



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:14 PM UTC

PDB ID : 2ZA3 / pdb_00002za3
Title : Crystal Structure of orotidine 5'-monophosphate decarboxylase complexed with uridine 5'-monophosphate from P.falciparum
Authors : Tokuoka, K.; Inoue, T.
Deposited on : 2007-09-26
Resolution : 2.65 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

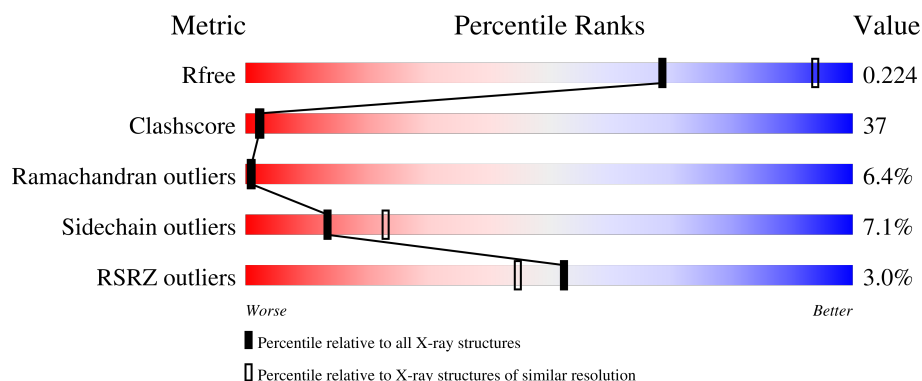
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	323	2% 43% 44% 11% ..
1	B	323	3% 46% 40% 12% ..

2 Entry composition [i](#)

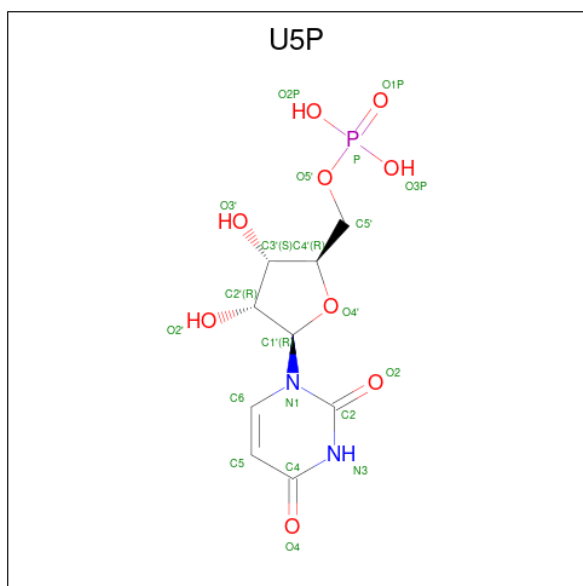
There are 3 unique types of molecules in this entry. The entry contains 5187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2566	1653	412	486	15			
1	B	316	Total	C	N	O	S	0	0	0
			2532	1633	407	477	15			

- 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		
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

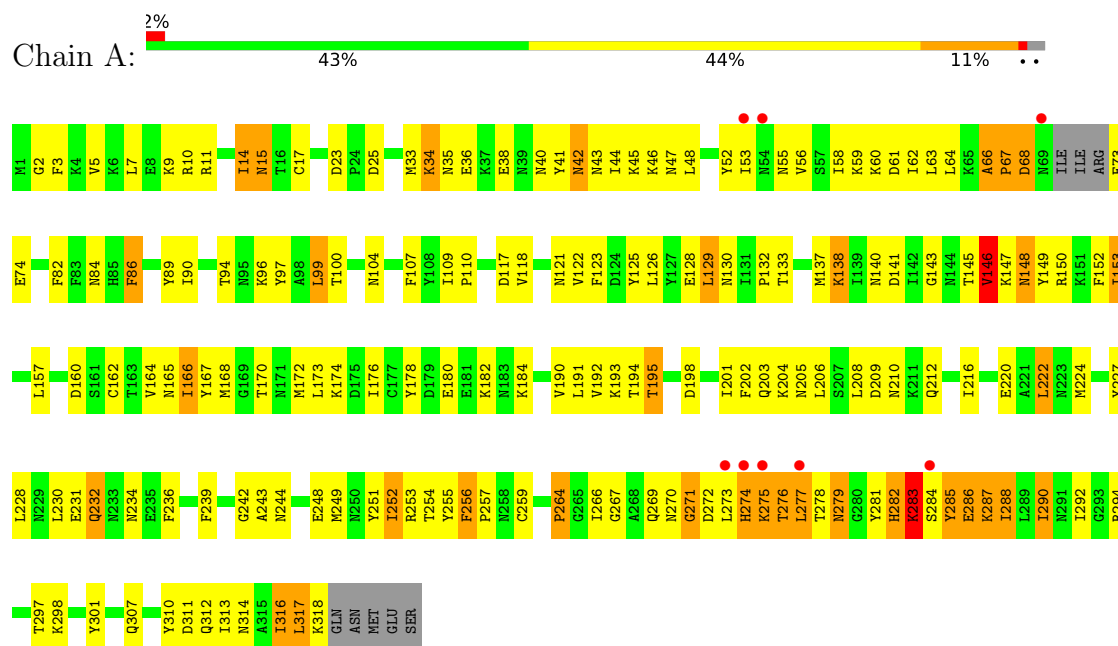
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total 22	O 22	0	0
3	B	25	Total 25	O 25	0	0

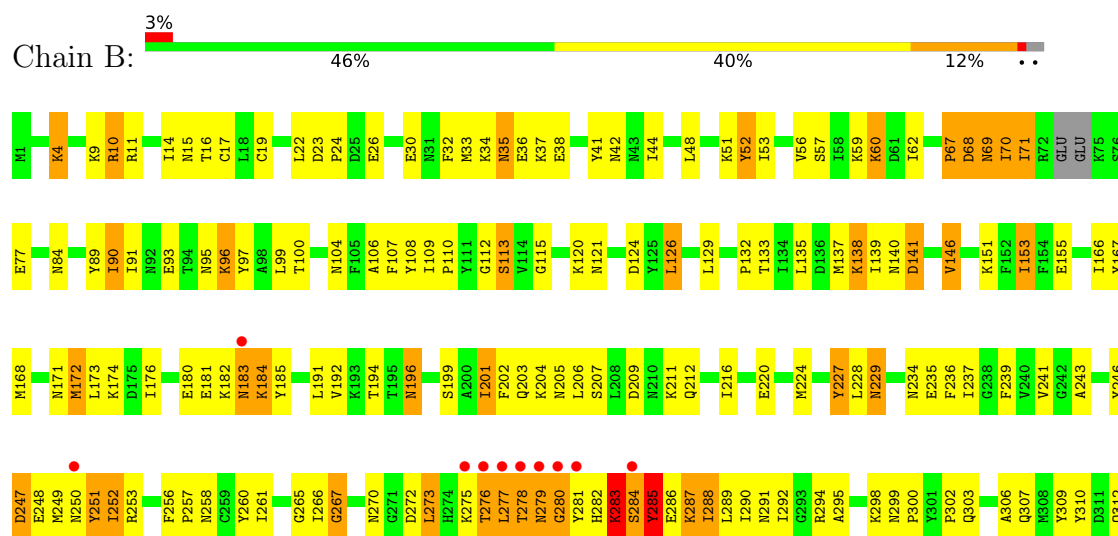
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Orotidine 5'-phosphate decarboxylase



• Molecule 1: Orotidine 5'-phosphate decarboxylase



I313	I314	A315	I316	I317	K318	GLN	ASN	MET	GLU	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	202.50Å 202.50Å 44.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.27 – 2.65 38.27 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.27-2.65) 99.0 (38.27-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.287 0.217 , 0.224	Depositor DCC
R_{free} test set	1060 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5187	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: 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	0.46	0/2620	1.04	15/3536 (0.4%)
1	B	0.44	0/2585	1.02	14/3496 (0.4%)
All	All	0.45	0/5205	1.03	29/7032 (0.4%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	THR	N-CA-C	-14.91	93.39	114.12
1	B	71	ILE	N-CA-C	-11.66	101.09	112.17
1	B	276	THR	N-CA-C	-9.39	100.07	113.21
1	B	227	TYR	N-CA-C	-8.35	98.72	110.50
1	B	252	ILE	N-CA-C	-7.53	102.99	110.30
1	A	149	TYR	N-CA-C	-7.18	103.53	111.36
1	A	66	ALA	N-CA-C	-6.91	100.24	109.84
1	A	301	TYR	CA-C-N	6.74	126.25	119.24
1	A	301	TYR	C-N-CA	6.74	126.25	119.24
1	B	287	LYS	N-CA-C	-6.66	104.90	113.16
1	A	99	LEU	N-CA-C	-6.37	104.55	112.90
1	B	153	ILE	N-CA-C	6.30	116.42	110.30
1	A	195	THR	N-CA-C	6.17	120.81	113.16
1	B	265	GLY	N-CA-C	6.10	123.55	114.95
1	B	10	ARG	N-CA-C	-5.84	105.04	111.82
1	B	52	TYR	N-CA-C	5.76	119.78	112.87
1	A	35	ASN	N-CA-C	-5.67	106.03	113.12
1	A	287	LYS	N-CA-C	-5.61	105.94	112.89
1	B	139	ILE	N-CA-C	5.59	116.53	110.21
1	A	94	THR	N-CA-C	5.50	122.58	113.89
1	A	153	ILE	N-CA-C	5.42	116.20	110.72
1	B	299	ASN	CA-C-N	5.41	125.12	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	ASN	C-N-CA	5.41	125.12	119.82
1	A	129	LEU	N-CA-C	-5.40	106.53	113.01
1	B	207	SER	N-CA-C	5.34	116.92	108.96
1	B	280	GLY	N-CA-C	-5.26	102.76	110.97
1	A	256	PHE	CA-C-N	5.18	125.48	119.47
1	A	256	PHE	C-N-CA	5.18	125.48	119.47
1	A	86	PHE	N-CA-C	-5.13	105.58	111.07

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	2566	0	2502	195	0
1	B	2532	0	2439	186	0
2	A	21	0	11	1	0
2	B	21	0	11	1	0
3	A	22	0	0	3	0
3	B	25	0	0	3	0
All	All	5187	0	4963	370	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 37.

All (370) 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:60:LYS:H	1:B:60:LYS:HD2	1.20	1.05
1:B:204:LYS:HE2	1:B:212:GLN:HE22	1.27	0.99
1:A:166:ILE:HD11	1:A:170:THR:HG22	1.45	0.97
1:A:100:THR:HG22	1:A:132:PRO:HB2	1.46	0.94
1:A:166:ILE:HA	1:A:172:MET:HE1	1.49	0.94
1:B:62:ILE:HD13	1:B:77:GLU:HG2	1.51	0.93
1:A:194:THR:HG21	1:B:168:MET:HG2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LYS:HD2	1:A:284:SER:H	1.37	0.89
1:B:249:MET:HE1	1:B:261:ILE:HG21	1.55	0.89
1:B:204:LYS:HE2	1:B:212:GLN:NE2	1.89	0.88
1:A:165:ASN:HD22	1:B:140:ASN:ND2	1.74	0.84
1:A:283:LYS:CD	1:A:284:SER:H	1.91	0.84
1:A:170:THR:HG21	1:A:220:GLU:HB3	1.61	0.83
1:A:313:ILE:O	1:A:317:LEU:HD13	1.78	0.81
1:B:283:LYS:C	1:B:285:TYR:H	1.88	0.81
1:B:60:LYS:HD2	1:B:60:LYS:N	1.96	0.81
1:B:224:MET:HE1	1:B:227:TYR:HD2	1.46	0.80
1:A:84:ASN:HD21	1:A:121:ASN:HD22	1.31	0.78
1:A:193:LYS:HA	1:A:203:GLN:NE2	2.00	0.76
1:A:192:VAL:HG21	1:A:239:PHE:HB3	1.68	0.76
1:B:266:ILE:HD11	1:B:292:ILE:HD11	1.69	0.75
1:A:52:TYR:HD1	1:A:55:ASN:ND2	1.85	0.75
1:A:283:LYS:HE2	1:A:287:LYS:HE3	1.68	0.75
1:A:269:GLN:C	1:A:271:GLY:H	1.94	0.74
1:B:93:GLU:HG3	1:B:303:GLN:HB2	1.68	0.74
1:B:243:ALA:HB1	1:B:276:THR:HG22	1.69	0.74
1:B:32:PHE:O	1:B:36:GLU:HB2	1.89	0.72
1:B:60:LYS:H	1:B:60:LYS:CD	1.92	0.72
1:A:275:LYS:HB3	1:A:316:ILE:HD13	1.71	0.72
1:A:59:LYS:HD3	1:A:62:ILE:HD11	1.72	0.71
1:A:138:LYS:HD3	3:B:611:HOH:O	1.89	0.71
1:B:292:ILE:HG23	1:B:295:ALA:HB3	1.71	0.71
1:A:86:PHE:CE1	1:A:90:ILE:HD11	2.25	0.71
1:B:277:LEU:O	1:B:279:ASN:N	2.24	0.70
1:A:248:GLU:O	1:A:252:ILE:HG22	1.92	0.70
1:A:36:GLU:HB3	1:A:41:TYR:HD1	1.55	0.70
1:B:68:ASP:O	1:B:71:ILE:HG12	1.91	0.69
1:B:285:TYR:C	1:B:287:LYS:H	1.98	0.69
1:B:288:ILE:HG23	1:B:288:ILE:O	1.92	0.69
1:B:17:CYS:HB3	1:B:285:TYR:HD2	1.58	0.69
1:A:166:ILE:HA	1:A:172:MET:CE	2.21	0.69
1:B:138:LYS:HD3	1:B:138:LYS:N	2.08	0.69
1:A:193:LYS:HD2	1:A:203:GLN:HE21	1.58	0.68
1:B:84:ASN:HD21	1:B:121:ASN:HD22	1.40	0.68
1:A:192:VAL:CG2	1:A:239:PHE:HB3	2.23	0.68
1:A:164:VAL:CG1	1:A:172:MET:HE3	2.23	0.68
1:A:194:THR:H	1:A:203:GLN:HE22	1.40	0.67
1:A:86:PHE:CZ	1:A:90:ILE:HD11	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ASN:C	1:B:292:ILE:HD12	2.18	0.67
1:A:55:ASN:CB	1:A:128:GLU:HG3	2.25	0.67
1:A:288:ILE:O	1:A:288:ILE:HG23	1.93	0.67
1:A:42:ASN:O	1:A:46:LYS:HG3	1.94	0.67
1:B:283:LYS:CD	1:B:284:SER:H	2.08	0.67
1:B:243:ALA:HB1	1:B:276:THR:CG2	2.26	0.66
1:B:23:ASP:HB3	1:B:107:PHE:CE2	2.31	0.66
1:B:275:LYS:HA	1:B:279:ASN:HB3	1.77	0.66
1:A:285:TYR:O	1:A:286:GLU:HB3	1.95	0.66
1:B:99:LEU:HG	1:B:100:THR:HG23	1.78	0.65
1:B:109:ILE:N	1:B:110:PRO:HD2	2.12	0.65
1:A:274:HIS:CE1	1:A:276:THR:HG21	2.32	0.65
1:B:275:LYS:CB	1:B:279:ASN:HD22	2.09	0.65
1:A:316:ILE:C	1:A:318:LYS:H	2.05	0.64
1:A:252:ILE:HD13	1:A:252:ILE:C	2.22	0.64
1:A:23:ASP:HB3	1:A:107:PHE:CD2	2.32	0.64
1:B:276:THR:HG22	1:B:276:THR:O	1.97	0.64
1:A:164:VAL:HG11	1:A:172:MET:HE3	1.80	0.63
1:B:283:LYS:C	1:B:285:TYR:N	2.54	0.63
1:A:55:ASN:CG	1:A:128:GLU:HG3	2.24	0.63
1:A:109:ILE:N	1:A:110:PRO:HD2	2.14	0.62
1:A:23:ASP:HB3	1:A:107:PHE:CE2	2.34	0.62
1:B:59:LYS:HD2	1:B:62:ILE:HD12	1.82	0.62
1:B:196:ASN:HB2	1:B:199:SER:HB3	1.80	0.62
1:B:266:ILE:HG13	1:B:267:GLY:N	2.15	0.62
1:A:44:ILE:O	1:A:48:LEU:HD23	2.00	0.61
1:B:91:ILE:O	1:B:95:ASN:HB3	2.00	0.61
1:B:266:ILE:HD13	1:B:273:LEU:HD13	1.81	0.61
1:B:283:LYS:HG3	1:B:284:SER:N	2.15	0.61
1:A:168:MET:HG2	1:B:194:THR:HG21	1.82	0.61
1:A:266:ILE:HG22	1:A:273:LEU:H	1.64	0.61
1:B:201:ILE:O	1:B:205:ASN:HB2	2.00	0.61
1:B:183:ASN:O	1:B:184:LYS:O	2.18	0.61
1:B:272:ASP:O	1:B:273:LEU:C	2.44	0.61
1:B:273:LEU:HD23	1:B:312:GLN:HG2	1.83	0.61
1:B:283:LYS:HZ3	1:B:283:LYS:HB2	1.66	0.61
1:A:269:GLN:C	1:A:271:GLY:N	2.56	0.60
1:B:224:MET:HE3	1:B:227:TYR:HB3	1.83	0.60
1:A:152:PHE:HB2	1:B:110:PRO:HA	1.83	0.60
1:B:267:GLY:HA3	1:B:295:ALA:HB2	1.82	0.60
1:B:109:ILE:N	1:B:110:PRO:CD	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:HG13	1:A:292:ILE:CD1	2.32	0.60
1:A:143:GLY:O	1:A:147:LYS:HG3	2.01	0.60
1:A:193:LYS:HE3	1:A:204:LYS:HD3	1.85	0.59
1:A:204:LYS:HE2	1:A:212:GLN:HE22	1.68	0.59
1:B:53:ILE:O	1:B:56:VAL:HG23	2.02	0.59
1:A:41:TYR:O	1:A:42:ASN:CB	2.51	0.59
1:A:317:LEU:N	1:A:317:LEU:HD12	2.18	0.59
1:B:146:VAL:HG11	1:B:176:ILE:HG13	1.85	0.59
1:A:63:LEU:HD13	1:A:63:LEU:O	2.02	0.58
1:A:104:ASN:ND2	2:A:500:U5P:O2'	2.35	0.58
1:A:231:GLU:HB3	1:A:232:GLN:HE21	1.66	0.58
1:A:269:GLN:O	1:A:271:GLY:N	2.36	0.58
1:B:283:LYS:HB2	1:B:283:LYS:NZ	2.18	0.58
1:B:14:ILE:HD11	1:B:99:LEU:HA	1.85	0.58
1:B:266:ILE:CD1	1:B:292:ILE:HD11	2.33	0.58
1:A:44:ILE:HG21	1:A:67:PRO:HG3	1.86	0.58
1:A:166:ILE:HG22	3:A:506:HOH:O	2.04	0.58
1:A:283:LYS:HE2	1:A:287:LYS:CE	2.34	0.58
1:B:283:LYS:CG	1:B:284:SER:N	2.67	0.58
1:A:3:PHE:CD1	1:A:160:ASP:HB3	2.39	0.58
1:A:278:THR:CG2	1:A:316:ILE:HG21	2.34	0.58
1:B:23:ASP:HB3	1:B:107:PHE:CD2	2.39	0.57
1:B:192:VAL:HG21	1:B:239:PHE:HB3	1.86	0.57
1:A:275:LYS:CB	1:A:316:ILE:HD13	2.34	0.57
1:A:66:ALA:O	1:A:67:PRO:O	2.21	0.57
1:A:118:VAL:O	1:A:122:VAL:HG23	2.03	0.57
1:A:52:TYR:HD1	1:A:55:ASN:HD21	1.51	0.57
1:A:109:ILE:N	1:A:110:PRO:CD	2.68	0.57
1:A:198:ASP:CG	1:B:171:ASN:HD22	2.12	0.57
1:B:57:SER:O	1:B:60:LYS:HE3	2.04	0.57
1:B:224:MET:HE1	1:B:227:TYR:CD2	2.34	0.56
1:B:291:ASN:O	1:B:292:ILE:HD12	2.05	0.56
1:A:266:ILE:CD1	1:A:292:ILE:HD11	2.35	0.56
1:A:267:GLY:H	1:A:272:ASP:HA	1.69	0.56
1:A:145:THR:O	1:A:148:ASN:OD1	2.24	0.56
1:B:282:HIS:CG	1:B:283:LYS:H	2.23	0.56
1:B:104:ASN:ND2	2:B:600:U5P:O2'	2.38	0.56
1:B:290:ILE:HG22	1:B:292:ILE:CD1	2.36	0.56
1:B:227:TYR:O	1:B:228:LEU:HB2	2.06	0.56
1:A:208:LEU:HB3	1:A:216:ILE:HD11	1.86	0.55
1:A:202:PHE:O	1:A:206:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:LYS:O	1:B:285:TYR:N	2.32	0.55
1:A:58:ILE:HG21	1:A:117:ASP:OD1	2.07	0.55
1:A:97:TYR:CZ	1:A:307:GLN:HB3	2.42	0.55
1:A:2:GLY:HA3	1:A:234:ASN:HB3	1.89	0.54
1:B:314:ASN:C	1:B:316:ILE:H	2.15	0.54
1:A:178:TYR:CE2	1:A:180:GLU:HG2	2.43	0.54
1:B:146:VAL:CG1	1:B:176:ILE:HG13	2.38	0.54
1:B:285:TYR:C	1:B:287:LYS:N	2.66	0.54
1:B:283:LYS:HD3	1:B:284:SER:H	1.72	0.53
1:B:91:ILE:HD13	1:B:126:LEU:CD1	2.38	0.53
1:A:271:GLY:O	1:A:272:ASP:C	2.50	0.53
1:A:59:LYS:HB3	1:A:62:ILE:HD11	1.91	0.53
1:B:196:ASN:H	1:B:196:ASN:HD22	1.56	0.53
1:A:25:ASP:OD2	1:A:298:LYS:NZ	2.41	0.53
1:A:193:LYS:HE2	1:A:204:LYS:HG2	1.91	0.53
1:B:41:TYR:CD2	1:B:67:PRO:HB2	2.44	0.53
1:B:192:VAL:CG2	1:B:239:PHE:HB3	2.39	0.53
1:A:193:LYS:CE	1:A:204:LYS:HD3	2.39	0.53
1:B:26:GLU:O	1:B:30:GLU:HG2	2.09	0.53
1:A:228:LEU:HB2	1:A:230:LEU:HD13	1.91	0.53
1:A:41:TYR:CE2	1:A:67:PRO:HB2	2.45	0.52
1:A:273:LEU:O	1:A:274:HIS:ND1	2.41	0.52
1:B:282:HIS:CG	1:B:283:LYS:N	2.77	0.52
1:B:284:SER:O	1:B:285:TYR:O	2.27	0.52
1:A:194:THR:N	1:A:203:GLN:HE22	2.06	0.52
1:A:266:ILE:HD11	1:A:290:ILE:CG2	2.40	0.52
1:B:19:CYS:O	1:B:291:ASN:HA	2.09	0.52
1:A:285:TYR:O	1:A:286:GLU:CB	2.57	0.52
1:B:126:LEU:HD23	1:B:133:THR:HG22	1.90	0.52
1:A:86:PHE:O	1:A:89:TYR:HB3	2.09	0.52
1:B:15:ASN:O	1:B:314:ASN:ND2	2.42	0.52
1:A:11:ARG:C	1:A:11:ARG:HD2	2.35	0.52
1:A:52:TYR:CD1	1:A:55:ASN:ND2	2.72	0.52
1:A:222:LEU:HD23	1:A:239:PHE:CZ	2.45	0.51
1:A:232:GLN:H	1:A:232:GLN:NE2	2.09	0.51
1:B:250:ASN:O	1:B:251:TYR:HB2	2.10	0.51
1:A:243:ALA:CB	1:A:266:ILE:HG23	2.41	0.51
1:A:166:ILE:CA	1:A:172:MET:HE1	2.32	0.51
1:A:278:THR:HG21	1:A:316:ILE:HG21	1.93	0.51
1:A:100:THR:HG22	1:A:132:PRO:CB	2.31	0.51
1:A:249:MET:HE3	1:A:277:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:O	1:B:48:LEU:HD22	2.10	0.51
1:B:246:TYR:CE1	1:B:276:THR:HA	2.46	0.51
1:B:224:MET:HE3	1:B:224:MET:O	2.11	0.51
1:A:294:ARG:HA	1:A:297:THR:OG1	2.11	0.51
1:A:317:LEU:N	1:A:317:LEU:CD1	2.74	0.51
1:B:211:LYS:CB	1:B:216:ILE:HD11	2.40	0.51
1:B:17:CYS:HB3	1:B:285:TYR:CD2	2.41	0.50
1:A:25:ASP:HA	3:A:502:HOH:O	2.10	0.50
1:A:252:ILE:HD11	1:A:259:CYS:SG	2.52	0.50
1:B:227:TYR:O	1:B:228:LEU:CB	2.59	0.50
1:B:294:ARG:HG2	1:B:298:LYS:HE2	1.94	0.50
1:A:198:ASP:CG	1:B:171:ASN:ND2	2.69	0.50
1:B:243:ALA:O	1:B:276:THR:HG23	2.11	0.50
1:B:266:ILE:CD1	1:B:273:LEU:HD13	2.41	0.50
1:B:283:LYS:CG	1:B:284:SER:H	2.25	0.50
1:A:253:ARG:O	1:A:257:PRO:HA	2.12	0.49
1:B:211:LYS:HB2	1:B:216:ILE:HD11	1.94	0.49
1:A:283:LYS:HE2	1:A:287:LYS:CD	2.42	0.49
1:B:309:TYR:O	1:B:313:ILE:HG13	2.11	0.49
1:A:123:PHE:CE1	1:A:133:THR:HB	2.48	0.49
1:B:292:ILE:CG2	1:B:295:ALA:HB3	2.40	0.49
1:B:67:PRO:O	1:B:68:ASP:C	2.55	0.49
1:A:201:ILE:HA	1:A:205:ASN:HD22	1.78	0.49
1:A:273:LEU:O	1:A:274:HIS:HB3	2.13	0.48
1:B:84:ASN:ND2	1:B:121:ASN:HD22	2.07	0.48
1:B:146:VAL:HG13	1:B:176:ILE:HG12	1.96	0.48
1:A:86:PHE:O	1:A:90:ILE:HD12	2.13	0.48
1:A:266:ILE:HD11	1:A:292:ILE:HD11	1.94	0.48
1:B:14:ILE:HG13	1:B:16:THR:HG22	1.95	0.48
1:A:153:ILE:HG21	1:A:162:CYS:HB3	1.94	0.48
1:B:33:MET:O	1:B:37:LYS:HG3	2.14	0.48
1:B:209:ASP:C	1:B:211:LYS:H	2.21	0.48
1:A:84:ASN:ND2	1:A:121:ASN:HD22	2.07	0.48
1:B:194:THR:H	1:B:203:GLN:HE22	1.62	0.48
1:B:35:ASN:HA	1:B:38:GLU:HG2	1.95	0.48
1:A:17:CYS:HB3	1:A:285:TYR:HB2	1.96	0.48
1:A:243:ALA:HB1	1:A:266:ILE:HG23	1.95	0.48
1:A:288:ILE:HD13	1:A:288:ILE:C	2.39	0.47
1:B:202:PHE:O	1:B:206:LEU:HB2	2.14	0.47
1:A:137:MET:O	1:A:138:LYS:HG2	2.14	0.47
1:A:193:LYS:HD2	1:A:203:GLN:NE2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:O	1:A:318:LYS:N	2.44	0.47
1:B:266:ILE:HD11	1:B:292:ILE:CD1	2.43	0.47
1:A:53:ILE:O	1:A:56:VAL:HG22	2.14	0.47
1:A:99:LEU:HG	1:A:100:THR:HG23	1.97	0.47
1:A:33:MET:HG3	1:A:82:PHE:CZ	2.49	0.47
1:A:109:ILE:HG13	1:A:109:ILE:O	2.14	0.47
1:B:68:ASP:OD2	1:B:68:ASP:N	2.47	0.47
1:B:272:ASP:HB3	1:B:276:THR:OG1	2.14	0.47
1:B:185:TYR:CE1	1:B:228:LEU:O	2.68	0.47
1:B:224:MET:HE2	1:B:228:LEU:HD11	1.95	0.47
1:A:146:VAL:HG21	1:A:176:ILE:HD11	1.97	0.47
1:A:267:GLY:H	1:A:272:ASP:CA	2.27	0.47
1:A:288:ILE:O	1:A:288:ILE:CG2	2.63	0.47
1:B:91:ILE:HD13	1:B:126:LEU:HD11	1.95	0.47
1:B:137:MET:O	1:B:138:LYS:C	2.57	0.47
1:B:68:ASP:O	1:B:70:ILE:N	2.43	0.47
1:B:272:ASP:O	1:B:276:THR:OG1	2.33	0.47
1:A:251:TYR:O	1:A:255:TYR:HD2	1.97	0.47
1:B:252:ILE:O	1:B:256:PHE:HB2	2.15	0.47
1:A:267:GLY:O	1:A:271:GLY:HA2	2.14	0.46
1:B:100:THR:HG22	1:B:132:PRO:HB2	1.97	0.46
1:A:67:PRO:O	1:A:68:ASP:HB2	2.14	0.46
1:B:171:ASN:OD1	1:B:174:LYS:HE3	2.15	0.46
1:A:166:ILE:HG22	1:A:190:VAL:HG13	1.97	0.46
1:A:243:ALA:HA	1:A:277:LEU:HG	1.97	0.46
1:B:151:LYS:O	1:B:155:GLU:HB2	2.15	0.46
1:B:288:ILE:O	1:B:288:ILE:CG2	2.62	0.46
1:A:273:LEU:O	1:A:274:HIS:CB	2.63	0.46
1:B:173:LEU:HD13	1:B:237:ILE:HD13	1.97	0.46
1:B:70:ILE:O	1:B:70:ILE:HG22	2.14	0.46
1:B:11:ARG:O	1:B:15:ASN:N	2.46	0.46
1:B:67:PRO:HA	1:B:70:ILE:HD12	1.97	0.46
1:B:216:ILE:HD12	1:B:216:ILE:H	1.81	0.46
1:B:258:ASN:HB3	1:B:287:LYS:HZ2	1.80	0.46
1:A:52:TYR:CD1	1:A:128:GLU:HB3	2.51	0.46
1:A:137:MET:C	1:A:138:LYS:HG2	2.41	0.46
1:A:283:LYS:CD	1:A:284:SER:N	2.71	0.46
1:B:106:ALA:O	1:B:110:PRO:HD3	2.16	0.46
1:A:67:PRO:O	1:A:68:ASP:CB	2.63	0.45
1:B:146:VAL:HG13	1:B:176:ILE:CG1	2.45	0.45
1:A:307:GLN:HA	1:A:310:TYR:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:O	1:A:184:LYS:HG2	2.17	0.45
1:A:249:MET:HE3	1:A:277:LEU:CD2	2.47	0.45
1:B:253:ARG:HG2	1:B:281:TYR:HA	1.97	0.45
1:A:140:ASN:O	1:B:138:LYS:HG3	2.15	0.45
1:A:283:LYS:CD	1:A:287:LYS:HD2	2.47	0.45
1:B:135:LEU:HD23	1:B:153:ILE:HG12	1.98	0.45
1:A:165:ASN:HD22	1:B:140:ASN:HD22	1.60	0.45
1:B:62:ILE:HG21	1:B:77:GLU:HG2	1.99	0.45
1:A:284:SER:O	1:A:285:TYR:C	2.59	0.45
1:A:294:ARG:HA	1:A:297:THR:HG1	1.82	0.45
1:B:108:TYR:O	1:B:115:GLY:HA3	2.16	0.45
1:B:236:PHE:CE2	1:B:260:TYR:HB2	2.52	0.45
1:A:254:THR:O	1:A:257:PRO:HD3	2.16	0.45
1:A:266:ILE:HG13	1:A:292:ILE:HD13	1.99	0.45
1:B:185:TYR:HE1	1:B:228:LEU:O	2.00	0.45
1:A:222:LEU:HD23	1:A:239:PHE:HZ	1.82	0.45
1:B:276:THR:O	1:B:277:LEU:CB	2.65	0.44
1:A:173:LEU:HB2	1:A:224:MET:HG2	1.98	0.44
1:A:193:LYS:HA	1:A:203:GLN:HE21	1.81	0.44
1:B:16:THR:HB	1:B:310:TYR:CE1	2.51	0.44
1:B:228:LEU:O	1:B:229:ASN:C	2.60	0.44
1:B:266:ILE:HG13	1:B:267:GLY:H	1.81	0.44
1:A:166:ILE:HG13	1:A:170:THR:HA	1.99	0.44
1:A:201:ILE:HD13	1:B:220:GLU:OE2	2.18	0.44
1:A:3:PHE:O	1:A:7:LEU:HB2	2.17	0.44
1:A:36:GLU:OE2	1:A:43:ASN:HB2	2.18	0.44
1:A:274:HIS:CE1	1:A:276:THR:CG2	2.99	0.44
1:A:282:HIS:CG	1:A:283:LYS:N	2.86	0.44
1:A:311:ASP:O	1:A:314:ASN:HB3	2.18	0.44
1:B:273:LEU:HD23	1:B:312:GLN:HE21	1.81	0.44
1:B:166:ILE:O	1:B:167:TYR:C	2.60	0.44
1:B:249:MET:HE3	1:B:249:MET:HA	2.00	0.44
1:A:117:ASP:OD1	1:B:113:SER:OG	2.34	0.44
1:B:96:LYS:HE2	1:B:97:TYR:CE2	2.53	0.44
1:A:55:ASN:ND2	1:A:128:GLU:HG3	2.33	0.44
1:A:178:TYR:HE2	1:A:180:GLU:HG2	1.83	0.43
1:B:141:ASP:H	1:B:172:MET:HE2	1.82	0.43
1:A:232:GLN:NE2	1:A:232:GLN:N	2.66	0.43
1:B:22:LEU:C	1:B:24:PRO:HD3	2.43	0.43
1:A:209:ASP:O	1:A:210:ASN:HB2	2.18	0.43
1:B:246:TYR:HE1	1:B:276:THR:OG1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PRO:HG2	1:B:258:ASN:H	1.84	0.43
1:B:288:ILE:C	1:B:288:ILE:HD13	2.43	0.43
1:A:9:LYS:HE3	1:A:9:LYS:HB2	1.82	0.43
1:A:10:ARG:O	1:A:14:ILE:HG12	2.18	0.43
1:B:69:ASN:O	1:B:70:ILE:HG13	2.17	0.43
1:B:247:ASP:O	1:B:250:ASN:O	2.36	0.43
1:B:275:LYS:CA	1:B:279:ASN:HB3	2.45	0.43
1:A:25:ASP:C	1:A:25:ASP:OD1	2.62	0.43
1:A:97:TYR:CE2	1:A:307:GLN:HB3	2.53	0.43
1:A:125:TYR:O	1:A:129:LEU:HD23	2.18	0.43
1:B:115:GLY:HA3	3:B:604:HOH:O	2.17	0.43
1:B:120:LYS:HE3	1:B:124:ASP:OD2	2.18	0.43
1:A:195:THR:HG22	1:A:242:GLY:HA3	1.99	0.43
1:A:267:GLY:H	1:A:272:ASP:N	2.16	0.43
1:A:272:ASP:O	1:A:273:LEU:C	2.62	0.43
1:B:314:ASN:C	1:B:316:ILE:N	2.77	0.43
1:A:2:GLY:HA3	1:A:234:ASN:CB	2.48	0.43
1:A:194:THR:CG2	1:B:168:MET:HE3	2.49	0.43
1:A:275:LYS:NZ	1:A:312:GLN:NE2	2.67	0.43
1:B:185:TYR:O	1:B:235:GLU:HG3	2.19	0.43
1:A:14:ILE:O	1:A:15:ASN:C	2.62	0.42
1:A:47:ASN:O	1:A:53:ILE:HG13	2.18	0.42
1:A:222:LEU:HD22	1:A:222:LEU:HA	1.88	0.42
1:B:300:PRO:C	1:B:302:PRO:HD3	2.44	0.42
1:A:41:TYR:HD2	1:A:45:LYS:HE2	1.85	0.42
1:B:258:ASN:HB3	1:B:287:LYS:NZ	2.34	0.42
1:A:128:GLU:C	1:A:130:ASN:N	2.78	0.42
1:A:147:LYS:O	1:A:150:ARG:HB3	2.18	0.42
1:B:89:TYR:CD2	1:B:90:ILE:HD12	2.55	0.42
1:B:250:ASN:O	1:B:251:TYR:CB	2.67	0.42
1:A:33:MET:HB2	1:A:82:PHE:CG	2.54	0.42
1:B:241:VAL:HG11	1:B:249:MET:HE3	2.00	0.42
1:B:248:GLU:O	1:B:252:ILE:HG12	2.20	0.42
1:B:257:PRO:O	1:B:283:LYS:NZ	2.53	0.42
1:B:51:LYS:HE2	1:B:52:TYR:CE1	2.54	0.42
1:A:236:PHE:CD2	1:A:236:PHE:C	2.98	0.42
1:B:112:GLY:O	1:B:113:SER:C	2.62	0.42
1:B:196:ASN:H	1:B:196:ASN:ND2	2.17	0.42
1:B:280:GLY:O	1:B:281:TYR:CB	2.67	0.42
1:A:34:LYS:O	1:A:38:GLU:HG3	2.20	0.42
1:A:36:GLU:HB3	1:A:41:TYR:CD1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MET:C	1:B:138:LYS:HD3	2.44	0.42
1:A:128:GLU:C	1:A:130:ASN:H	2.27	0.42
1:B:180:GLU:O	1:B:182:LYS:N	2.53	0.42
1:A:40:ASN:OD1	1:A:45:LYS:HE3	2.20	0.41
1:A:256:PHE:N	1:A:257:PRO:CD	2.83	0.41
1:A:266:ILE:HD11	1:A:290:ILE:HG21	2.02	0.41
1:B:96:LYS:HE2	1:B:97:TYR:CZ	2.55	0.41
1:B:109:ILE:H	1:B:110:PRO:CD	2.31	0.41
1:B:278:THR:HG23	1:B:290:ILE:HD11	2.01	0.41
1:A:174:LYS:HE2	1:A:227:TYR:CE2	2.55	0.41
1:B:52:TYR:CD2	1:B:129:LEU:HD23	2.54	0.41
1:A:201:ILE:HA	1:A:205:ASN:ND2	2.35	0.41
1:A:316:ILE:C	1:A:318:LYS:N	2.74	0.41
1:A:40:ASN:OD1	1:A:40:ASN:O	2.39	0.41
1:A:166:ILE:CG2	3:A:506:HOH:O	2.66	0.41
1:B:4:LYS:HB2	1:B:234:ASN:O	2.20	0.41
1:B:14:ILE:O	1:B:310:TYR:OH	2.31	0.41
1:B:306:ALA:O	1:B:307:GLN:C	2.63	0.41
1:B:276:THR:CG2	1:B:276:THR:O	2.67	0.41
1:B:182:LYS:O	1:B:183:ASN:HB2	2.19	0.41
1:B:191:LEU:HB2	3:B:603:HOH:O	2.21	0.41
1:A:193:LYS:HA	1:A:203:GLN:HE22	1.80	0.41
1:B:314:ASN:O	1:B:316:ILE:N	2.48	0.41
1:A:90:ILE:HD12	1:A:90:ILE:H	1.86	0.41
1:A:279:ASN:C	1:A:281:TYR:H	2.29	0.41
1:B:146:VAL:CG1	1:B:176:ILE:CG1	2.99	0.40
1:B:146:VAL:HG21	1:B:172:MET:HG3	2.02	0.40
1:B:277:LEU:CB	1:B:288:ILE:HD11	2.51	0.40
1:A:60:LYS:HG2	1:A:64:LEU:HD22	2.02	0.40
1:B:10:ARG:O	1:B:14:ILE:HG12	2.20	0.40
1:A:137:MET:O	1:A:138:LYS:C	2.65	0.40
1:A:275:LYS:HZ3	1:A:312:GLN:NE2	2.20	0.40
1:B:10:ARG:HG2	1:B:99:LEU:O	2.22	0.40
1:A:73:GLU:HB3	1:A:74:GLU:H	1.62	0.40
1:A:96:LYS:HE3	1:A:97:TYR:CZ	2.56	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	311/323 (96%)	268 (86%)	24 (8%)	19 (6%)	1	1
1	B	312/323 (97%)	249 (80%)	42 (14%)	21 (7%)	1	0
All	All	623/646 (96%)	517 (83%)	66 (11%)	40 (6%)	1	1

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	67	PRO
1	A	274	HIS
1	B	184	LYS
1	B	277	LEU
1	B	278	THR
1	B	285	TYR
1	A	15	ASN
1	A	42	ASN
1	A	270	ASN
1	A	282	HIS
1	A	283	LYS
1	A	285	TYR
1	A	286	GLU
1	A	317	LEU
1	B	70	ILE
1	B	181	GLU
1	B	251	TYR
1	B	267	GLY
1	B	283	LYS
1	B	34	LYS
1	B	42	ASN
1	B	67	PRO
1	B	284	SER
1	B	141	ASP

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Mol	Chain	Res	Type
1	B	183	ASN
1	B	270	ASN
1	B	273	LEU
1	A	68	ASP
1	A	167	TYR
1	B	69	ASN
1	B	279	ASN
1	A	141	ASP
1	A	316	ILE
1	B	68	ASP
1	B	113	SER
1	A	264	PRO
1	A	271	GLY
1	A	14	ILE
1	A	146	VAL

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	280/295 (95%)	260 (93%)	20 (7%)	13	23
1	B	270/295 (92%)	251 (93%)	19 (7%)	14	24
All	All	550/590 (93%)	511 (93%)	39 (7%)	13	23

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	61	ASP
1	A	126	LEU
1	A	138	LYS
1	A	146	VAL
1	A	148	ASN
1	A	157	LEU
1	A	166	ILE

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Mol	Chain	Res	Type
1	A	191	LEU
1	A	222	LEU
1	A	232	GLN
1	A	244	ASN
1	A	252	ILE
1	A	264	PRO
1	A	275	LYS
1	A	277	LEU
1	A	279	ASN
1	A	283	LYS
1	A	288	ILE
1	A	290	ILE
1	B	4	LYS
1	B	9	LYS
1	B	35	ASN
1	B	60	LYS
1	B	90	ILE
1	B	96	LYS
1	B	126	LEU
1	B	138	LYS
1	B	146	VAL
1	B	172	MET
1	B	196	ASN
1	B	201	ILE
1	B	229	ASN
1	B	247	ASP
1	B	283	LYS
1	B	285	TYR
1	B	286	GLU
1	B	288	ILE
1	B	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	35	ASN
1	A	55	ASN
1	A	84	ASN
1	A	92	ASN
1	A	95	ASN
1	A	130	ASN

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Mol	Chain	Res	Type
1	A	140	ASN
1	A	196	ASN
1	A	203	GLN
1	A	205	ASN
1	A	212	GLN
1	A	229	ASN
1	A	234	ASN
1	A	270	ASN
1	A	312	GLN
1	B	84	ASN
1	B	140	ASN
1	B	144	ASN
1	B	171	ASN
1	B	196	ASN
1	B	203	GLN
1	B	212	GLN
1	B	223	ASN
1	B	232	GLN
1	B	279	ASN
1	B	282	HIS
1	B	291	ASN
1	B	303	GLN
1	B	307	GLN
1	B	312	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 oligosaccharides 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	$\# Z > 2$
2	U5P	A	500	-	22,22,22	0.81	0	32,33,33	1.71	8 (25%)
2	U5P	B	600	-	22,22,22	0.90	0	32,33,33	1.80	8 (25%)

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	A	500	-	-	2/10/26/26	0/2/2/2
2	U5P	B	600	-	-	2/10/26/26	0/2/2/2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	U5P	C4-N3-C2	-4.52	121.00	126.61
2	A	500	U5P	C4-N3-C2	-4.38	121.18	126.61
2	B	600	U5P	C5-C4-N3	3.73	120.02	114.80
2	A	500	U5P	N3-C2-N1	3.64	119.63	114.89
2	A	500	U5P	C5-C4-N3	3.64	119.89	114.80
2	B	600	U5P	N3-C2-N1	3.53	119.48	114.89
2	B	600	U5P	O4-C4-C5	-3.14	119.75	125.16
2	A	500	U5P	O4-C4-C5	-3.09	119.84	125.16
2	B	600	U5P	C5'-C4'-C3'	-2.96	104.54	115.21
2	A	500	U5P	C1'-N1-C2	2.82	122.66	117.59
2	B	600	U5P	C2'-C3'-C4'	2.82	108.05	102.61
2	B	600	U5P	C1'-N1-C2	2.62	122.30	117.59
2	B	600	U5P	O4'-C1'-N1	2.33	113.64	108.36
2	A	500	U5P	O4'-C1'-N1	2.20	113.35	108.36
2	A	500	U5P	C2'-C3'-C4'	2.07	106.60	102.61
2	A	500	U5P	C5'-C4'-C3'	-2.06	107.79	115.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

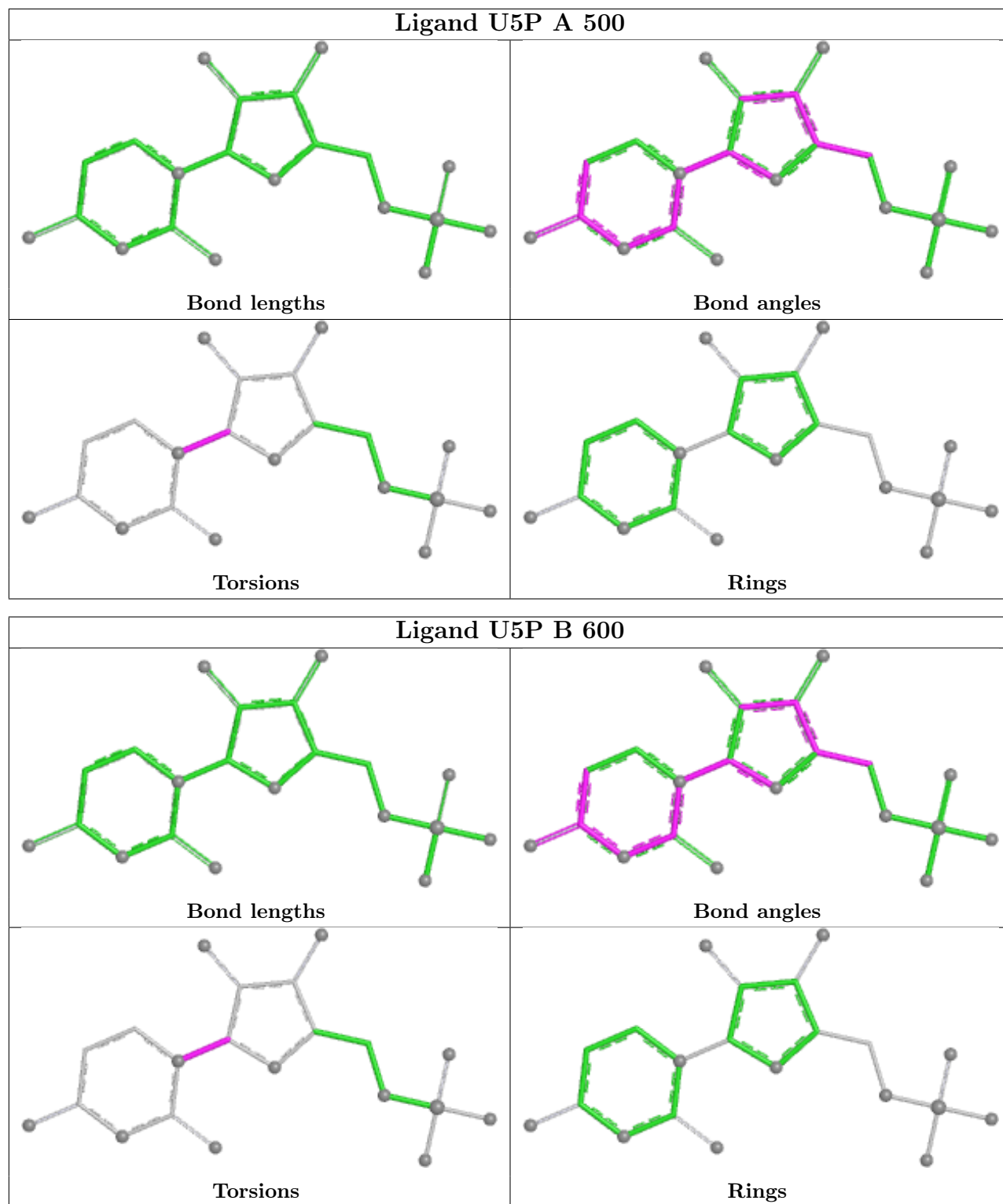
Mol	Chain	Res	Type	Atoms
2	A	500	U5P	O4'-C1'-N1-C2
2	A	500	U5P	O4'-C1'-N1-C6
2	B	600	U5P	O4'-C1'-N1-C2
2	B	600	U5P	O4'-C1'-N1-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	U5P	1	0
2	B	600	U5P	1	0

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



5.7 Other polymers ⓘ

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	315/323 (97%)	0.17	8 (2%) 58 52	25, 50, 87, 124	0
1	B	316/323 (97%)	0.19	11 (3%) 47 38	25, 49, 82, 107	0
All	All	631/646 (97%)	0.18	19 (3%) 52 45	25, 49, 84, 124	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	LEU	4.9
1	B	318	LYS	3.5
1	A	53	ILE	3.4
1	B	276	THR	3.2
1	B	280	GLY	3.2
1	B	281	TYR	3.1
1	A	54	ASN	2.9
1	A	275	LYS	2.8
1	A	277	LEU	2.7
1	B	278	THR	2.7
1	A	273	LEU	2.4
1	B	183	ASN	2.4
1	B	284	SER	2.4
1	B	250	ASN	2.3
1	B	275	LYS	2.2
1	A	284	SER	2.2
1	B	279	ASN	2.1
1	A	69	ASN	2.1
1	A	274	HIS	2.1

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](#)

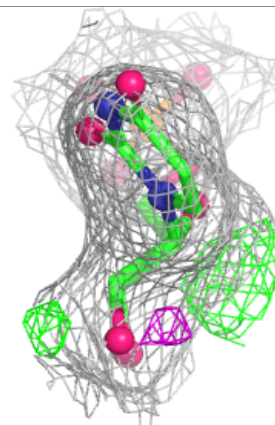
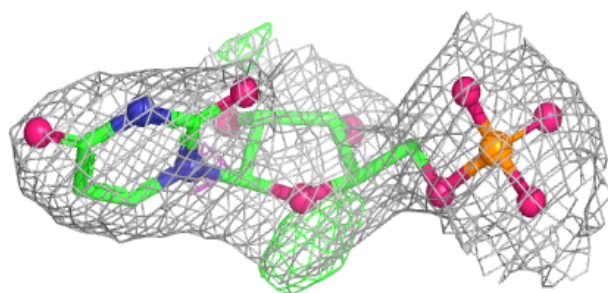
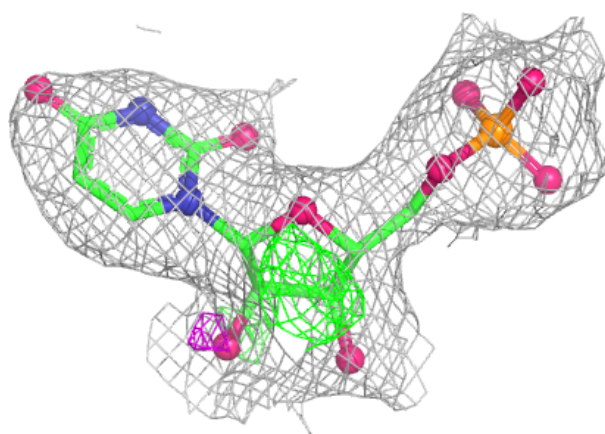
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	U5P	B	600	21/21	0.92	0.11	37,48,58,74	0
2	U5P	A	500	21/21	0.94	0.09	29,46,56,61	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.

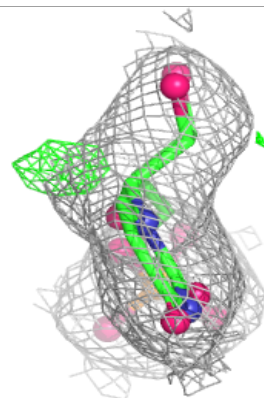
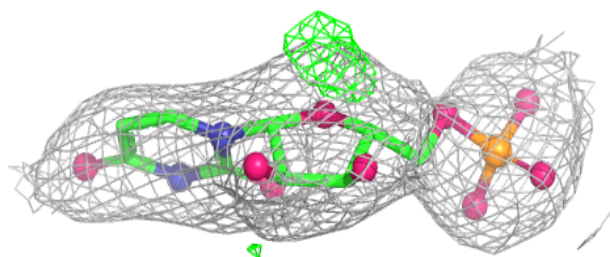
Electron density around U5P B 600:

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 500:

$2mF_o-DF_c$ (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.