



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 09:31 AM EDT

PDB ID : 5HHF
Title : Crystal structure of *Aspergillus fumigatus* UDP-Galactopyranose mutase mutant H63A with covalent FAD-Galactopyranose and bound UDP
Authors : Tanner, J.J.
Deposited on : 2016-01-10
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-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

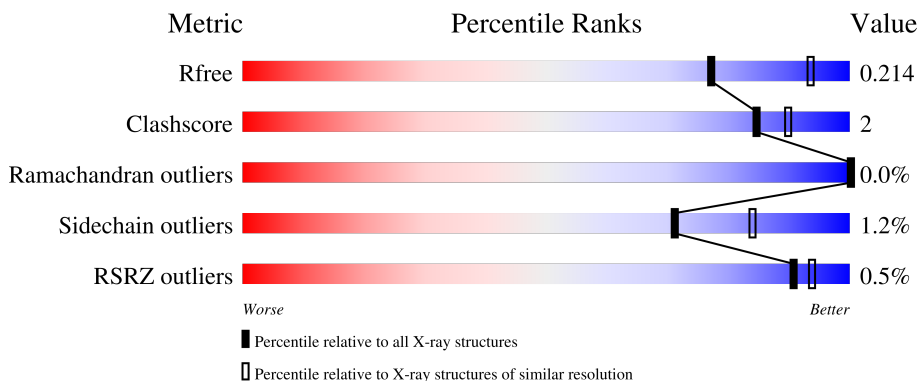
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

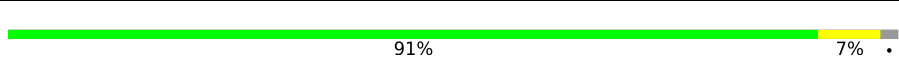
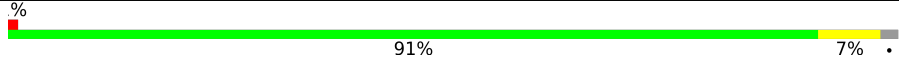
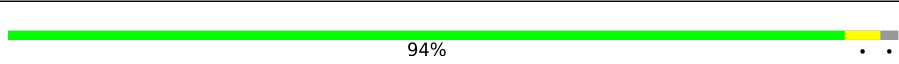
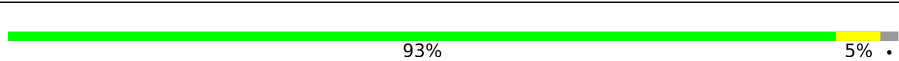
The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	 91% 7%
1	B	513	 91% 7%
1	C	513	 94%
1	D	513	 93% 5%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16554 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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	505	3872	2459	657	735	21	0	0	0
1	B	505	3873	2458	658	736	21	0	0	0
1	C	502	3848	2445	652	730	21	0	0	0
1	D	503	3855	2450	651	733	21	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

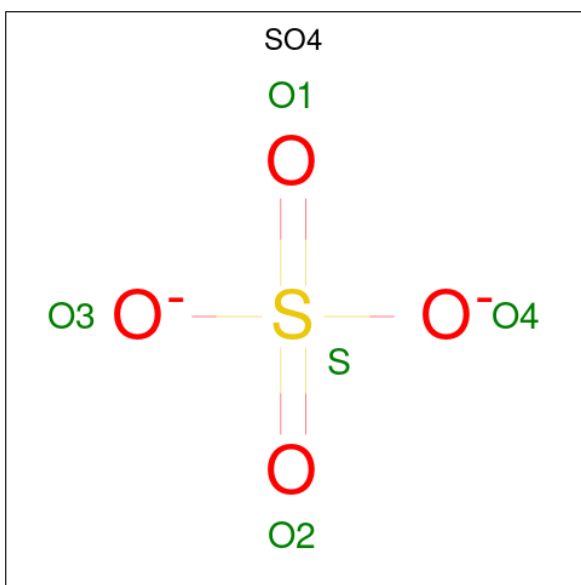
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP Q4W1X2
A	-1	ILE	-	expression tag	UNP Q4W1X2
A	0	ALA	-	expression tag	UNP Q4W1X2
A	63	ALA	HIS	engineered mutation	UNP Q4W1X2
A	344	ALA	LYS	engineered mutation	UNP Q4W1X2
A	345	ALA	LYS	engineered mutation	UNP Q4W1X2
A	429	THR	ALA	see REMARK 999	UNP Q4W1X2
B	-2	ALA	-	expression tag	UNP Q4W1X2
B	-1	ILE	-	expression tag	UNP Q4W1X2
B	0	ALA	-	expression tag	UNP Q4W1X2
B	63	ALA	HIS	engineered mutation	UNP Q4W1X2
B	344	ALA	LYS	engineered mutation	UNP Q4W1X2
B	345	ALA	LYS	engineered mutation	UNP Q4W1X2
B	429	THR	ALA	see REMARK 999	UNP Q4W1X2
C	-2	ALA	-	expression tag	UNP Q4W1X2
C	-1	ILE	-	expression tag	UNP Q4W1X2
C	0	ALA	-	expression tag	UNP Q4W1X2
C	63	ALA	HIS	engineered mutation	UNP Q4W1X2
C	344	ALA	LYS	engineered mutation	UNP Q4W1X2
C	345	ALA	LYS	engineered mutation	UNP Q4W1X2
C	429	THR	ALA	see REMARK 999	UNP Q4W1X2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ALA	-	expression tag	UNP Q4W1X2
D	-1	ILE	-	expression tag	UNP Q4W1X2
D	0	ALA	-	expression tag	UNP Q4W1X2
D	63	ALA	HIS	engineered mutation	UNP Q4W1X2
D	344	ALA	LYS	engineered mutation	UNP Q4W1X2
D	345	ALA	LYS	engineered mutation	UNP Q4W1X2
D	429	THR	ALA	see REMARK 999	UNP Q4W1X2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



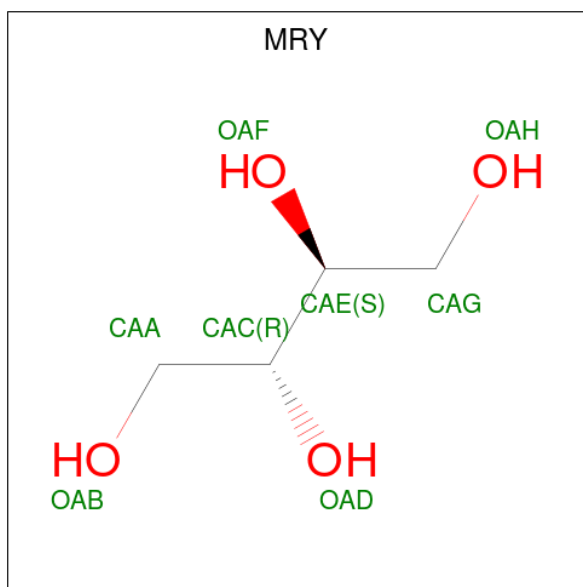
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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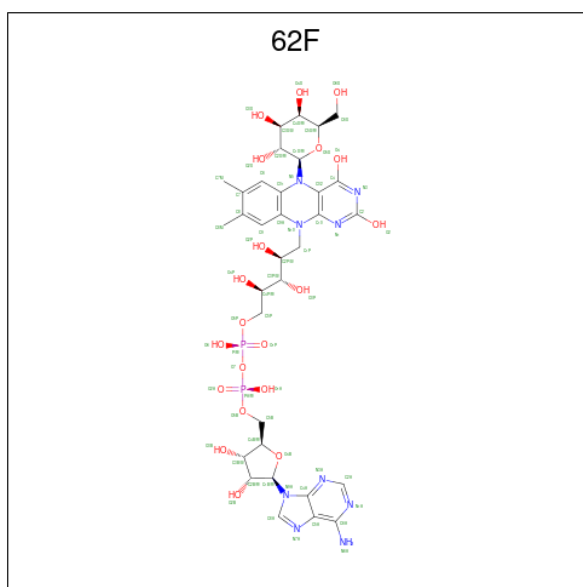
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MESO-ERYTHRITOL (three-letter code: MRY) (formula: C₄H₁₀O₄).



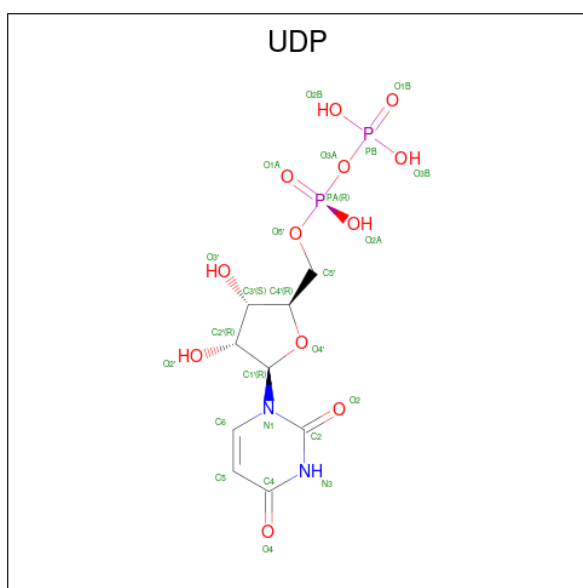
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	B	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl [(2 {R},3 {S},4 {S})-5-[5-[(2 {R},3 {R},4 {S},5 {R},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]-7,8-dimethyl-2,4-bis(oxidanyl)benz o[g]pteridin-10-yl]-2,3,4-tris(oxidanyl)pentyl] hydrogen phosphate (three-letter code: 62F) (formula: C₃₃H₄₅N₉O₂₀P₂).



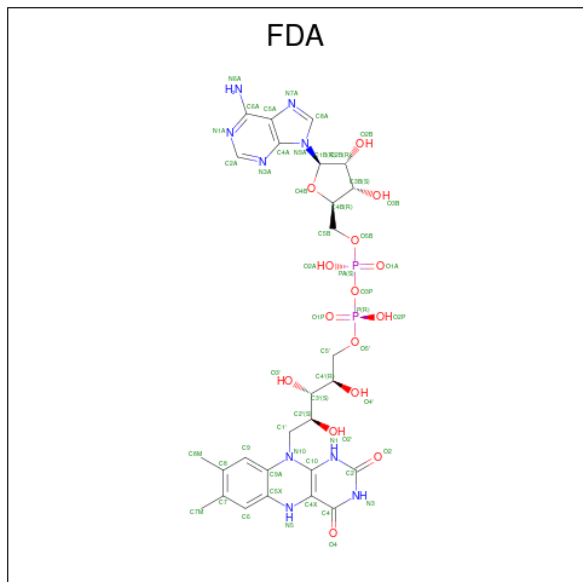
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
4	A	1	Total	64	33	9	20	2	0	0
4	B	1	Total	64	33	9	20	2	0	0

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
5	A	1	Total	25	9	2	12	2	0	0
5	B	1	Total	25	9	2	12	2	0	0

- Molecule 6 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	C	1	53	27	9	15	2	0	0
6	D	1	53	27	9	15	2	0	0

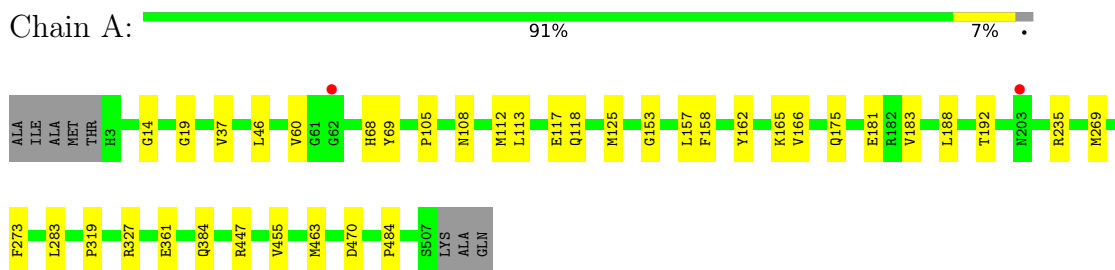
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	172	Total	O	0	0
			172	172		
7	B	202	Total	O	0	0
			202	202		
7	C	177	Total	O	0	0
			177	177		
7	D	189	Total	O	0	0
			189	189		

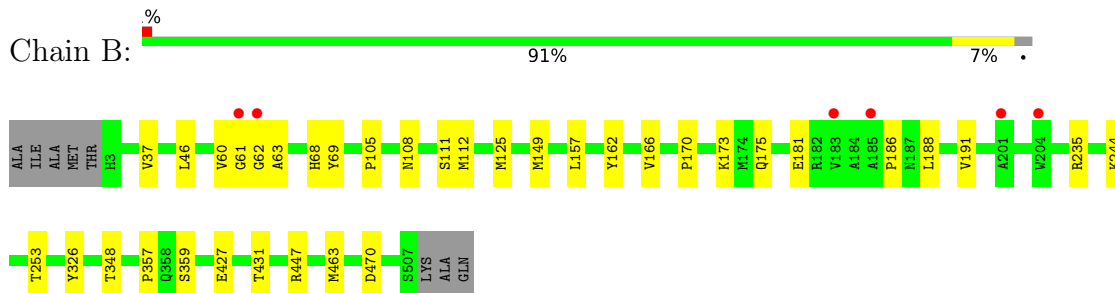
3 Residue-property plots [i](#)

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.

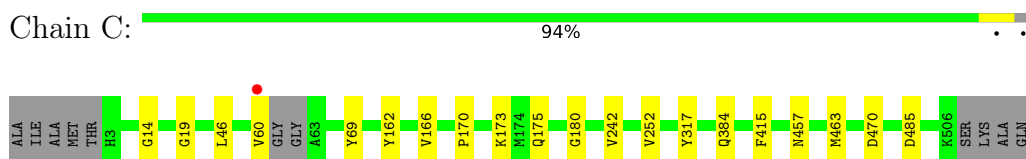
- Molecule 1: UDP-galactopyranose mutase



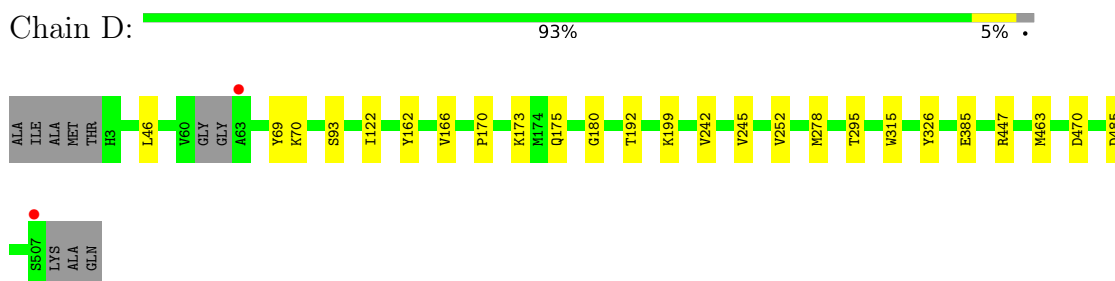
- Molecule 1: UDP-galactopyranose mutase



- Molecule 1: UDP-galactopyranose mutase



- Molecule 1: UDP-galactopyranose mutase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	217.51Å 217.51Å 319.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.61 – 2.30 61.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.61-2.30) 100.0 (61.61-2.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.184 , 0.213 0.185 , 0.214	Depositor DCC
R_{free} test set	3849 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtrriage
Anisotropy	0.466	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16554	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 62F, FDA, UDP, MRY, 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	0.41	0/3969	0.58	0/5416
1	B	0.43	0/3970	0.58	0/5418
1	C	0.39	0/3944	0.55	0/5383
1	D	0.39	0/3951	0.54	0/5391
All	All	0.41	0/15834	0.56	0/21608

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3872	0	3702	21	0
1	B	3873	0	3702	18	0
1	C	3848	0	3667	11	0
1	D	3855	0	3679	15	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	20	0	0	0	0
2	D	15	0	0	0	0
3	A	8	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	10	0	0
3	C	8	0	10	0	0
3	D	8	0	10	0	0
4	A	64	0	41	3	0
4	B	64	0	41	3	0
5	A	25	0	11	4	0
5	B	25	0	11	0	0
6	C	53	0	33	3	0
6	D	53	0	33	6	0
7	A	172	0	0	0	0
7	B	202	0	0	0	0
7	C	177	0	0	0	0
7	D	189	0	0	0	0
All	All	16554	0	14960	71	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 2.

All (71) 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:D:46:LEU:HD13	6:D:605:FDA:HM81	1.71	0.72
1:B:125:MET:HE3	1:B:186:PRO:HB2	1.75	0.69
1:C:457:ASN:HA	6:C:606:FDA:H1'2	1.77	0.65
1:D:180:GLY:HA2	1:D:485:ASP:OD1	1.99	0.62
1:C:170:PRO:HG2	1:C:173:LYS:HG2	1.81	0.62
1:B:170:PRO:HG2	1:B:173:LYS:HG2	1.82	0.62
6:D:605:FDA:O4'	6:D:605:FDA:O2'	2.18	0.60
4:B:604:62F:O4P	4:B:604:62F:O2P	2.06	0.59
1:B:68:HIS:NE2	1:B:181:GLU:OE2	2.28	0.58
1:D:122:ILE:HD12	1:D:192:THR:HG22	1.87	0.57
1:B:348:THR:O	1:B:357:PRO:HG3	2.05	0.56
1:A:183:VAL:HG22	5:A:604:UDP:H1'	1.87	0.56
1:D:170:PRO:HG2	1:D:173:LYS:HG2	1.88	0.55
1:A:192:THR:HG21	1:D:122:ILE:HG21	1.89	0.54
1:B:105:PRO:HG2	1:B:108:ASN:HB2	1.90	0.53
1:A:447:ARG:HB2	4:A:603:62F:H20	1.91	0.52
1:D:242:VAL:HG13	1:D:252:VAL:HG13	1.91	0.52
1:B:447:ARG:HB2	4:B:604:62F:H20	1.91	0.52
1:D:69:TYR:CG	1:D:463:MET:HG3	2.45	0.51
6:D:605:FDA:H2'	6:D:605:FDA:HN1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLY:O	1:B:63:ALA:N	2.44	0.51
1:D:69:TYR:CD2	1:D:463:MET:HG3	2.46	0.51
6:C:606:FDA:O2'	6:C:606:FDA:O4'	2.20	0.51
1:A:46:LEU:HD22	1:A:60:VAL:HG11	1.94	0.50
1:A:162:TYR:CZ	1:A:166:VAL:HG21	2.47	0.50
1:A:68:HIS:NE2	1:A:181:GLU:OE2	2.32	0.50
1:A:69:TYR:CG	1:A:463:MET:HG3	2.47	0.49
1:A:327:ARG:NH2	5:A:604:UDP:O3B	2.38	0.49
1:B:61:GLY:HA3	4:B:604:62F:H5	1.95	0.49
4:A:603:62F:O4P	4:A:603:62F:O2P	2.21	0.49
1:A:69:TYR:CD2	1:A:463:MET:HG3	2.48	0.49
1:A:455:VAL:HG13	1:A:484:PRO:HB3	1.95	0.49
1:B:244:LYS:HB3	1:B:253:THR:HB	1.95	0.49
1:D:162:TYR:O	1:D:166:VAL:HG23	2.13	0.48
1:B:427:GLU:O	1:B:431:THR:HG23	2.13	0.48
1:C:180:GLY:HA2	1:C:485:ASP:OD1	2.13	0.48
1:B:69:TYR:CG	1:B:463:MET:HG3	2.49	0.47
1:B:125:MET:HE2	1:B:188:LEU:HA	1.95	0.47
1:B:125:MET:HE1	1:B:191:VAL:HB	1.96	0.47
1:C:162:TYR:HH	1:C:317:TYR:HD2	1.63	0.47
1:C:60:VAL:HG13	1:C:415:PHE:CZ	2.50	0.47
1:B:149:MET:O	1:B:186:PRO:HD2	2.15	0.46
1:D:295:THR:HG21	6:D:605:FDA:C7M	2.45	0.46
1:C:69:TYR:CG	1:C:463:MET:HG3	2.51	0.46
1:A:37:VAL:HG12	1:A:235:ARG:HB3	1.98	0.46
1:C:46:LEU:HD13	6:C:606:FDA:HM81	1.97	0.46
1:C:14:GLY:O	1:C:19:GLY:HA3	2.16	0.46
1:D:245:VAL:O	1:D:278:MET:HA	2.16	0.46
1:D:447:ARG:HB2	6:D:605:FDA:H5'2	1.98	0.45
1:B:162:TYR:CZ	1:B:166:VAL:HG21	2.52	0.45
1:B:46:LEU:HD22	1:B:60:VAL:HG11	1.99	0.45
1:A:105:PRO:HG2	1:A:108:ASN:HB2	2.00	0.44
1:A:153:GLY:O	1:A:157:LEU:HB2	2.18	0.44
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.82	0.43
1:C:69:TYR:CD2	1:C:463:MET:HG3	2.54	0.43
1:B:166:VAL:HG22	1:B:326:TYR:CD1	2.54	0.42
1:A:158:PHE:CE2	5:A:604:UDP:C4	3.07	0.42
1:A:14:GLY:O	1:A:19:GLY:HA3	2.19	0.42
1:D:166:VAL:HG22	1:D:326:TYR:CD2	2.54	0.42
1:A:162:TYR:HB2	1:A:319:PRO:HB3	2.01	0.42
6:D:605:FDA:H9	6:D:605:FDA:H1'1	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:TYR:O	1:C:166:VAL:HG23	2.20	0.42
1:C:242:VAL:HG13	1:C:252:VAL:HG13	2.02	0.41
1:A:125:MET:HE2	1:A:188:LEU:HA	2.02	0.41
1:A:113:LEU:O	1:A:118:GLN:NE2	2.42	0.41
1:A:117:GLU:HG2	1:A:157:LEU:HD11	2.01	0.41
1:D:199:LYS:HE3	1:D:199:LYS:HB2	1.77	0.41
1:A:269:MET:HE2	1:A:273:PHE:HB3	2.01	0.41
1:B:37:VAL:HG12	1:B:235:ARG:HB3	2.04	0.40
4:A:603:62F:H40	5:A:604:UDP:O3A	2.21	0.40
1:D:93:SER:HA	1:D:315:TRP:O	2.22	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	503/513 (98%)	489 (97%)	14 (3%)	0	100	100
1	B	503/513 (98%)	489 (97%)	13 (3%)	1 (0%)	47	58
1	C	498/513 (97%)	490 (98%)	8 (2%)	0	100	100
1	D	499/513 (97%)	491 (98%)	8 (2%)	0	100	100
All	All	2003/2052 (98%)	1959 (98%)	43 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	62	GLY

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	404/431 (94%)	398 (98%)	6 (2%)	65	79
1	B	405/431 (94%)	399 (98%)	6 (2%)	65	79
1	C	400/431 (93%)	397 (99%)	3 (1%)	81	91
1	D	402/431 (93%)	398 (99%)	4 (1%)	76	87
All	All	1611/1724 (93%)	1592 (99%)	19 (1%)	71	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	MET
1	A	165	LYS
1	A	175	GLN
1	A	361	GLU
1	A	384	GLN
1	A	470	ASP
1	B	111	SER
1	B	112	MET
1	B	157	LEU
1	B	175	GLN
1	B	359	SER
1	B	470	ASP
1	C	175	GLN
1	C	384	GLN
1	C	470	ASP
1	D	70	LYS
1	D	175	GLN
1	D	385	GLU
1	D	470	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

20 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	SO4	D	602	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	A	601	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	C	604	-	4,4,4	0.17	0	6,6,6	0.22	0
6	FDA	C	606	-	52,58,58	2.82	23 (44%)	60,89,89	1.47	12 (20%)
2	SO4	C	601	-	4,4,4	0.13	0	6,6,6	0.27	0
2	SO4	B	601	-	4,4,4	0.14	0	6,6,6	0.17	0
3	MRY	B	603	-	7,7,7	0.76	0	8,8,8	1.29	1 (12%)
4	62F	A	603	-	61,70,70	2.35	16 (26%)	72,108,108	2.22	27 (37%)
6	FDA	D	605	-	52,58,58	2.78	22 (42%)	60,89,89	1.77	13 (21%)
2	SO4	C	602	-	4,4,4	0.13	0	6,6,6	0.12	0
4	62F	B	604	-	61,70,70	2.51	20 (32%)	72,108,108	2.14	24 (33%)
2	SO4	D	601	-	4,4,4	0.16	0	6,6,6	0.22	0
3	MRY	A	602	-	7,7,7	0.81	0	8,8,8	1.30	1 (12%)
2	SO4	C	603	-	4,4,4	0.12	0	6,6,6	0.14	0
2	SO4	B	602	-	4,4,4	0.15	0	6,6,6	0.12	0
5	UDP	B	605	-	24,26,26	3.58	15 (62%)	37,40,40	1.51	6 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	603	-	4,4,4	0.15	0	6,6,6	0.10	0
3	MRY	D	604	-	7,7,7	0.69	0	8,8,8	1.30	1 (12%)
5	UDP	A	604	-	24,26,26	3.59	16 (66%)	37,40,40	1.62	9 (24%)
3	MRY	C	605	-	7,7,7	0.65	0	8,8,8	1.40	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MRY	B	603	-	-	1/8/8/8	-
4	62F	A	603	-	-	12/36/76/76	0/6/7/7
6	FDA	D	605	-	-	19/30/50/50	0/6/6/6
4	62F	B	604	-	-	14/36/76/76	0/6/7/7
3	MRY	A	602	-	-	2/8/8/8	-
6	FDA	C	606	-	-	11/30/50/50	0/6/6/6
3	MRY	D	604	-	-	0/8/8/8	-
5	UDP	A	604	-	-	2/16/32/32	0/2/2/2
3	MRY	C	605	-	-	0/8/8/8	-
5	UDP	B	605	-	-	0/16/32/32	0/2/2/2

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	62F	C01-N5	8.92	1.53	1.41
6	C	606	FDA	O4-C4	8.09	1.39	1.23
6	D	605	FDA	O4-C4	8.09	1.39	1.23
4	B	604	62F	C1X-N5	7.50	1.57	1.45
5	A	604	UDP	C2-N1	7.48	1.50	1.38
4	A	603	62F	C01-N5	7.48	1.51	1.41
5	B	605	UDP	C3'-C2'	-7.47	1.32	1.53
5	A	604	UDP	C3'-C2'	-7.42	1.33	1.53
5	B	605	UDP	C2-N1	7.39	1.50	1.38
6	C	606	FDA	O2-C2	7.36	1.38	1.23
6	D	605	FDA	O2-C2	7.28	1.38	1.23
4	A	603	62F	C1X-N5	7.23	1.57	1.45
6	C	606	FDA	C6-C5X	6.41	1.49	1.39
5	B	605	UDP	C2-N3	6.36	1.49	1.38
5	A	604	UDP	C2-N3	6.22	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	UDP	C6-C5	6.13	1.49	1.35
5	B	605	UDP	C6-C5	5.98	1.48	1.35
6	C	606	FDA	C9-C9A	5.92	1.49	1.39
6	D	605	FDA	C9-C9A	5.78	1.49	1.39
6	D	605	FDA	C6-C5X	5.77	1.48	1.39
5	B	605	UDP	O4'-C1'	-4.95	1.30	1.42
5	A	604	UDP	O4'-C1'	-4.87	1.30	1.42
4	A	603	62F	O4B-C1B	4.79	1.47	1.41
4	A	603	62F	C6-C01	4.71	1.47	1.39
4	B	604	62F	O4B-C1B	4.70	1.47	1.41
6	D	605	FDA	C10-N1	4.70	1.45	1.37
4	B	604	62F	C6-C01	4.62	1.47	1.39
6	C	606	FDA	C10-N1	4.55	1.45	1.37
6	C	606	FDA	C4X-N5	4.47	1.45	1.35
5	A	604	UDP	O4'-C4'	4.19	1.54	1.45
6	C	606	FDA	C5X-N5	4.13	1.46	1.39
6	D	605	FDA	C4X-N5	4.12	1.44	1.35
5	B	605	UDP	C4-N3	4.12	1.45	1.38
4	B	604	62F	C9-C9A	4.11	1.46	1.39
4	A	603	62F	O4P-C4P	4.07	1.52	1.43
4	B	604	62F	C9-C8	-4.04	1.33	1.39
6	D	605	FDA	C5X-C9A	-3.99	1.36	1.40
5	B	605	UDP	O4'-C4'	3.98	1.53	1.45
4	A	603	62F	O3P-C3P	3.82	1.52	1.43
5	A	604	UDP	C4-N3	3.77	1.45	1.38
4	B	604	62F	C6-C7	3.75	1.45	1.39
4	A	603	62F	C9-C8	-3.72	1.34	1.39
4	B	604	62F	O3P-C3P	3.71	1.51	1.43
4	B	604	62F	O4P-C4P	3.66	1.51	1.43
6	C	606	FDA	C5X-C9A	-3.63	1.36	1.40
6	D	605	FDA	C2-N1	3.63	1.43	1.37
6	C	606	FDA	C2-N1	3.59	1.43	1.37
4	A	603	62F	C10-N1	3.56	1.38	1.34
6	D	605	FDA	C5X-N5	3.53	1.45	1.39
4	A	603	62F	C9-C9A	3.51	1.45	1.39
4	B	604	62F	C02-N5	3.49	1.48	1.42
6	D	605	FDA	C2B-C1B	-3.48	1.48	1.53
4	B	604	62F	C2X-C1X	3.38	1.57	1.52
5	A	604	UDP	C6-N1	3.32	1.46	1.38
6	D	605	FDA	C2-N3	3.29	1.43	1.37
4	B	604	62F	C4P-C3P	-3.26	1.47	1.53
5	B	605	UDP	C6-N1	3.19	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	62F	C02-N5	3.18	1.48	1.42
6	D	605	FDA	C10-N10	3.17	1.44	1.38
6	C	606	FDA	C2B-C1B	-3.15	1.49	1.53
6	D	605	FDA	C2A-N3A	3.15	1.37	1.32
6	C	606	FDA	C6A-N6A	3.15	1.45	1.34
6	C	606	FDA	C10-N10	3.11	1.44	1.38
4	A	603	62F	C2X-C1X	3.09	1.56	1.52
5	A	604	UDP	C5'-C4'	-3.07	1.42	1.51
5	B	605	UDP	C5'-C4'	-3.07	1.42	1.51
6	C	606	FDA	C9A-N10	3.06	1.46	1.41
6	C	606	FDA	C4X-C4	3.00	1.50	1.42
6	C	606	FDA	C2A-N3A	3.00	1.36	1.32
4	A	603	62F	C4P-C3P	-3.00	1.47	1.53
6	C	606	FDA	C2-N3	2.99	1.42	1.37
4	A	603	62F	C6-C7	2.97	1.43	1.39
5	B	605	UDP	C5-C4	2.96	1.50	1.43
4	B	604	62F	O5X-C5X	2.91	1.51	1.44
6	D	605	FDA	C6A-N6A	2.89	1.44	1.34
4	B	604	62F	C10-N1	2.89	1.37	1.34
5	A	604	UDP	C5-C4	2.86	1.50	1.43
4	A	603	62F	C1P-N10	-2.76	1.42	1.46
6	D	605	FDA	PA-O5B	-2.75	1.48	1.59
5	A	604	UDP	O4-C4	-2.71	1.19	1.24
4	A	603	62F	O5X-C5X	2.61	1.50	1.44
6	C	606	FDA	PA-O5B	-2.60	1.48	1.59
5	B	605	UDP	O3'-C3'	2.55	1.49	1.43
5	A	604	UDP	O3'-C3'	2.55	1.49	1.43
5	B	605	UDP	C2'-C1'	2.55	1.61	1.53
6	D	605	FDA	O2'-C2'	-2.52	1.38	1.43
6	D	605	FDA	C4X-C4	2.51	1.48	1.42
4	B	604	62F	O5X-C1X	2.50	1.46	1.42
5	A	604	UDP	C2'-C1'	2.48	1.61	1.53
5	B	605	UDP	O4-C4	-2.45	1.19	1.24
4	B	604	62F	C1P-N10	-2.43	1.43	1.46
5	A	604	UDP	O2-C2	-2.40	1.18	1.23
6	C	606	FDA	O4'-C4'	-2.38	1.38	1.43
5	B	605	UDP	O2-C2	-2.36	1.18	1.23
4	B	604	62F	C9A-C01	2.35	1.44	1.40
6	D	605	FDA	C9A-N10	2.35	1.45	1.41
5	A	604	UDP	PA-O5'	2.33	1.68	1.59
4	B	604	62F	P-O5P	2.33	1.68	1.59
6	C	606	FDA	O2'-C2'	-2.32	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	UDP	PA-O5'	2.31	1.68	1.59
4	B	604	62F	C8-C7	2.25	1.46	1.40
6	D	605	FDA	P-O1P	2.22	1.58	1.50
6	C	606	FDA	O3B-C3B	-2.22	1.37	1.43
6	D	605	FDA	O3B-C3B	-2.22	1.37	1.43
4	A	603	62F	C8-C7	2.21	1.46	1.40
6	C	606	FDA	P-O1P	2.16	1.58	1.50
6	D	605	FDA	PA-O2A	-2.13	1.45	1.55
6	C	606	FDA	PA-O2A	-2.13	1.45	1.55
6	D	605	FDA	O4'-C4'	-2.12	1.38	1.43
4	B	604	62F	C1P-C2P	2.11	1.55	1.52
6	C	606	FDA	C2B-C3B	-2.08	1.47	1.53
5	A	604	UDP	O2'-C2'	2.06	1.47	1.43

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	62F	C01-C9A-N10	6.83	124.87	118.80
4	B	604	62F	O3P-C3P-C4P	-6.53	93.05	108.81
6	D	605	FDA	N3A-C2A-N1A	-6.00	119.30	128.68
4	A	603	62F	O3P-C3P-C4P	-5.68	95.09	108.81
4	B	604	62F	C01-C9A-N10	5.55	123.73	118.80
6	C	606	FDA	N3A-C2A-N1A	-5.41	120.22	128.68
4	A	603	62F	C5X-O5X-C1X	4.71	121.09	112.45
4	B	604	62F	C3X-C2X-C1X	4.68	115.85	108.98
5	B	605	UDP	C4-N3-C2	-4.59	120.53	126.58
5	A	604	UDP	C4-N3-C2	-4.51	120.64	126.58
4	A	603	62F	C3X-C2X-C1X	4.27	115.26	108.98
4	A	603	62F	N3A-C2A-N1A	-4.18	122.15	128.68
4	A	603	62F	C2X-C1X-N5	4.15	118.13	112.88
4	B	604	62F	N3A-C2A-N1A	-3.95	122.50	128.68
4	A	603	62F	C2X-C3X-C4X	3.71	117.30	110.82
4	B	604	62F	C2A-N1A-C6A	3.71	125.10	118.75
4	B	604	62F	C5X-O5X-C1X	3.70	119.25	112.45
4	A	603	62F	C9-C9A-C01	-3.69	114.49	120.11
4	A	603	62F	C2A-N1A-C6A	3.56	124.84	118.75
5	A	604	UDP	C5-C4-N3	3.55	120.15	114.84
4	B	604	62F	C2X-C1X-N5	3.49	117.30	112.88
5	A	604	UDP	N3-C2-N1	3.47	119.49	114.89
4	B	604	62F	C2X-C3X-C4X	3.47	116.87	110.82
6	D	605	FDA	C5'-C4'-C3'	-3.44	105.57	112.20
6	D	605	FDA	C4-N3-C2	-3.43	121.40	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	605	FDA	C1B-N9A-C4A	-3.42	120.64	126.64
6	D	605	FDA	O4-C4-C4X	-3.37	119.52	127.24
5	B	605	UDP	N3-C2-N1	3.37	119.36	114.89
4	A	603	62F	O5X-C5X-C4X	3.29	115.66	109.69
5	B	605	UDP	C5-C4-N3	3.27	119.74	114.84
4	B	604	62F	C5A-C6A-N1A	-3.26	112.97	120.35
6	C	606	FDA	C4-N3-C2	-3.16	121.79	126.34
4	A	603	62F	C6-C01-C9A	3.15	124.90	120.11
4	A	603	62F	O4B-C1B-C2B	-3.10	102.40	106.93
6	D	605	FDA	N3-C2-N1	3.04	120.69	115.80
4	B	604	62F	C8M-C8-C9	2.96	124.96	119.49
3	D	604	MRY	CAA-CAC-CAE	-2.94	106.73	113.11
4	A	603	62F	C8M-C8-C9	2.91	124.87	119.49
4	A	603	62F	C5A-C6A-N1A	-2.90	113.77	120.35
4	A	603	62F	C2B-C3B-C4B	2.85	108.17	102.64
4	B	604	62F	C02-N5-C01	-2.83	112.35	119.22
4	B	604	62F	O4B-C1B-C2B	-2.81	102.82	106.93
4	B	604	62F	C2B-C3B-C4B	2.80	108.08	102.64
6	D	605	FDA	C9-C9A-N10	-2.78	118.07	121.84
4	A	603	62F	C8M-C8-C7	-2.77	115.06	120.74
4	B	604	62F	PA-O7-P	2.76	142.30	132.83
4	B	604	62F	C5A-C6A-N6A	2.74	124.52	120.35
3	A	602	MRY	CAA-CAC-CAE	-2.73	107.18	113.11
6	D	605	FDA	O2P-P-O5'	-2.72	95.12	107.75
4	A	603	62F	O3X-C3X-C4X	-2.70	104.10	110.35
5	B	605	UDP	O4-C4-C5	-2.70	120.41	125.16
6	D	605	FDA	O2A-PA-O5B	-2.63	95.55	107.75
6	D	605	FDA	O5'-P-O1P	2.61	119.27	109.07
3	C	605	MRY	CAA-CAC-CAE	-2.61	107.45	113.11
4	A	603	62F	C9A-C9-C8	2.60	124.53	119.30
6	C	606	FDA	N3-C2-N1	2.59	119.97	115.80
4	A	603	62F	N6A-C6A-N1A	2.55	123.87	118.57
6	C	606	FDA	O2A-PA-O5B	-2.54	95.97	107.75
5	A	604	UDP	O4-C4-C5	-2.52	120.72	125.16
4	B	604	62F	C8M-C8-C7	-2.51	115.59	120.74
6	C	606	FDA	O5B-PA-O1A	2.47	118.70	109.07
6	C	606	FDA	O4-C4-C4X	-2.44	121.65	127.24
4	A	603	62F	O6-P-O1P	2.42	124.19	112.24
5	B	605	UDP	C3'-C2'-C1'	2.40	105.99	101.43
4	B	604	62F	O4P-C4P-C3P	-2.40	103.27	109.10
6	D	605	FDA	O5B-PA-O1A	2.39	118.41	109.07
4	A	603	62F	C4P-C3P-C2P	2.38	118.32	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	UDP	O4'-C4'-C3'	-2.38	100.40	105.11
6	C	606	FDA	C5X-N5-C4X	-2.37	115.41	121.02
4	B	604	62F	O3X-C3X-C4X	-2.37	104.87	110.35
3	C	605	MRY	OAH-CAG-CAE	-2.36	105.93	111.07
6	D	605	FDA	O3'-C3'-C2'	2.36	114.51	108.81
4	A	603	62F	C02-N5-C01	-2.33	113.57	119.22
4	A	603	62F	C01-C6-C7	-2.30	114.67	119.30
4	A	603	62F	C2-N3-C4	2.29	120.37	115.49
4	B	604	62F	O6-P-O1P	2.27	123.46	112.24
5	B	605	UDP	O4'-C4'-C3'	-2.27	100.63	105.11
6	C	606	FDA	O2P-P-O5'	-2.27	97.22	107.75
4	B	604	62F	C9-C9A-C01	-2.26	116.66	120.11
4	B	604	62F	C9A-C9-C8	2.21	123.75	119.30
5	A	604	UDP	O2B-PB-O3A	2.20	112.03	104.64
6	C	606	FDA	O3'-C3'-C2'	2.20	114.14	108.81
6	C	606	FDA	C1B-N9A-C4A	-2.19	122.79	126.64
5	A	604	UDP	C2'-C3'-C4'	2.19	106.89	102.64
5	A	604	UDP	C3'-C2'-C1'	2.17	105.55	101.43
3	B	603	MRY	CAA-CAC-CAE	-2.15	108.44	113.11
4	B	604	62F	O3P-C3P-C2P	2.13	113.95	108.81
4	A	603	62F	O5P-C5P-C4P	-2.11	103.73	109.36
6	D	605	FDA	C5X-N5-C4X	-2.10	116.06	121.02
4	A	603	62F	PA-O7-P	2.08	139.98	132.83
4	B	604	62F	C01-C6-C7	-2.08	115.12	119.30
6	C	606	FDA	C2A-N1A-C6A	2.07	122.30	118.75
5	A	604	UDP	C4'-O4'-C1'	-2.06	104.93	109.47
4	B	604	62F	C2-N3-C4	2.05	119.85	115.49
4	A	603	62F	O4X-C4X-C3X	2.01	114.99	110.35
6	C	606	FDA	C4X-C4-N3	2.00	118.27	112.31

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	62F	C2X-C1X-N5-C02
4	A	603	62F	C1P-C2P-C3P-O3P
4	A	603	62F	O3P-C3P-C4P-C5P
4	A	603	62F	C3P-C4P-C5P-O5P
4	A	603	62F	O4P-C4P-C5P-O5P
4	B	604	62F	C2X-C1X-N5-C02
4	B	604	62F	C1P-C2P-C3P-O3P
4	B	604	62F	O2P-C2P-C3P-O3P

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Mol	Chain	Res	Type	Atoms
4	B	604	62F	C3P-C4P-C5P-O5P
4	B	604	62F	O4P-C4P-C5P-O5P
4	B	604	62F	C5P-O5P-P-O7
6	C	606	FDA	C1'-C2'-C3'-O3'
6	C	606	FDA	C1'-C2'-C3'-C4'
6	C	606	FDA	O2'-C2'-C3'-O3'
6	C	606	FDA	O2'-C2'-C3'-C4'
6	C	606	FDA	C5'-O5'-P-O1P
6	C	606	FDA	C5'-O5'-P-O2P
6	C	606	FDA	C5'-O5'-P-O3P
6	D	605	FDA	C5B-O5B-PA-O1A
6	D	605	FDA	P-O3P-PA-O5B
6	D	605	FDA	C1'-C2'-C3'-O3'
6	D	605	FDA	C1'-C2'-C3'-C4'
6	D	605	FDA	O2'-C2'-C3'-O3'
6	D	605	FDA	O2'-C2'-C3'-C4'
6	D	605	FDA	C3'-C4'-C5'-O5'
6	D	605	FDA	O4'-C4'-C5'-O5'
6	D	605	FDA	C5'-O5'-P-O3P
4	A	603	62F	O3P-C3P-C4P-O4P
4	A	603	62F	C2P-C3P-C4P-O4P
4	A	603	62F	C4X-C5X-C6X-O6X
4	A	603	62F	O2P-C2P-C3P-O3P
4	B	604	62F	O3P-C3P-C4P-C5P
4	A	603	62F	C2P-C3P-C4P-C5P
4	B	604	62F	O2P-C2P-C3P-C4P
4	A	603	62F	O5X-C5X-C6X-O6X
4	B	604	62F	C2P-C3P-C4P-C5P
4	B	604	62F	C2P-C3P-C4P-O4P
5	A	604	UDP	PA-O3A-PB-O1B
6	C	606	FDA	C2'-C3'-C4'-O4'
6	D	605	FDA	O4B-C4B-C5B-O5B
6	C	606	FDA	C2'-C3'-C4'-C5'
4	B	604	62F	O3P-C3P-C4P-O4P
6	D	605	FDA	C2'-C3'-C4'-O4'
6	D	605	FDA	C2'-C3'-C4'-C5'
5	A	604	UDP	PA-O3A-PB-O2B
6	D	605	FDA	C2'-C1'-N10-C10
6	D	605	FDA	P-O3P-PA-O1A
4	B	604	62F	C5P-O5P-P-O1P
6	D	605	FDA	C5B-O5B-PA-O2A
6	D	605	FDA	C5'-O5'-P-O1P

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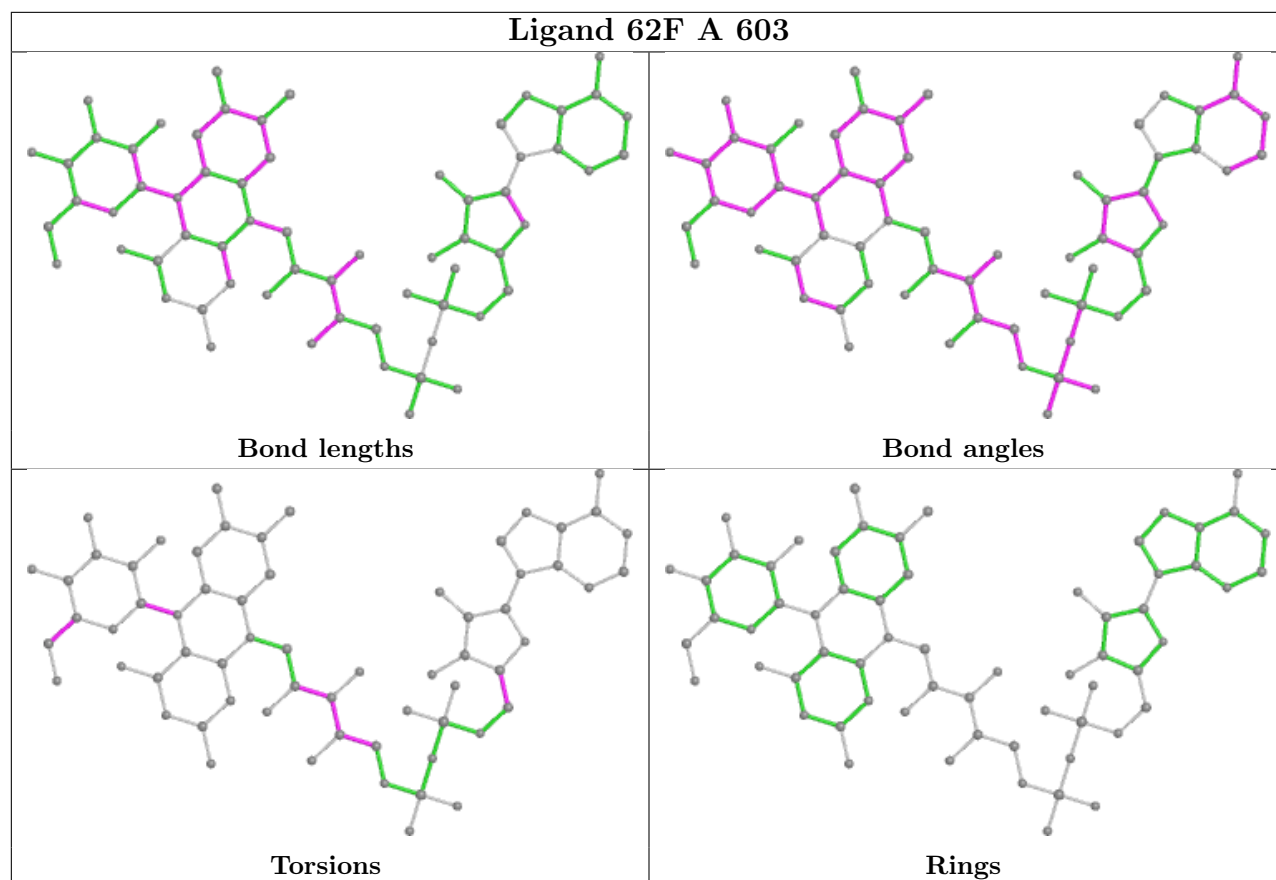
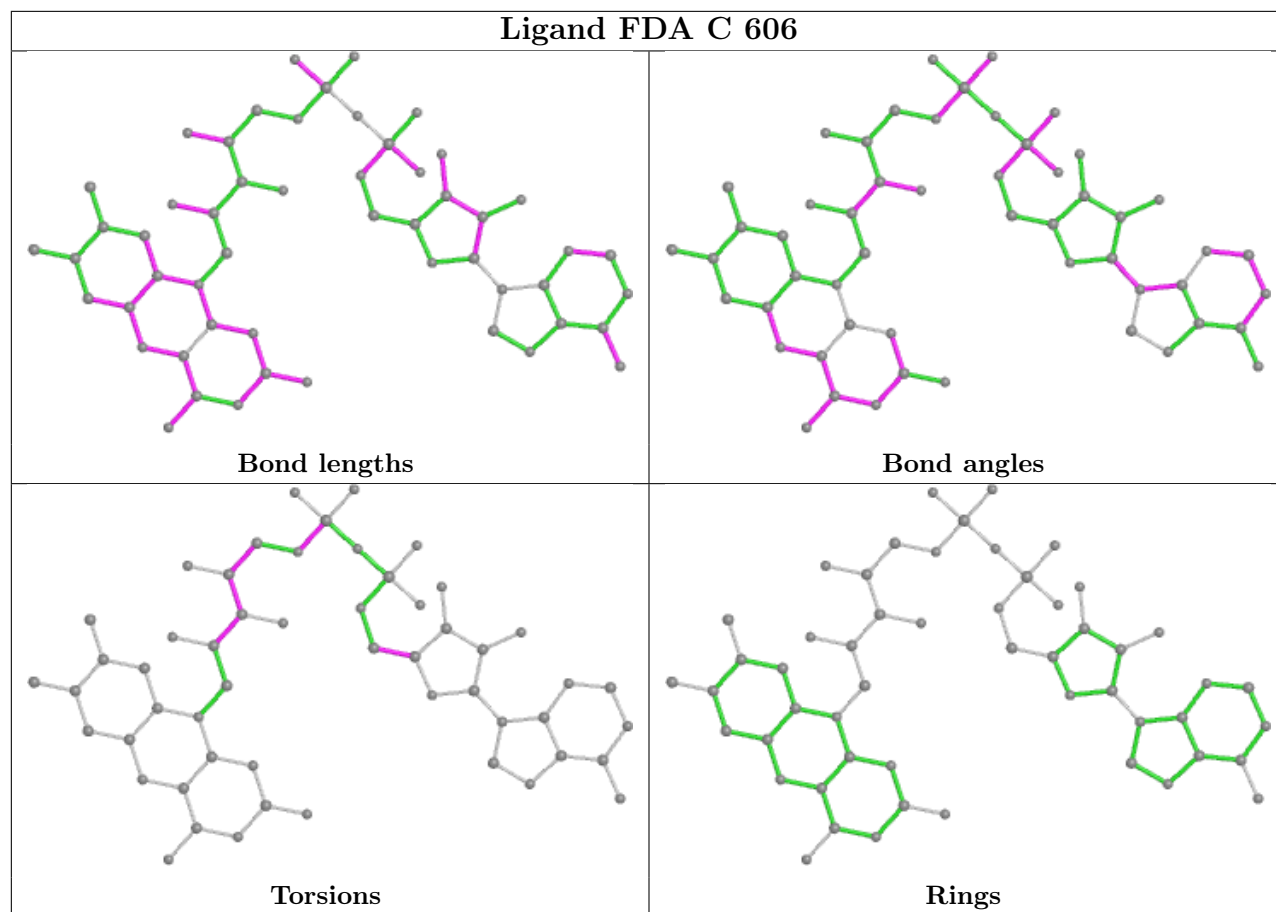
Mol	Chain	Res	Type	Atoms
6	D	605	FDA	C5'-O5'-P-O2P
3	A	602	MRY	OAF-CAE-CAG-OAH
6	C	606	FDA	C3'-C4'-C5'-O5'
4	A	603	62F	O4B-C4B-C5B-O5B
6	D	605	FDA	C3B-C4B-C5B-O5B
4	B	604	62F	O4B-C4B-C5B-O5B
3	A	602	MRY	OAD-CAC-CAE-OAF
3	B	603	MRY	OAD-CAC-CAE-OAF
6	D	605	FDA	C5B-O5B-PA-O3P
6	C	606	FDA	O4B-C4B-C5B-O5B
4	B	604	62F	C5P-O5P-P-O6

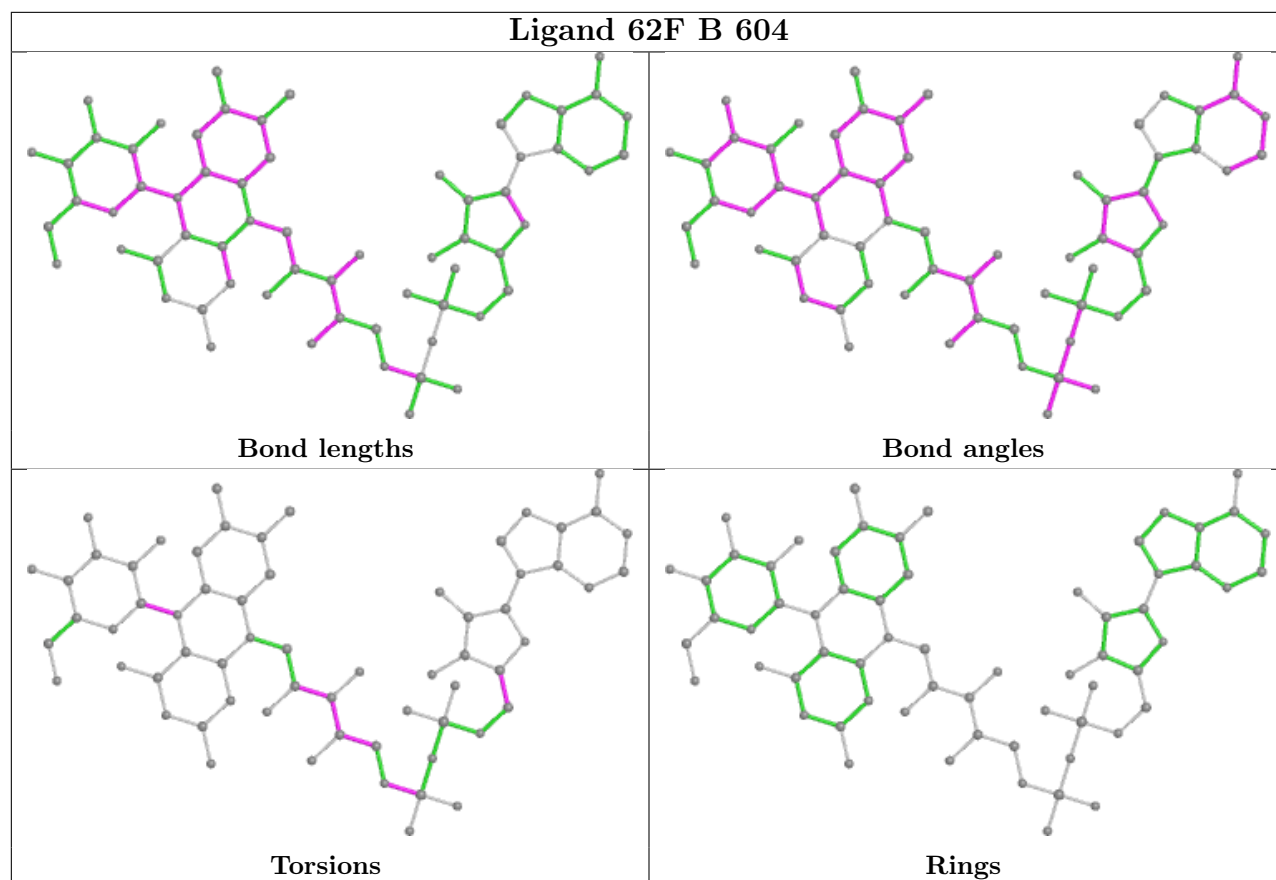
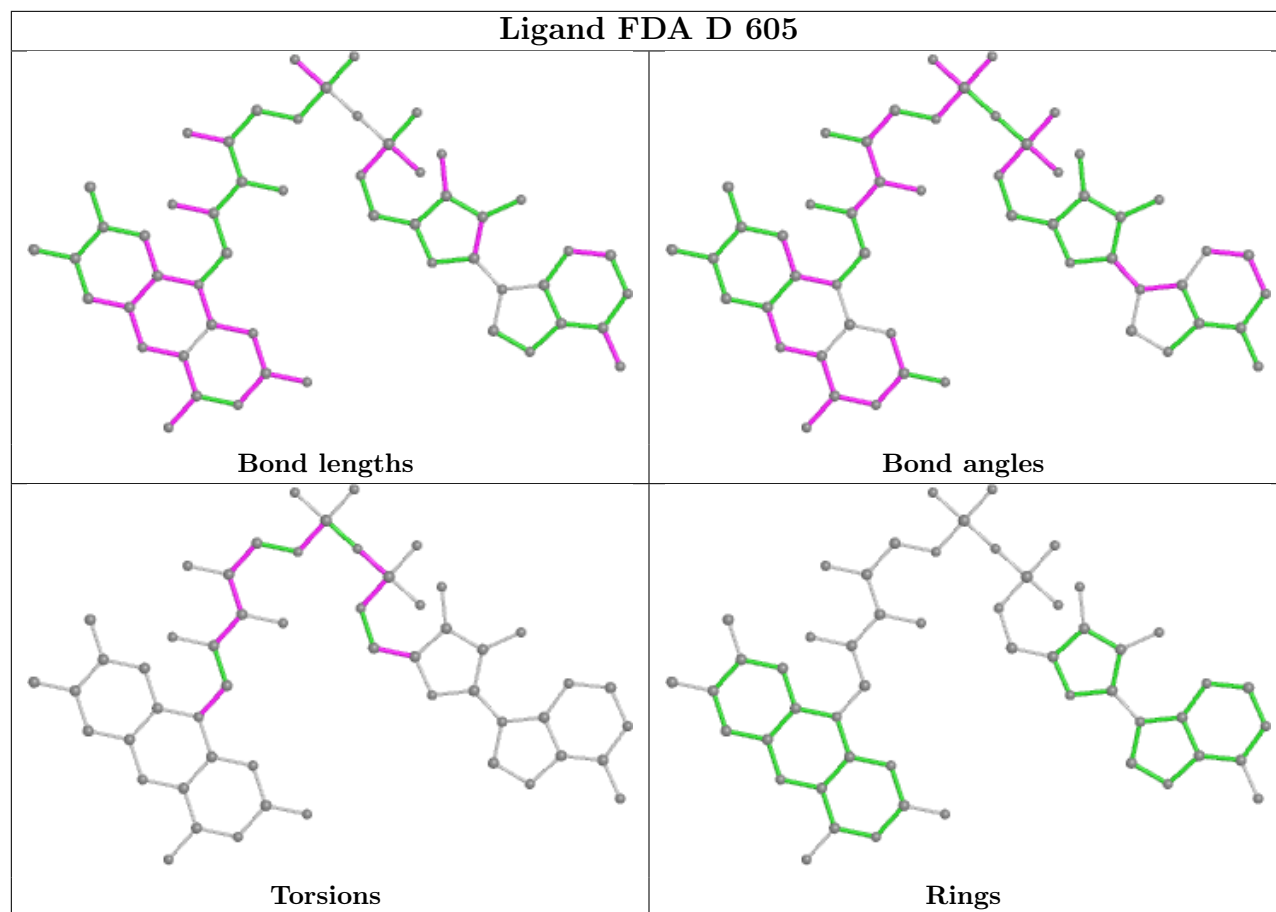
There are no ring outliers.

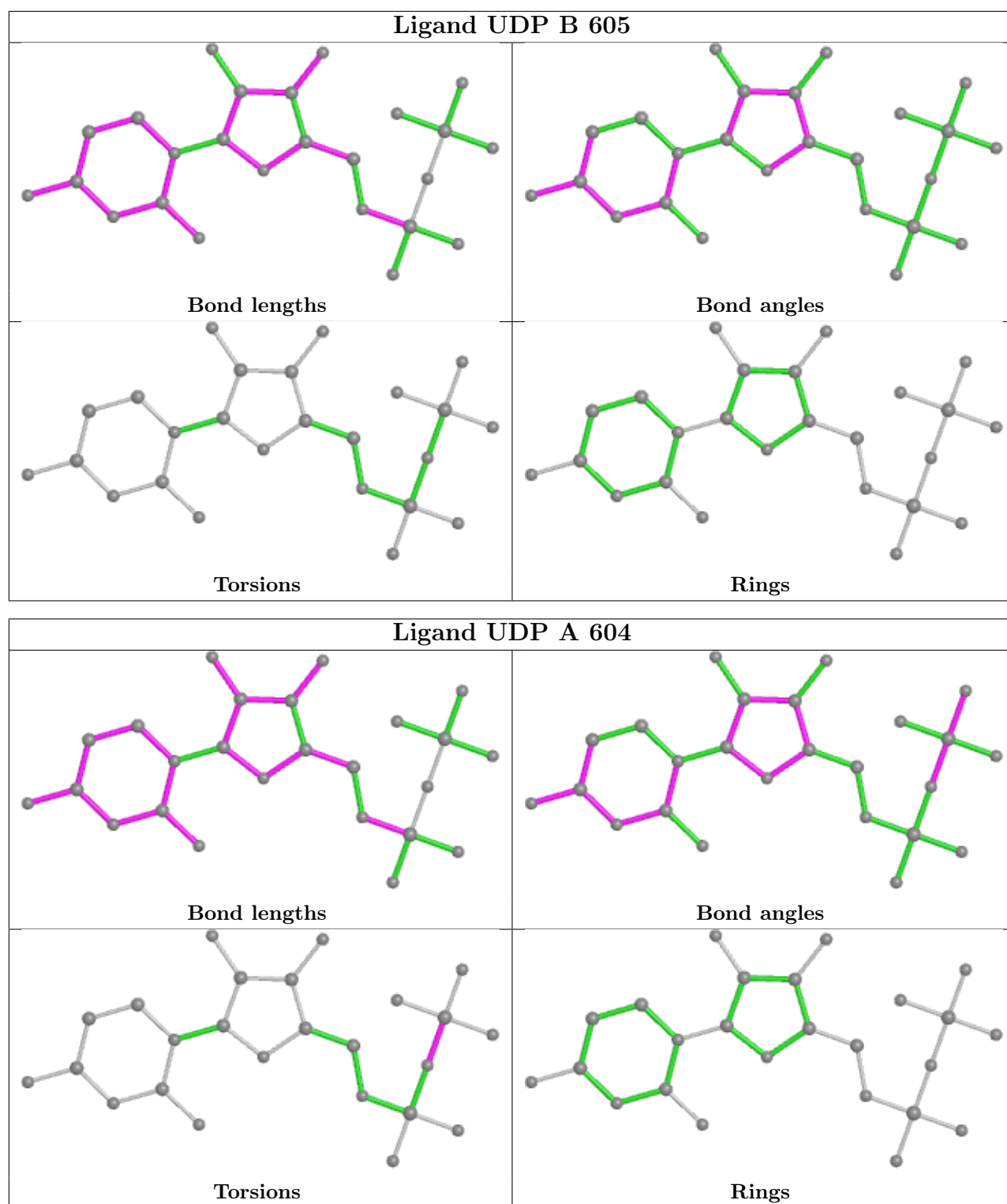
5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	606	FDA	3	0
4	A	603	62F	3	0
6	D	605	FDA	6	0
4	B	604	62F	3	0
5	A	604	UDP	4	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	505/513 (98%)	-0.33	2 (0%) 92 95	25, 38, 60, 99	0
1	B	505/513 (98%)	-0.38	6 (1%) 79 83	24, 34, 57, 99	0
1	C	502/513 (97%)	-0.46	1 (0%) 95 96	23, 39, 61, 81	0
1	D	503/513 (98%)	-0.48	2 (0%) 92 95	21, 38, 61, 91	0
All	All	2015/2052 (98%)	-0.41	11 (0%) 91 94	21, 37, 61, 99	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	TRP	3.2
1	A	62	GLY	2.9
1	B	61	GLY	2.7
1	B	185	ALA	2.6
1	D	63	ALA	2.4
1	C	60	VAL	2.3
1	B	183	VAL	2.2
1	D	507	SER	2.1
1	B	201	ALA	2.1
1	A	203	ASN	2.0
1	B	62	GLY	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

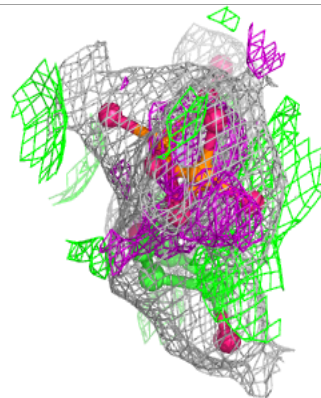
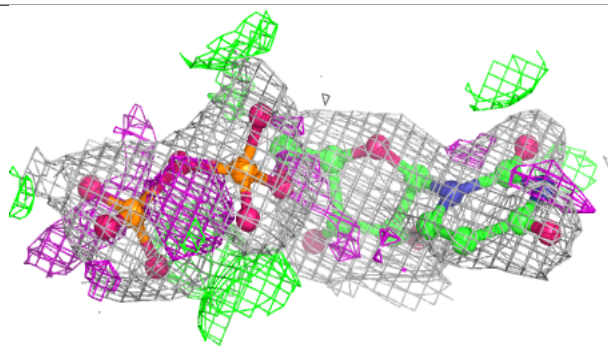
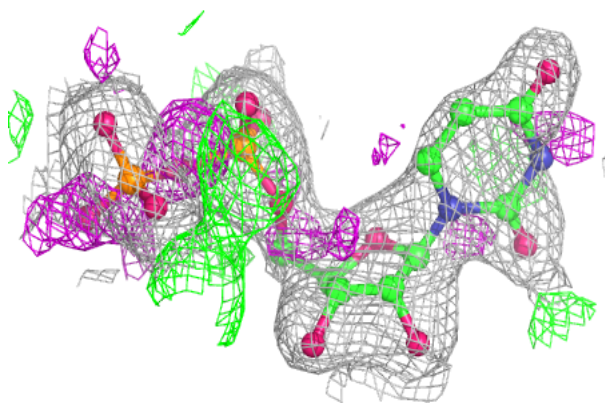
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	C	602	5/5	0.80	0.29	120,123,125,127	0
2	SO4	D	603	5/5	0.84	0.23	110,114,116,117	0
2	SO4	C	603	5/5	0.85	0.14	100,100,103,104	0
2	SO4	B	602	5/5	0.91	0.12	100,101,102,102	0
2	SO4	C	604	5/5	0.92	0.18	92,95,99,99	0
3	MRY	A	602	8/8	0.93	0.17	49,58,59,59	0
2	SO4	A	601	5/5	0.94	0.17	81,82,88,89	0
2	SO4	D	602	5/5	0.94	0.18	80,84,86,91	0
5	UDP	B	605	25/25	0.94	0.18	38,57,65,73	0
6	FDA	D	605	53/53	0.94	0.14	36,53,63,74	0
3	MRY	D	604	8/8	0.95	0.10	40,47,51,55	0
2	SO4	C	601	5/5	0.95	0.15	73,73,75,81	0
3	MRY	C	605	8/8	0.95	0.08	34,46,48,54	0
5	UDP	A	604	25/25	0.96	0.16	41,48,59,65	0
4	62F	A	603	64/64	0.96	0.13	30,43,62,68	0
6	FDA	C	606	53/53	0.96	0.12	33,45,59,64	0
4	62F	B	604	64/64	0.96	0.13	28,39,72,78	0
2	SO4	D	601	5/5	0.97	0.12	75,77,80,81	0
3	MRY	B	603	8/8	0.97	0.14	31,44,50,50	0
2	SO4	B	601	5/5	0.98	0.12	58,65,71,71	0

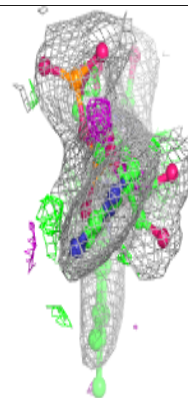
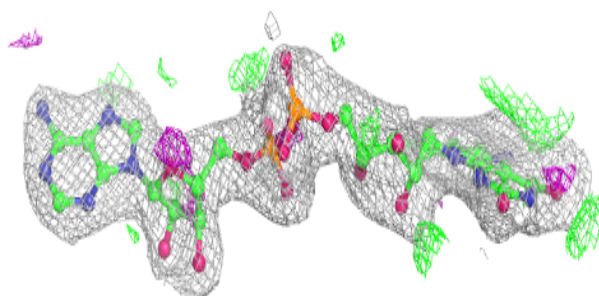
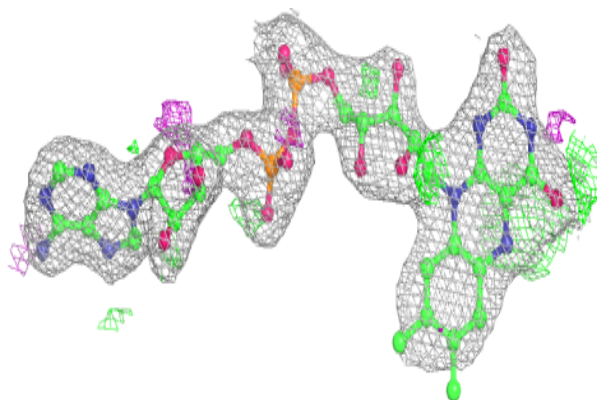
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP B 605:

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

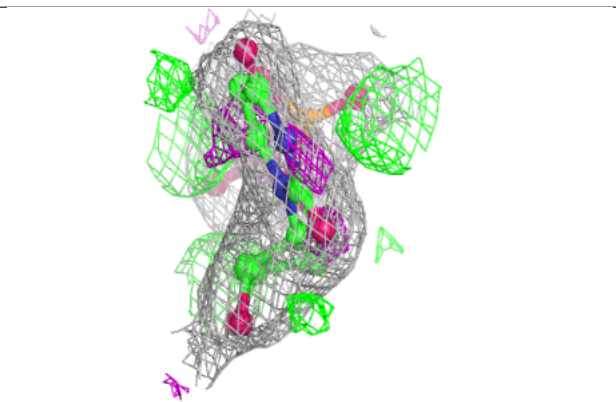
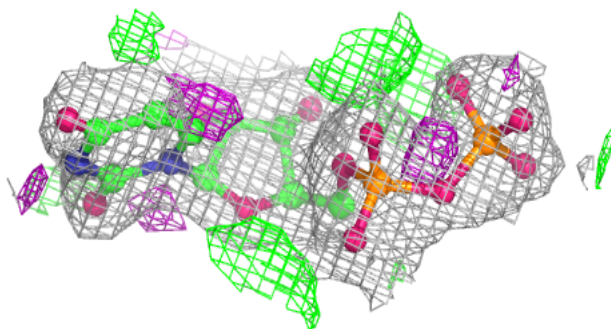
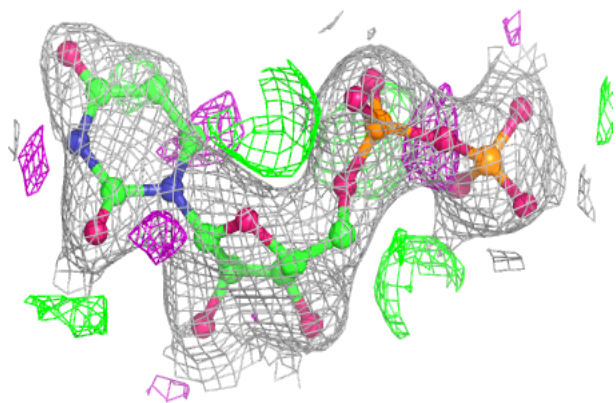
**Electron density around FDA D 605:**

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

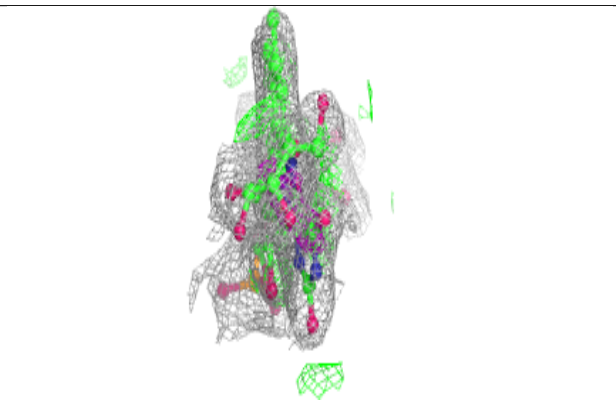
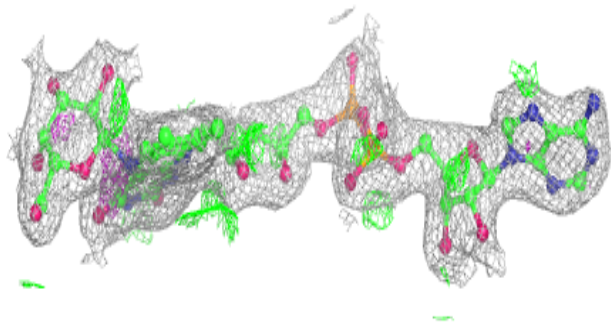
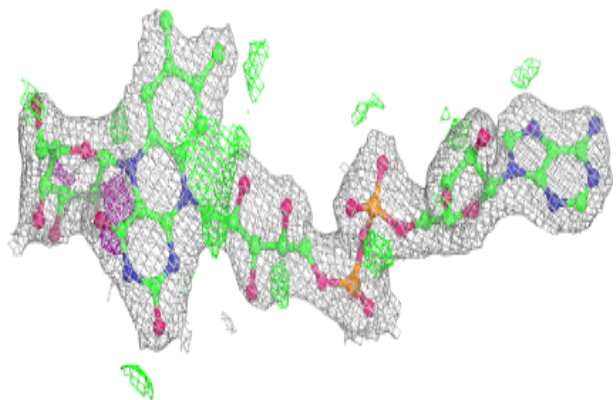


Electron density around UDP A 604:

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

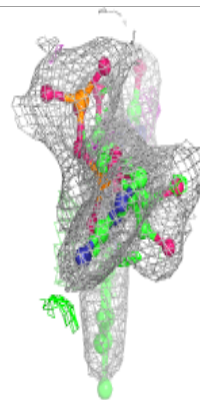
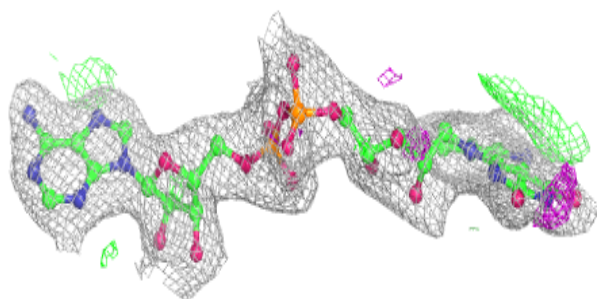
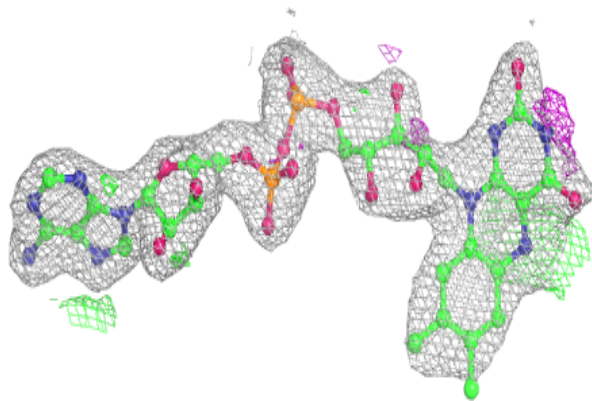
**Electron density around 62F A 603:**

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

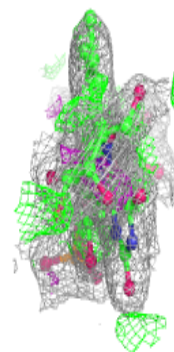
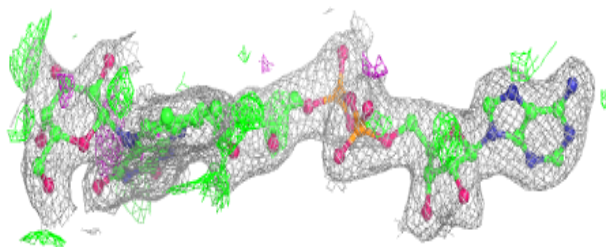
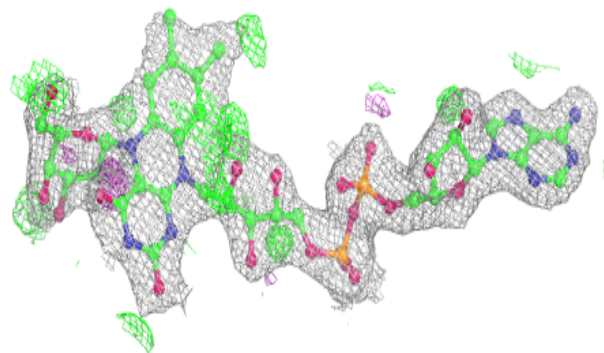


Electron density around FDA C 606:

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

**Electron density around 62F B 604:**

$2mF_o-DF_c$ (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.