



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:28 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

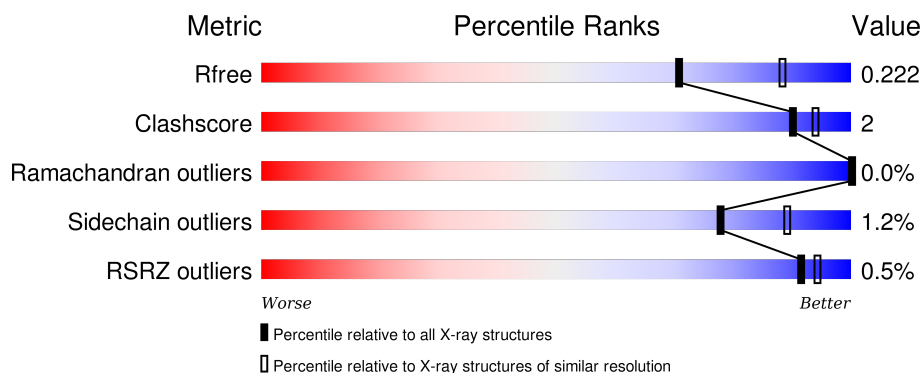
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>91%</div> <div>7% •</div> </div>
1	B	513	<div> <div>%</div> <div>91%</div> <div>7% •</div> </div>
1	C	513	<div> <div>94%</div> <div>• •</div> </div>
1	D	513	<div> <div>93%</div> <div>5% •</div> </div>

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
3	MRY	A	602	-	-	-	X

## 2 Entry composition

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

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: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



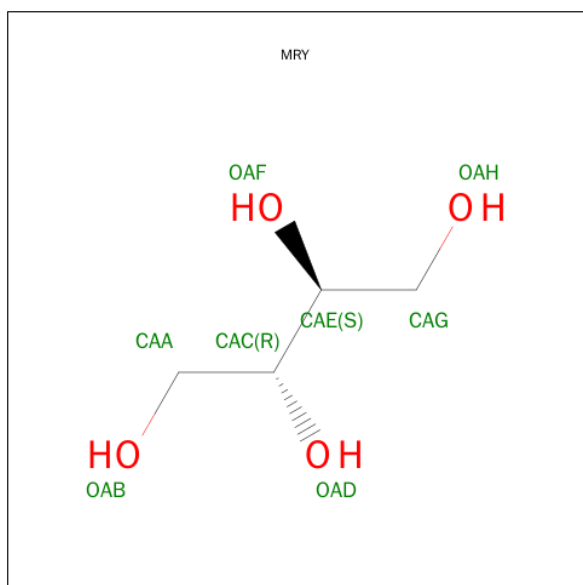
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

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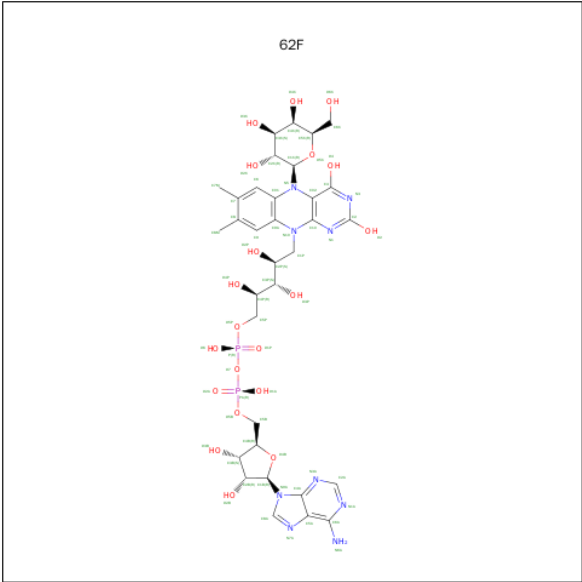
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MESO-ERYTHRITOL (three-letter code: MRY) (formula:  $C_4H_{10}O_4$ ).



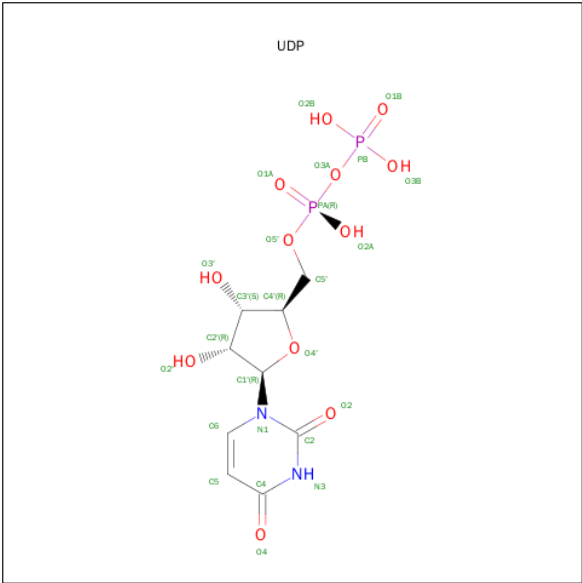
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	4	4		
3	B	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		

- 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:  $C_{33}H_{45}N_9O_{20}P_2$ ).



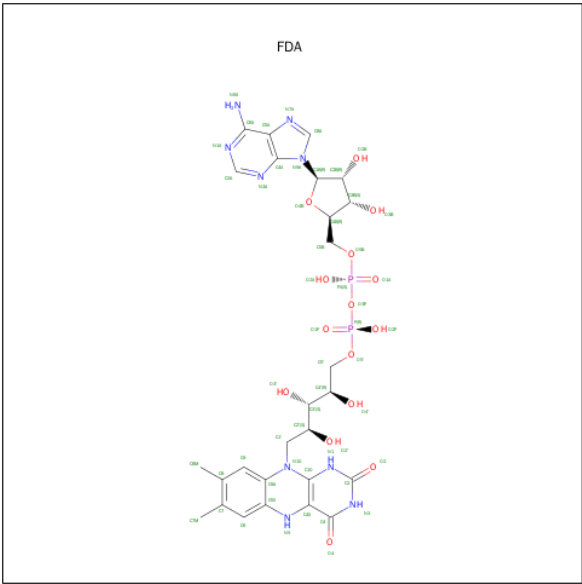
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			64	33	9	20	2		
4	B	1	Total	C	N	O	P	0	0
			64	33	9	20	2		

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>2</sub>O<sub>12</sub>P<sub>2</sub>).



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

- Molecule 6 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: C<sub>27</sub>H<sub>35</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

- Molecule 7 is water.

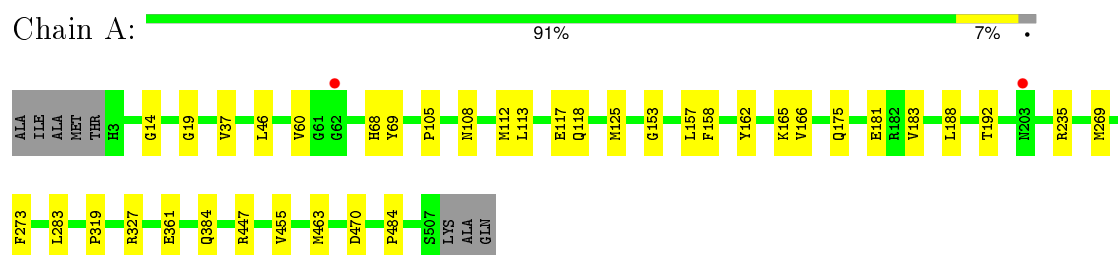
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	172	Total	O	0	0
			172	172		
7	B	202	Total	O	0	0
			202	202		
7	C	177	Total	O	0	0
			177	177		
7	D	189	Total	O	0	0
			189	189		



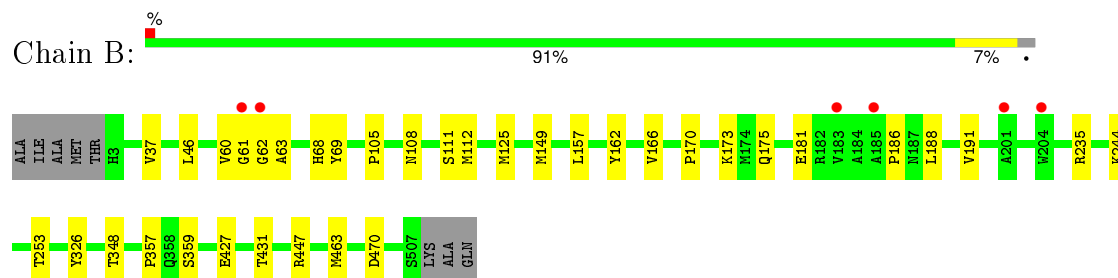
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

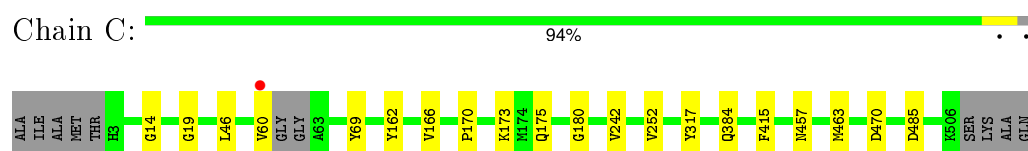
#### • Molecule 1: UDP-galactopyranose mutase



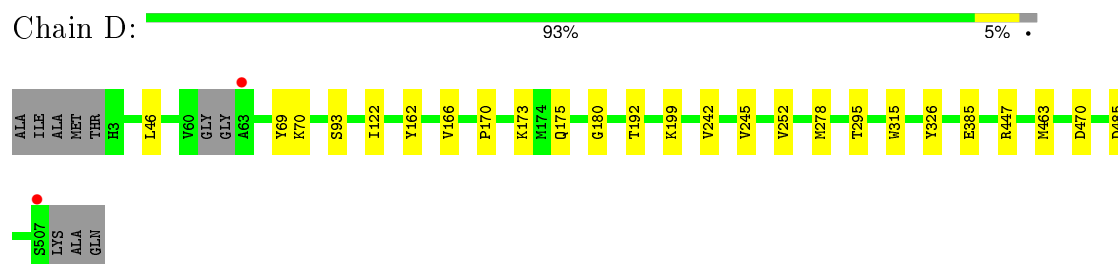
#### • Molecule 1: UDP-galactopyranose mutase



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.184 , 0.213 0.193 , 0.222	Depositor DCC
$R_{free}$ test set	3849 reflections (2.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 195942 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage'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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: FDA, SO4, UDP, MRY, 62F

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:O2'	6:D:605:FDA:O4'	2.18	0.60
4:B:604:62F:O2P	4:B:604:62F:O4P	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
6:D:605:FDA:HN1	6:D:605:FDA:H2'	1.75	0.51
1:D:69:TYR:CG	1:D:463:MET:HG3	2.45	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:O4'	6:C:606:FDA:O2'	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:327:ARG:NH2	5:A:604:UDP:O3B	2.38	0.49
1:A:69:TYR:CG	1:A:463:MET:HG3	2.47	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:C:180:GLY:HA2	1:C:485:ASP:OD1	2.13	0.48
1:B:427:GLU:O	1:B:431:THR:HG23	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:D:295:THR:HG21	6:D:605:FDA:C7M	2.45	0.46
1:B:149:MET:O	1:B:186:PRO:HD2	2.15	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:153:GLY:O	1:A:157:LEU:HB2	2.18	0.44
1:A:105:PRO:HG2	1:A:108:ASN:HB2	2.00	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
6:D:605:FDA:H1'1	6:D:605:FDA:H9	1.79	0.42
1:A:162:TYR:HB2	1:A:319:PRO:HB3	2.01	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:HB2	1:D:199:LYS:HE3	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%)	52	64
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 ⓘ

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%)	72	85
1	B	405/431 (94%)	399 (98%)	6 (2%)	72	85
1	C	400/431 (93%)	397 (99%)	3 (1%)	86	94
1	D	402/431 (93%)	398 (99%)	4 (1%)	82	91
All	All	1611/1724 (93%)	1592 (99%)	19 (1%)	78	89

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

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	601	-	4,4,4	0.11	0	6,6,6	0.24	0
3	MRY	A	602	-	7,7,7	0.77	0	6,8,8	0.89	0
4	62F	A	603	-	59,70,70	2.16	13 (22%)	69,108,108	2.87	22 (31%)
5	UDP	A	604	-	20,26,26	4.18	13 (65%)	24,40,40	1.88	4 (16%)
2	SO4	B	601	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	B	602	-	4,4,4	0.20	0	6,6,6	0.12	0
3	MRY	B	603	-	7,7,7	0.72	0	6,8,8	0.91	0
4	62F	B	604	-	59,70,70	2.31	15 (25%)	69,108,108	2.72	23 (33%)
5	UDP	B	605	-	20,26,26	4.19	11 (55%)	24,40,40	1.75	3 (12%)
2	SO4	C	601	-	4,4,4	0.15	0	6,6,6	0.32	0
2	SO4	C	602	-	4,4,4	0.22	0	6,6,6	0.10	0
2	SO4	C	603	-	4,4,4	0.20	0	6,6,6	0.18	0
2	SO4	C	604	-	4,4,4	0.22	0	6,6,6	0.18	0
3	MRY	C	605	-	7,7,7	0.61	0	6,8,8	1.07	1 (16%)
6	FDA	C	606	-	52,58,58	2.83	22 (42%)	52,89,89	2.47	12 (23%)
2	SO4	D	601	-	4,4,4	0.18	0	6,6,6	0.16	0



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	0.16	0
2	SO4	D	603	-	4,4,4	0.21	0	6,6,6	0.09	0
3	MRY	D	604	-	7,7,7	0.65	0	6,8,8	0.73	0
6	FDA	D	605	-	52,58,58	2.75	22 (42%)	52,89,89	2.65	13 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	601	-	-	0/0/0/0	0/0/0/0
3	MRY	A	602	-	-	0/8/8/8	0/0/0/0
4	62F	A	603	-	-	0/32/76/76	0/7/7/7
5	UDP	A	604	-	-	0/12/32/32	0/2/2/2
2	SO4	B	601	-	-	0/0/0/0	0/0/0/0
2	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	MRY	B	603	-	-	0/8/8/8	0/0/0/0
4	62F	B	604	-	-	0/32/76/76	0/7/7/7
5	UDP	B	605	-	-	0/12/32/32	0/2/2/2
2	SO4	C	601	-	-	0/0/0/0	0/0/0/0
2	SO4	C	602	-	-	0/0/0/0	0/0/0/0
2	SO4	C	603	-	-	0/0/0/0	0/0/0/0
2	SO4	C	604	-	-	0/0/0/0	0/0/0/0
3	MRY	C	605	-	-	0/8/8/8	0/0/0/0
6	FDA	C	606	-	-	0/30/50/50	0/6/6/6
2	SO4	D	601	-	-	0/0/0/0	0/0/0/0
2	SO4	D	602	-	-	0/0/0/0	0/0/0/0
2	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	MRY	D	604	-	-	0/8/8/8	0/0/0/0
6	FDA	D	605	-	-	0/30/50/50	0/6/6/6

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	UDP	O4'-C1'	-7.68	1.30	1.41
5	B	605	UDP	C3'-C2'	-7.61	1.32	1.53
5	A	604	UDP	C3'-C2'	-7.55	1.33	1.53
5	A	604	UDP	O4'-C1'	-7.55	1.30	1.41
4	A	603	62F	C1P-N10	-5.30	1.42	1.48
4	B	604	62F	C1P-N10	-4.87	1.43	1.48
6	D	605	FDA	C2B-C1B	-3.25	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	62F	C4P-C3P	-3.11	1.47	1.53
6	D	605	FDA	C9A-C5X	-3.08	1.36	1.42
5	A	604	UDP	C5'-C4'	-2.97	1.42	1.51
5	B	605	UDP	C5'-C4'	-2.96	1.42	1.51
6	C	606	FDA	C2B-C1B	-2.93	1.49	1.53
6	C	606	FDA	C9A-C5X	-2.88	1.36	1.42
4	A	603	62F	C4P-C3P	-2.86	1.47	1.53
6	D	605	FDA	PA-O5B	-2.58	1.48	1.59
6	C	606	FDA	PA-O5B	-2.44	1.48	1.59
6	D	605	FDA	O2'-C2'	-2.40	1.38	1.43
6	D	605	FDA	PA-O2A	-2.30	1.45	1.55
6	C	606	FDA	PA-O2A	-2.29	1.45	1.55
6	C	606	FDA	O4'-C4'	-2.27	1.38	1.43
6	C	606	FDA	O2'-C2'	-2.21	1.38	1.43
6	C	606	FDA	O3B-C3B	-2.21	1.37	1.43
6	D	605	FDA	O3B-C3B	-2.21	1.37	1.43
6	C	606	FDA	C2B-C3B	-2.14	1.47	1.53
5	A	604	UDP	O4-C4	-2.11	1.19	1.24
6	D	605	FDA	O4'-C4'	-2.02	1.38	1.43
4	A	603	62F	C7-C8	2.02	1.46	1.41
6	D	605	FDA	P-O1P	2.06	1.58	1.51
4	B	604	62F	C7-C8	2.06	1.46	1.41
5	A	604	UDP	O2'-C2'	2.07	1.47	1.43
4	A	603	62F	C9-C9A	2.10	1.45	1.40
6	C	606	FDA	C2-N3	2.14	1.42	1.38
4	A	603	62F	C6-C7	2.22	1.43	1.37
5	B	605	UDP	PA-O5'	2.23	1.68	1.59
4	B	604	62F	P-O5P	2.24	1.68	1.59
5	A	604	UDP	PA-O5'	2.25	1.68	1.59
6	D	605	FDA	C2-N3	2.39	1.43	1.38
4	A	603	62F	O5X-C5X	2.52	1.50	1.44
4	B	604	62F	C9-C9A	2.54	1.46	1.40
4	B	604	62F	O2-C2	2.56	1.34	1.24
6	D	605	FDA	C6A-N6A	2.56	1.44	1.34
5	A	604	UDP	O3'-C3'	2.56	1.49	1.43
5	B	605	UDP	O3'-C3'	2.56	1.49	1.43
4	A	603	62F	O2-C2	2.62	1.34	1.24
4	B	604	62F	C6-C7	2.62	1.45	1.37
6	C	606	FDA	C2-N1	2.63	1.43	1.38
6	D	605	FDA	C2-N1	2.67	1.43	1.38
4	B	604	62F	O5X-C1X	2.69	1.46	1.42
6	C	606	FDA	C2A-N3A	2.70	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	62F	C2-N3	2.78	1.41	1.37
6	C	606	FDA	C6A-N6A	2.78	1.45	1.34
4	B	604	62F	O5X-C5X	2.82	1.51	1.44
6	D	605	FDA	C2A-N3A	2.83	1.37	1.32
4	B	604	62F	C2-N3	2.92	1.42	1.37
4	B	604	62F	C6-C01	2.92	1.47	1.40
4	A	603	62F	C6-C01	2.99	1.47	1.40
4	B	604	62F	O4P-C4P	3.46	1.51	1.43
6	D	605	FDA	C4-C4X	3.70	1.48	1.41
4	B	604	62F	O3P-C3P	3.71	1.51	1.43
6	D	605	FDA	C9-C9A	3.79	1.49	1.40
4	A	603	62F	O3P-C3P	3.83	1.52	1.43
4	A	603	62F	O4P-C4P	3.85	1.52	1.43
5	B	605	UDP	O4'-C4'	3.87	1.53	1.45
6	C	606	FDA	C9-C9A	3.90	1.49	1.40
5	A	604	UDP	O4'-C4'	4.08	1.54	1.45
6	C	606	FDA	C10-N10	4.18	1.44	1.39
6	D	605	FDA	C10-N10	4.28	1.44	1.39
6	C	606	FDA	C4-C4X	4.32	1.50	1.41
6	D	605	FDA	C6-C5X	4.42	1.48	1.41
4	B	604	62F	O4B-C1B	4.48	1.47	1.41
6	D	605	FDA	C9A-N10	4.55	1.45	1.38
4	A	603	62F	O4B-C1B	4.56	1.47	1.41
6	C	606	FDA	C4-N3	4.56	1.41	1.33
6	D	605	FDA	C4-N3	4.71	1.41	1.33
5	A	604	UDP	C2'-C1'	4.89	1.61	1.53
5	B	605	UDP	C6-C5	4.98	1.48	1.38
5	B	605	UDP	C2'-C1'	5.03	1.61	1.53
6	C	606	FDA	C6-C5X	5.07	1.49	1.41
5	A	604	UDP	C6-C5	5.15	1.49	1.38
5	A	604	UDP	C2-N3	5.23	1.49	1.38
5	B	605	UDP	C2-N3	5.35	1.49	1.38
6	C	606	FDA	C9A-N10	5.44	1.46	1.38
6	D	605	FDA	O4-C4	5.68	1.39	1.24
6	C	606	FDA	O4-C4	5.68	1.39	1.24
6	C	606	FDA	C10-N1	5.78	1.45	1.35
6	D	605	FDA	C10-N1	5.94	1.45	1.35
6	D	605	FDA	C5X-N5	6.72	1.45	1.35
5	A	604	UDP	C4-N3	6.80	1.45	1.33
5	B	605	UDP	C4-N3	7.15	1.45	1.33
6	D	605	FDA	C4X-N5	7.35	1.44	1.33
6	C	606	FDA	C5X-N5	7.38	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	UDP	C6-N1	7.69	1.45	1.35
6	C	606	FDA	C4X-N5	7.84	1.45	1.33
5	A	604	UDP	C6-N1	7.93	1.46	1.35
4	A	603	62F	C01-N5	9.59	1.51	1.40
4	B	604	62F	C01-N5	11.26	1.53	1.40

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	605	FDA	N3A-C2A-N1A	-12.18	119.30	128.87
6	C	606	FDA	N3A-C2A-N1A	-11.02	120.22	128.87
4	B	604	62F	C02-N5-C01	-9.06	112.35	121.72
4	A	603	62F	N3A-C2A-N1A	-8.55	122.15	128.87
4	B	604	62F	N3A-C2A-N1A	-8.11	122.50	128.87
4	A	603	62F	C02-N5-C01	-7.88	113.57	121.72
4	B	604	62F	O3P-C3P-C4P	-6.05	93.05	108.73
4	A	603	62F	C4B-O4B-C1B	-6.00	103.29	109.64
6	D	605	FDA	C1B-N9A-C4A	-5.53	120.64	126.81
4	B	604	62F	C4B-O4B-C1B	-5.38	103.94	109.64
4	A	603	62F	O3P-C3P-C4P	-5.26	95.09	108.73
4	A	603	62F	O5X-C1X-N5	-4.91	99.29	107.07
6	C	606	FDA	N3-C2-N1	-4.59	119.97	127.69
4	A	603	62F	C9-C9A-C01	-4.57	114.49	119.05
5	A	604	UDP	C4'-O4'-C1'	-4.44	104.93	109.64
6	D	605	FDA	C4X-C4-N3	-4.42	117.74	123.52
6	D	605	FDA	N3-C2-N1	-4.16	120.69	127.69
5	B	605	UDP	C4'-O4'-C1'	-4.03	105.37	109.64
6	C	606	FDA	C4X-C4-N3	-4.02	118.27	123.52
6	C	606	FDA	C1B-N9A-C4A	-3.60	122.79	126.81
4	B	604	62F	O5X-C1X-N5	-3.49	101.53	107.07
6	C	606	FDA	O2P-P-O3P	-3.38	90.78	105.27
6	D	605	FDA	O2A-PA-O3P	-3.34	90.97	105.27
4	A	603	62F	O3X-C3X-C4X	-2.78	104.10	110.36
6	D	605	FDA	O2P-P-O5'	-2.75	95.12	108.24
6	D	605	FDA	O2A-PA-O5B	-2.66	95.55	108.24
4	A	603	62F	C8M-C8-C7	-2.64	115.06	120.73
6	C	606	FDA	O2A-PA-O5B	-2.57	95.97	108.24
4	B	604	62F	O3X-C3X-C4X	-2.43	104.87	110.36
4	B	604	62F	C9-C9A-C01	-2.39	116.66	119.05
4	B	604	62F	C8M-C8-C7	-2.39	115.59	120.73
5	A	604	UDP	O4'-C4'-C3'	-2.35	100.40	105.16
3	C	605	MRY	OAH-CAG-CAE	-2.32	105.93	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	606	FDA	O2P-P-O5'	-2.31	97.22	108.24
5	B	605	UDP	O4'-C4'-C3'	-2.24	100.63	105.16
4	B	604	62F	O4P-C4P-C3P	-2.21	103.27	108.96
4	B	604	62F	O4X-C4X-C3X	2.01	114.90	110.36
4	B	604	62F	O3P-C3P-C2P	2.01	113.95	108.73
4	A	603	62F	O4X-C4X-C3X	2.05	114.99	110.36
5	A	604	UDP	C2'-C3'-C4'	2.08	106.89	102.64
6	C	606	FDA	O3'-C3'-C2'	2.09	114.14	108.73
4	B	604	62F	O6-P-O1P	2.09	123.46	112.56
6	D	605	FDA	O3'-C3'-C2'	2.23	114.51	108.73
4	A	603	62F	O6-P-O1P	2.23	124.19	112.56
6	D	605	FDA	O5B-PA-O1A	2.25	118.41	109.21
6	C	606	FDA	O5B-PA-O1A	2.32	118.70	109.21
6	D	605	FDA	O4B-C1B-N9A	2.37	112.58	108.11
4	B	604	62F	N6A-C6A-N1A	2.38	122.51	118.52
4	B	604	62F	C2-N3-C4	2.43	119.85	115.41
6	D	605	FDA	O5'-P-O1P	2.46	119.27	109.21
4	B	604	62F	C01-C9A-N10	2.64	123.73	120.03
4	B	604	62F	C2B-C3B-C4B	2.66	108.08	102.64
4	A	603	62F	C2B-C3B-C4B	2.71	108.17	102.64
4	A	603	62F	C2-N3-C4	2.71	120.37	115.41
6	C	606	FDA	O4B-C1B-N9A	2.90	113.58	108.11
4	A	603	62F	O5X-C5X-C4X	3.14	115.66	109.67
4	A	603	62F	N6A-C6A-N1A	3.19	123.87	118.52
4	B	604	62F	C4X-C3X-C2X	3.31	116.87	110.79
4	A	603	62F	C2A-N1A-C6A	3.41	124.84	118.77
4	A	603	62F	C01-C9A-N10	3.46	124.87	120.03
6	C	606	FDA	C5X-C9A-N10	3.50	120.20	117.58
4	A	603	62F	C4X-C3X-C2X	3.54	117.30	110.79
4	B	604	62F	C2A-N1A-C6A	3.55	125.10	118.77
4	B	604	62F	C6-C01-C9A	3.57	122.61	119.05
6	D	605	FDA	C5X-C9A-N10	3.59	120.27	117.58
4	A	603	62F	C3X-C2X-C1X	3.70	115.26	109.18
4	B	604	62F	C3X-C2X-C1X	4.06	115.85	109.18
4	B	604	62F	C10-C02-N5	5.72	124.77	120.54
4	A	603	62F	C6-C01-C9A	5.86	124.90	119.05
5	B	605	UDP	C4-N3-C2	6.00	120.53	114.21
5	A	604	UDP	C4-N3-C2	6.10	120.64	114.21
4	A	603	62F	O4-C4-C02	6.39	131.28	119.88
4	B	604	62F	C5X-O5X-C1X	6.44	119.25	108.62
4	A	603	62F	C10-C02-N5	6.48	125.33	120.54
4	B	604	62F	O4-C4-C02	7.01	132.38	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	D	605	FDA	C4-N3-C2	7.48	121.40	115.16
4	A	603	62F	C5X-O5X-C1X	7.56	121.09	108.62
6	C	606	FDA	C4-N3-C2	7.95	121.79	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

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

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	505/513 (98%)	-0.33	2 (0%) 93 95	25, 38, 60, 99	0
1	B	505/513 (98%)	-0.38	6 (1%) 81 85	24, 34, 57, 99	0
1	C	502/513 (97%)	-0.46	1 (0%) 95 97	23, 39, 61, 81	0
1	D	503/513 (98%)	-0.48	2 (0%) 93 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	2.3
1	D	507	SER	2.1
1	A	203	ASN	2.1
1	B	201	ALA	2.1
1	B	62	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MRY	A	602	8/8	0.93	0.17	3.14	49,58,59,59	0
5	UDP	A	604	25/25	0.96	0.16	1.47	41,48,59,65	0
5	UDP	B	605	25/25	0.94	0.18	1.09	38,57,65,73	0
6	FDA	D	605	53/53	0.94	0.14	0.51	36,53,63,74	0
3	MRY	B	603	8/8	0.97	0.14	0.28	31,44,50,50	0
4	62F	B	604	64/64	0.96	0.13	0.12	28,39,72,78	0
6	FDA	C	606	53/53	0.96	0.12	0.11	33,45,59,64	0
4	62F	A	603	64/64	0.96	0.13	0.07	30,43,62,68	0
3	MRY	D	604	8/8	0.95	0.10	-1.44	40,47,51,55	0
3	MRY	C	605	8/8	0.95	0.08	-3.72	34,46,48,54	0
2	SO4	C	602	5/5	0.80	0.29	-	120,123,125,127	0
2	SO4	B	601	5/5	0.98	0.12	-	58,65,71,71	0
2	SO4	C	603	5/5	0.85	0.14	-	100,100,103,104	0
2	SO4	A	601	5/5	0.94	0.17	-	81,82,88,89	0
2	SO4	D	603	5/5	0.84	0.23	-	110,114,116,117	0
2	SO4	C	601	5/5	0.95	0.15	-	73,73,75,81	0
2	SO4	D	602	5/5	0.94	0.18	-	80,84,86,91	0
2	SO4	D	601	5/5	0.97	0.12	-	75,77,80,81	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

## 6.5 Other polymers [i](#)

There are no such residues in this entry.