Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 04:26 AM EDT

PDB ID	:	4HO8
Title	:	Crystal structure of glucose 1-phosphate thymidylyltransferase from Aneurinibacillus thermoaerophilus complexed with UDP-glucose and thymidine
Authors	:	Chen, T.J.; Chien, W.T.; Lin, C.C.; Wang, W.C.
Deposited on	:	2012-10-22
Resolution	:	2.60 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:

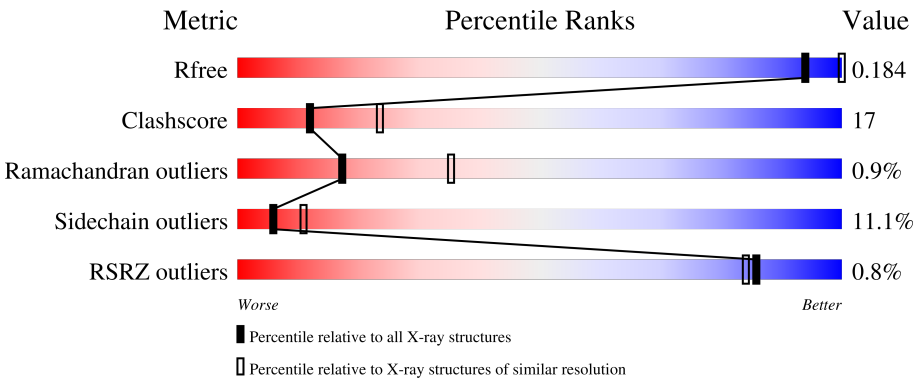
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	297	.% 69% 23% 5% • •
1	B	297	64% 27% 6% •
1	C	297	68% 23% 6% •
1	D	297	2% 65% 29% • •

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	302	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9462 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.

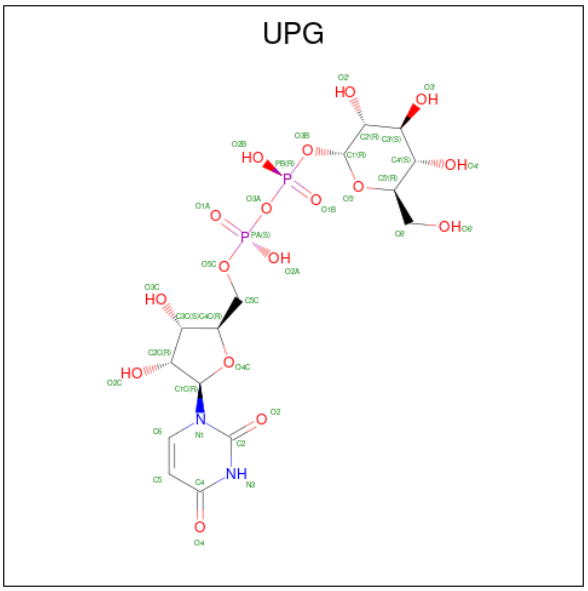
- Molecule 1 is a protein called Glucose-1-phosphate thymidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2256	1449	370	430	7	0	0	0
1	B	288	2256	1449	370	430	7	0	0	0
1	C	288	2256	1449	370	430	7	0	0	0
1	D	288	2256	1449	370	430	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

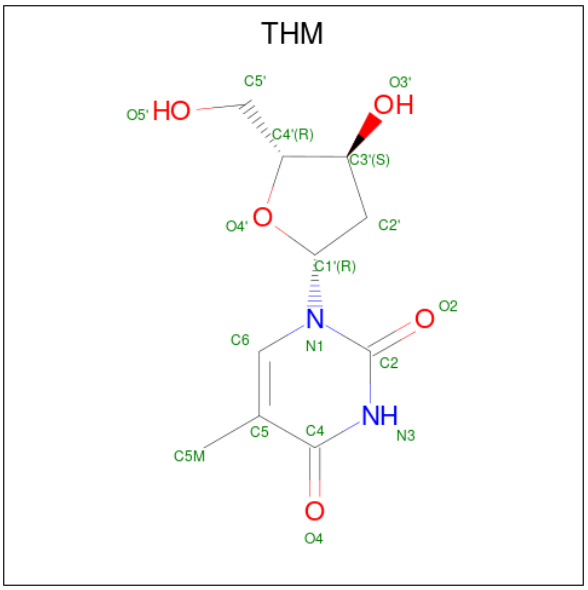
Chain	Residue	Modelled	Actual	Comment	Reference
A	297	GLY	-	expression tag	UNP Q9AGY4
B	297	GLY	-	expression tag	UNP Q9AGY4
C	297	GLY	-	expression tag	UNP Q9AGY4
D	297	GLY	-	expression tag	UNP Q9AGY4

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



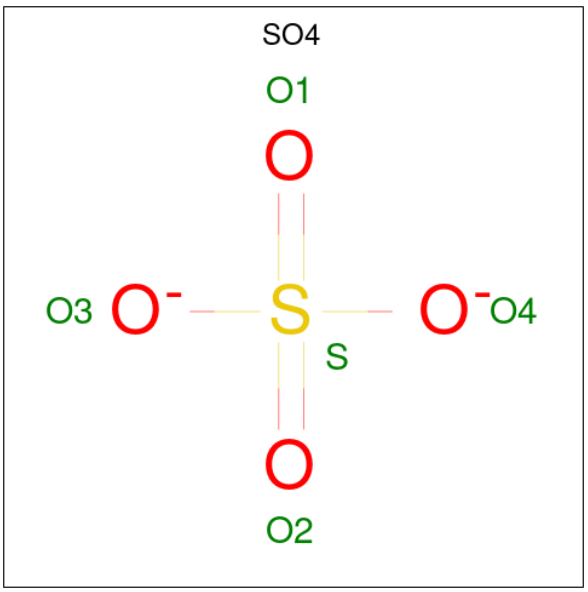
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	36	15	2	17	2	0	0
			Total	C	N	O	P		
2	B	1	36	15	2	17	2	0	0
			Total	C	N	O	P		
2	C	1	36	15	2	17	2	0	0
			Total	C	N	O	P		
2	D	1	36	15	2	17	2	0	0

- Molecule 3 is THYMIDINE (three-letter code: THM) (formula: $C_{10}H_{14}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	10	2	5	0	0
3	B	1	17	10	2	5	0	0
3	C	1	17	10	2	5	0	0
3	D	1	17	10	2	5	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	A	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	C	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0

- Molecule 5 is water.

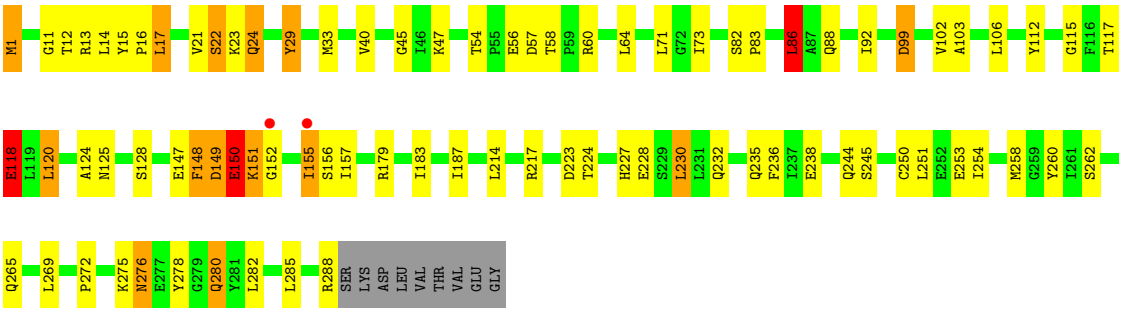
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	44	44	44	0	0
			Total	O		
5	B	40	40	40	0	0
			Total	O		
5	C	36	36	36	0	0
			Total	O		
5	D	36	36	36	0	0

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.

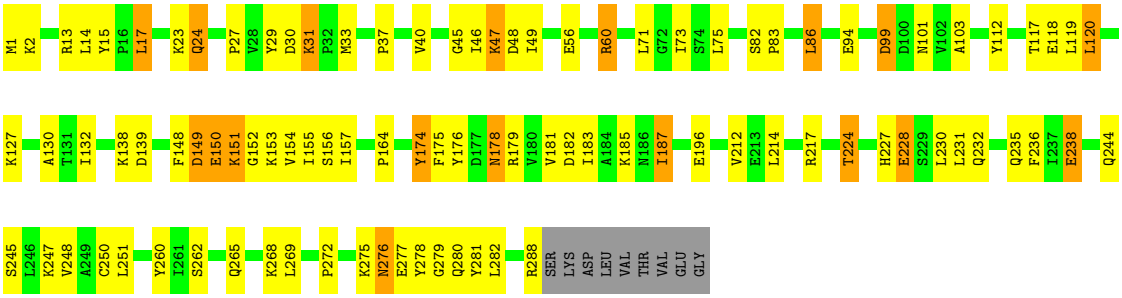
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain A:



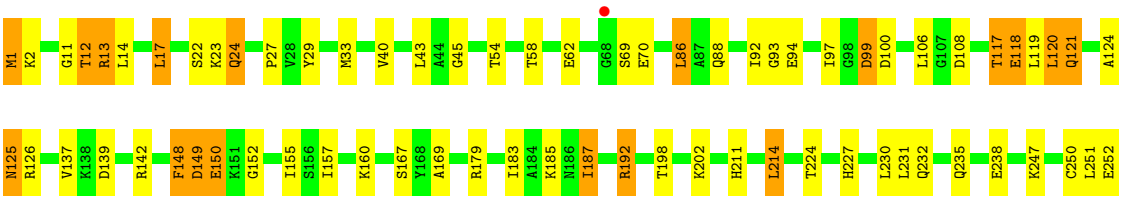
• Molecule 1: Glucose-1-phosphate thymidylyltransferase

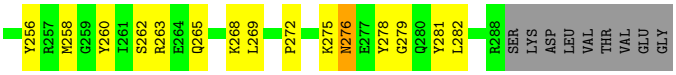
Chain B:



• Molecule 1: Glucose-1-phosphate thymidylyltransferase

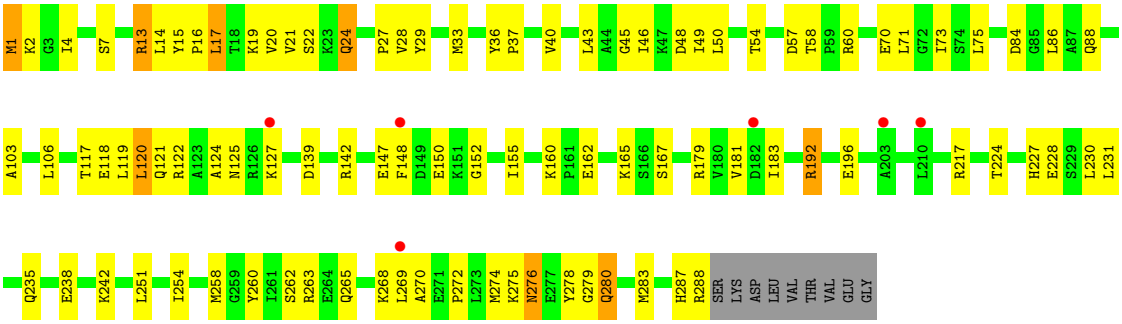
Chain C:





• Molecule 1: Glucose-1-phosphate thymidylyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.02Å 91.25Å 91.23Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 25.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.60) 97.9 (25.30-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.185 , 0.240 0.187 , 0.184	Depositor DCC
R_{free} test set	1761 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 26.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.469 for -h,-l,-k 0.458 for -h,l,k 0.459 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9462	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UPG, THM, SO4

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	0.85	1/2299 (0.0%)	0.61	1/3107 (0.0%)
1	B	0.85	2/2299 (0.1%)	0.58	0/3107
1	C	0.85	1/2299 (0.0%)	0.63	1/3107 (0.0%)
1	D	0.82	1/2299 (0.0%)	0.58	0/3107
All	All	0.84	5/9196 (0.1%)	0.60	2/12428 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	118	GLU	CG-CD	6.07	1.61	1.51
1	B	228	GLU	CG-CD	6.03	1.60	1.51
1	A	118	GLU	CB-CG	5.52	1.62	1.52
1	B	56	GLU	CG-CD	5.30	1.59	1.51
1	C	118	GLU	CG-CD	5.03	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	LEU	CA-CB-CG	5.71	128.43	115.30
1	C	214	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	148	PHE	Peptide
1	B	149	ASP	Peptide
1	C	12	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2256	0	2277	70	0
1	B	2256	0	2277	104	0
1	C	2256	0	2277	96	0
1	D	2256	0	2277	74	0
2	A	36	0	22	0	0
2	B	36	0	22	1	0
2	C	36	0	22	3	0
2	D	36	0	22	5	0
3	A	17	0	14	0	0
3	B	17	0	14	0	0
3	C	17	0	14	1	0
3	D	17	0	14	0	0
4	A	15	0	0	3	0
4	B	20	0	0	0	0
4	C	20	0	0	0	0
4	D	15	0	0	0	0
5	A	44	0	0	3	0
5	B	40	0	0	2	0
5	C	36	0	0	8	0
5	D	36	0	0	2	0
All	All	9462	0	9252	319	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 17.

All (319) 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:31:LYS:NZ	1:B:248:VAL:O	1.77	1.18
1:D:43:LEU:HA	1:D:258:MET:CE	1.86	1.04
1:D:33:MET:CE	1:D:224:THR:HG21	1.93	0.98
1:D:33:MET:HE2	1:D:224:THR:HG21	1.46	0.95
1:A:224:THR:HG22	1:A:224:THR:O	1.66	0.94
1:B:235:GLN:HE21	1:C:235:GLN:HG2	1.30	0.94
1:D:224:THR:HG22	1:D:224:THR:O	1.68	0.93
1:A:24:GLN:H	1:A:24:GLN:HE21	0.97	0.93
1:C:124:ALA:O	1:C:125:ASN:HB2	1.66	0.92
1:C:43:LEU:HD23	1:C:258:MET:HE1	1.52	0.91
1:A:24:GLN:H	1:A:24:GLN:NE2	1.67	0.91
1:B:235:GLN:HE21	1:C:235:GLN:CG	1.85	0.90
1:B:24:GLN:H	1:B:24:GLN:HE21	1.15	0.90
1:B:228:GLU:HG3	5:C:410:HOH:O	1.73	0.89
1:A:275:LYS:HB2	5:A:430:HOH:O	1.73	0.88
1:A:24:GLN:HE21	1:A:24:GLN:N	1.71	0.87
1:B:262:SER:H	1:B:265:GLN:HE21	1.19	0.87
1:C:33:MET:CE	1:C:224:THR:HG21	2.05	0.86
1:C:139:ASP:HB2	1:C:142:ARG:HE	1.42	0.85
1:D:262:SER:H	1:D:265:GLN:HE21	1.22	0.85
1:B:235:GLN:NE2	1:C:235:GLN:HG2	1.91	0.84
1:D:43:LEU:HA	1:D:258:MET:HE3	1.59	0.83
1:C:276:ASN:HD22	1:C:278:TYR:H	1.26	0.83
1:B:33:MET:SD	1:B:224:THR:HG21	2.19	0.82
1:C:13:ARG:HD2	5:C:415:HOH:O	1.78	0.82
1:D:224:THR:O	1:D:224:THR:CG2	2.27	0.82
1:A:33:MET:HE2	1:A:224:THR:HG21	1.64	0.80
1:A:262:SER:H	1:A:265:GLN:HE21	1.29	0.80
1:B:276:ASN:HD22	1:B:278:TYR:H	1.25	0.80
1:C:224:THR:O	1:C:224:THR:HG22	1.80	0.80
1:D:274:MET:HE1	1:D:283:MET:HB2	1.63	0.80
1:B:24:GLN:H	1:B:24:GLN:NE2	1.79	0.79
1:A:60:ARG:HD2	1:D:60:ARG:HH21	1.47	0.79
1:B:13:ARG:O	1:B:14:LEU:HB2	1.81	0.78
1:C:148:PHE:CD1	1:C:148:PHE:N	2.49	0.78
1:C:13:ARG:O	1:C:14:LEU:HB2	1.83	0.77
2:D:300:UPG:H6	2:D:300:UPG:H5C2	1.68	0.75
1:D:276:ASN:HD22	1:D:278:TYR:H	1.34	0.75
1:C:179:ARG:O	1:C:183:ILE:HD12	1.87	0.75
1:B:1:MET:HE1	1:B:46:ILE:HD11	1.68	0.74
1:D:24:GLN:H	1:D:24:GLN:NE2	1.85	0.74
1:C:148:PHE:HD1	1:C:148:PHE:H	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ASP:HA	1:B:150:GLU:CB	2.18	0.73
1:B:33:MET:CE	1:B:224:THR:HG21	2.18	0.73
1:B:149:ASP:HA	1:B:150:GLU:HB3	1.69	0.73
1:B:1:MET:CE	1:B:46:ILE:HD11	2.18	0.73
1:B:262:SER:OG	1:B:265:GLN:HG3	1.89	0.73
1:D:13:ARG:HD2	5:D:407:HOH:O	1.88	0.72
1:D:262:SER:H	1:D:265:GLN:NE2	1.87	0.72
1:D:14:LEU:O	1:D:17:LEU:HB2	1.90	0.72
1:C:24:GLN:H	1:C:24:GLN:NE2	1.88	0.71
1:C:33:MET:HE1	1:C:224:THR:HG21	1.72	0.71
1:B:127:LYS:O	1:B:127:LYS:HG3	1.90	0.71
1:B:231:LEU:CD2	1:C:238:GLU:HG2	2.20	0.70
1:D:24:GLN:H	1:D:24:GLN:HE21	1.39	0.70
1:A:224:THR:O	1:A:224:THR:CG2	2.39	0.70
1:C:256:TYR:OH	1:C:263:ARG:HG3	1.90	0.70
1:A:262:SER:H	1:A:265:GLN:NE2	1.90	0.69
1:B:235:GLN:HG2	1:C:235:GLN:NE2	2.06	0.69
1:C:117:THR:HG22	5:C:426:HOH:O	1.93	0.69
1:C:150:GLU:HA	1:C:150:GLU:OE2	1.92	0.69
1:A:33:MET:CE	1:A:224:THR:HG21	2.22	0.69
1:C:276:ASN:ND2	1:C:279:GLY:H	1.91	0.69
1:C:148:PHE:O	1:C:149:ASP:HB3	1.91	0.69
1:B:196:GLU:HA	1:B:196:GLU:OE1	1.92	0.69
1:B:262:SER:H	1:B:265:GLN:NE2	1.90	0.68
1:A:288:ARG:C	5:A:433:HOH:O	2.31	0.68
1:C:124:ALA:O	1:C:125:ASN:CB	2.40	0.68
1:B:47:LYS:HB3	1:B:73:ILE:HG22	1.77	0.67
1:B:276:ASN:ND2	1:B:279:GLY:H	1.93	0.67
1:A:147:GLU:OE2	1:A:155:ILE:HG12	1.95	0.67
1:D:274:MET:CE	1:D:283:MET:HB2	2.24	0.67
1:C:14:LEU:O	1:C:17:LEU:HB2	1.95	0.66
1:B:262:SER:N	1:B:265:GLN:HE21	1.93	0.66
1:B:275:LYS:HB2	5:B:403:HOH:O	1.94	0.66
1:B:235:GLN:HG2	1:C:235:GLN:HE21	1.60	0.66
1:C:276:ASN:HD22	1:C:278:TYR:N	1.93	0.66
1:A:14:LEU:O	1:A:17:LEU:HB2	1.96	0.66
1:B:149:ASP:HB2	1:B:153:LYS:H	1.61	0.66
1:D:2:LYS:HD3	1:D:48:ASP:OD2	1.97	0.65
1:B:150:GLU:O	1:B:151:LYS:HB2	1.96	0.65
1:C:262:SER:H	1:C:265:GLN:HE21	1.43	0.65
1:D:147:GLU:OE1	1:D:165:LYS:HD3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:NE2	1:A:24:GLN:N	2.37	0.64
1:D:40:VAL:HG13	1:D:120:LEU:HD21	1.80	0.64
1:B:14:LEU:HA	1:B:227:HIS:NE2	2.12	0.64
1:B:276:ASN:HD22	1:B:278:TYR:N	1.96	0.64
1:C:139:ASP:HB2	1:C:142:ARG:NE	2.11	0.64
1:B:224:THR:O	1:B:224:THR:CG2	2.46	0.64
1:B:33:MET:HE2	1:B:224:THR:HG21	1.80	0.63
1:A:11:GLY:HA2	4:A:302:SO4:O4	1.98	0.63
1:C:33:MET:HE2	1:C:224:THR:HG21	1.80	0.62
1:C:54:THR:O	1:C:58:THR:OG1	2.16	0.62
1:A:276:ASN:HD22	1:A:278:TYR:H	1.45	0.62
1:C:24:GLN:H	1:C:24:GLN:HE21	1.47	0.62
1:C:183:ILE:O	1:C:187:ILE:HG23	2.00	0.62
1:A:147:GLU:OE2	1:A:155:ILE:CG1	2.47	0.62
1:A:112:TYR:OH	1:B:217:ARG:O	2.15	0.62
1:A:40:VAL:HG13	1:A:120:LEU:HD21	1.81	0.61
1:B:149:ASP:HB3	1:B:150:GLU:O	2.00	0.61
1:A:54:THR:O	1:A:58:THR:OG1	2.16	0.61
1:B:276:ASN:HD21	1:B:278:TYR:HB3	1.65	0.61
1:C:149:ASP:HB2	1:C:150:GLU:HA	1.83	0.61
1:D:160:LYS:NZ	2:D:300:UPG:O2B	2.34	0.61
1:D:228:GLU:HB2	5:D:419:HOH:O	2.00	0.61
1:C:121:GLN:O	1:C:124:ALA:O	2.19	0.60
1:A:244:GLN:HE22	1:B:217:ARG:HA	1.66	0.60
1:B:24:GLN:HE21	1:B:24:GLN:N	1.95	0.60
1:C:202:LYS:HE3	5:C:434:HOH:O	2.01	0.60
1:B:99:ASP:C	1:B:178:ASN:OD1	2.40	0.60
1:D:124:ALA:O	1:D:125:ASN:HB2	2.00	0.60
1:C:276:ASN:ND2	1:C:278:TYR:HB3	2.17	0.60
1:B:99:ASP:OD1	1:B:99:ASP:N	2.28	0.59
1:D:45:GLY:HA2	1:D:260:TYR:OH	2.02	0.59
1:B:101:ASN:HD21	1:B:127:LYS:HD3	1.68	0.59
1:D:86:LEU:HD13	1:D:106:LEU:HD21	1.84	0.59
1:B:183:ILE:O	1:B:187:ILE:HG23	2.03	0.59
1:D:276:ASN:HD22	1:D:278:TYR:N	2.01	0.59
1:D:270:ALA:HB1	1:D:274:MET:CE	2.33	0.59
1:D:270:ALA:HB1	1:D:274:MET:HE3	1.85	0.59
1:B:235:GLN:NE2	1:C:235:GLN:HE21	2.01	0.58
1:B:1:MET:HE1	1:B:103:ALA:HB2	1.84	0.58
1:B:276:ASN:ND2	1:B:278:TYR:HB3	2.17	0.58
1:C:150:GLU:C	1:C:152:GLY:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:THR:O	1:C:224:THR:CG2	2.52	0.58
1:C:126:ARG:NH1	1:C:211:HIS:CE1	2.71	0.58
1:A:1:MET:HE1	1:A:102:VAL:C	2.24	0.58
1:B:1:MET:CE	1:B:103:ALA:HB2	2.34	0.58
1:D:1:MET:HE2	1:D:46:ILE:HD11	1.85	0.58
1:A:238:GLU:HG2	1:D:231:LEU:CD2	2.34	0.58
1:C:276:ASN:HD21	1:C:278:TYR:HB3	1.69	0.57
1:D:1:MET:HE1	1:D:103:ALA:N	2.18	0.57
1:B:14:LEU:O	1:B:17:LEU:HB2	2.04	0.57
1:D:33:MET:SD	1:D:224:THR:HG21	2.44	0.57
1:A:228:GLU:HB2	5:A:419:HOH:O	2.03	0.56
1:A:11:GLY:CA	4:A:302:SO4:O4	2.53	0.56
1:B:2:LYS:HG2	1:B:48:ASP:OD2	2.05	0.56
1:B:33:MET:SD	1:B:224:THR:CG2	2.92	0.56
1:B:71:LEU:HB2	1:B:73:ILE:HG12	1.87	0.56
1:C:117:THR:CG2	5:C:426:HOH:O	2.52	0.56
1:B:149:ASP:O	1:B:152:GLY:N	2.38	0.56
1:C:40:VAL:HG13	1:C:120:LEU:HD21	1.87	0.56
1:C:269:LEU:O	1:C:272:PRO:HD2	2.05	0.56
1:A:262:SER:N	1:A:265:GLN:HE21	2.01	0.56
1:C:99:ASP:OD1	1:C:99:ASP:N	2.35	0.56
1:B:47:LYS:CB	1:B:73:ILE:HG22	2.36	0.55
1:C:276:ASN:ND2	1:C:278:TYR:H	2.01	0.55
1:C:247:LYS:HD2	1:C:281:TYR:CD2	2.42	0.54
1:C:276:ASN:HD21	1:C:279:GLY:H	1.52	0.54
1:A:149:ASP:O	1:A:151:LYS:N	2.40	0.54
1:A:217:ARG:O	1:B:112:TYR:OH	2.21	0.54
1:C:12:THR:H	1:C:13:ARG:HB2	1.72	0.54
1:B:86:LEU:HD21	2:B:300:UPG:H1'	1.90	0.54
1:D:1:MET:CE	1:D:2:LYS:O	2.56	0.54
1:B:149:ASP:O	1:B:152:GLY:CA	2.55	0.53
1:A:45:GLY:HA2	1:A:260:TYR:OH	2.08	0.53
1:D:33:MET:CE	1:D:224:THR:CG2	2.78	0.53
1:A:17:LEU:HD11	1:D:27:PRO:HB3	1.90	0.53
1:B:269:LEU:O	1:B:272:PRO:HD2	2.09	0.53
1:C:43:LEU:HD23	1:C:258:MET:CE	2.34	0.53
1:B:130:ALA:HA	1:B:175:PHE:O	2.09	0.53
1:D:276:ASN:HD22	1:D:276:ASN:C	2.11	0.53
1:A:148:PHE:N	1:A:148:PHE:CD2	2.76	0.53
1:D:276:ASN:ND2	1:D:278:TYR:H	2.03	0.53
1:D:22:SER:HB2	1:D:57:ASP:CG	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:O	1:A:152:GLY:N	2.38	0.52
1:B:238:GLU:HG2	1:C:231:LEU:CD2	2.39	0.52
1:B:150:GLU:O	1:B:151:LYS:CB	2.56	0.52
1:C:275:LYS:HB2	5:C:407:HOH:O	2.08	0.52
1:A:11:GLY:N	4:A:302:SO4:O4	2.43	0.52
1:B:224:THR:O	1:B:224:THR:HG23	2.09	0.52
1:D:86:LEU:HD21	2:D:300:UPG:H5C1	1.91	0.52
1:A:250:CYS:SG	1:A:282:LEU:HD21	2.50	0.52
1:C:252:GLU:OE1	1:C:252:GLU:N	2.38	0.52
1:A:60:ARG:HD2	1:D:60:ARG:NH2	2.21	0.52
1:B:33:MET:O	1:B:37:PRO:HD2	2.10	0.51
1:B:149:ASP:C	1:B:152:GLY:H	2.13	0.51
1:D:43:LEU:HA	1:D:258:MET:HE1	1.86	0.51
1:D:269:LEU:O	1:D:272:PRO:HD2	2.11	0.51
1:A:23:LYS:O	1:A:33:MET:HE3	2.11	0.51
1:B:60:ARG:NH2	5:B:412:HOH:O	2.43	0.51
1:D:20:VAL:HG23	1:D:21:VAL:HG23	1.93	0.51
1:D:43:LEU:HD23	1:D:258:MET:CE	2.41	0.51
1:D:150:GLU:CD	1:D:150:GLU:H	2.14	0.51
1:C:148:PHE:N	1:C:148:PHE:HD1	1.94	0.51
1:D:287:HIS:O	1:D:288:ARG:HG2	2.11	0.50
1:A:99:ASP:OD2	1:A:99:ASP:N	2.37	0.50
1:A:29:TYR:CD1	1:A:238:GLU:HB3	2.47	0.50
1:B:24:GLN:NE2	1:B:24:GLN:N	2.56	0.50
1:C:93:GLY:O	1:C:97:ILE:HG13	2.11	0.50
1:C:69:SER:HB3	5:C:435:HOH:O	2.12	0.50
1:C:160:LYS:NZ	2:C:300:UPG:O2B	2.44	0.50
1:D:276:ASN:C	1:D:276:ASN:ND2	2.65	0.49
1:D:139:ASP:HB2	1:D:142:ARG:NH1	2.26	0.49
1:A:269:LEU:O	1:A:272:PRO:HD2	2.12	0.49
1:A:1:MET:HE1	1:A:103:ALA:N	2.27	0.49
1:A:224:THR:HG23	1:A:230:LEU:HG	1.94	0.49
1:B:235:GLN:HE21	1:C:235:GLN:HE21	1.60	0.49
1:B:235:GLN:CG	1:C:235:GLN:HE21	2.25	0.49
1:D:1:MET:HE2	1:D:46:ILE:CD1	2.42	0.49
1:D:43:LEU:HD23	1:D:258:MET:HE2	1.95	0.49
2:D:300:UPG:H3C	2:D:300:UPG:O1A	2.13	0.49
1:D:43:LEU:CA	1:D:258:MET:HE3	2.38	0.48
1:A:1:MET:HG3	1:A:124:ALA:O	2.13	0.48
1:A:21:VAL:HG13	1:A:60:ARG:NH2	2.28	0.48
1:A:47:LYS:HE2	1:A:260:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASP:OD1	1:B:31:LYS:CE	2.62	0.48
1:C:12:THR:N	1:C:13:ARG:HB2	2.28	0.48
1:B:13:ARG:O	1:B:14:LEU:CB	2.51	0.48
1:C:157:ILE:HG12	1:C:198:THR:HG23	1.94	0.48
1:B:231:LEU:HD21	1:C:238:GLU:HG2	1.94	0.48
1:A:47:LYS:HE2	1:A:260:TYR:CD1	2.49	0.48
1:B:1:MET:HE2	1:B:46:ILE:HD11	1.93	0.48
1:C:23:LYS:NZ	1:C:108:ASP:OD2	2.43	0.48
1:C:86:LEU:HD13	1:C:106:LEU:HD21	1.96	0.48
2:D:300:UPG:H6	2:D:300:UPG:C5C	2.39	0.48
1:B:132:ILE:HG22	1:B:174:TYR:HD2	1.79	0.47
1:A:235:GLN:CD	1:D:235:GLN:HE21	2.17	0.47
1:B:247:LYS:HD2	1:B:281:TYR:CD2	2.49	0.47
1:C:247:LYS:O	1:D:217:ARG:NH2	2.45	0.47
1:D:84:ASP:HB2	1:D:88:GLN:OE1	2.14	0.47
1:B:1:MET:HG3	1:B:101:ASN:HB2	1.96	0.47
1:D:179:ARG:O	1:D:183:ILE:HG13	2.14	0.47
1:B:27:PRO:HG3	1:C:17:LEU:HG	1.97	0.47
1:C:12:THR:CA	1:C:13:ARG:HB2	2.44	0.47
1:A:17:LEU:HD22	1:A:227:HIS:CD2	2.50	0.47
1:A:244:GLN:NE2	1:B:217:ARG:HA	2.30	0.47
1:B:178:ASN:O	1:B:178:ASN:ND2	2.42	0.47
1:A:235:GLN:HG2	1:D:235:GLN:NE2	2.30	0.46
1:B:49:ILE:HB	1:B:75:LEU:HD23	1.97	0.46
1:A:82:SER:HB2	1:A:83:PRO:CD	2.45	0.46
1:B:149:ASP:CA	1:B:150:GLU:CB	2.93	0.46
1:D:254:ILE:O	1:D:258:MET:HB2	2.16	0.46
1:A:244:GLN:O	1:A:245:SER:HB3	2.15	0.45
1:C:17:LEU:HD22	1:C:227:HIS:CD2	2.51	0.45
1:D:28:VAL:HB	1:D:36:TYR:CE1	2.52	0.45
1:C:45:GLY:HA2	1:C:260:TYR:OH	2.16	0.45
1:D:1:MET:HE3	1:D:2:LYS:O	2.16	0.45
1:B:33:MET:CE	1:B:224:THR:CG2	2.91	0.45
1:C:12:THR:HG23	5:C:430:HOH:O	2.15	0.45
1:C:13:ARG:O	1:C:14:LEU:CB	2.55	0.45
1:A:15:TYR:CG	1:A:16:PRO:HA	2.52	0.45
1:A:86:LEU:HD13	1:A:106:LEU:HD21	1.99	0.45
1:C:1:MET:CE	1:C:2:LYS:O	2.65	0.45
1:D:4:ILE:HG12	1:D:50:LEU:HB3	1.99	0.44
1:C:94:GLU:OE2	1:C:185:LYS:NZ	2.47	0.44
1:A:147:GLU:OE2	1:A:155:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:O	1:A:183:ILE:HG13	2.18	0.44
1:A:254:ILE:O	1:A:258:MET:HB2	2.17	0.44
1:C:150:GLU:C	1:C:152:GLY:N	2.70	0.44
1:C:258:MET:HG2	1:C:260:TYR:CZ	2.53	0.44
1:B:47:LYS:HB2	1:B:47:LYS:HE3	1.89	0.44
1:B:94:GLU:OE1	1:B:185:LYS:NZ	2.51	0.44
1:B:17:LEU:HG	1:C:27:PRO:HG3	1.98	0.44
1:B:138:LYS:HD3	1:B:139:ASP:OD2	2.18	0.44
1:B:149:ASP:O	1:B:152:GLY:HA2	2.18	0.44
1:B:231:LEU:HD11	1:C:235:GLN:HG3	2.00	0.44
1:D:276:ASN:ND2	1:D:279:GLY:H	2.15	0.44
1:C:149:ASP:CB	1:C:150:GLU:HA	2.46	0.44
1:C:192:ARG:HH22	2:C:300:UPG:PB	2.40	0.43
3:C:301:THM:H6	3:C:301:THM:O5'	2.18	0.43
1:A:149:ASP:O	1:A:150:GLU:C	2.56	0.43
1:B:40:VAL:HG13	1:B:120:LEU:HD21	2.00	0.43
1:A:147:GLU:HG2	1:A:156:SER:OG	2.18	0.43
1:B:179:ARG:O	1:B:183:ILE:HG12	2.19	0.43
1:C:137:VAL:HG21	1:C:169:ALA:HB2	2.00	0.43
1:B:149:ASP:HB3	1:B:150:GLU:C	2.38	0.43
1:B:244:GLN:O	1:B:245:SER:HB3	2.18	0.43
1:C:1:MET:HE2	1:C:1:MET:HB3	1.91	0.43
1:D:49:ILE:HB	1:D:75:LEU:HD23	2.01	0.43
1:A:115:GLY:HA2	1:A:118:GLU:OE1	2.19	0.42
1:B:276:ASN:HD21	1:B:279:GLY:H	1.64	0.42
2:C:300:UPG:H3C	2:C:300:UPG:O1A	2.18	0.42
1:B:82:SER:HB2	1:B:83:PRO:HD2	2.01	0.42
1:C:14:LEU:HA	1:C:227:HIS:NE2	2.35	0.42
1:B:45:GLY:HA2	1:B:260:TYR:OH	2.19	0.42
1:D:4:ILE:HA	1:D:50:LEU:O	2.20	0.42
1:D:71:LEU:HB2	1:D:73:ILE:HG12	2.02	0.42
1:C:125:ASN:HD22	1:C:125:ASN:HA	1.62	0.42
1:A:64:LEU:HD12	1:D:19:LYS:HD3	2.01	0.42
1:B:14:LEU:O	1:B:15:TYR:C	2.58	0.42
1:B:235:GLN:HE21	1:C:235:GLN:NE2	2.17	0.42
1:C:139:ASP:H	1:C:142:ARG:HH21	1.68	0.42
1:D:17:LEU:HD22	1:D:227:HIS:CD2	2.54	0.42
1:D:148:PHE:CD2	1:D:148:PHE:N	2.88	0.42
1:A:22:SER:OG	1:A:57:ASP:HB3	2.20	0.42
1:A:88:GLN:HG2	1:A:92:ILE:HD12	2.01	0.42
1:A:236:PHE:CE1	1:B:236:PHE:CE1	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HD12	1:B:23:LYS:HG3	2.00	0.42
1:A:64:LEU:HB2	1:D:20:VAL:HG11	2.02	0.42
1:B:178:ASN:O	1:B:181:VAL:HG12	2.20	0.42
1:A:276:ASN:O	1:A:280:GLN:HG2	2.19	0.42
1:D:15:TYR:CG	1:D:16:PRO:HA	2.54	0.41
1:B:99:ASP:O	1:B:178:ASN:OD1	2.37	0.41
1:C:88:GLN:O	1:C:92:ILE:HD12	2.20	0.41
1:B:127:LYS:O	1:B:127:LYS:CG	2.65	0.41
1:D:150:GLU:C	1:D:152:GLY:H	2.24	0.41
1:B:154:VAL:HG22	1:B:212:VAL:CG2	2.51	0.41
1:C:150:GLU:OE2	1:C:150:GLU:CA	2.66	0.41
1:C:276:ASN:ND2	1:C:278:TYR:N	2.63	0.41
1:B:250:CYS:SG	1:B:282:LEU:HD21	2.60	0.41
1:B:1:MET:HE2	1:B:1:MET:HB3	1.94	0.41
1:A:253:GLU:HG3	1:A:285:LEU:CD2	2.50	0.41
1:B:30:ASP:OD1	1:B:31:LYS:HE2	2.21	0.41
1:C:11:GLY:C	1:C:13:ARG:O	2.59	0.41
1:C:250:CYS:SG	1:C:282:LEU:HD21	2.61	0.41
1:C:256:TYR:CZ	1:C:263:ARG:HG3	2.56	0.41
1:D:280:GLN:H	1:D:280:GLN:HG2	1.56	0.41
1:C:276:ASN:HD22	1:C:276:ASN:C	2.24	0.41
1:B:101:ASN:HB3	1:B:176:TYR:O	2.21	0.40
1:C:12:THR:N	1:C:13:ARG:O	2.54	0.40
1:D:192:ARG:HD3	1:D:196:GLU:OE2	2.20	0.40
1:C:148:PHE:O	1:C:149:ASP:CB	2.67	0.40
1:C:148:PHE:HB2	1:C:152:GLY:HA2	2.04	0.40
1:D:36:TYR:N	1:D:37:PRO:HD2	2.36	0.40
1:A:12:THR:HG21	1:D:275:LYS:HG3	2.03	0.40
1:A:276:ASN:HD22	1:A:278:TYR:N	2.16	0.40
1:A:71:LEU:HB2	1:A:73:ILE:HG12	2.03	0.40
1:D:54:THR:O	1:D:58:THR:OG1	2.27	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	286/297 (96%)	272 (95%)	11 (4%)	3 (1%)	15	32
1	B	286/297 (96%)	272 (95%)	11 (4%)	3 (1%)	15	32
1	C	286/297 (96%)	270 (94%)	13 (4%)	3 (1%)	15	32
1	D	286/297 (96%)	272 (95%)	13 (4%)	1 (0%)	41	64
All	All	1144/1188 (96%)	1086 (95%)	48 (4%)	10 (1%)	17	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	GLU
1	C	149	ASP
1	C	125	ASN
1	B	29	TYR
1	C	29	TYR
1	D	29	TYR
1	A	29	TYR
1	A	157	ILE
1	B	151	LYS
1	B	157	ILE

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	243/251 (97%)	217 (89%)	26 (11%)	6	12
1	B	243/251 (97%)	213 (88%)	30 (12%)	4	9
1	C	243/251 (97%)	216 (89%)	27 (11%)	6	11
1	D	243/251 (97%)	218 (90%)	25 (10%)	7	13
All	All	972/1004 (97%)	864 (89%)	108 (11%)	6	11

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	13	ARG
1	A	17	LEU
1	A	22	SER
1	A	24	GLN
1	A	56	GLU
1	A	86	LEU
1	A	99	ASP
1	A	117	THR
1	A	118	GLU
1	A	120	LEU
1	A	125	ASN
1	A	128	SER
1	A	148	PHE
1	A	149	ASP
1	A	150	GLU
1	A	151	LYS
1	A	155	ILE
1	A	187	ILE
1	A	214	LEU
1	A	223	ASP
1	A	230	LEU
1	A	232	GLN
1	A	251	LEU
1	A	276	ASN
1	A	280	GLN
1	B	17	LEU
1	B	24	GLN
1	B	31	LYS
1	B	47	LYS
1	B	60	ARG
1	B	86	LEU
1	B	99	ASP
1	B	117	THR
1	B	118	GLU
1	B	119	LEU
1	B	120	LEU
1	B	150	GLU
1	B	155	ILE
1	B	156	SER
1	B	164	PRO
1	B	174	TYR
1	B	178	ASN

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Mol	Chain	Res	Type
1	B	182	ASP
1	B	187	ILE
1	B	214	LEU
1	B	224	THR
1	B	230	LEU
1	B	232	GLN
1	B	238	GLU
1	B	251	LEU
1	B	268	LYS
1	B	276	ASN
1	B	277	GLU
1	B	280	GLN
1	B	288	ARG
1	C	1	MET
1	C	13	ARG
1	C	17	LEU
1	C	22	SER
1	C	24	GLN
1	C	62	GLU
1	C	70	GLU
1	C	86	LEU
1	C	99	ASP
1	C	100	ASP
1	C	117	THR
1	C	118	GLU
1	C	119	LEU
1	C	120	LEU
1	C	121	GLN
1	C	148	PHE
1	C	150	GLU
1	C	155	ILE
1	C	167	SER
1	C	187	ILE
1	C	192	ARG
1	C	214	LEU
1	C	230	LEU
1	C	232	GLN
1	C	251	LEU
1	C	268	LYS
1	C	276	ASN
1	D	1	MET
1	D	7	SER

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Mol	Chain	Res	Type
1	D	13	ARG
1	D	17	LEU
1	D	24	GLN
1	D	70	GLU
1	D	117	THR
1	D	119	LEU
1	D	120	LEU
1	D	121	GLN
1	D	122	ARG
1	D	127	LYS
1	D	155	ILE
1	D	162	GLU
1	D	167	SER
1	D	181	VAL
1	D	192	ARG
1	D	230	LEU
1	D	238	GLU
1	D	242	LYS
1	D	251	LEU
1	D	263	ARG
1	D	268	LYS
1	D	276	ASN
1	D	280	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	211	HIS
1	A	232	GLN
1	A	244	GLN
1	A	265	GLN
1	A	276	ASN
1	A	280	GLN
1	B	24	GLN
1	B	211	HIS
1	B	235	GLN
1	B	265	GLN
1	B	276	ASN
1	B	280	GLN
1	C	24	GLN
1	C	125	ASN

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Mol	Chain	Res	Type
1	C	211	HIS
1	C	232	GLN
1	C	235	GLN
1	C	265	GLN
1	C	276	ASN
1	D	24	GLN
1	D	125	ASN
1	D	186	ASN
1	D	211	HIS
1	D	232	GLN
1	D	235	GLN
1	D	265	GLN
1	D	276	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

22 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	$\#\|Z\| > 2$
4	SO4	B	302	-	4,4,4	0.19	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	C	305	-	4,4,4	0.09	0	6,6,6	0.14	0
2	UPG	C	300	-	35,38,38	0.89	1 (2%)	53,58,58	1.66	10 (18%)
4	SO4	A	303	-	4,4,4	0.17	0	6,6,6	0.13	0
3	THM	B	301	-	18,18,18	1.65	4 (22%)	26,26,26	2.14	7 (26%)
4	SO4	B	304	-	4,4,4	0.43	0	6,6,6	0.35	0
4	SO4	B	305	-	4,4,4	0.23	0	6,6,6	0.18	0
4	SO4	C	302	-	4,4,4	0.08	0	6,6,6	0.26	0
2	UPG	A	300	-	35,38,38	0.99	3 (8%)	53,58,58	1.43	5 (9%)
4	SO4	A	302	-	4,4,4	0.20	0	6,6,6	0.24	0
4	SO4	D	303	-	4,4,4	0.13	0	6,6,6	0.14	0
3	THM	D	301	-	18,18,18	1.67	5 (27%)	26,26,26	2.13	8 (30%)
4	SO4	C	304	-	4,4,4	0.26	0	6,6,6	0.21	0
4	SO4	D	304	-	4,4,4	0.35	0	6,6,6	0.23	0
3	THM	C	301	-	18,18,18	1.68	4 (22%)	26,26,26	2.22	6 (23%)
2	UPG	D	300	-	35,38,38	0.91	1 (2%)	53,58,58	1.58	8 (15%)
2	UPG	B	300	-	35,38,38	1.00	2 (5%)	53,58,58	1.48	8 (15%)
3	THM	A	301	-	18,18,18	1.71	6 (33%)	26,26,26	2.24	8 (30%)
4	SO4	B	303	-	4,4,4	0.15	0	6,6,6	0.18	0
4	SO4	D	302	-	4,4,4	0.10	0	6,6,6	0.17	0
4	SO4	A	304	-	4,4,4	0.39	0	6,6,6	0.30	0
4	SO4	C	303	-	4,4,4	0.18	0	6,6,6	0.19	0

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	THM	D	301	-	-	0/6/18/18	0/2/2/2
2	UPG	C	300	-	-	2/23/59/59	0/3/3/3
2	UPG	B	300	-	-	5/23/59/59	0/3/3/3
2	UPG	A	300	-	-	5/23/59/59	0/3/3/3
2	UPG	D	300	-	-	11/23/59/59	0/3/3/3
3	THM	C	301	-	-	0/6/18/18	0/2/2/2
3	THM	B	301	-	-	0/6/18/18	0/2/2/2
3	THM	A	301	-	-	0/6/18/18	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	THM	C6-C5	3.75	1.40	1.34
3	B	301	THM	C6-C5	3.45	1.40	1.34
3	A	301	THM	C2-N1	-3.31	1.33	1.38
3	A	301	THM	C4-N3	-3.10	1.33	1.38
3	B	301	THM	C2-N1	-2.85	1.33	1.38
3	D	301	THM	C6-C5	2.80	1.39	1.34
3	C	301	THM	C4-C5	-2.74	1.40	1.44
3	D	301	THM	C6-N1	-2.69	1.33	1.38
3	C	301	THM	C2-N3	-2.67	1.33	1.38
2	A	300	UPG	C2-N1	2.66	1.42	1.38
3	D	301	THM	C4-C5	-2.57	1.40	1.44
3	C	301	THM	C4-N3	-2.53	1.34	1.38
3	A	301	THM	C6-C5	2.50	1.38	1.34
3	D	301	THM	C2-N1	-2.46	1.34	1.38
3	D	301	THM	C4-N3	-2.41	1.34	1.38
3	B	301	THM	O4-C4	2.40	1.28	1.23
3	A	301	THM	C2-N3	-2.35	1.33	1.38
3	B	301	THM	C4-N3	-2.33	1.34	1.38
2	B	300	UPG	C6-C5	2.25	1.40	1.35
3	A	301	THM	C4-C5	-2.19	1.41	1.44
2	B	300	UPG	C2-N3	-2.18	1.34	1.38
2	A	300	UPG	C2-N3	-2.17	1.34	1.38
2	D	300	UPG	C6-C5	2.16	1.40	1.35
3	A	301	THM	C6-N1	-2.07	1.34	1.38
2	C	300	UPG	C6-C5	2.04	1.39	1.35
2	A	300	UPG	O2-C2	2.04	1.26	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	THM	C5-C4-N3	5.56	120.06	115.31
2	C	300	UPG	C4-N3-C2	-5.12	119.83	126.58
3	D	301	THM	C4-N3-C2	-5.02	120.86	127.35
3	A	301	THM	C4-N3-C2	-4.84	121.08	127.35
3	B	301	THM	N3-C2-N1	4.81	121.28	114.89
3	C	301	THM	C4-N3-C2	-4.80	121.13	127.35
3	A	301	THM	C5-C4-N3	4.69	119.31	115.31
2	A	300	UPG	C4-N3-C2	-4.65	120.45	126.58
3	C	301	THM	N3-C2-N1	4.63	121.03	114.89
2	B	300	UPG	C4-N3-C2	-4.62	120.48	126.58
3	D	301	THM	C5-C4-N3	4.59	119.23	115.31
2	D	300	UPG	C4-N3-C2	-4.51	120.63	126.58
3	A	301	THM	N3-C2-N1	4.51	120.88	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	THM	C5-C6-N1	-4.48	118.73	123.34
3	B	301	THM	C4-N3-C2	-4.44	121.61	127.35
2	D	300	UPG	N3-C2-N1	4.42	120.76	114.89
2	A	300	UPG	C5-C4-N3	4.39	121.41	114.84
3	D	301	THM	N3-C2-N1	4.33	120.64	114.89
3	B	301	THM	C5M-C5-C4	4.26	123.46	118.77
2	C	300	UPG	N3-C2-N1	4.23	120.51	114.89
3	A	301	THM	C5-C6-N1	-4.23	118.99	123.34
2	A	300	UPG	PB-O3A-PA	-3.99	119.12	132.83
2	B	300	UPG	N3-C2-N1	3.96	120.14	114.89
2	C	300	UPG	C5-C4-N3	3.85	120.60	114.84
2	C	300	UPG	PB-O3A-PA	-3.83	119.67	132.83
3	B	301	THM	C5-C4-N3	3.79	118.54	115.31
2	B	300	UPG	C5-C4-N3	3.79	120.50	114.84
2	D	300	UPG	C5-C4-N3	3.76	120.47	114.84
3	C	301	THM	O4-C4-C5	-3.53	120.81	124.90
2	D	300	UPG	PB-O3A-PA	-3.47	120.93	132.83
2	A	300	UPG	N3-C2-N1	3.44	119.46	114.89
3	D	301	THM	C5-C6-N1	-3.40	119.84	123.34
3	B	301	THM	C5-C6-N1	-3.40	119.84	123.34
3	D	301	THM	C5M-C5-C4	3.31	122.42	118.77
3	A	301	THM	C5M-C5-C4	3.31	122.41	118.77
3	B	301	THM	C5M-C5-C6	-3.25	118.51	122.85
2	B	300	UPG	PB-O3A-PA	-3.24	121.72	132.83
2	A	300	UPG	O4-C4-C5	-3.22	119.50	125.16
2	C	300	UPG	O4-C4-C5	-3.10	119.70	125.16
3	A	301	THM	O2-C2-N1	-3.01	118.78	122.79
2	D	300	UPG	O2-C2-N1	-2.90	118.93	122.79
3	B	301	THM	O2-C2-N1	-2.87	118.97	122.79
2	B	300	UPG	C6'-C5'-C4'	-2.84	106.34	113.00
3	D	301	THM	C5M-C5-C6	-2.68	119.27	122.85
2	C	300	UPG	O5'-C5'-C4'	2.67	114.54	109.69
2	D	300	UPG	O4-C4-C5	-2.66	120.48	125.16
3	C	301	THM	C5'-C4'-C3'	-2.65	108.12	114.81
2	C	300	UPG	C6'-C5'-C4'	-2.64	106.83	113.00
3	A	301	THM	C5M-C5-C6	-2.62	119.35	122.85
2	C	300	UPG	O2-C2-N1	-2.51	119.45	122.79
2	B	300	UPG	O4-C4-C5	-2.47	120.82	125.16
3	D	301	THM	O4-C4-C5	-2.46	122.05	124.90
3	A	301	THM	O4-C4-C5	-2.38	122.15	124.90
2	D	300	UPG	O3A-PB-O3B	2.36	107.25	102.48
2	B	300	UPG	O2'-C2'-C3'	-2.33	104.95	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	300	UPG	O2-C2-N1	-2.16	119.91	122.79
2	C	300	UPG	O3C-C3C-C4C	-2.13	104.90	111.05
2	C	300	UPG	C1'-C2'-C3'	2.10	114.37	110.00
3	D	301	THM	C2'-C3'-C4'	2.10	107.13	102.76
2	D	300	UPG	C6'-C5'-C4'	-2.01	108.29	113.00

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	300	UPG	C5C-O5C-PA-O1A
2	A	300	UPG	O5'-C5'-C6'-O6'
2	A	300	UPG	C4'-C5'-C6'-O6'
2	D	300	UPG	O5'-C5'-C6'-O6'
2	D	300	UPG	C3C-C4C-C5C-O5C
2	A	300	UPG	O4C-C4C-C5C-O5C
2	D	300	UPG	PB-O3A-PA-O5C
2	D	300	UPG	C1'-O3B-PB-O3A
2	B	300	UPG	C3C-C4C-C5C-O5C
2	B	300	UPG	O4C-C4C-C5C-O5C
2	D	300	UPG	PA-O3A-PB-O1B
2	D	300	UPG	C4C-C5C-O5C-PA
2	D	300	UPG	O5'-C1'-O3B-PB
2	B	300	UPG	PB-O3A-PA-O2A
2	A	300	UPG	C4C-C5C-O5C-PA
2	C	300	UPG	C4C-C5C-O5C-PA
2	A	300	UPG	C3C-C4C-C5C-O5C
2	D	300	UPG	O4C-C4C-C5C-O5C
2	B	300	UPG	PB-O3A-PA-O1A
2	D	300	UPG	C5C-O5C-PA-O3A
2	C	300	UPG	O4C-C4C-C5C-O5C
2	B	300	UPG	C5C-O5C-PA-O1A
2	D	300	UPG	C4'-C5'-C6'-O6'

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	300	UPG	3	0
4	A	302	SO4	3	0
3	C	301	THM	1	0

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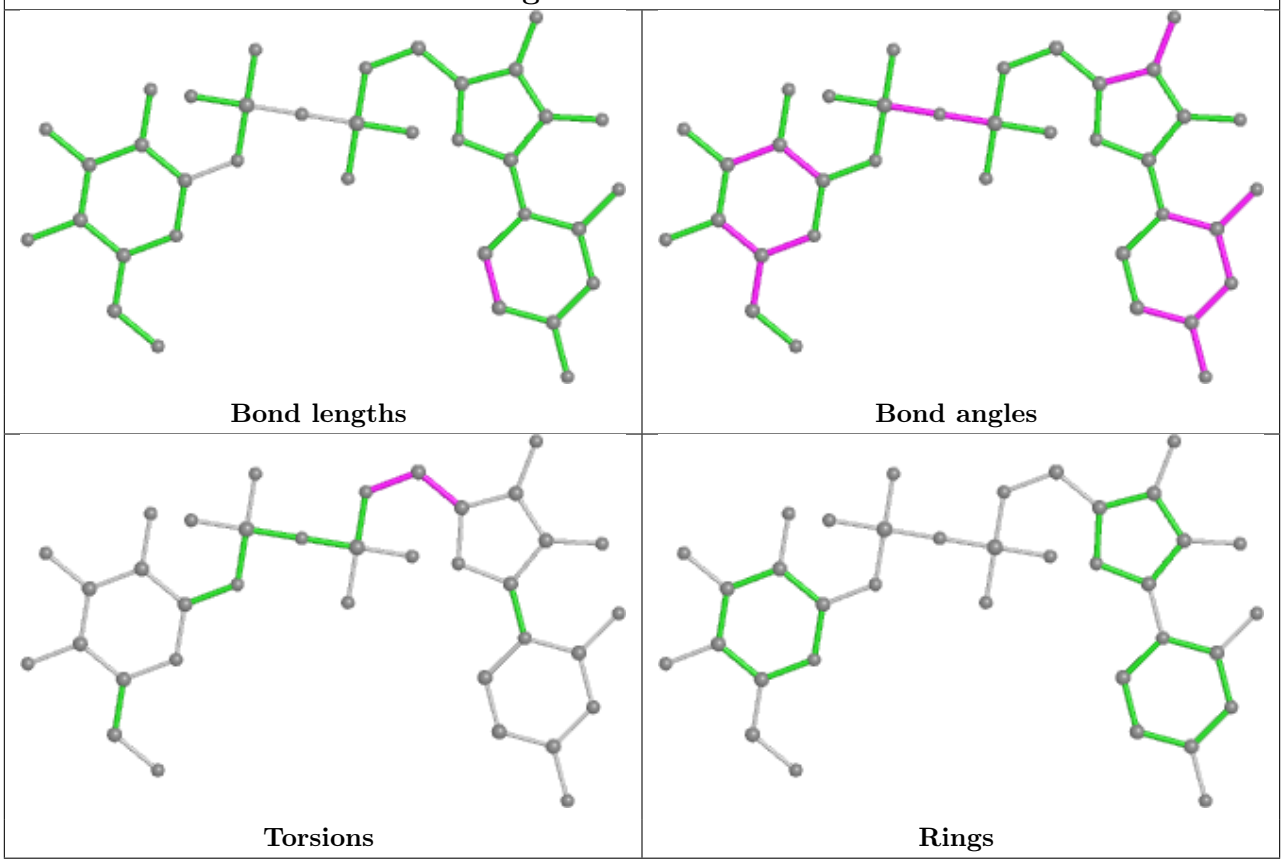
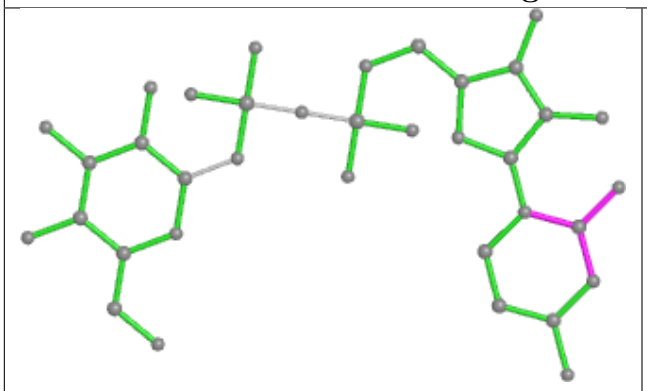
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	300	UPG	5	0
2	B	300	UPG	1	0

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 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.

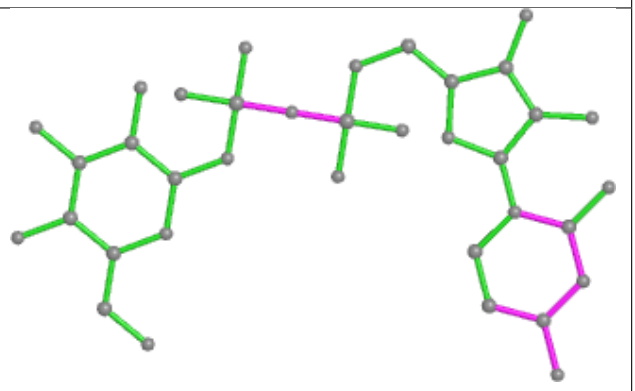
Ligand UPG C 300



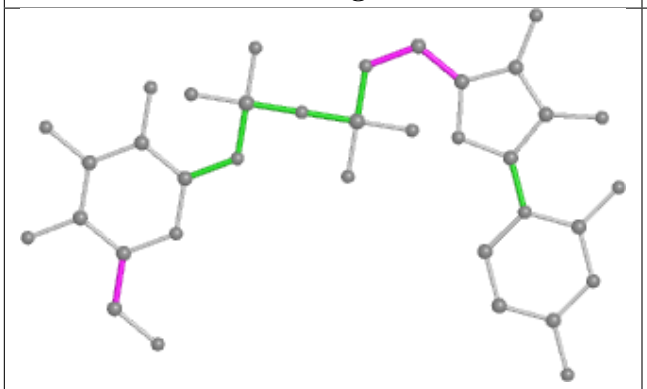
Ligand UPG A 300



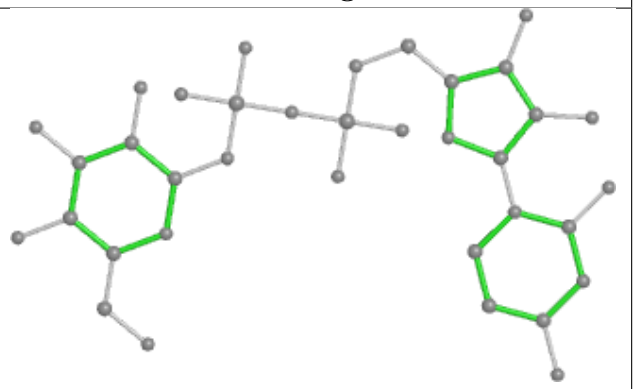
Bond lengths



Bond angles

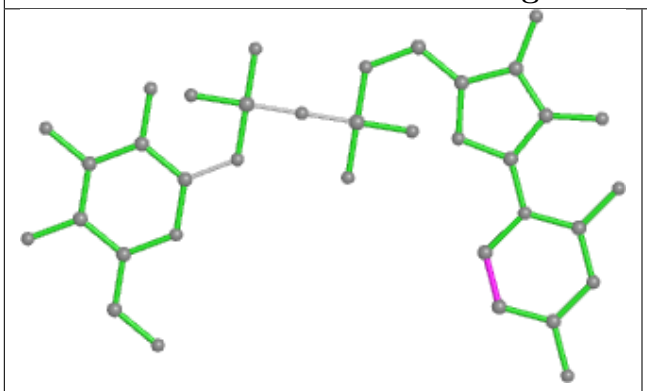


Torsions

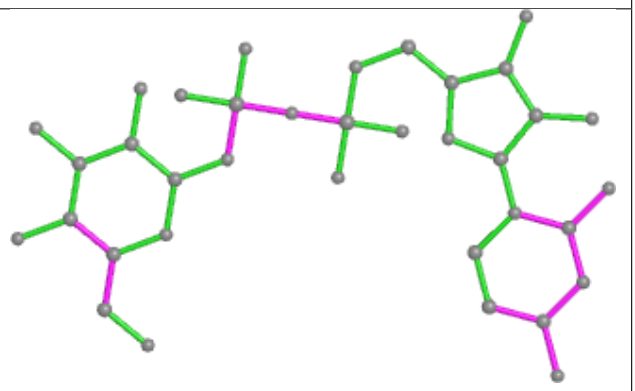


Rings

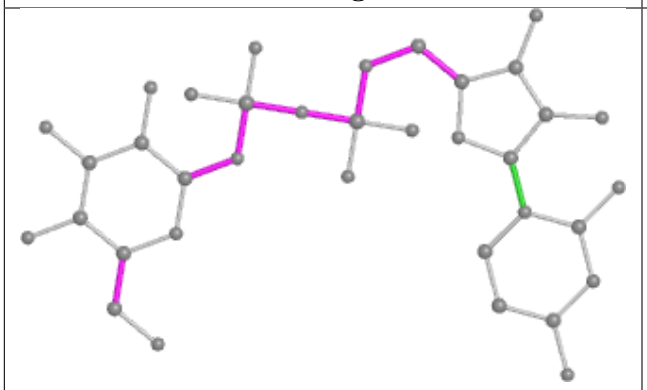
Ligand UPG D 300



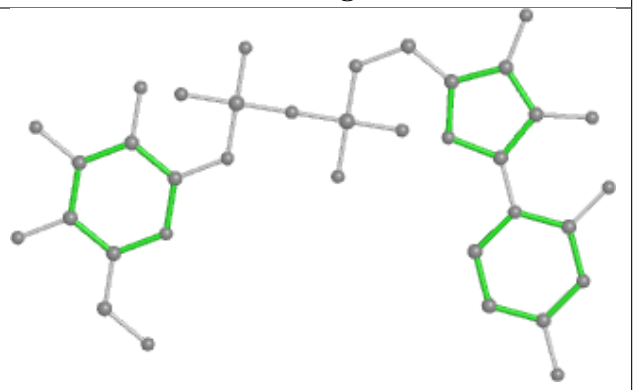
Bond lengths



Bond angles

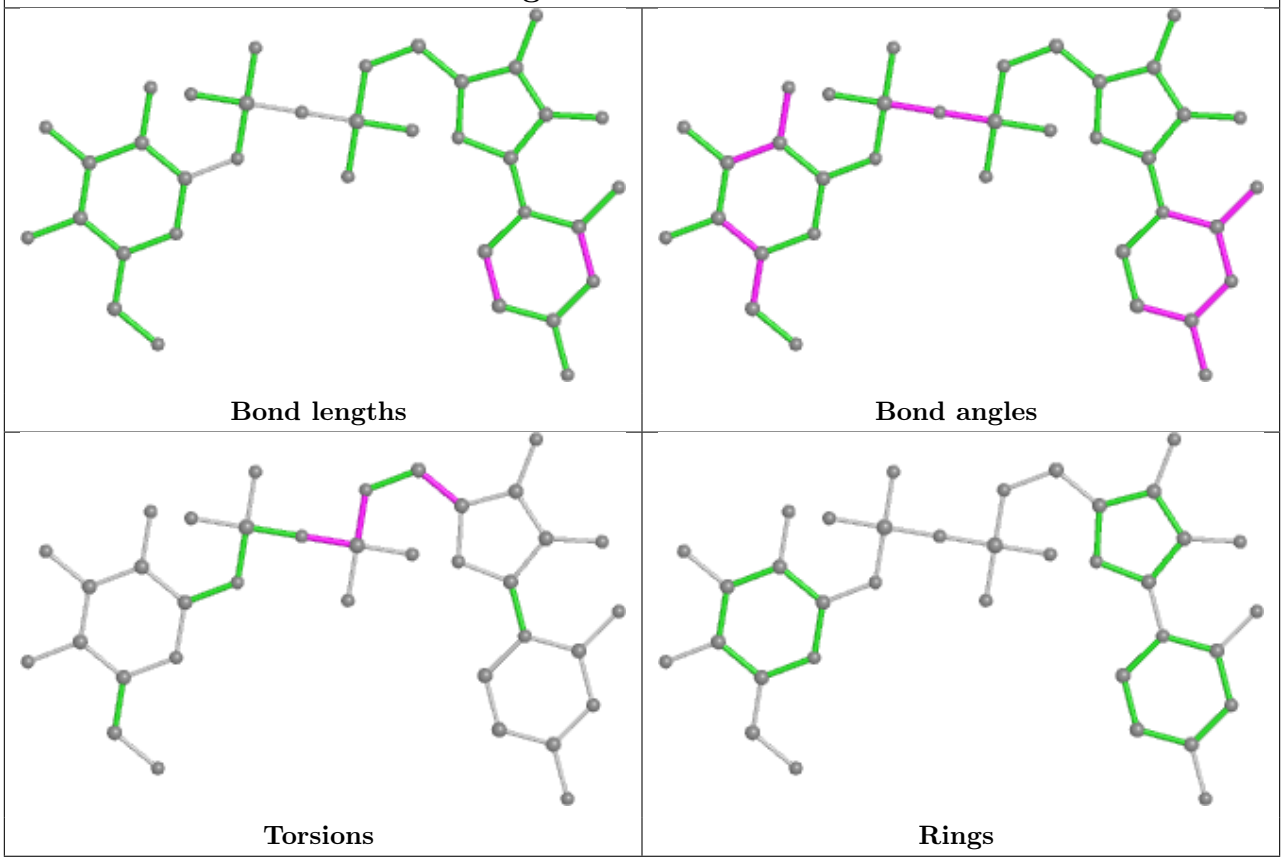


Torsions



Rings

Ligand UPG B 300



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	288/297 (96%)	-0.18	2 (0%) 87 86	34, 48, 65, 81	0
1	B	288/297 (96%)	-0.12	0 100 100	32, 49, 64, 84	0
1	C	288/297 (96%)	-0.16	1 (0%) 94 93	32, 48, 64, 77	0
1	D	288/297 (96%)	-0.13	6 (2%) 63 58	32, 49, 66, 76	0
All	All	1152/1188 (96%)	-0.15	9 (0%) 86 84	32, 49, 65, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	210	LEU	4.1
1	D	148	PHE	3.1
1	C	68	GLY	3.0
1	D	203	ALA	2.6
1	A	155	ILE	2.4
1	D	127	LYS	2.4
1	D	182	ASP	2.3
1	A	152	GLY	2.1
1	D	269	LEU	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)

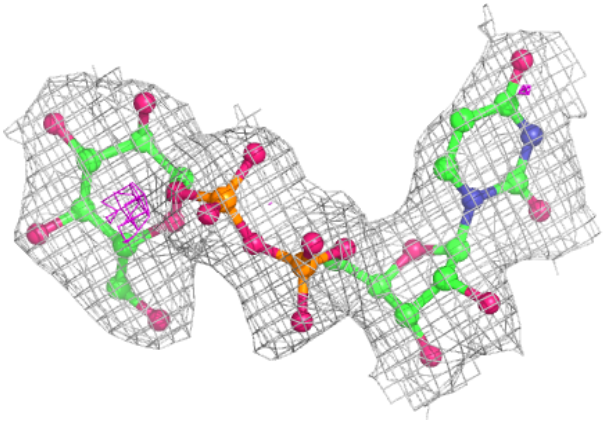
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

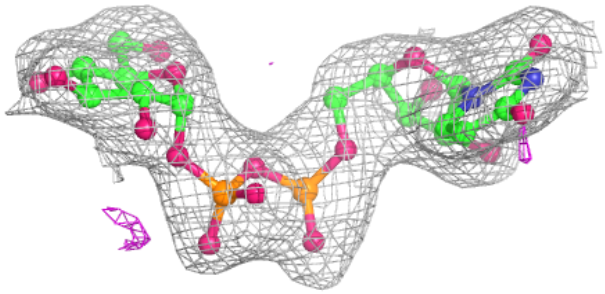
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	303	5/5	0.71	0.22	126,126,127,127	0
4	SO4	A	303	5/5	0.82	0.21	105,107,107,107	0
4	SO4	C	303	5/5	0.87	0.13	112,112,113,113	0
4	SO4	D	303	5/5	0.90	0.14	107,107,108,108	0
4	SO4	A	302	5/5	0.93	0.13	80,81,83,83	0
2	UPG	B	300	36/36	0.95	0.14	36,45,48,49	0
2	UPG	D	300	36/36	0.95	0.14	40,45,50,51	0
4	SO4	C	305	5/5	0.95	0.14	86,87,88,89	0
4	SO4	D	302	5/5	0.95	0.11	81,81,83,83	0
4	SO4	A	304	5/5	0.95	0.13	58,59,60,63	0
4	SO4	D	304	5/5	0.95	0.14	49,50,53,54	0
3	THM	B	301	17/17	0.96	0.14	29,33,37,37	0
4	SO4	B	304	5/5	0.96	0.12	53,56,57,58	0
4	SO4	B	305	5/5	0.96	0.12	81,81,82,83	0
4	SO4	C	302	5/5	0.96	0.11	74,75,77,77	0
3	THM	C	301	17/17	0.96	0.16	31,33,39,43	0
4	SO4	C	304	5/5	0.96	0.12	52,53,56,57	0
2	UPG	C	300	36/36	0.96	0.13	38,43,47,49	0
2	UPG	A	300	36/36	0.96	0.14	40,44,48,49	0
3	THM	A	301	17/17	0.96	0.15	26,31,37,38	0
4	SO4	B	302	5/5	0.96	0.10	80,81,81,81	0
3	THM	D	301	17/17	0.97	0.15	31,34,39,42	0

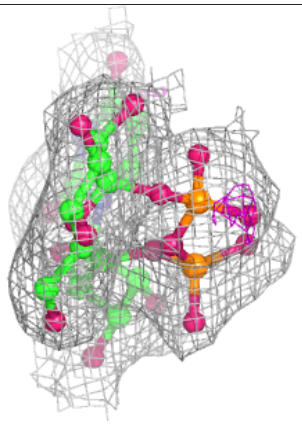
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UPG B 300:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around UPG D 300:

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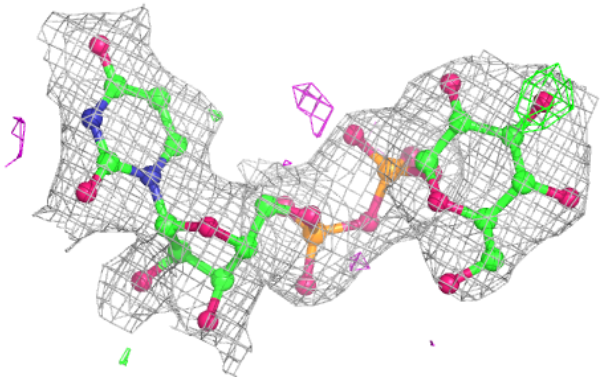
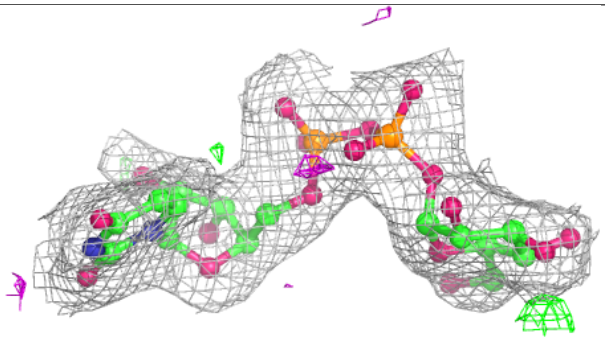
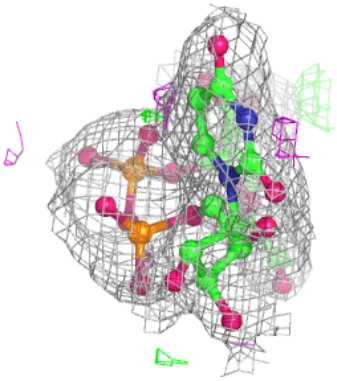
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

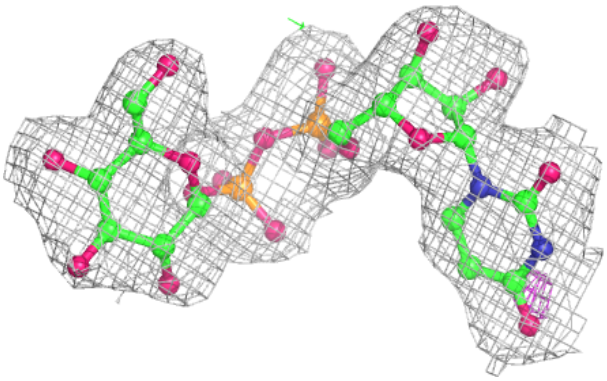


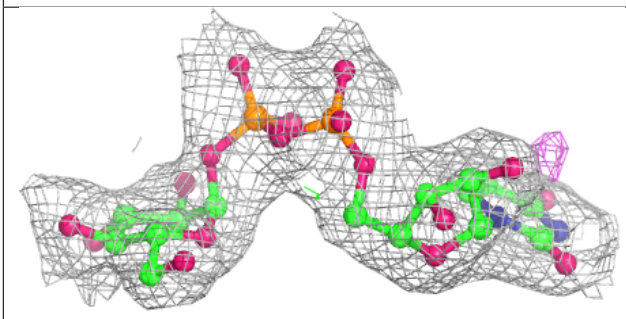


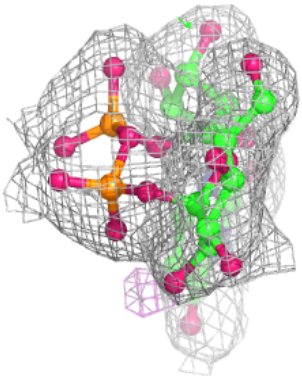


Electron density around UPG C 300:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

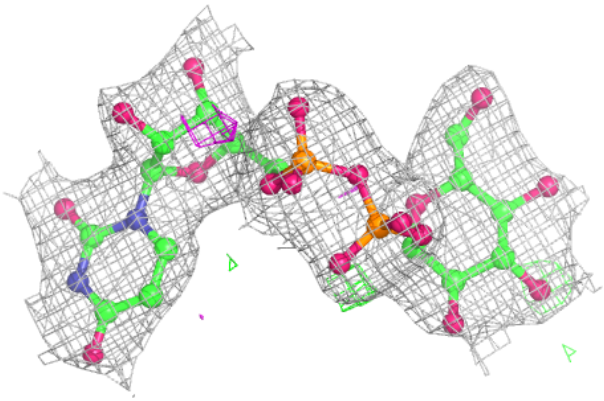


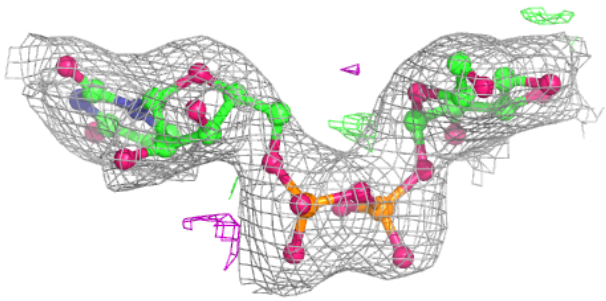


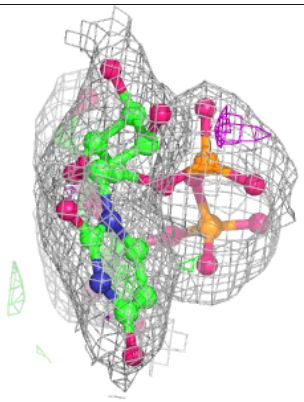


Electron density around UPG A 300:

$2mF_o$-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.