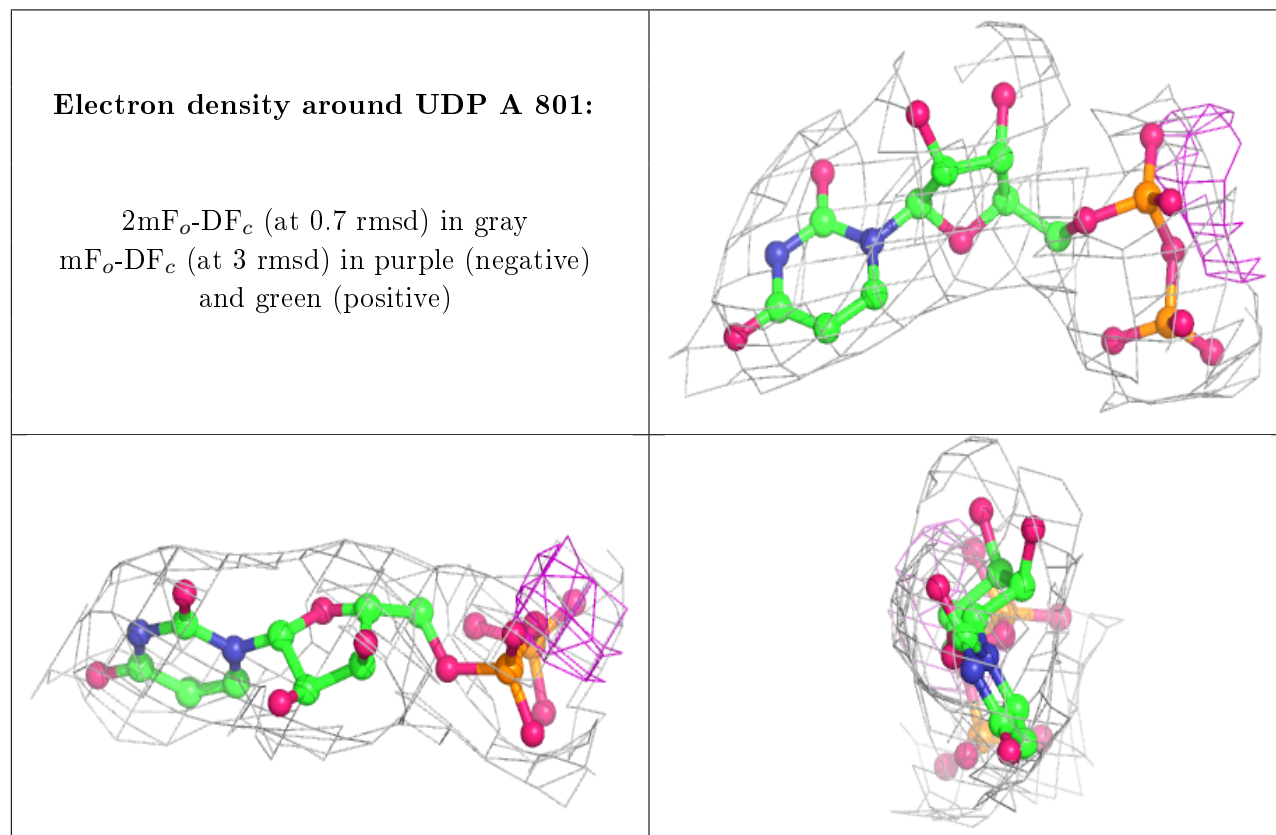
There are no carbohydrates in this entry.

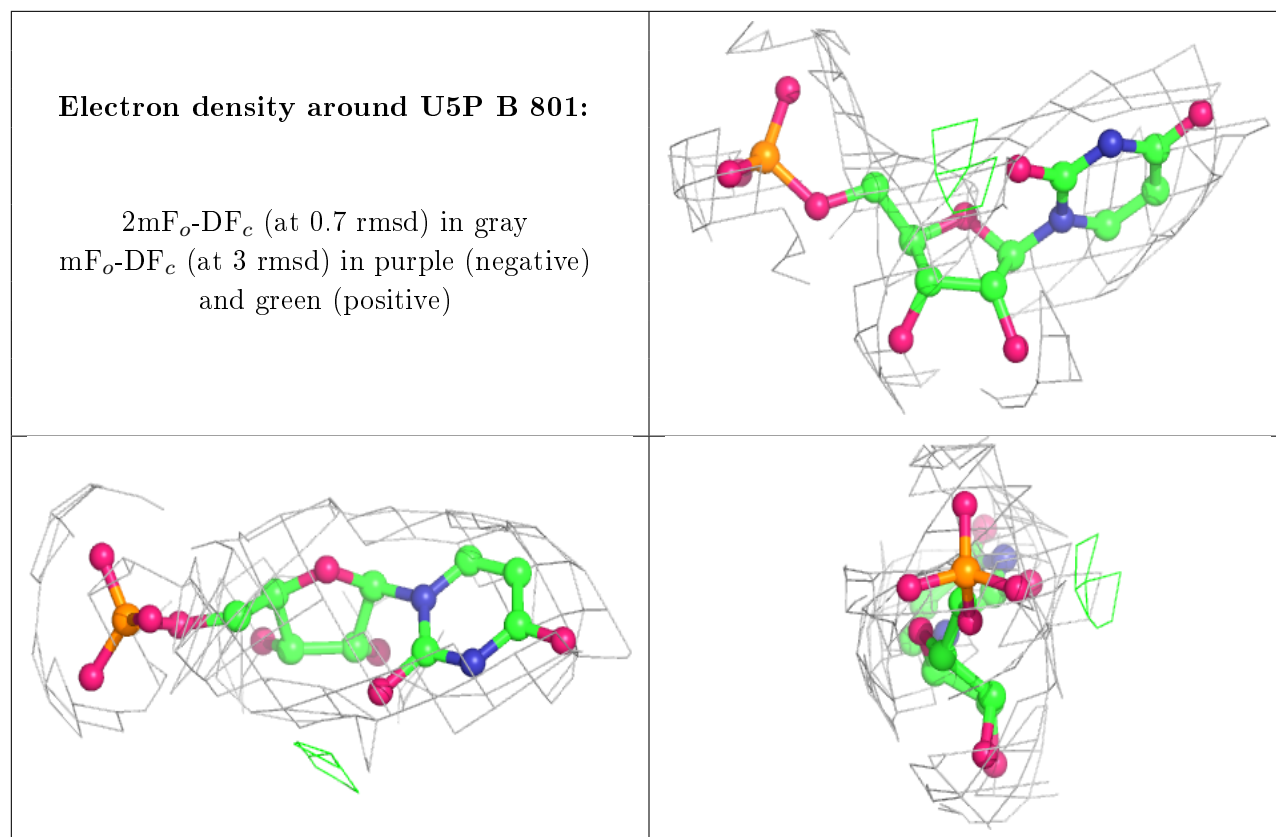
6.4 Ligands [i](#)

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	0.94	0.18	92,121,165,169	0
3	U5P	B	801	21/21	0.96	0.16	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.