Full wwPDB X-ray Structure Validation Report (i)

Jun 9, 2025 – 02:16 PM JST

PDB ID	:	8ZWQ / pdb_00008zwq
Title	:	pseudorabies virus dUTPase structure
Authors	:	Wang, Y.
Deposited on	:	2024-06-13
Resolution	:	2.23 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 (i) 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 (i)) were used in the production of this report:

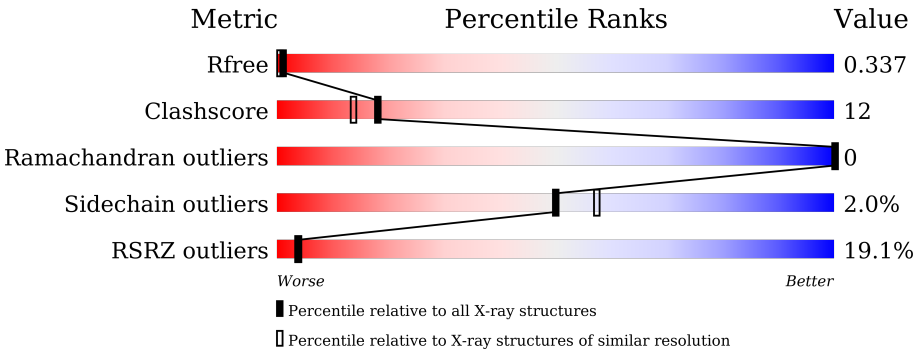
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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}	164625	3139 (2.26-2.22)
Clashscore	180529	3381 (2.26-2.22)
Ramachandran outliers	177936	3334 (2.26-2.22)
Sidechain outliers	177891	3335 (2.26-2.22)
RSRZ outliers	164620	3138 (2.26-2.22)

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 <=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	276	20% 60% 21% · 19%
1	B	276	12% 59% 21% · 19%
1	C	276	15% 61% 20% 19%
1	D	276	16% 65% 16% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UMP	A	402	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7214 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 dUTPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1717	1100	315	295	7			
1	C	224	Total	C	N	O	S	0	0	0
			1717	1100	315	295	7			
1	B	224	Total	C	N	O	S	0	0	0
			1717	1100	315	295	7			
1	D	224	Total	C	N	O	S	0	0	0
			1717	1100	315	295	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	PRO	conflict	UNP G3G945
A	269	LEU	-	expression tag	UNP G3G945
A	270	GLU	-	expression tag	UNP G3G945
A	271	HIS	-	expression tag	UNP G3G945
A	272	HIS	-	expression tag	UNP G3G945
A	273	HIS	-	expression tag	UNP G3G945
A	274	HIS	-	expression tag	UNP G3G945
A	275	HIS	-	expression tag	UNP G3G945
A	276	HIS	-	expression tag	UNP G3G945
C	110	LEU	PRO	conflict	UNP G3G945
C	269	LEU	-	expression tag	UNP G3G945
C	270	GLU	-	expression tag	UNP G3G945
C	271	HIS	-	expression tag	UNP G3G945
C	272	HIS	-	expression tag	UNP G3G945
C	273	HIS	-	expression tag	UNP G3G945
C	274	HIS	-	expression tag	UNP G3G945
C	275	HIS	-	expression tag	UNP G3G945
C	276	HIS	-	expression tag	UNP G3G945
B	110	LEU	PRO	conflict	UNP G3G945
B	269	LEU	-	expression tag	UNP G3G945
B	270	GLU	-	expression tag	UNP G3G945

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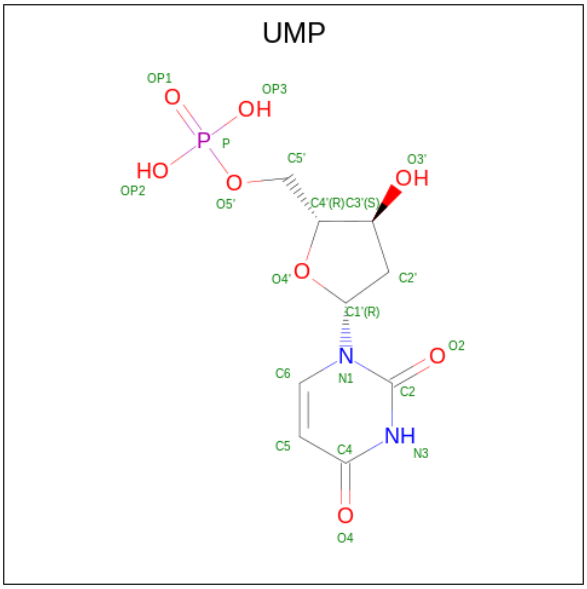
Chain	Residue	Modelled	Actual	Comment	Reference
B	271	HIS	-	expression tag	UNP G3G945
B	272	HIS	-	expression tag	UNP G3G945
B	273	HIS	-	expression tag	UNP G3G945
B	274	HIS	-	expression tag	UNP G3G945
B	275	HIS	-	expression tag	UNP G3G945
B	276	HIS	-	expression tag	UNP G3G945
D	110	LEU	PRO	conflict	UNP G3G945
D	269	LEU	-	expression tag	UNP G3G945
D	270	GLU	-	expression tag	UNP G3G945
D	271	HIS	-	expression tag	UNP G3G945
D	272	HIS	-	expression tag	UNP G3G945
D	273	HIS	-	expression tag	UNP G3G945
D	274	HIS	-	expression tag	UNP G3G945
D	275	HIS	-	expression tag	UNP G3G945
D	276	HIS	-	expression tag	UNP G3G945

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 4 is water.

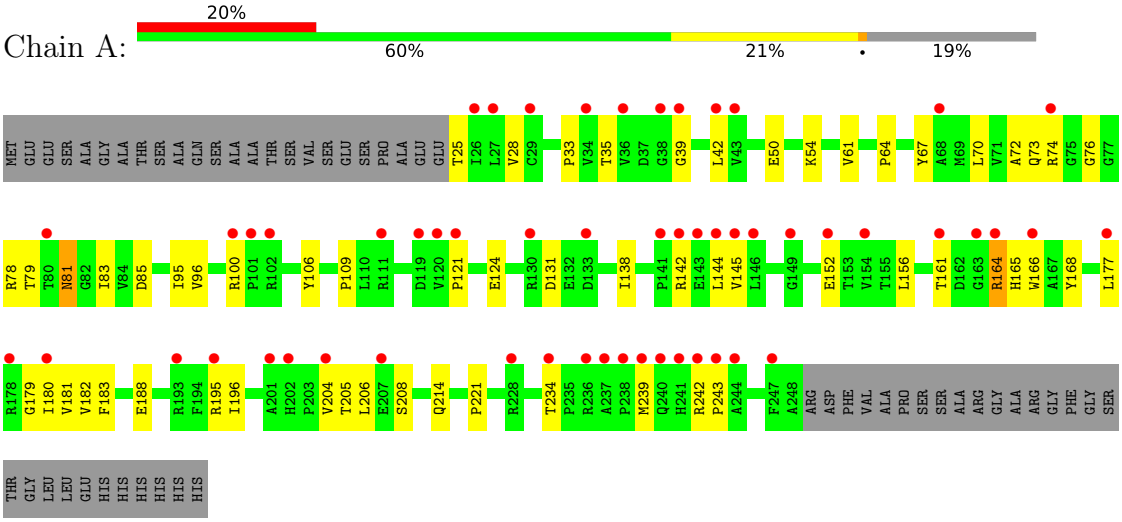
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	C	77	Total	O	0	0
			77	77		
4	B	83	Total	O	0	0
			83	83		
4	D	84	Total	O	0	0
			84	84		

3 Residue-property plots (i)

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.

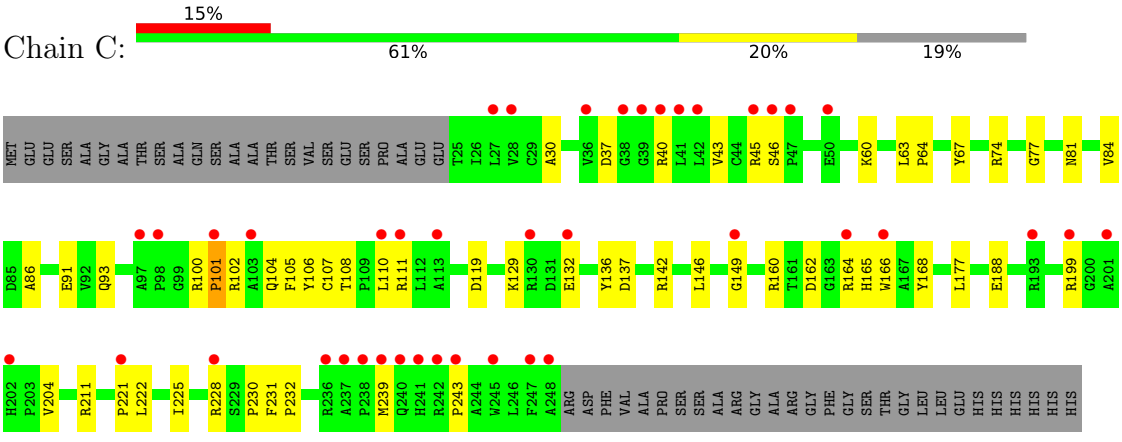
- Molecule 1: dUTPase

Chain A:



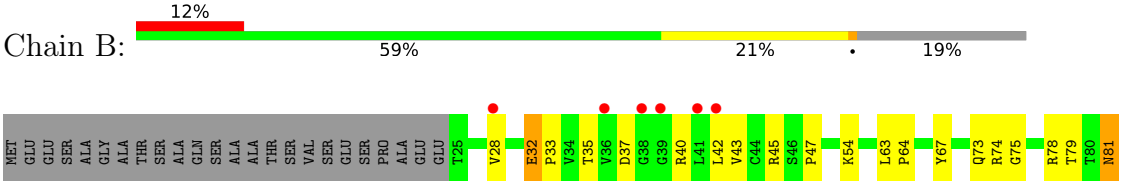
- Molecule 1: dUTPase

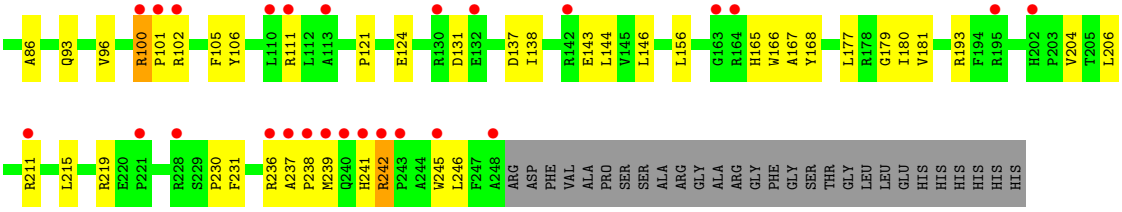
Chain C:



- Molecule 1: dUTPase

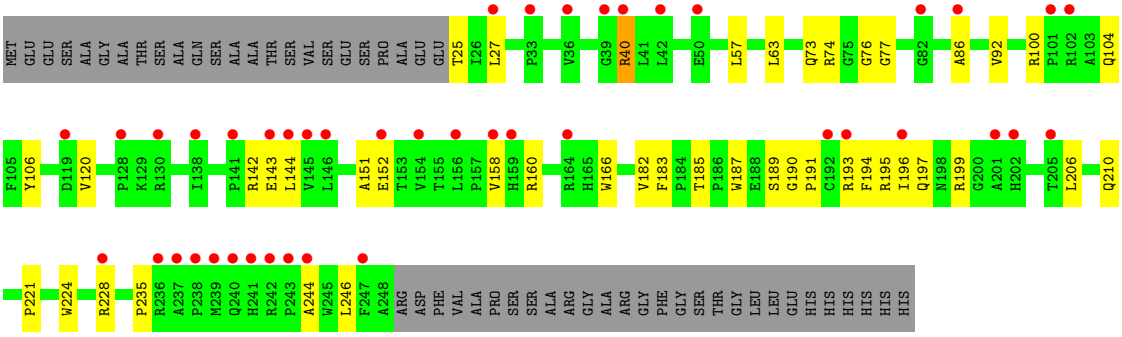
Chain B:





• Molecule 1: dUTPase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	98.25Å 103.26Å 98.73Å 90.00° 99.47° 90.00°	Depositor
Resolution (Å)	48.45 – 2.23 48.45 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.45-2.23) 99.4 (48.45-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.277 , 0.339 0.277 , 0.337	Depositor DCC
R_{free} test set	2362 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.56$, $< L^2 > = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7214	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0955e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UMP, MG

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	0.51	0/1770	0.69	0/2420
1	B	0.39	0/1770	0.60	0/2420
1	C	0.44	0/1770	0.66	1/2420 (0.0%)
1	D	0.43	0/1770	0.62	0/2420
All	All	0.44	0/7080	0.64	1/9680 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	101	PRO	N-CA-C	7.13	123.11	113.84

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	1717	0	1724	49	0
1	B	1717	0	1724	44	1
1	C	1717	0	1724	39	1
1	D	1717	0	1724	34	0
2	A	1	0	0	0	0
3	A	20	0	9	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	81	0	0	8	0
4	B	83	0	0	9	0
4	C	77	0	0	14	0
4	D	84	0	0	10	0
All	All	7214	0	6905	165	1

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 12.

All (165) 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:C:63:LEU:HB2	1:C:86:ALA:HA	1.71	0.72
1:D:57:LEU:HD12	1:D:92:VAL:HG12	1.73	0.69
1:B:40:ARG:NH1	1:B:237:ALA:O	2.23	0.69
1:D:144:LEU:HB2	1:D:206:LEU:HB2	1.75	0.68
1:C:102:ARG:NH1	4:C:305:HOH:O	2.25	0.68
1:A:78:ARG:NH1	1:A:100:ARG:O	2.26	0.68
1:A:54:LYS:HE3	1:A:177:LEU:HD11	1.75	0.67
1:A:214:GLN:OE1	3:A:402:UMP:OP3	2.11	0.67
1:B:219:ARG:NH1	4:B:306:HOH:O	2.28	0.66
1:A:180:ILE:HG22	1:A:196:ILE:HD11	1.77	0.66
1:B:121:PRO:HB2	1:B:124:GLU:HG3	1.76	0.66
1:A:188:GLU:OE2	4:A:501:HOH:O	2.13	0.66
1:A:33:PRO:O	4:A:502:HOH:O	2.14	0.64
1:B:63:LEU:HB2	1:B:86:ALA:HA	1.80	0.64
1:B:193:ARG:O	4:B:302:HOH:O	2.15	0.64
1:A:28:VAL:HG22	1:A:61:VAL:HG12	1.81	0.63
1:C:46:SER:HB3	1:C:102:ARG:HG2	1.81	0.63
1:A:72:ALA:HB3	1:A:234:THR:HG23	1.82	0.62
1:A:142:ARG:HH12	1:A:208:SER:HB3	1.64	0.62
1:A:145:VAL:HG22	1:A:205:THR:HG22	1.80	0.61
1:B:74:ARG:HG3	1:B:106:TYR:CE2	2.35	0.61
1:C:165:HIS:N	4:C:301:HOH:O	2.12	0.61
1:C:30:ALA:O	4:C:302:HOH:O	2.16	0.60
1:B:131:ASP:O	4:B:303:HOH:O	2.16	0.60
1:D:74:ARG:NH1	1:D:104:GLN:OE1	2.34	0.60
1:D:142:ARG:HH22	1:D:152:GLU:HG3	1.67	0.60
1:B:242:ARG:HH11	1:B:242:ARG:HG3	1.66	0.59
1:A:131:ASP:HB2	4:A:537:HOH:O	2.03	0.58
1:D:193:ARG:NH1	4:D:305:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:PHE:HE2	1:D:196:ILE:HD11	1.67	0.58
1:A:183:PHE:CE2	1:A:195:ARG:HD2	2.39	0.58
1:A:234:THR:HG21	4:A:505:HOH:O	2.04	0.58
1:D:193:ARG:NH2	4:D:306:HOH:O	2.36	0.58
1:A:124:GLU:O	4:A:503:HOH:O	2.17	0.58
1:D:63:LEU:HB2	1:D:86:ALA:HA	1.86	0.57
1:A:166:TRP:CD1	1:A:168:TYR:HH	2.23	0.56
1:C:160:ARG:NH1	1:C:188:GLU:OE1	2.38	0.56
1:B:236:ARG:H	1:B:236:ARG:HD2	1.71	0.56
1:A:142:ARG:NH1	1:A:208:SER:HB3	2.20	0.56
1:C:129:LYS:HE3	1:C:136:TYR:CZ	2.40	0.56
1:C:104:GLN:NE2	4:C:306:HOH:O	2.25	0.56
1:B:64:PRO:HG2	1:B:67:TYR:CD1	2.41	0.55
1:C:100:ARG:HG2	1:C:101:PRO:HD2	1.88	0.55
1:A:70:LEU:HD11	1:A:81:ASN:HB3	1.88	0.55
1:C:166:TRP:CE2	1:C:221:PRO:HB3	2.43	0.54
1:B:43:VAL:HG23	1:B:105:PHE:HB2	1.89	0.54
1:B:238:PRO:HB2	1:B:242:ARG:HH21	1.73	0.54
1:B:32:GLU:HG3	1:B:33:PRO:HD2	1.90	0.54
1:D:197:GLN:HG2	1:D:199:ARG:HG3	1.89	0.53
1:A:79:THR:HG23	1:A:96:VAL:HG12	1.91	0.53
1:C:74:ARG:HD2	1:C:106:TYR:CZ	2.43	0.53
1:C:84:VAL:HG22	4:C:373:HOH:O	2.09	0.52
1:C:132:GLU:O	4:C:303:HOH:O	2.19	0.52
1:D:40:ARG:NH2	1:D:224:TRP:CH2	2.78	0.52
1:C:45:ARG:NE	4:C:312:HOH:O	2.42	0.52
1:A:138:ILE:HG23	1:A:156:LEU:HD21	1.92	0.52
1:A:144:LEU:HD12	1:A:206:LEU:HD12	1.91	0.52
1:A:85:ASP:HB3	3:A:402:UMP:H5"	1.92	0.52
1:C:43:VAL:HG23	1:C:105:PHE:HB2	1.91	0.52
1:D:185:THR:OG1	4:D:302:HOH:O	2.15	0.52
1:A:166:TRP:NE1	1:A:221:PRO:HB3	2.25	0.51
1:C:146:LEU:HB2	1:C:204:VAL:HG22	1.91	0.51
1:A:83:ILE:O	3:A:402:UMP:H5'	2.11	0.51
1:B:238:PRO:HB2	1:B:242:ARG:NH2	2.26	0.51
1:A:121:PRO:HB2	1:A:124:GLU:HG3	1.92	0.50
1:C:37:ASP:OD2	4:C:304:HOH:O	2.19	0.50
1:B:179:GLY:O	1:B:181:VAL:HG23	2.12	0.50
1:B:246:LEU:HD11	1:D:244:ALA:HB1	1.92	0.50
1:B:35:THR:HB	1:B:42:LEU:HB3	1.94	0.50
1:A:166:TRP:CE2	1:A:221:PRO:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:GLN:NE2	1:D:76:GLY:HA3	2.28	0.49
1:C:228:ARG:NH1	4:C:314:HOH:O	2.44	0.49
1:B:146:LEU:HB2	1:B:204:VAL:HG22	1.95	0.49
1:A:81:ASN:N	1:A:81:ASN:HD22	2.11	0.49
1:D:27:LEU:HD21	1:D:246:LEU:HD23	1.94	0.49
1:D:40:ARG:NH1	1:D:235:PRO:O	2.46	0.49
1:A:95:ILE:HD13	1:A:177:LEU:HG	1.94	0.49
1:D:190:GLY:N	4:D:308:HOH:O	2.46	0.49
1:A:64:PRO:HG2	1:A:67:TYR:CD1	2.49	0.48
1:A:72:ALA:HB1	4:A:536:HOH:O	2.13	0.48
1:D:142:ARG:NH2	1:D:152:GLU:HG3	2.27	0.48
1:B:237:ALA:HB3	4:B:308:HOH:O	2.12	0.48
1:D:100:ARG:NE	4:D:309:HOH:O	2.43	0.48
1:A:109:PRO:HG3	1:A:243:PRO:HG3	1.96	0.48
1:C:43:VAL:CG2	1:C:105:PHE:HB2	2.44	0.48
1:C:40:ARG:HB3	1:C:107:CYS:O	2.13	0.48
1:A:179:GLY:O	1:A:181:VAL:HG23	2.14	0.47
1:C:81:ASN:ND2	1:C:232:PRO:HG2	2.28	0.47
1:D:228:ARG:O	1:D:228:ARG:HG2	2.14	0.47
1:D:74:ARG:HD2	1:D:106:TYR:CZ	2.49	0.47
1:D:160:ARG:HG3	1:D:187:TRP:CE2	2.49	0.47
1:D:182:VAL:HG22	1:D:196:ILE:HG12	1.96	0.47
1:A:109:PRO:CG	1:A:243:PRO:HG3	2.44	0.47
1:B:144:LEU:HD12	1:B:206:LEU:HD12	1.96	0.47
1:B:236:ARG:HD2	1:B:236:ARG:N	2.30	0.47
1:D:151:ALA:HB3	4:D:313:HOH:O	2.14	0.47
1:C:45:ARG:CZ	4:C:312:HOH:O	2.62	0.46
1:B:230:PRO:HG2	1:B:231:PHE:CD2	2.51	0.46
1:B:43:VAL:CG2	1:B:105:PHE:HB2	2.44	0.46
1:D:189:SER:O	4:D:303:HOH:O	2.21	0.46
1:B:102:ARG:HD3	4:B:367:HOH:O	2.14	0.46
1:C:40:ARG:NH1	1:C:239:MET:SD	2.88	0.46
1:C:45:ARG:NH2	4:C:312:HOH:O	2.48	0.46
1:C:77:GLY:HA2	4:C:323:HOH:O	2.14	0.46
1:A:35:THR:HB	1:A:42:LEU:HB3	1.97	0.46
1:B:81:ASN:HD22	1:B:81:ASN:N	2.14	0.45
1:C:64:PRO:HG2	1:C:67:TYR:CD1	2.51	0.45
1:A:144:LEU:HD22	1:A:152:GLU:CD	2.42	0.45
1:B:138:ILE:HG23	1:B:156:LEU:HD21	1.99	0.45
1:D:77:GLY:HA2	4:D:321:HOH:O	2.16	0.45
1:A:73:GLN:HB2	1:A:79:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:C	1:A:196:ILE:HD12	2.42	0.45
1:C:67:TYR:CZ	1:C:111:ARG:HG2	2.52	0.45
1:B:239:MET:O	1:B:242:ARG:NE	2.45	0.44
1:D:195:ARG:NH1	4:D:313:HOH:O	2.50	0.44
1:D:158:VAL:O	1:D:191:PRO:HA	2.17	0.44
1:C:166:TRP:HB3	1:C:168:TYR:CE2	2.53	0.44
1:C:177:LEU:O	1:C:177:LEU:HD13	2.18	0.44
1:A:73:GLN:NE2	1:A:76:GLY:HA3	2.33	0.43
1:C:110:LEU:HD22	1:C:222:LEU:HD11	2.00	0.43
1:D:144:LEU:O	1:D:206:LEU:N	2.27	0.43
1:B:165:HIS:N	4:B:301:HOH:O	1.95	0.43
1:B:45:ARG:O	1:B:47:PRO:HD3	2.18	0.43
1:B:73:GLN:HB2	1:B:79:THR:OG1	2.18	0.43
1:A:109:PRO:HG2	1:A:239:MET:HE1	2.01	0.43
1:B:75:GLY:HA3	1:B:236:ARG:HH21	1.83	0.43
1:A:182:VAL:CG2	1:A:196:ILE:HD13	2.49	0.43
1:A:142:ARG:NH1	1:A:142:ARG:HA	2.34	0.43
1:A:164:ARG:HG2	1:A:165:HIS:NE2	2.33	0.43
1:B:111:ARG:NH1	4:B:309:HOH:O	2.38	0.42
1:B:167:ALA:HB1	1:B:215:LEU:HD11	2.01	0.42
1:C:40:ARG:CZ	1:C:239:MET:HG2	2.49	0.42
1:C:243:PRO:HB3	4:C:322:HOH:O	2.19	0.42
1:B:79:THR:HG23	1:B:96:VAL:HG12	2.00	0.42
1:D:142:ARG:CZ	1:D:144:LEU:HD21	2.49	0.42
1:D:183:PHE:CZ	1:D:195:ARG:HD2	2.55	0.42
1:C:199:ARG:HB3	4:C:360:HOH:O	2.18	0.42
1:D:27:LEU:HD23	1:D:27:LEU:HA	1.86	0.42
1:B:166:TRP:HB3	1:B:168:TYR:CE2	2.55	0.42
1:A:85:ASP:CG	3:A:402:UMP:H5"	2.45	0.42
1:C:119:ASP:N	1:C:119:ASP:OD1	2.51	0.42
1:B:78:ARG:NH1	1:B:100:ARG:O	2.52	0.42
1:B:180:ILE:HD11	1:B:204:VAL:HG11	2.01	0.42
1:A:25:THR:N	4:A:514:HOH:O	2.53	0.42
1:A:180:ILE:HD13	1:A:204:VAL:HG11	2.01	0.42
1:B:28:VAL:HG21	1:B:245:TRP:HE3	1.85	0.42
1:B:37:ASP:OD1	1:B:37:ASP:C	2.63	0.41
1:A:39:GLY:HA2	1:A:242:ARG:HE	1.85	0.41
1:B:241:HIS:HB2	4:B:363:HOH:O	2.18	0.41
1:B:219:ARG:O	4:B:304:HOH:O	2.22	0.41
1:C:60:LYS:HG2	1:C:91:GLU:HA	2.02	0.41
1:C:230:PRO:HG2	1:C:231:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:THR:N	4:D:317:HOH:O	2.53	0.41
1:A:50:GLU:H	1:A:50:GLU:CD	2.29	0.41
1:A:74:ARG:HD2	1:A:106:TYR:CZ	2.56	0.41
1:A:234:THR:CG2	4:A:541:HOH:O	2.68	0.41
1:B:137:ASP:OD2	1:B:211:ARG:HD3	2.21	0.41
1:D:143:GLU:HA	1:D:206:LEU:O	2.21	0.41
1:C:40:ARG:HD3	1:C:108:THR:OG1	2.21	0.41
1:B:143:GLU:HA	1:B:206:LEU:O	2.22	0.40
1:D:166:TRP:CD2	1:D:221:PRO:HB3	2.56	0.40
1:C:137:ASP:OD2	1:C:211:ARG:HD2	2.22	0.40
1:C:162:ASP:OD2	1:C:164:ARG:NH1	2.54	0.40
1:A:85:ASP:CB	3:A:402:UMP:H5"	2.50	0.40
1:B:54:LYS:HE3	1:B:177:LEU:HD11	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:GLY:N	1:B:101:PRO:CG[3_445]	2.16	0.04

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	222/276 (80%)	217 (98%)	5 (2%)	0	100	100
1	B	222/276 (80%)	216 (97%)	6 (3%)	0	100	100
1	C	222/276 (80%)	219 (99%)	3 (1%)	0	100	100
1	D	222/276 (80%)	214 (96%)	8 (4%)	0	100	100
All	All	888/1104 (80%)	866 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	179/217 (82%)	176 (98%)	3 (2%)	56	64
1	B	179/217 (82%)	174 (97%)	5 (3%)	38	44
1	C	179/217 (82%)	176 (98%)	3 (2%)	56	64
1	D	179/217 (82%)	176 (98%)	3 (2%)	56	64
All	All	716/868 (82%)	702 (98%)	14 (2%)	50	57

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	161	THR
1	A	164	ARG
1	C	93	GLN
1	C	142	ARG
1	C	225	ILE
1	B	32	GLU
1	B	81	ASN
1	B	93	GLN
1	B	100	ARG
1	B	242	ARG
1	D	40	ARG
1	D	120	VAL
1	D	210	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	C	214	GLN
1	B	81	ASN
1	B	214	GLN
1	D	93	GLN

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Mol	Chain	Res	Type
1	D	197	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	UMP	A	402	-	21,21,21	4.21	14 (66%)	31,31,31	3.99	16 (51%)

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	UMP	A	402	-	-	4/10/22/22	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	UMP	C2-N3	7.99	1.52	1.38
3	A	402	UMP	C2-N1	7.69	1.50	1.38
3	A	402	UMP	O4'-C4'	7.65	1.62	1.45
3	A	402	UMP	C6-C5	6.95	1.51	1.35
3	A	402	UMP	C4-N3	5.88	1.49	1.38
3	A	402	UMP	C3'-C4'	-5.78	1.37	1.53
3	A	402	UMP	O2-C2	-3.65	1.16	1.23
3	A	402	UMP	P-OP3	-3.27	1.42	1.54
3	A	402	UMP	O3'-C3'	2.99	1.49	1.43
3	A	402	UMP	O4'-C1'	-2.92	1.35	1.42
3	A	402	UMP	C6-N1	2.74	1.44	1.38
3	A	402	UMP	P-OP2	-2.35	1.45	1.54
3	A	402	UMP	C5-C4	2.18	1.48	1.43
3	A	402	UMP	O4-C4	-2.12	1.20	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	UMP	C4'-O4'-C1'	-11.66	81.26	109.45
3	A	402	UMP	O4'-C1'-N1	10.60	126.81	107.86
3	A	402	UMP	C6-C5-C4	6.20	127.99	119.52
3	A	402	UMP	O5'-P-OP1	5.59	122.15	106.47
3	A	402	UMP	N3-C2-N1	5.58	122.29	114.89
3	A	402	UMP	C2'-C1'-N1	4.63	124.42	113.77
3	A	402	UMP	O4-C4-N3	3.94	125.09	119.31
3	A	402	UMP	C3'-C2'-C1'	-3.92	92.71	102.54
3	A	402	UMP	OP3-P-OP1	-3.61	96.55	110.68
3	A	402	UMP	C4-N3-C2	-3.36	122.15	126.58
3	A	402	UMP	C6-N1-C2	-3.16	116.95	120.99
3	A	402	UMP	C1'-N1-C2	3.01	123.58	117.64
3	A	402	UMP	O5'-C5'-C4'	3.00	119.30	108.99
3	A	402	UMP	O2-C2-N1	-2.94	118.88	122.79
3	A	402	UMP	O4'-C4'-C5'	2.07	116.19	109.37
3	A	402	UMP	C5-C4-N3	-2.02	111.83	114.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

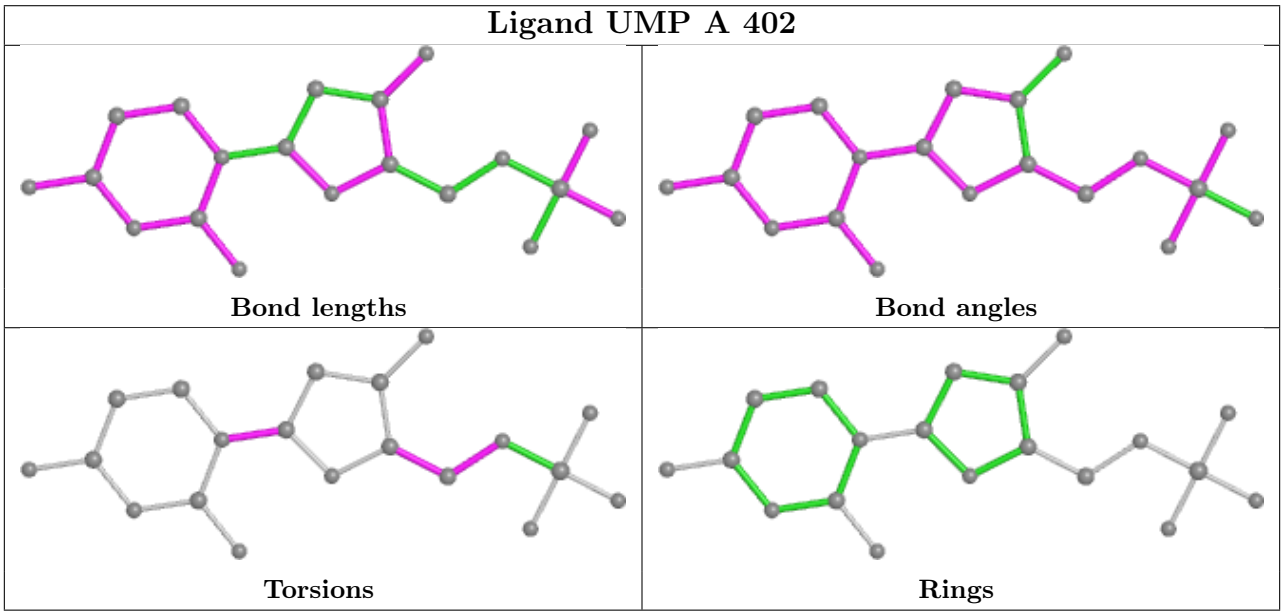
Mol	Chain	Res	Type	Atoms
3	A	402	UMP	O4'-C1'-N1-C2
3	A	402	UMP	O4'-C1'-N1-C6
3	A	402	UMP	C4'-C5'-O5'-P
3	A	402	UMP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	UMP	5	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 then 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	224/276 (81%)	1.38	55 (24%)	2	2	17, 34, 67, 95	0
1	B	224/276 (81%)	1.06	32 (14%)	7	7	20, 35, 70, 96	0
1	C	224/276 (81%)	1.21	41 (18%)	4	4	20, 36, 71, 92	0
1	D	224/276 (81%)	1.30	43 (19%)	4	4	19, 35, 66, 105	0
All	All	896/1104 (81%)	1.24	171 (19%)	4	4	17, 35, 70, 105	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	PRO	8.5
1	A	239	MET	7.1
1	D	239	MET	6.8
1	C	40	ARG	6.5
1	D	40	ARG	6.4
1	A	193	ARG	5.7
1	C	242	ARG	5.6
1	A	163	GLY	5.6
1	A	228	ARG	5.6
1	C	239	MET	5.4
1	B	100	ARG	5.2
1	B	243	PRO	5.2
1	D	228	ARG	5.1
1	B	164	ARG	4.8
1	A	243	PRO	4.8
1	C	111	ARG	4.8
1	A	242	ARG	4.7
1	D	201	ALA	4.6
1	C	241	HIS	4.6
1	A	154	VAL	4.4
1	D	236	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	111	ARG	4.3
1	B	102	ARG	4.3
1	A	101	PRO	4.3
1	B	241	HIS	4.3
1	C	36	VAL	4.2
1	C	101	PRO	4.2
1	A	142	ARG	4.1
1	C	243	PRO	4.1
1	A	36	VAL	4.0
1	C	248	ALA	4.0
1	A	74	ARG	4.0
1	A	234	THR	3.9
1	A	164	ARG	3.9
1	C	193	ARG	3.9
1	C	201	ALA	3.9
1	A	161	THR	3.8
1	B	239	MET	3.8
1	C	45	ARG	3.8
1	C	46	SER	3.7
1	C	164	ARG	3.7
1	B	39	GLY	3.7
1	A	201	ALA	3.7
1	D	243	PRO	3.7
1	A	102	ARG	3.6
1	A	39	GLY	3.6
1	C	110	LEU	3.6
1	D	152	GLU	3.4
1	C	240	GLN	3.4
1	B	195	ARG	3.4
1	C	130	ARG	3.4
1	D	241	HIS	3.3
1	B	236	ARG	3.3
1	B	237	ALA	3.3
1	D	164	ARG	3.3
1	D	202	HIS	3.3
1	B	238	PRO	3.3
1	D	240	GLN	3.3
1	B	242	ARG	3.2
1	C	47	PRO	3.2
1	D	196	ILE	3.2
1	A	146	LEU	3.2
1	A	177	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	145	VAL	3.2
1	B	228	ARG	3.2
1	A	100	ARG	3.1
1	A	130	ARG	3.1
1	A	202	HIS	3.1
1	C	38	GLY	3.1
1	D	237	ALA	3.1
1	A	241	HIS	3.0
1	A	143	GLU	3.0
1	A	166	TRP	3.0
1	C	50	GLU	3.0
1	D	101	PRO	3.0
1	B	110	LEU	3.0
1	B	240	GLN	3.0
1	B	38	GLY	2.9
1	C	41	LEU	2.9
1	C	113	ALA	2.9
1	A	152	GLU	2.8
1	C	97	ALA	2.8
1	B	211	ARG	2.8
1	A	238	PRO	2.8
1	A	68	ALA	2.8
1	D	102	ARG	2.8
1	D	158	VAL	2.8
1	A	195	ARG	2.7
1	D	50	GLU	2.7
1	D	193	ARG	2.7
1	D	141	PRO	2.7
1	D	154	VAL	2.7
1	D	244	ALA	2.7
1	C	166	TRP	2.7
1	D	205	THR	2.7
1	D	146	LEU	2.7
1	A	204	VAL	2.6
1	A	38	GLY	2.6
1	C	245	TRP	2.6
1	A	207	GLU	2.6
1	A	178	ARG	2.6
1	B	132	GLU	2.5
1	D	82	GLY	2.5
1	C	28	VAL	2.5
1	D	130	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	29	CYS	2.5
1	D	39	GLY	2.5
1	A	144	LEU	2.5
1	D	27	LEU	2.5
1	C	202	HIS	2.5
1	C	228	ARG	2.5
1	D	242	ARG	2.5
1	B	41	LEU	2.5
1	C	236	ARG	2.5
1	A	121	PRO	2.5
1	A	26	ILE	2.4
1	D	238	PRO	2.4
1	D	192	CYS	2.4
1	D	36	VAL	2.4
1	C	238	PRO	2.4
1	B	221	PRO	2.4
1	B	202	HIS	2.4
1	B	42	LEU	2.4
1	D	144	LEU	2.4
1	A	43	VAL	2.3
1	B	245	TRP	2.3
1	C	221	PRO	2.3
1	A	120	VAL	2.3
1	A	141	PRO	2.3
1	C	39	GLY	2.3
1	A	237	ALA	2.3
1	D	145	VAL	2.3
1	C	199	ARG	2.3
1	B	130	ARG	2.3
1	C	149	GLY	2.3
1	C	27	LEU	2.2
1	A	34	VAL	2.2
1	D	159	HIS	2.2
1	D	143	GLU	2.2
1	A	111	ARG	2.2
1	A	236	ARG	2.2
1	A	180	ILE	2.2
1	A	27	LEU	2.2
1	D	86	ALA	2.2
1	A	133	ASP	2.2
1	D	42	LEU	2.2
1	D	156	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	244	ALA	2.2
1	A	247	PHE	2.2
1	D	247	PHE	2.2
1	B	163	GLY	2.1
1	D	138	ILE	2.1
1	A	240	GLN	2.1
1	B	113	ALA	2.1
1	B	28	VAL	2.1
1	A	80	THR	2.1
1	C	237	ALA	2.1
1	B	36	VAL	2.1
1	A	42	LEU	2.1
1	C	103	ALA	2.1
1	C	247	PHE	2.1
1	A	119	ASP	2.1
1	C	42	LEU	2.1
1	D	128	PRO	2.1
1	B	248	ALA	2.1
1	B	142	ARG	2.0
1	D	119	ASP	2.0
1	C	98	PRO	2.0
1	C	132	GLU	2.0
1	A	149	GLY	2.0
1	D	33	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

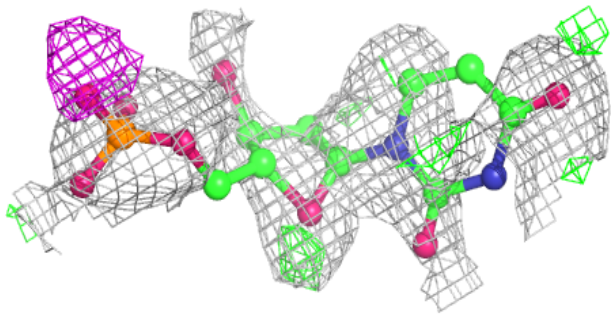
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

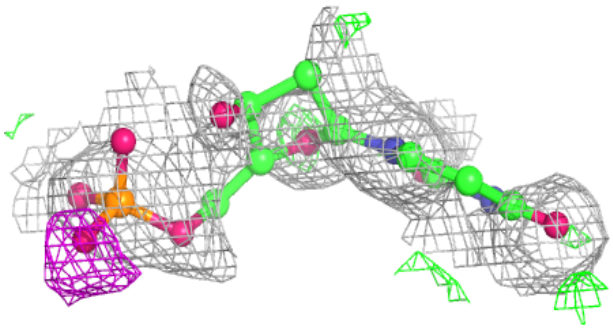
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UMP	A	402	20/20	0.55	0.32	71,93,112,119	0
2	MG	A	401	1/1	0.92	0.14	53,53,53,53	0

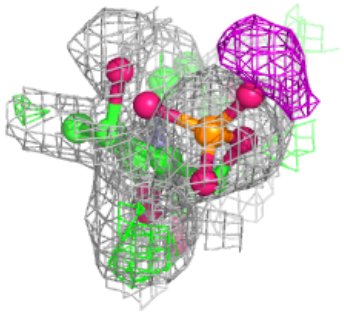
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UMP A 402:

$2mF_o$-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

There are no such residues in this entry.