



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:59 pm BST

PDB ID : 2ZA1  
Title : Crystal Structure of orotidine 5'-monophosphate decarboxylase complexed with orotidine 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](mailto: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.

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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

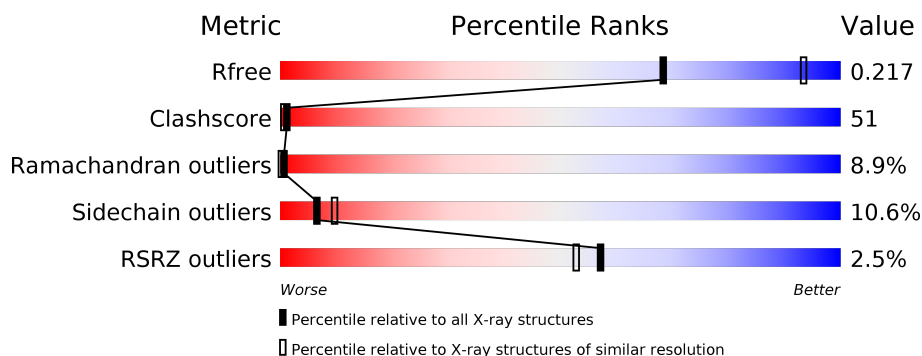
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>35%</div> <div>52%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	323	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>47%</div> <div>13%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

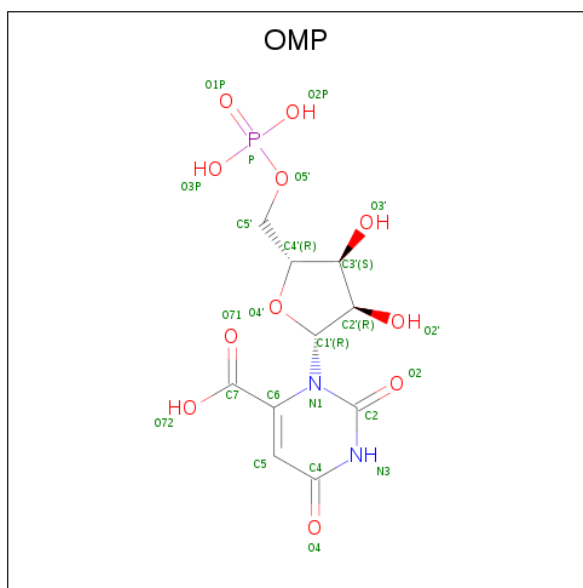
There are 3 unique types of molecules in this entry. The entry contains 5275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	318	Total	C	N	O	S	0	0	0
			2574	1664	414	481	15			
1	B	315	Total	C	N	O	S	0	0	0
			2535	1635	406	479	15			

- Molecule 2 is OROTIDINE-5'-MONOPHOSPHATE (three-letter code: OMP) (formula:  $C_{10}H_{13}N_2O_{11}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	2	11	1		
2	B	1	Total	C	N	O	P	0	0
			24	10	2	11	1		

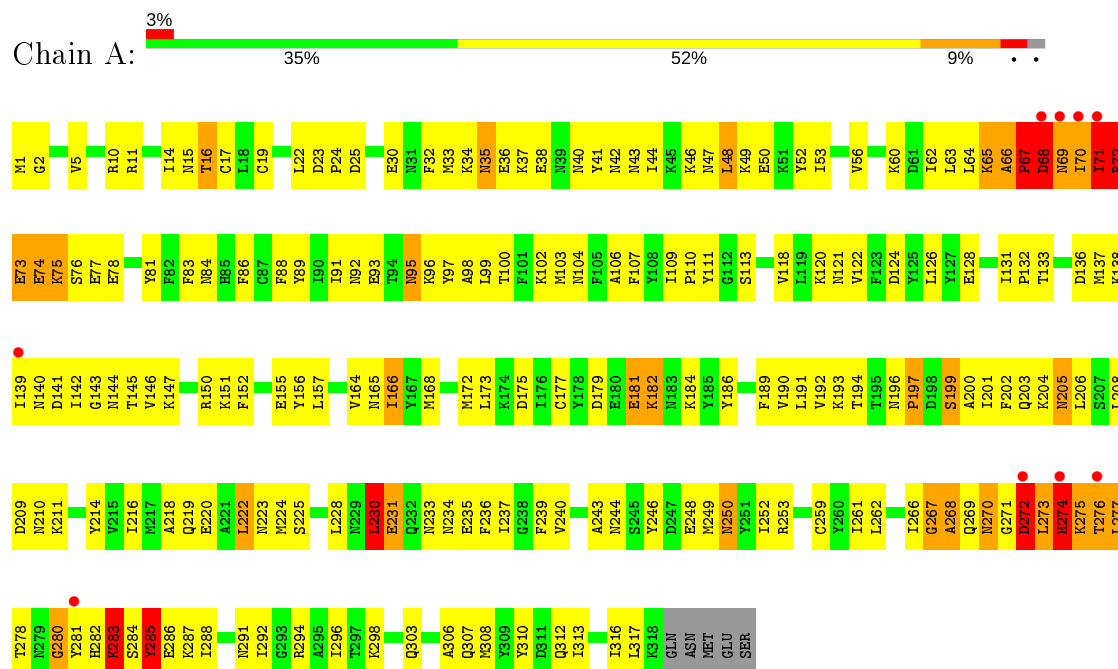
- Molecule 3 is water.

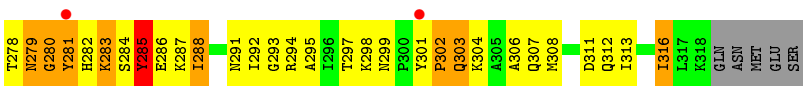
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total 64	O 64	0	0
3	B	54	Total 54	O 54	0	0

### 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: Orotidine 5'-phosphate decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.80 Å   201.80 Å   44.20 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	38.14 – 2.65 38.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (38.14-2.65) 98.7 (38.14-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.79 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.210 , 0.292 0.218 , 0.217	Depositor DCC
$R_{free}$ test set	1049 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OMP

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	0/2629	0.78	7/3550 (0.2%)
1	B	0.47	0/2589	0.79	3/3501 (0.1%)
All	All	0.46	0/5218	0.78	10/7051 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LEU	N-CA-C	-6.96	92.20	111.00
1	A	230	LEU	CA-CB-CG	6.41	130.03	115.30
1	A	285	TYR	N-CA-C	6.37	128.21	111.00
1	B	280	GLY	N-CA-C	-6.22	97.54	113.10
1	B	277	LEU	N-CA-C	-6.02	94.74	111.00
1	A	69	ASN	N-CA-C	-5.97	94.87	111.00
1	A	280	GLY	N-CA-C	-5.79	98.63	113.10
1	A	72	ARG	N-CA-C	-5.52	96.11	111.00
1	A	71	ILE	N-CA-C	-5.46	96.27	111.00
1	A	68	ASP	N-CA-C	5.42	125.62	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	251	TYR	Sidechain

## 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	2574	0	2520	253	0
1	B	2535	0	2439	283	0
2	A	24	0	11	3	0
2	B	24	0	11	3	0
3	A	64	0	0	13	0
3	B	54	0	0	13	0
All	All	5275	0	4981	519	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 51.

All (519) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:THR:HG22	1:A:132:PRO:HB2	1.34	1.09
1:B:232:GLN:O	1:B:234:ASN:N	1.86	1.08
1:A:283:LYS:HD2	1:A:284:SER:H	1.19	1.06
1:B:273:LEU:HD12	1:B:312:GLN:HE21	1.26	1.00
1:A:113:SER:HB2	1:B:113:SER:HB2	1.42	1.00
1:B:174:LYS:HG3	1:B:228:LEU:HD21	1.45	0.99
1:A:166:ILE:HD11	1:A:173:LEU:HG	1.40	0.97
1:A:196:ASN:HB2	1:A:199:SER:HB2	1.44	0.97
1:B:196:ASN:O	1:B:199:SER:HB2	1.68	0.94
1:B:232:GLN:C	1:B:234:ASN:H	1.71	0.93
1:A:68:ASP:C	1:A:70:ILE:H	1.69	0.93
1:B:294:ARG:HG2	1:B:298:LYS:HE2	1.49	0.93
1:A:283:LYS:HE2	1:A:287:LYS:HE3	1.51	0.92
1:A:282:HIS:O	1:A:283:LYS:HB2	1.68	0.91
1:B:147:LYS:HA	3:B:629:HOH:O	1.75	0.87
1:A:230:LEU:HD23	1:A:230:LEU:O	1.74	0.86
1:B:50:GLU:O	1:B:51:LYS:HB3	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD13	1:A:77:GLU:HG2	1.57	0.86
1:A:312:GLN:O	1:A:316:ILE:HD13	1.77	0.85
1:B:283:LYS:HG3	1:B:284:SER:H	1.41	0.85
1:A:266:ILE:HD11	1:A:277:LEU:HD13	1.57	0.84
1:A:243:ALA:HB1	1:A:277:LEU:HD11	1.58	0.84
1:A:151:LYS:HE3	1:B:110:PRO:HB2	1.60	0.84
1:B:283:LYS:HG3	1:B:284:SER:N	1.92	0.84
1:A:283:LYS:CD	1:A:284:SER:H	1.91	0.84
1:A:17:CYS:HB3	1:A:285:TYR:HB2	1.58	0.83
1:A:272:ASP:O	1:A:275:LYS:HD3	1.79	0.83
1:A:173:LEU:HD13	1:A:237:ILE:HD13	1.61	0.82
1:A:84:ASN:HD21	1:A:121:ASN:HD22	1.27	0.82
1:B:56:VAL:HG21	1:B:88:PHE:HZ	1.44	0.80
1:A:69:ASN:O	1:A:71:ILE:N	2.13	0.79
1:B:276:THR:OG1	1:B:280:GLY:HA3	1.82	0.79
1:B:276:THR:HA	1:B:280:GLY:H	1.47	0.79
1:A:182:LYS:HG3	1:A:184:LYS:HG3	1.63	0.79
1:B:275:LYS:O	1:B:277:LEU:N	2.15	0.79
1:B:200:ALA:CB	1:B:203:GLN:HB2	2.14	0.78
1:A:283:LYS:HD2	1:A:284:SER:N	1.96	0.78
1:A:313:ILE:O	1:A:317:LEU:HB2	1.83	0.78
1:B:279:ASN:N	1:B:279:ASN:HD22	1.80	0.78
1:B:81:TYR:O	1:B:82:PHE:HB2	1.84	0.78
1:A:271:GLY:O	1:A:272:ASP:HB2	1.84	0.77
1:A:138:LYS:HD2	1:B:140:ASN:O	1.84	0.77
1:A:273:LEU:HA	1:A:277:LEU:CB	2.14	0.77
1:B:32:PHE:O	1:B:36:GLU:HB2	1.84	0.77
1:B:193:LYS:HA	1:B:203:GLN:NE2	2.00	0.76
1:B:227:TYR:HD2	1:B:228:LEU:N	1.83	0.76
1:A:74:GLU:O	1:A:76:SER:N	2.18	0.76
1:A:294:ARG:HG2	1:A:298:LYS:HD2	1.67	0.75
1:A:62:ILE:HD13	1:A:77:GLU:CG	2.17	0.75
1:A:184:LYS:HE3	1:A:186:TYR:OH	1.86	0.74
1:A:273:LEU:HA	1:A:277:LEU:HB2	1.68	0.74
1:B:249:MET:HE2	1:B:261:ILE:HD13	1.68	0.73
1:B:202:PHE:HA	1:B:206:LEU:HD22	1.70	0.73
1:B:266:ILE:HD11	1:B:277:LEU:HD13	1.72	0.72
1:A:17:CYS:HA	1:A:99:LEU:HD23	1.72	0.71
1:B:11:ARG:HD3	1:B:286:GLU:HG2	1.73	0.71
1:B:11:ARG:O	1:B:15:ASN:N	2.24	0.70
1:B:44:ILE:HD13	1:B:67:PRO:HG3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASP:C	1:A:70:ILE:N	2.44	0.70
1:A:166:ILE:HD12	1:A:172:MET:CE	2.21	0.70
1:A:273:LEU:HD13	1:A:274:HIS:H	1.57	0.70
1:A:84:ASN:ND2	1:A:121:ASN:HD22	1.88	0.70
1:A:100:THR:HG22	1:A:132:PRO:CB	2.19	0.69
1:B:243:ALA:HB1	1:B:277:LEU:HD11	1.75	0.69
1:B:230:LEU:O	1:B:232:GLN:O	2.11	0.69
1:B:51:LYS:HG2	1:B:52:TYR:H	1.57	0.69
1:B:227:TYR:O	1:B:228:LEU:HB2	1.91	0.69
1:B:56:VAL:HG21	1:B:88:PHE:CZ	2.28	0.69
1:B:251:TYR:HD2	1:B:252:ILE:HD12	1.58	0.68
1:A:41:TYR:HD1	1:A:44:ILE:HD12	1.59	0.68
1:A:197:PRO:C	1:A:199:SER:H	1.96	0.68
1:B:52:TYR:CD2	1:B:129:LEU:HD11	2.29	0.67
1:A:91:ILE:O	1:A:95:ASN:HB3	1.95	0.67
1:B:55:ASN:HB2	1:B:128:GLU:CG	2.26	0.66
1:B:51:LYS:HG2	1:B:52:TYR:N	2.10	0.66
1:B:50:GLU:O	1:B:51:LYS:CB	2.43	0.66
1:B:245:SER:HB3	1:B:248:GLU:CG	2.26	0.66
1:B:249:MET:CE	1:B:261:ILE:HD13	2.25	0.65
1:A:42:ASN:O	1:A:46:LYS:HG3	1.96	0.65
1:A:71:ILE:HG22	1:A:71:ILE:O	1.96	0.65
1:B:283:LYS:HG2	1:B:287:LYS:HD2	1.78	0.65
1:B:266:ILE:HD11	1:B:277:LEU:CD1	2.26	0.65
1:A:307:GLN:O	1:A:310:TYR:N	2.27	0.65
1:B:56:VAL:HG13	1:B:121:ASN:CG	2.17	0.65
1:B:17:CYS:HB3	1:B:285:TYR:HB2	1.79	0.65
1:B:292:ILE:HG23	1:B:295:ALA:HB3	1.78	0.65
1:B:294:ARG:HA	1:B:297:THR:CG2	2.27	0.65
1:B:299:ASN:O	1:B:302:PRO:HD3	1.97	0.65
1:A:182:LYS:HE2	1:A:182:LYS:O	1.97	0.64
1:A:166:ILE:HD12	1:A:172:MET:HE2	1.79	0.64
1:A:68:ASP:HA	1:A:81:TYR:CE2	2.33	0.64
1:A:152:PHE:HB2	1:B:110:PRO:HA	1.80	0.64
1:A:73:GLU:O	1:A:74:GLU:HB2	1.98	0.64
1:A:84:ASN:HB3	3:A:554:HOH:O	1.97	0.64
1:A:196:ASN:CB	1:A:199:SER:HB2	2.25	0.64
1:B:283:LYS:HZ3	1:B:284:SER:H	1.44	0.64
1:A:70:ILE:O	1:A:71:ILE:HB	1.98	0.63
1:B:229:ASN:HB2	3:B:625:HOH:O	1.98	0.63
1:B:280:GLY:O	1:B:281:TYR:CB	2.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASN:HA	1:B:224:MET:HE3	1.78	0.63
1:A:209:ASP:O	1:A:210:ASN:HB2	1.98	0.62
1:A:60:LYS:O	1:A:64:LEU:HD23	2.00	0.62
1:A:72:ARG:O	1:A:73:GLU:CB	2.47	0.62
1:B:51:LYS:CG	1:B:52:TYR:N	2.61	0.62
1:A:121:ASN:HA	3:A:533:HOH:O	1.98	0.62
1:B:41:TYR:HB3	1:B:44:ILE:CG2	2.30	0.62
1:B:293:GLY:O	1:B:297:THR:HG22	1.98	0.62
1:B:138:LYS:HD2	1:B:191:LEU:HD21	1.82	0.62
1:A:243:ALA:CB	1:A:277:LEU:HD21	2.30	0.62
1:A:282:HIS:CG	1:A:283:LYS:H	2.18	0.62
1:B:273:LEU:HD12	1:B:312:GLN:NE2	2.08	0.62
1:A:208:LEU:HB3	1:A:216:ILE:CD1	2.30	0.61
1:B:282:HIS:NE2	3:B:624:HOH:O	2.28	0.61
1:B:200:ALA:HB1	1:B:203:GLN:HB2	1.83	0.61
1:B:283:LYS:NZ	1:B:284:SER:H	1.99	0.61
1:A:266:ILE:HB	1:A:292:ILE:CD1	2.30	0.61
1:B:316:ILE:O	1:B:316:ILE:HG22	2.00	0.61
1:A:230:LEU:O	1:A:231:GLU:HB2	2.00	0.61
1:B:109:ILE:N	1:B:110:PRO:HD2	2.16	0.60
1:A:150:ARG:HD2	3:A:552:HOH:O	2.01	0.60
1:A:196:ASN:HB2	1:A:199:SER:CB	2.26	0.60
1:B:20:ILE:HD13	1:B:94:THR:HB	1.84	0.60
1:A:16:THR:O	1:A:99:LEU:HD22	2.02	0.60
1:B:55:ASN:HB2	1:B:128:GLU:HG3	1.83	0.60
1:B:275:LYS:O	1:B:277:LEU:HB2	2.01	0.60
1:B:44:ILE:CD1	1:B:67:PRO:HG3	2.31	0.60
1:B:171:ASN:HA	1:B:224:MET:CE	2.32	0.60
1:B:302:PRO:O	1:B:303:GLN:HB3	2.01	0.60
1:A:266:ILE:HD11	1:A:277:LEU:CD1	2.30	0.59
1:B:67:PRO:O	1:B:68:ASP:CG	2.40	0.59
1:A:273:LEU:HD13	1:A:274:HIS:N	2.16	0.59
1:B:258:ASN:O	1:B:287:LYS:HE3	2.02	0.59
1:A:33:MET:HE3	1:A:78:GLU:CG	2.32	0.59
1:A:109:ILE:N	1:A:110:PRO:HD2	2.17	0.59
1:B:39:ASN:ND2	1:B:39:ASN:O	2.36	0.59
1:B:60:LYS:NZ	1:B:60:LYS:HB2	2.17	0.59
1:A:274:HIS:HA	1:A:316:ILE:HG12	1.85	0.59
1:B:23:ASP:OD1	2:B:600:OMP:O3'	2.18	0.59
1:A:273:LEU:HA	1:A:277:LEU:HB3	1.85	0.59
1:B:245:SER:HB3	1:B:248:GLU:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ILE:HG12	1:B:53:ILE:O	2.02	0.59
1:A:165:ASN:HD22	1:B:140:ASN:ND2	2.01	0.59
1:B:109:ILE:N	1:B:110:PRO:CD	2.66	0.58
1:A:316:ILE:H	1:A:316:ILE:CD1	2.16	0.58
1:B:196:ASN:O	1:B:199:SER:CB	2.49	0.58
1:B:200:ALA:HB2	1:B:203:GLN:HB2	1.85	0.58
1:A:268:ALA:HB3	3:A:564:HOH:O	2.02	0.58
1:A:164:VAL:HG11	1:A:172:MET:HE3	1.86	0.58
1:B:294:ARG:HA	1:B:297:THR:HG22	1.84	0.58
1:B:6:LYS:HE3	1:B:130:ASN:ND2	2.18	0.58
1:B:47:ASN:O	1:B:50:GLU:HB2	2.04	0.58
1:B:193:LYS:HD2	1:B:203:GLN:HE21	1.69	0.57
1:B:4:LYS:HB3	1:B:4:LYS:NZ	2.19	0.57
1:A:109:ILE:HG13	1:B:152:PHE:CD1	2.39	0.57
1:B:135:LEU:HD23	1:B:153:ILE:HG12	1.86	0.57
1:B:172:MET:HE2	1:B:176:ILE:CD1	2.34	0.57
1:B:285:TYR:CD1	1:B:285:TYR:N	2.71	0.57
1:B:56:VAL:HG13	1:B:121:ASN:OD1	2.04	0.57
1:B:276:THR:HA	1:B:280:GLY:N	2.18	0.57
1:A:166:ILE:HD11	1:A:173:LEU:CG	2.25	0.57
1:B:60:LYS:HG2	1:B:64:LEU:HD11	1.86	0.57
1:A:208:LEU:HB3	1:A:216:ILE:HD13	1.86	0.57
1:A:110:PRO:HA	1:B:152:PHE:HB2	1.86	0.57
1:B:150:ARG:HD3	1:B:175:ASP:O	2.04	0.57
1:B:55:ASN:O	1:B:56:VAL:C	2.42	0.57
1:A:201:ILE:HD12	1:B:170:THR:HG22	1.86	0.57
1:A:282:HIS:CG	1:A:283:LYS:N	2.72	0.57
1:A:211:LYS:CE	1:A:219:GLN:HE22	2.18	0.56
1:A:107:PHE:CE2	1:B:145:THR:HG23	2.41	0.56
1:B:102:LYS:HE3	1:B:291:ASN:ND2	2.20	0.56
1:A:164:VAL:O	1:A:190:VAL:HA	2.06	0.56
1:A:274:HIS:CD2	1:A:275:LYS:HG3	2.40	0.56
1:A:73:GLU:O	1:A:74:GLU:CB	2.54	0.56
1:A:151:LYS:HA	1:A:155:GLU:HG3	1.88	0.56
1:A:273:LEU:C	1:A:273:LEU:HD22	2.26	0.56
1:A:44:ILE:HG22	1:A:48:LEU:HD22	1.88	0.56
1:B:180:GLU:O	1:B:181:GLU:C	2.44	0.56
1:A:205:ASN:O	1:B:208:LEU:HD13	2.05	0.56
1:B:41:TYR:CD1	1:B:67:PRO:HB3	2.40	0.56
1:A:214:TYR:HE2	1:A:252:ILE:CD1	2.18	0.56
1:A:274:HIS:CG	1:A:275:LYS:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TYR:HD1	1:A:285:TYR:H	1.54	0.56
1:A:41:TYR:CG	1:A:67:PRO:HB3	2.41	0.56
1:B:267:GLY:O	1:B:268:ALA:HB3	2.06	0.56
1:A:11:ARG:HD3	1:A:286:GLU:CD	2.26	0.56
1:B:54:ASN:O	1:B:54:ASN:ND2	2.39	0.56
1:A:182:LYS:HG3	1:A:184:LYS:CG	2.36	0.56
1:A:41:TYR:CD2	1:A:67:PRO:HB3	2.41	0.56
1:B:292:ILE:CG2	1:B:295:ALA:HB3	2.35	0.56
1:B:294:ARG:CG	1:B:298:LYS:HE2	2.31	0.56
1:B:50:GLU:HA	1:B:50:GLU:OE2	2.03	0.56
1:A:109:ILE:N	1:A:110:PRO:CD	2.69	0.55
1:A:288:ILE:HG23	1:A:288:ILE:O	2.06	0.55
1:A:36:GLU:HG3	1:A:41:TYR:HA	1.87	0.55
1:A:273:LEU:O	1:A:274:HIS:C	2.44	0.55
1:B:183:ASN:O	1:B:184:LYS:O	2.25	0.55
1:A:285:TYR:CG	1:A:317:LEU:HD21	2.41	0.55
1:A:50:GLU:O	1:A:53:ILE:HG22	2.07	0.55
1:A:253:ARG:HH22	1:A:287:LYS:HB3	1.72	0.55
1:A:316:ILE:HD12	1:A:316:ILE:N	2.22	0.55
1:B:44:ILE:HD11	1:B:81:TYR:OH	2.07	0.55
1:B:20:ILE:CD1	1:B:94:THR:HB	2.37	0.54
1:B:249:MET:HE1	1:B:261:ILE:HG21	1.89	0.54
1:A:23:ASP:HB3	1:A:107:PHE:CE2	2.43	0.54
1:A:204:LYS:O	1:A:206:LEU:N	2.40	0.54
1:A:196:ASN:O	1:A:199:SER:HB3	2.07	0.54
1:A:250:ASN:HD22	1:A:250:ASN:N	2.06	0.54
1:A:281:TYR:CB	1:A:288:ILE:HD13	2.37	0.54
1:B:34:LYS:O	1:B:38:GLU:HG2	2.07	0.54
1:A:173:LEU:HD13	1:A:237:ILE:CD1	2.36	0.54
1:B:123:PHE:CE1	1:B:133:THR:HB	2.43	0.54
1:B:15:ASN:O	1:B:16:THR:HG22	2.07	0.54
1:A:36:GLU:OE2	1:A:43:ASN:N	2.40	0.54
1:B:109:ILE:H	1:B:110:PRO:CD	2.20	0.54
1:B:173:LEU:HD22	1:B:173:LEU:H	1.73	0.54
1:A:19:CYS:O	1:A:291:ASN:HA	2.06	0.54
1:A:136:ASP:OD2	2:A:500:OMP:O71	2.26	0.54
1:A:109:ILE:HG13	1:A:109:ILE:O	2.08	0.54
1:A:285:TYR:CD2	1:A:317:LEU:HD21	2.43	0.54
1:B:232:GLN:C	1:B:234:ASN:N	2.43	0.54
1:B:245:SER:HB3	1:B:248:GLU:HG2	1.89	0.54
1:B:303:GLN:O	1:B:306:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:TYR:HB3	1:B:44:ILE:HG23	1.90	0.54
1:A:204:LYS:C	1:A:206:LEU:H	2.11	0.53
1:B:11:ARG:HD3	1:B:286:GLU:CG	2.37	0.53
1:B:172:MET:HE2	1:B:176:ILE:HD11	1.89	0.53
1:B:164:VAL:O	1:B:191:LEU:HD13	2.07	0.53
1:A:17:CYS:HA	1:A:99:LEU:CD2	2.38	0.53
1:B:283:LYS:HG2	1:B:287:LYS:CD	2.37	0.53
1:A:71:ILE:CG2	1:A:71:ILE:O	2.56	0.53
1:B:275:LYS:O	1:B:276:THR:C	2.46	0.53
1:B:182:LYS:O	1:B:183:ASN:HB2	2.09	0.53
1:A:208:LEU:HD13	1:B:205:ASN:O	2.08	0.53
1:B:243:ALA:HA	1:B:277:LEU:HD21	1.90	0.53
1:B:81:TYR:O	1:B:82:PHE:CB	2.53	0.53
1:A:113:SER:HB2	1:B:113:SER:CB	2.29	0.53
1:A:177:CYS:HB3	1:A:230:LEU:CD1	2.39	0.53
1:B:60:LYS:HZ2	1:B:60:LYS:HB2	1.72	0.53
1:B:3:PHE:HE1	1:B:132:PRO:HB3	1.74	0.53
1:A:25:ASP:HA	3:A:550:HOH:O	2.08	0.53
1:B:99:LEU:HG	1:B:100:THR:HG23	1.90	0.53
1:B:172:MET:CE	1:B:176:ILE:HD11	2.38	0.52
1:A:316:ILE:H	1:A:316:ILE:HD12	1.75	0.52
1:B:52:TYR:CE2	1:B:129:LEU:HD11	2.44	0.52
1:B:65:LYS:O	1:B:66:ALA:O	2.27	0.52
1:A:189:PHE:CD1	1:A:262:LEU:HB2	2.44	0.52
2:A:500:OMP:H1'	2:A:500:OMP:O71	2.10	0.52
1:A:96:LYS:HE3	1:A:97:TYR:CZ	2.45	0.52
1:B:277:LEU:O	1:B:280:GLY:O	2.28	0.52
1:A:156:TYR:HD2	1:A:157:LEU:CD1	2.23	0.52
1:A:233:ASN:O	1:A:234:ASN:HB2	2.10	0.52
1:B:202:PHE:O	1:B:206:LEU:HB2	2.09	0.52
1:B:200:ALA:HB1	1:B:203:GLN:N	2.25	0.51
1:B:253:ARG:HB2	1:B:281:TYR:HA	1.92	0.51
1:A:16:THR:N	1:A:285:TYR:HE2	2.09	0.51
1:A:37:LYS:HD3	1:A:41:TYR:OH	2.09	0.51
1:B:227:TYR:O	1:B:228:LEU:CB	2.58	0.51
1:B:173:LEU:HG	1:B:237:ILE:HD13	1.93	0.51
1:A:166:ILE:CD1	1:A:172:MET:HE2	2.40	0.51
1:B:95:ASN:HB2	1:B:131:ILE:CD1	2.40	0.51
1:A:224:MET:CE	1:A:228:LEU:HG	2.40	0.51
1:B:193:LYS:HE3	1:B:204:LYS:HD2	1.91	0.51
1:A:118:VAL:O	1:A:122:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HD3	1:A:99:LEU:O	2.11	0.51
1:B:41:TYR:CG	1:B:67:PRO:HB3	2.45	0.51
1:B:278:THR:HG22	1:B:279:ASN:ND2	2.26	0.51
1:B:313:ILE:O	1:B:316:ILE:CD1	2.59	0.50
1:A:285:TYR:CD1	1:A:285:TYR:N	2.79	0.50
1:A:17:CYS:CB	1:A:285:TYR:HB2	2.36	0.50
1:B:179:ASP:O	1:B:183:ASN:O	2.29	0.50
1:A:65:LYS:O	1:A:66:ALA:C	2.50	0.50
1:B:95:ASN:HB2	1:B:131:ILE:HD11	1.93	0.50
1:B:249:MET:HE3	1:B:249:MET:HA	1.93	0.50
1:A:23:ASP:HB3	1:A:107:PHE:CD2	2.46	0.50
1:A:259:CYS:HA	3:A:528:HOH:O	2.11	0.50
1:A:141:ASP:OD2	1:B:138:LYS:NZ	2.41	0.50
1:A:259:CYS:O	1:A:259:CYS:SG	2.68	0.50
1:A:250:ASN:ND2	1:A:280:GLY:HA3	2.26	0.50
1:B:197:PRO:C	1:B:199:SER:H	2.13	0.50
1:B:200:ALA:HB1	1:B:203:GLN:CB	2.41	0.50
1:A:218:ALA:HB1	1:A:239:PHE:CZ	2.47	0.50
1:A:307:GLN:O	1:A:308:MET:C	2.49	0.50
1:B:276:THR:CA	1:B:280:GLY:H	2.21	0.50
1:A:164:VAL:CG1	1:A:172:MET:CE	2.90	0.50
1:A:243:ALA:HB1	1:A:277:LEU:CD1	2.34	0.50
1:A:65:LYS:NZ	1:A:74:GLU:OE2	2.41	0.50
1:A:86:PHE:O	1:A:89:TYR:HB3	2.11	0.50
1:B:10:ARG:HH11	1:B:10:ARG:HG3	1.77	0.49
1:B:55:ASN:O	1:B:55:ASN:ND2	2.45	0.49
1:A:43:ASN:O	1:A:46:LYS:HB2	2.11	0.49
1:B:268:ALA:C	1:B:270:ASN:N	2.65	0.49
1:A:267:GLY:O	1:A:268:ALA:CB	2.59	0.49
1:B:268:ALA:C	1:B:270:ASN:H	2.15	0.49
1:A:202:PHE:O	1:A:206:LEU:HB2	2.12	0.49
1:A:22:LEU:O	1:A:24:PRO:HD3	2.13	0.49
1:B:191:LEU:HD11	3:B:648:HOH:O	2.13	0.49
1:B:272:ASP:O	1:B:274:HIS:O	2.31	0.49
1:B:41:TYR:HB3	1:B:44:ILE:HG21	1.95	0.49
1:B:227:TYR:CD2	1:B:228:LEU:N	2.73	0.49
1:A:120:LYS:HE3	1:A:124:ASP:OD1	2.13	0.49
1:A:25:ASP:OD1	1:A:25:ASP:C	2.51	0.49
1:B:183:ASN:HD22	1:B:183:ASN:N	2.10	0.49
1:B:166:ILE:HG21	1:B:173:LEU:HD21	1.95	0.49
1:A:124:ASP:HB2	3:A:533:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LYS:HD3	1:A:203:GLN:NE2	2.28	0.48
1:A:192:VAL:HG21	1:A:239:PHE:HB3	1.95	0.48
1:A:34:LYS:HE2	3:A:560:HOH:O	2.12	0.48
1:B:135:LEU:CD2	1:B:153:ILE:HG12	2.42	0.48
1:B:282:HIS:CE1	3:B:624:HOH:O	2.65	0.48
1:B:46:LYS:NZ	1:B:46:LYS:HB3	2.28	0.48
1:A:164:VAL:CG1	1:A:172:MET:HE3	2.43	0.48
1:A:147:LYS:HE3	1:A:175:ASP:OD1	2.12	0.48
1:B:191:LEU:HG	3:B:648:HOH:O	2.12	0.48
1:B:51:LYS:NZ	1:B:52:TYR:CE1	2.81	0.48
1:A:248:GLU:N	1:A:248:GLU:OE2	2.30	0.48
1:A:93:GLU:O	1:A:303:GLN:HG3	2.14	0.48
1:B:109:ILE:HG13	1:B:109:ILE:O	2.13	0.48
1:B:285:TYR:H	1:B:285:TYR:HD1	1.59	0.48
1:B:283:LYS:O	1:B:285:TYR:N	2.46	0.48
1:B:38:GLU:HG2	3:B:643:HOH:O	2.12	0.48
1:A:99:LEU:O	1:A:132:PRO:HD2	2.13	0.48
1:B:113:SER:HB3	3:B:644:HOH:O	2.14	0.48
1:B:32:PHE:O	1:B:36:GLU:CB	2.59	0.48
1:A:274:HIS:CD2	1:A:274:HIS:C	2.86	0.48
1:A:316:ILE:N	1:A:316:ILE:CD1	2.77	0.48
1:A:197:PRO:C	1:A:199:SER:N	2.65	0.48
1:A:243:ALA:O	1:A:277:LEU:HD11	2.14	0.47
1:A:71:ILE:O	1:A:72:ARG:CB	2.62	0.47
1:A:274:HIS:CE1	1:A:275:LYS:HG3	2.48	0.47
1:A:202:PHE:HE1	1:B:216:ILE:HG22	1.80	0.47
1:B:56:VAL:HG11	1:B:63:LEU:HD13	1.95	0.47
1:B:255:TYR:N	1:B:255:TYR:CD1	2.81	0.47
1:A:252:ILE:HG22	1:A:253:ARG:N	2.27	0.47
1:A:64:LEU:N	1:A:64:LEU:HD22	2.30	0.47
1:B:293:GLY:C	1:B:297:THR:HG22	2.35	0.47
1:B:86:PHE:O	1:B:90:ILE:HD13	2.15	0.47
1:A:179:ASP:OD1	1:A:181:GLU:HG2	2.14	0.47
1:B:10:ARG:O	1:B:14:ILE:HG12	2.15	0.47
1:B:247:ASP:OD1	1:B:248:GLU:OE2	2.32	0.47
1:A:273:LEU:HD22	1:A:274:HIS:N	2.30	0.47
1:B:278:THR:C	1:B:279:ASN:HD22	2.18	0.47
1:B:54:ASN:ND2	1:B:60:LYS:HD3	2.30	0.47
1:B:200:ALA:C	1:B:202:PHE:H	2.15	0.47
1:B:279:ASN:N	1:B:279:ASN:ND2	2.51	0.47
1:B:97:TYR:CZ	1:B:307:GLN:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ILE:HD13	1:A:306:ALA:HA	1.95	0.47
1:B:253:ARG:O	1:B:257:PRO:HA	2.15	0.47
1:A:52:TYR:CD1	1:A:128:GLU:HG3	2.50	0.47
1:B:278:THR:CG2	1:B:279:ASN:ND2	2.78	0.47
1:A:62:ILE:CD1	1:A:77:GLU:HG2	2.38	0.47
1:B:93:GLU:O	1:B:303:GLN:HB2	2.15	0.47
1:A:266:ILE:CD1	1:A:277:LEU:HD13	2.38	0.46
1:A:44:ILE:HG22	1:A:48:LEU:CD2	2.44	0.46
1:B:101:PHE:HD2	1:B:131:ILE:HG21	1.80	0.46
1:B:65:LYS:O	1:B:66:ALA:C	2.52	0.46
1:A:151:LYS:O	1:A:155:GLU:HB2	2.16	0.46
1:A:208:LEU:HB3	1:A:216:ILE:HD11	1.97	0.46
1:B:169:GLY:O	1:B:172:MET:HG3	2.15	0.46
1:A:191:LEU:HD23	1:A:240:VAL:HG21	1.96	0.46
1:B:35:ASN:HA	1:B:38:GLU:CG	2.45	0.46
1:A:267:GLY:O	1:A:268:ALA:HB2	2.16	0.46
1:A:84:ASN:HD21	1:A:121:ASN:ND2	2.05	0.46
1:B:138:LYS:HA	1:B:163:THR:O	2.16	0.46
1:B:200:ALA:HB3	1:B:204:LYS:HG3	1.96	0.46
1:B:222:LEU:HA	1:B:222:LEU:HD12	1.74	0.46
1:B:276:THR:HG23	1:B:276:THR:O	2.15	0.46
1:A:139:ILE:O	1:A:140:ASN:HB3	2.15	0.46
1:A:249:MET:SD	1:A:281:TYR:CB	3.04	0.46
1:B:266:ILE:HG22	1:B:267:GLY:N	2.30	0.46
1:B:54:ASN:HD21	1:B:60:LYS:HD3	1.80	0.46
1:A:194:THR:H	1:A:203:GLN:HE22	1.64	0.46
1:A:199:SER:OG	1:A:199:SER:O	2.34	0.46
1:A:204:LYS:NZ	3:A:522:HOH:O	2.48	0.46
1:A:250:ASN:HD21	1:A:280:GLY:HA3	1.80	0.46
1:B:142:ILE:HD11	3:B:649:HOH:O	2.15	0.46
1:B:307:GLN:HG3	1:B:311:ASP:OD2	2.15	0.46
1:A:246:TYR:CE1	1:A:276:THR:HG23	2.51	0.46
1:B:19:CYS:SG	1:B:102:LYS:HB2	2.56	0.46
1:B:84:ASN:HD21	1:B:121:ASN:HD22	1.63	0.46
1:B:230:LEU:O	1:B:231:GLU:C	2.54	0.46
1:B:62:ILE:HD13	1:B:77:GLU:HG3	1.98	0.46
1:A:14:ILE:HD11	1:A:99:LEU:HA	1.97	0.45
1:B:251:TYR:O	1:B:255:TYR:HD1	1.99	0.45
1:A:104:ASN:ND2	2:A:500:OMP:O2'	2.48	0.45
1:A:200:ALA:HB1	1:A:204:LYS:HB2	1.97	0.45
1:A:235:GLU:OE1	1:A:235:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:O	1:A:275:LYS:N	2.49	0.45
1:A:261:ILE:N	1:A:287:LYS:O	2.39	0.45
1:B:288:ILE:O	1:B:288:ILE:HG13	2.16	0.45
1:A:164:VAL:HG12	1:A:172:MET:HE1	1.99	0.45
1:A:222:LEU:O	1:A:225:SER:N	2.49	0.45
1:B:33:MET:O	1:B:34:LYS:C	2.55	0.45
1:B:267:GLY:O	1:B:268:ALA:CB	2.64	0.45
1:A:2:GLY:O	1:A:5:VAL:CG1	2.64	0.45
1:B:164:VAL:HG12	1:B:165:ASN:N	2.31	0.45
1:B:16:THR:HG23	1:B:18:LEU:H	1.81	0.45
1:B:185:TYR:CE1	1:B:228:LEU:O	2.70	0.45
1:A:294:ARG:CG	1:A:298:LYS:HD2	2.41	0.45
1:B:140:ASN:O	1:B:141:ASP:HB2	2.16	0.45
1:B:313:ILE:O	1:B:316:ILE:HD13	2.17	0.45
1:B:36:GLU:OE2	1:B:44:ILE:HG22	2.16	0.45
1:B:50:GLU:CA	1:B:50:GLU:OE2	2.65	0.45
2:B:600:OMP:O71	2:B:600:OMP:H1'	2.16	0.45
1:A:191:LEU:HA	1:A:240:VAL:HB	1.99	0.45
1:B:191:LEU:CD1	3:B:648:HOH:O	2.64	0.45
1:B:58:ILE:HA	3:B:626:HOH:O	2.16	0.45
1:A:53:ILE:O	1:A:56:VAL:HG22	2.17	0.44
1:A:137:MET:O	1:A:138:LYS:C	2.55	0.44
1:A:78:GLU:O	1:A:81:TYR:HB3	2.16	0.44
1:B:256:PHE:N	1:B:257:PRO:CD	2.80	0.44
1:A:278:THR:CG2	1:A:316:ILE:HG21	2.48	0.44
1:A:35:ASN:O	1:A:38:GLU:N	2.47	0.44
1:A:193:LYS:HE3	1:A:204:LYS:HE2	1.99	0.44
1:B:273:LEU:O	1:B:274:HIS:O	2.36	0.44
1:A:266:ILE:HD12	1:A:272:ASP:HA	1.99	0.44
1:A:32:PHE:CD1	1:A:86:PHE:HD1	2.35	0.44
1:A:168:MET:HE3	1:B:194:THR:HG21	1.99	0.44
1:B:266:ILE:O	1:B:267:GLY:O	2.36	0.44
1:B:49:LYS:O	1:B:50:GLU:C	2.56	0.44
1:A:156:TYR:HA	3:A:516:HOH:O	2.17	0.44
1:A:307:GLN:O	1:A:310:TYR:HB3	2.17	0.44
1:A:30:GLU:O	1:A:34:LYS:HG2	2.18	0.44
1:B:196:ASN:OD1	1:B:199:SER:HA	2.17	0.44
1:B:214:TYR:HE2	1:B:252:ILE:HD11	1.83	0.44
1:B:58:ILE:HG21	1:B:117:ASP:CG	2.38	0.44
1:B:180:GLU:O	1:B:182:LYS:N	2.51	0.44
1:B:19:CYS:O	1:B:291:ASN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HD2	1:A:132:PRO:HD3	2.00	0.44
1:A:177:CYS:HB3	1:A:230:LEU:HD11	2.00	0.44
1:A:106:ALA:CB	1:B:145:THR:HG22	2.48	0.44
1:A:220:GLU:HG2	1:B:201:ILE:HD11	2.00	0.44
1:B:272:ASP:O	1:B:273:LEU:C	2.56	0.44
1:A:266:ILE:HB	1:A:292:ILE:HD11	1.99	0.43
1:B:104:ASN:OD1	1:B:106:ALA:HB3	2.18	0.43
1:A:168:MET:HG2	1:B:194:THR:HG21	1.99	0.43
1:B:211:LYS:O	1:B:216:ILE:HD11	2.17	0.43
1:B:61:ASP:OD1	1:B:62:ILE:HG13	2.17	0.43
1:A:266:ILE:HD12	1:A:272:ASP:CA	2.48	0.43
1:A:62:ILE:HD13	1:A:77:GLU:CD	2.38	0.43
1:A:166:ILE:HG23	1:A:166:ILE:O	2.17	0.43
1:B:151:LYS:O	1:B:155:GLU:HB2	2.18	0.43
1:B:174:LYS:HA	1:B:228:LEU:HD11	2.00	0.43
1:B:185:TYR:HE1	1:B:228:LEU:O	2.02	0.43
1:B:200:ALA:CB	1:B:203:GLN:CB	2.89	0.43
1:A:204:LYS:C	1:A:206:LEU:N	2.71	0.43
1:B:3:PHE:O	1:B:4:LYS:C	2.57	0.43
1:B:33:MET:HE1	1:B:78:GLU:HG2	2.01	0.43
1:A:34:LYS:O	1:A:38:GLU:HB2	2.18	0.43
1:B:67:PRO:O	1:B:68:ASP:OD1	2.37	0.43
1:A:44:ILE:O	1:A:48:LEU:HD22	2.18	0.43
1:A:68:ASP:CB	1:A:70:ILE:H	2.31	0.43
1:B:46:LYS:HB2	3:B:614:HOH:O	2.19	0.43
1:A:47:ASN:OD1	1:A:92:ASN:ND2	2.52	0.43
1:B:195:THR:OG1	2:B:600:OMP:N3	2.39	0.43
1:B:200:ALA:HB1	1:B:203:GLN:H	1.83	0.43
1:B:274:HIS:O	1:B:275:LYS:O	2.36	0.43
1:B:302:PRO:C	1:B:304:LYS:N	2.72	0.43
1:A:231:GLU:H	1:A:233:ASN:H	1.65	0.43
1:A:69:ASN:C	1:A:71:ILE:H	2.14	0.43
1:B:302:PRO:O	1:B:303:GLN:CB	2.66	0.43
1:B:302:PRO:C	1:B:304:LYS:H	2.22	0.43
1:A:189:PHE:CE1	1:A:262:LEU:HB2	2.54	0.42
1:A:1:MET:O	1:A:5:VAL:HG11	2.18	0.42
1:A:102:LYS:HE3	1:A:291:ASN:ND2	2.34	0.42
1:A:142:ILE:HG13	1:A:143:GLY:O	2.18	0.42
1:B:200:ALA:HB1	1:B:203:GLN:CA	2.49	0.42
1:B:18:LEU:HD13	1:B:313:ILE:CD1	2.50	0.42
1:B:194:THR:H	1:B:203:GLN:HE22	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD11	1:B:100:THR:CG2	2.49	0.42
1:B:182:LYS:HB3	1:B:182:LYS:HE2	1.91	0.42
1:B:231:GLU:HB2	3:B:619:HOH:O	2.18	0.42
1:B:230:LEU:CD1	1:B:237:ILE:HG13	2.49	0.42
1:B:283:LYS:CG	1:B:287:LYS:HD2	2.49	0.42
1:A:110:PRO:HG2	1:A:111:TYR:CE2	2.55	0.42
1:A:243:ALA:HB1	1:A:277:LEU:HD21	2.02	0.42
1:A:219:GLN:O	1:A:223:ASN:ND2	2.53	0.42
1:A:273:LEU:C	1:A:275:LYS:N	2.73	0.42
1:A:10:ARG:NE	1:A:98:ALA:O	2.45	0.42
1:B:66:ALA:HA	1:B:67:PRO:HD3	1.94	0.42
1:A:250:ASN:H	1:A:250:ASN:HD22	1.67	0.41
1:A:266:ILE:HB	1:A:292:ILE:HD13	2.02	0.41
1:A:269:GLN:O	1:A:270:ASN:CB	2.68	0.41
1:B:109:ILE:H	1:B:110:PRO:HD2	1.83	0.41
1:B:198:ASP:O	1:B:199:SER:C	2.57	0.41
1:B:201:ILE:O	1:B:205:ASN:HB2	2.20	0.41
1:B:301:TYR:HA	1:B:302:PRO:HD2	1.80	0.41
1:A:131:ILE:O	1:A:133:THR:HG23	2.18	0.41
1:A:49:LYS:HE2	3:A:551:HOH:O	2.21	0.41
1:B:212:GLN:OE1	1:B:214:TYR:HE1	2.04	0.41
1:B:236:PHE:C	1:B:236:PHE:CD2	2.93	0.41
1:A:143:GLY:O	1:A:144:ASN:C	2.57	0.41
1:A:214:TYR:HA	3:A:507:HOH:O	2.21	0.41
1:B:50:GLU:HG2	1:B:125:TYR:OH	2.20	0.41
1:B:253:ARG:HG2	1:B:281:TYR:HA	2.03	0.41
1:B:3:PHE:CE2	1:B:161:SER:HB3	2.56	0.41
1:B:47:ASN:O	1:B:50:GLU:N	2.53	0.41
1:B:274:HIS:CG	1:B:275:LYS:H	2.39	0.41
1:A:43:ASN:ND2	3:A:530:HOH:O	2.50	0.41
1:B:193:LYS:HG2	1:B:248:GLU:HG3	2.03	0.41
1:B:35:ASN:HA	1:B:38:GLU:HG3	2.01	0.41
1:A:103:MET:SD	1:A:103:MET:N	2.93	0.41
1:B:154:PHE:CE1	1:B:186:TYR:HB3	2.56	0.41
1:B:183:ASN:O	1:B:184:LYS:HB2	2.21	0.41
1:B:19:CYS:HA	1:B:100:THR:O	2.21	0.41
1:B:274:HIS:CD2	1:B:275:LYS:H	2.39	0.41
1:B:27:LYS:HA	1:B:30:GLU:HG2	2.03	0.41
1:B:55:ASN:C	1:B:55:ASN:ND2	2.72	0.41
1:A:201:ILE:O	1:A:205:ASN:HB2	2.21	0.40
1:A:137:MET:HG2	1:A:139:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LYS:HA	1:B:203:GLN:HE22	1.81	0.40
1:A:201:ILE:HD13	1:B:220:GLU:OE2	2.21	0.40
1:A:84:ASN:OD1	1:A:88:PHE:CE2	2.75	0.40
1:B:16:THR:HG21	1:B:97:TYR:O	2.21	0.40
1:A:235:GLU:O	1:A:236:PHE:HB3	2.21	0.40
1:B:273:LEU:C	1:B:274:HIS:O	2.60	0.40
1:A:211:LYS:HE2	1:A:219:GLN:HE22	1.85	0.40
1:A:2:GLY:O	1:A:5:VAL:HG13	2.20	0.40
1:B:12:ASN:O	1:B:14:ILE:N	2.55	0.40
1:B:48:LEU:HD12	1:B:48:LEU:HA	1.94	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	316/323 (98%)	242 (77%)	48 (15%)	26 (8%)	1	0
1	B	311/323 (96%)	239 (77%)	42 (14%)	30 (10%)	0	0
All	All	627/646 (97%)	481 (77%)	90 (14%)	56 (9%)	1	0

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	PRO
1	A	70	ILE
1	A	72	ARG
1	A	73	GLU
1	A	74	GLU
1	A	145	THR
1	A	231	GLU
1	A	272	ASP

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Mol	Chain	Res	Type
1	A	283	LYS
1	A	285	TYR
1	B	66	ALA
1	B	199	SER
1	B	232	GLN
1	B	233	ASN
1	B	251	TYR
1	B	274	HIS
1	B	276	THR
1	B	285	TYR
1	A	65	LYS
1	A	71	ILE
1	A	75	LYS
1	A	181	GLU
1	A	205	ASN
1	A	267	GLY
1	A	268	ALA
1	A	270	ASN
1	B	50	GLU
1	B	51	LYS
1	B	67	PRO
1	B	184	LYS
1	B	231	GLU
1	B	267	GLY
1	B	275	LYS
1	B	281	TYR
1	B	302	PRO
1	A	40	ASN
1	A	197	PRO
1	B	13	ALA
1	B	14	ILE
1	B	39	ASN
1	B	48	LEU
1	B	283	LYS
1	A	16	THR
1	A	199	SER
1	B	16	THR
1	B	56	VAL
1	B	82	PHE
1	B	141	ASP
1	B	270	ASN
1	A	15	ASN

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Mol	Chain	Res	Type
1	A	66	ALA
1	A	274	HIS
1	B	181	GLU
1	A	68	ASP
1	B	109	ILE
1	B	288	ILE

### 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	278/295 (94%)	254 (91%)	24 (9%)	10	15
1	B	271/295 (92%)	237 (88%)	34 (12%)	4	6
All	All	549/590 (93%)	491 (89%)	58 (11%)	6	10

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	48	LEU
1	A	63	LEU
1	A	67	PRO
1	A	71	ILE
1	A	75	LYS
1	A	83	PHE
1	A	95	ASN
1	A	126	LEU
1	A	146	VAL
1	A	166	ILE
1	A	182	LYS
1	A	222	LEU
1	A	230	LEU
1	A	244	ASN
1	A	250	ASN
1	A	272	ASP

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Mol	Chain	Res	Type
1	A	273	LEU
1	A	274	HIS
1	A	275	LYS
1	A	276	THR
1	A	277	LEU
1	A	283	LYS
1	A	285	TYR
1	B	3	PHE
1	B	16	THR
1	B	38	GLU
1	B	40	ASN
1	B	41	TYR
1	B	44	ILE
1	B	46	LYS
1	B	48	LEU
1	B	50	GLU
1	B	51	LYS
1	B	52	TYR
1	B	54	ASN
1	B	55	ASN
1	B	63	LEU
1	B	64	LEU
1	B	83	PHE
1	B	111	TYR
1	B	141	ASP
1	B	146	VAL
1	B	183	ASN
1	B	206	LEU
1	B	222	LEU
1	B	227	TYR
1	B	232	GLN
1	B	247	ASP
1	B	248	GLU
1	B	259	CYS
1	B	273	LEU
1	B	277	LEU
1	B	279	ASN
1	B	285	TYR
1	B	303	GLN
1	B	308	MET
1	B	316	ILE

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	35	ASN
1	A	40	ASN
1	A	84	ASN
1	A	140	ASN
1	A	148	ASN
1	A	171	ASN
1	A	203	GLN
1	A	223	ASN
1	A	244	ASN
1	A	250	ASN
1	A	269	GLN
1	A	274	HIS
1	A	291	ASN
1	A	307	GLN
1	B	35	ASN
1	B	54	ASN
1	B	84	ASN
1	B	130	ASN
1	B	140	ASN
1	B	183	ASN
1	B	203	GLN
1	B	223	ASN
1	B	232	GLN
1	B	234	ASN
1	B	269	GLN
1	B	274	HIS
1	B	279	ASN
1	B	291	ASN
1	B	307	GLN
1	B	312	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 carbohydrates 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	OMP	A	500	-	19,25,25	1.59	5 (26%)	21,38,38	1.65	4 (19%)
2	OMP	B	600	-	19,25,25	1.33	3 (15%)	21,38,38	1.57	3 (14%)

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	OMP	A	500	-	-	0/6/30/30	0/2/2/2
2	OMP	B	600	-	-	0/6/30/30	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	OMP	C6-N1	3.44	1.45	1.36
2	B	600	OMP	C6-N1	3.42	1.45	1.36
2	A	500	OMP	O4'-C1'	2.91	1.45	1.41
2	A	500	OMP	P-O3P	2.39	1.64	1.54
2	A	500	OMP	C1'-N1	2.28	1.56	1.49
2	B	600	OMP	P-O3P	2.09	1.62	1.54
2	A	500	OMP	P-O2P	2.07	1.62	1.54
2	B	600	OMP	P-O2P	2.07	1.62	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	OMP	C5-C4-N3	-4.48	118.85	124.08
2	A	500	OMP	C5-C4-N3	-4.26	119.10	124.08
2	B	600	OMP	P-O5'-C5'	-3.94	107.44	118.30
2	A	500	OMP	P-O5'-C5'	-3.80	107.84	118.30
2	A	500	OMP	C4-C5-C6	2.31	118.22	116.73
2	B	600	OMP	C4-C5-C6	2.22	118.17	116.73
2	A	500	OMP	C3'-C2'-C1'	2.21	104.31	100.98

There are no chirality outliers.

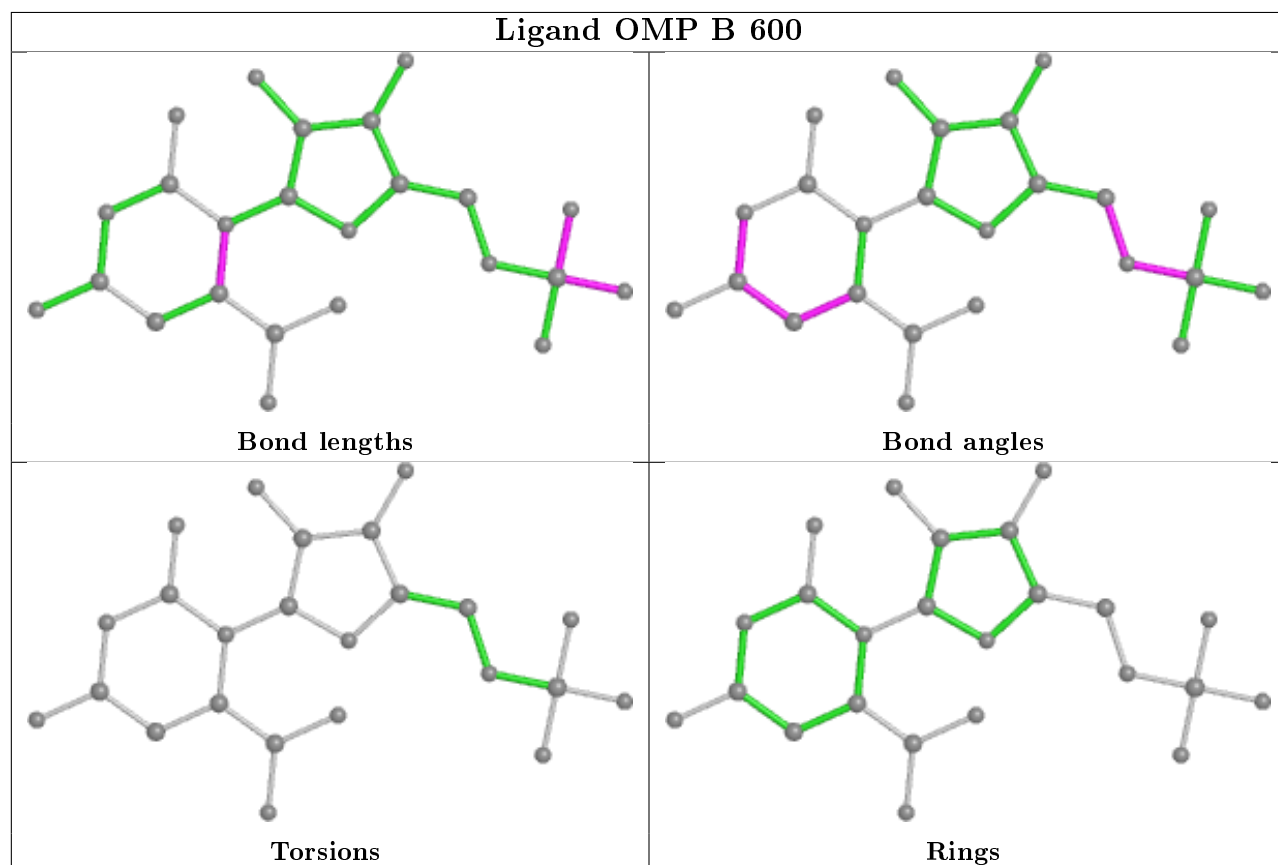
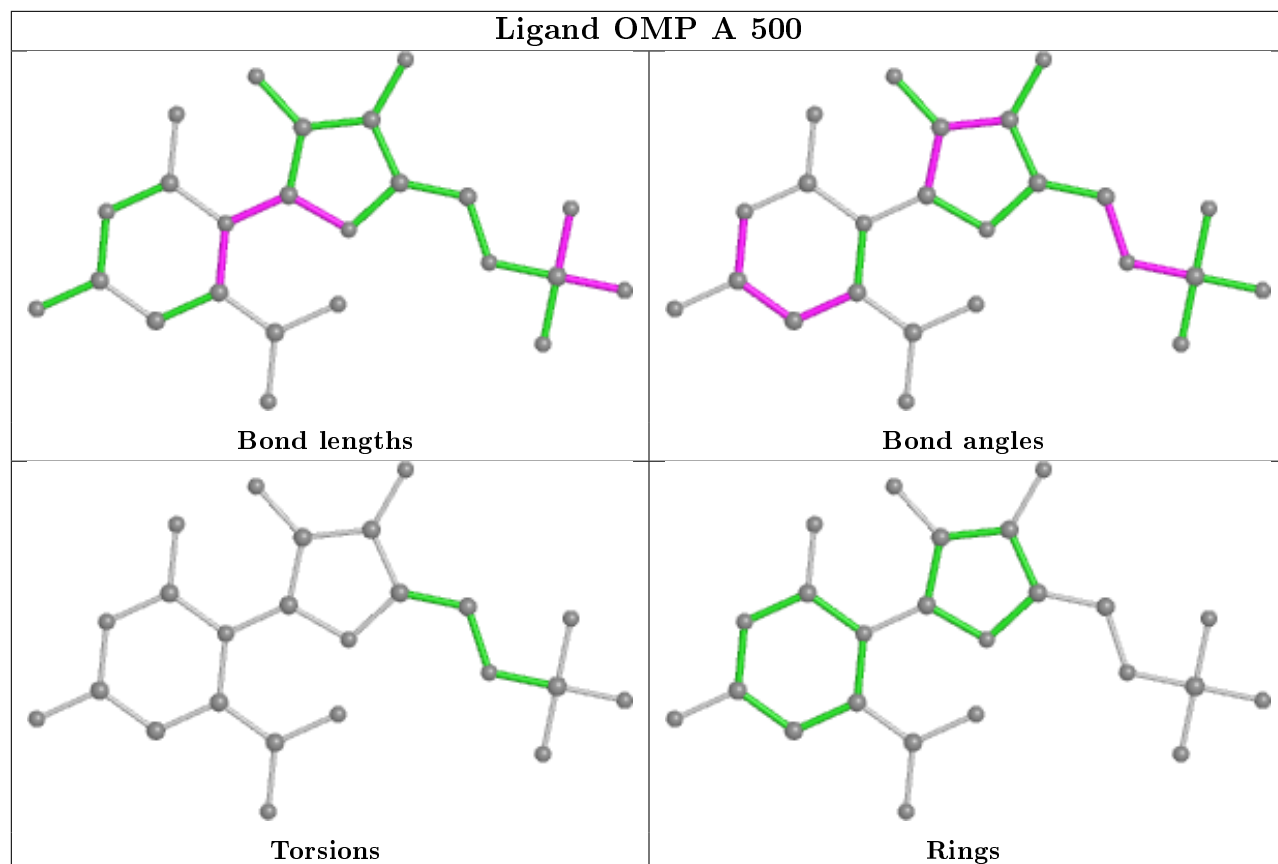
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	OMP	3	0
2	B	600	OMP	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	318/323 (98%)	-0.04	9 (2%) 53 49	28, 51, 84, 118	0
1	B	315/323 (97%)	-0.01	7 (2%) 62 57	26, 52, 78, 94	0
All	All	633/646 (97%)	-0.02	16 (2%) 57 53	26, 52, 80, 118	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ASP	5.9
1	A	71	ILE	4.8
1	A	70	ILE	3.6
1	B	276	THR	3.3
1	A	69	ASN	3.2
1	B	301	TYR	2.7
1	A	272	ASP	2.7
1	A	274	HIS	2.5
1	A	281	TYR	2.5
1	B	41	TYR	2.4
1	A	276	THR	2.3
1	A	139	ILE	2.3
1	B	74	GLU	2.2
1	B	37	LYS	2.1
1	B	281	TYR	2.1
1	B	75	LYS	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](#)

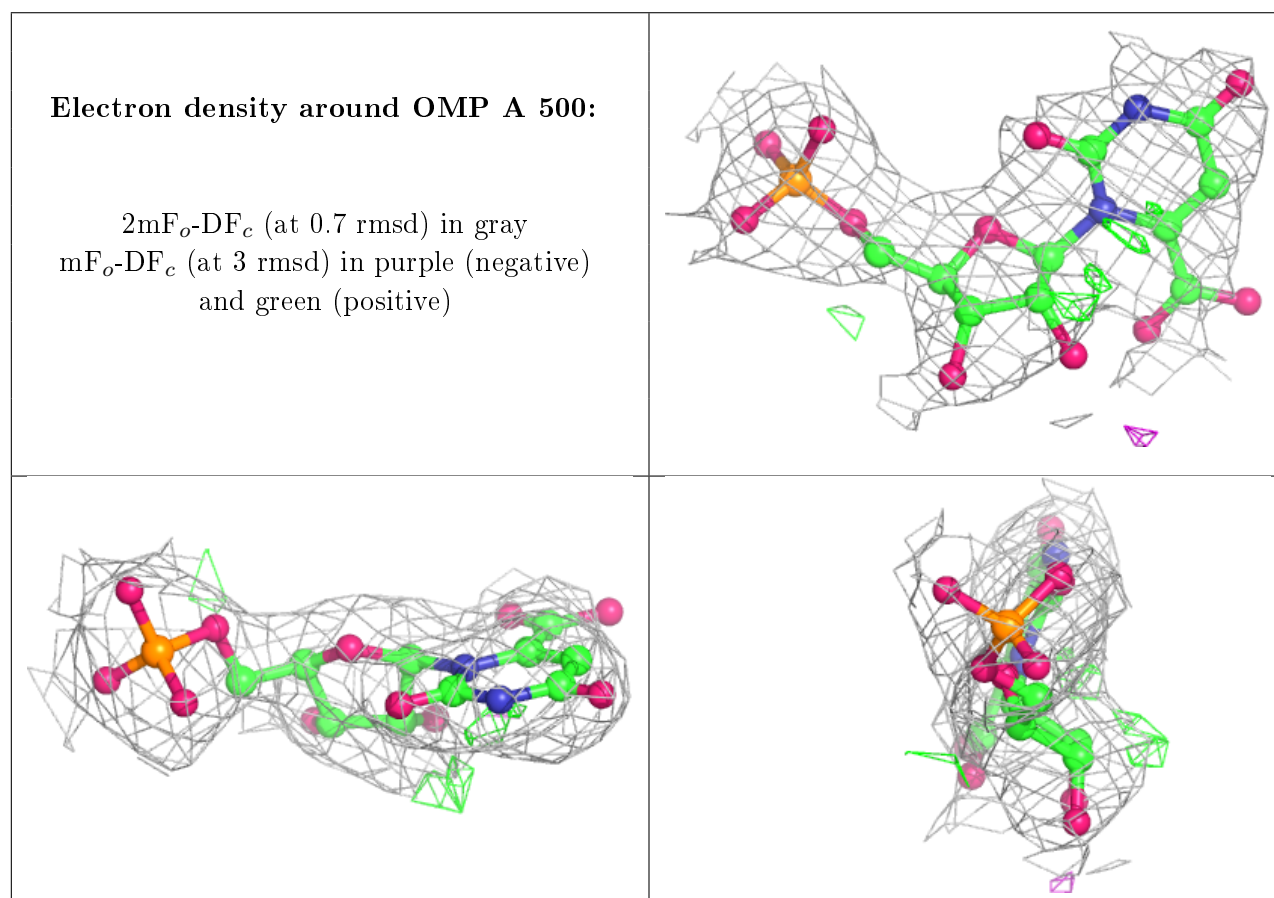
There are no carbohydrates in this entry.

### 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, 95<sup>th</sup> 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.

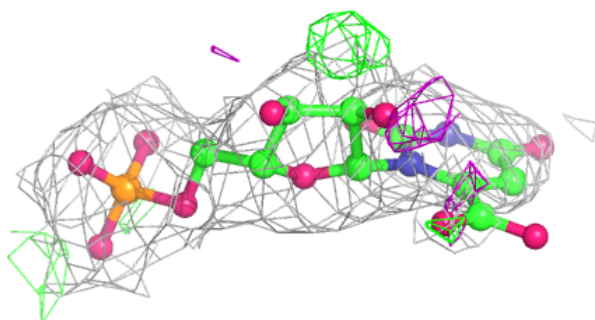
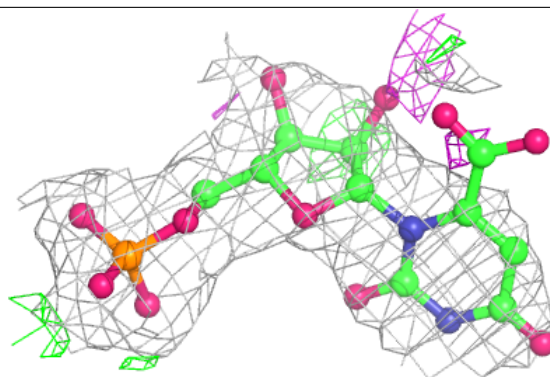
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OMP	A	500	24/24	0.92	0.18	55,67,77,88	0
2	OMP	B	600	24/24	0.93	0.21	51,74,105,113	0

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 OMP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.