



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2019 – 08:29 PM EDT

PDB ID : 6K5G  
Title : Structural and catalytic analysis of two diverse uridine phosphorylases in the oomycete *Phytophthora capsici*  
Authors : Yang, C.C.; Zhang, X.G.  
Deposited on : 2019-05-28  
Resolution : 1.57 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

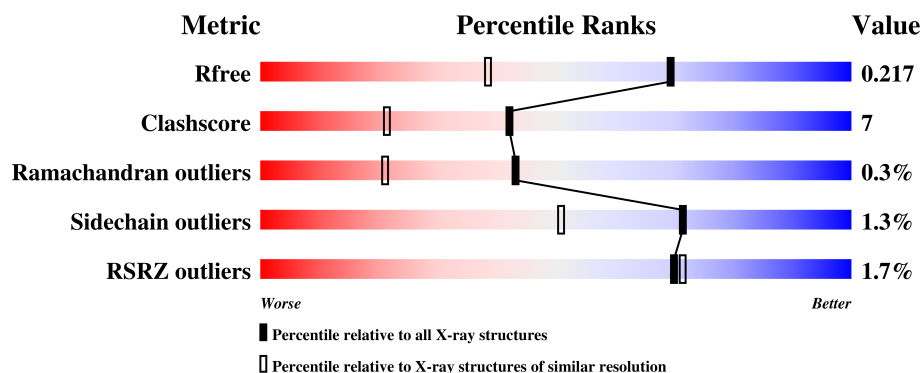
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.57 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))
$R_{free}$	111664	4679 (1.60-1.56)
Clashscore	122126	4976 (1.60-1.56)
Ramachandran outliers	120053	4851 (1.60-1.56)
Sidechain outliers	120020	4848 (1.60-1.56)
RSRZ outliers	108989	4581 (1.60-1.56)

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	309	 85% 12% •
1	B	309	 80% 13% • 6%
1	C	309	 83% 10% 7%
1	D	309	 85% 10% • •

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10178 atoms, of which 48 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2259	1407	395	444	13			
1	B	289	Total	C	N	O	S	0	0	0
			2160	1347	377	424	12			
1	C	288	Total	C	N	O	S	0	0	0
			2155	1344	376	423	12			
1	D	300	Total	C	N	O	S	0	0	0
			2240	1396	391	440	13			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP A0A410UCT3
A	0	GLY	-	expression tag	UNP A0A410UCT3
A	297	ALA	-	expression tag	UNP A0A410UCT3
A	298	ALA	-	expression tag	UNP A0A410UCT3
A	299	ALA	-	expression tag	UNP A0A410UCT3
A	300	LEU	-	expression tag	UNP A0A410UCT3
A	301	GLU	-	expression tag	UNP A0A410UCT3
A	302	HIS	-	expression tag	UNP A0A410UCT3
A	303	HIS	-	expression tag	UNP A0A410UCT3
A	304	HIS	-	expression tag	UNP A0A410UCT3
A	305	HIS	-	expression tag	UNP A0A410UCT3
A	306	HIS	-	expression tag	UNP A0A410UCT3
A	307	HIS	-	expression tag	UNP A0A410UCT3
B	-1	MET	-	expression tag	UNP A0A410UCT3
B	0	GLY	-	expression tag	UNP A0A410UCT3
B	297	ALA	-	expression tag	UNP A0A410UCT3
B	298	ALA	-	expression tag	UNP A0A410UCT3
B	299	ALA	-	expression tag	UNP A0A410UCT3
B	300	LEU	-	expression tag	UNP A0A410UCT3
B	301	GLU	-	expression tag	UNP A0A410UCT3
B	302	HIS	-	expression tag	UNP A0A410UCT3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	expression tag	UNP A0A410UCT3
B	304	HIS	-	expression tag	UNP A0A410UCT3
B	305	HIS	-	expression tag	UNP A0A410UCT3
B	306	HIS	-	expression tag	UNP A0A410UCT3
B	307	HIS	-	expression tag	UNP A0A410UCT3
C	-1	MET	-	expression tag	UNP A0A410UCT3
C	0	GLY	-	expression tag	UNP A0A410UCT3
C	297	ALA	-	expression tag	UNP A0A410UCT3
C	298	ALA	-	expression tag	UNP A0A410UCT3
C	299	ALA	-	expression tag	UNP A0A410UCT3
C	300	LEU	-	expression tag	UNP A0A410UCT3
C	301	GLU	-	expression tag	UNP A0A410UCT3
C	302	HIS	-	expression tag	UNP A0A410UCT3
C	303	HIS	-	expression tag	UNP A0A410UCT3
C	304	HIS	-	expression tag	UNP A0A410UCT3
C	305	HIS	-	expression tag	UNP A0A410UCT3
C	306	HIS	-	expression tag	UNP A0A410UCT3
C	307	HIS	-	expression tag	UNP A0A410UCT3
D	-1	MET	-	expression tag	UNP A0A410UCT3
D	0	GLY	-	expression tag	UNP A0A410UCT3
D	297	ALA	-	expression tag	UNP A0A410UCT3
D	298	ALA	-	expression tag	UNP A0A410UCT3
D	299	ALA	-	expression tag	UNP A0A410UCT3
D	300	LEU	-	expression tag	UNP A0A410UCT3
D	301	GLU	-	expression tag	UNP A0A410UCT3
D	302	HIS	-	expression tag	UNP A0A410UCT3
D	303	HIS	-	expression tag	UNP A0A410UCT3
D	304	HIS	-	expression tag	UNP A0A410UCT3
D	305	HIS	-	expression tag	UNP A0A410UCT3
D	306	HIS	-	expression tag	UNP A0A410UCT3
D	307	HIS	-	expression tag	UNP A0A410UCT3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

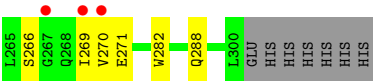
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	349	Total	O	0	0
			349	349		
3	B	297	Total	O	0	0
			297	297		
3	C	302	Total	O	0	0
			302	302		
3	D	332	Total	O	0	0
			332	332		



- Molecule 1: Uridine phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.25Å 153.06Å 67.28Å 90.00° 115.75° 90.00°	Depositor
Resolution (Å)	47.51 – 1.57 47.51 – 1.57	Depositor EDS
% Data completeness (in resolution range)	85.3 (47.51-1.57) 85.3 (47.51-1.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 1.58Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.186 , 0.217 0.186 , 0.217	Depositor DCC
$R_{free}$ test set	7284 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 29.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.408 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.38	0/2295	0.57	0/3117
1	B	0.35	0/2194	0.58	1/2979 (0.0%)
1	C	0.36	0/2189	0.56	0/2972
1	D	0.37	0/2275	0.57	1/3090 (0.0%)
All	All	0.36	0/8953	0.57	2/12158 (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	D	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	GLU	C-N-CA	-7.16	107.27	122.30
1	D	49	GLU	C-N-CA	-6.72	108.18	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	185	ASP	Peptide
1	D	50	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2259	0	2245	35	0
1	B	2160	0	2153	40	0
1	C	2155	0	2148	28	0
1	D	2240	0	2232	35	0
2	A	12	16	16	0	0
2	B	6	8	8	0	0
2	C	6	8	8	0	0
2	D	12	16	16	0	0
3	A	349	0	0	10	4
3	B	297	0	0	17	4
3	C	302	0	0	13	2
3	D	332	0	0	17	2
All	All	10130	48	8826	132	6

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 7.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLN:NE2	3:A:501:HOH:O	1.88	1.05
1:A:288:GLN:NE2	3:A:502:HOH:O	1.88	1.04
1:D:120:VAL:HG22	1:D:259:LEU:HD23	1.40	0.99
1:A:14:ASP:HB3	1:A:16:THR:HG23	1.44	0.99
1:B:288:GLN:HG2	3:B:710:HOH:O	1.70	0.91
1:B:97:ASN:OD1	3:B:501:HOH:O	1.88	0.91
1:C:97:ASN:OD1	3:C:501:HOH:O	1.87	0.91
1:D:120:VAL:HG21	1:D:282:TRP:CD1	2.07	0.88
1:A:120:VAL:HG11	1:A:282:TRP:CD1	2.09	0.88
1:D:192:PHE:HB3	3:D:517:HOH:O	1.73	0.88
1:D:120:VAL:HG22	1:D:259:LEU:CD2	2.05	0.86
1:A:13:SER:OG	3:A:503:HOH:O	1.94	0.84
1:A:101:THR:HG23	1:A:159:LEU:HD11	1.58	0.84
1:A:120:VAL:HG12	1:A:259:LEU:CD2	2.09	0.82
1:D:261:VAL:O	3:D:501:HOH:O	1.98	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:GLU:HB2	3:D:505:HOH:O	1.79	0.81
1:D:23:ARG:NH2	3:D:507:HOH:O	2.13	0.81
1:A:113:GLU:H	1:A:113:GLU:CD	1.85	0.80
1:C:101:THR:HG23	1:C:159:LEU:HD11	1.68	0.76
1:C:23:ARG:HD2	3:C:721:HOH:O	1.84	0.76
1:A:288:GLN:OE1	3:A:504:HOH:O	2.04	0.76
1:D:264:ARG:HG2	3:D:510:HOH:O	1.85	0.75
1:B:288:GLN:HG2	3:B:514:HOH:O	1.87	0.75
1:B:222:GLU:OE1	3:B:502:HOH:O	2.05	0.74
1:C:160:SER:O	1:C:164:VAL:HG23	1.87	0.74
1:D:270:VAL:HG12	3:D:501:HOH:O	1.89	0.73
1:A:49:GLU:OE1	3:A:505:HOH:O	2.06	0.72
1:B:190:ARG:HG2	3:B:535:HOH:O	1.87	0.72
1:D:271:GLU:OE2	3:D:503:HOH:O	2.06	0.72
1:B:193:ASP:OD2	3:B:503:HOH:O	2.06	0.72
1:D:270:VAL:N	3:D:501:HOH:O	2.09	0.71
1:B:289:THR:O	1:B:293:THR:HG23	1.92	0.70
1:A:14:ASP:CB	1:A:16:THR:HG23	2.22	0.69
1:B:151:ARG:NH2	3:B:508:HOH:O	2.26	0.69
1:B:50:GLY:HA3	1:D:26:GLN:NE2	2.08	0.68
1:D:142:SER:O	3:D:505:HOH:O	2.10	0.67
1:B:69:LYS:NZ	3:B:506:HOH:O	2.24	0.67
1:D:271:GLU:OE1	3:D:506:HOH:O	2.12	0.67
1:B:49:GLU:HB2	1:B:51:HIS:HD2	1.59	0.66
1:B:284:GLY:O	1:B:288:GLN:HG3	1.96	0.66
1:A:73:VAL:HG21	1:A:291:VAL:CG1	2.26	0.66
1:C:49:GLU:OE1	3:C:502:HOH:O	2.14	0.66
1:A:120:VAL:HG12	1:A:259:LEU:HD22	1.80	0.64
1:B:170:LYS:HD3	1:B:285:VAL:HG22	1.79	0.64
1:D:184:SER:O	1:D:186:CYS:N	2.32	0.63
1:C:14:ASP:OD2	3:C:503:HOH:O	2.15	0.63
1:D:264:ARG:N	3:D:510:HOH:O	2.31	0.63
1:B:174:LEU:HB2	1:B:281:PHE:CE2	2.35	0.62
1:C:247:ARG:NH1	3:C:506:HOH:O	2.31	0.62
1:D:12:HIS:HB2	1:D:14:ASP:HB3	1.82	0.61
1:B:9:MET:N	3:B:511:HOH:O	2.32	0.61
1:A:120:VAL:HG12	1:A:259:LEU:HD23	1.81	0.61
1:C:97:ASN:ND2	3:C:507:HOH:O	2.34	0.60
1:A:101:THR:HG23	1:A:159:LEU:CD1	2.30	0.60
1:C:273:GLU:CD	1:C:273:GLU:H	2.05	0.59
1:A:13:SER:N	3:A:503:HOH:O	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:VAL:HG21	1:D:282:TRP:NE1	2.17	0.58
1:A:6:THR:HB	1:B:269:ILE:HD11	1.85	0.58
1:A:14:ASP:N	3:A:503:HOH:O	2.08	0.58
1:B:101:THR:HG22	1:B:253:GLN:CG	2.34	0.58
1:B:69:LYS:CE	3:B:506:HOH:O	2.51	0.58
1:D:8:ALA:O	1:D:10:PRO:HD3	2.03	0.58
1:B:23:ARG:NH2	1:D:50:GLY:HA3	2.19	0.58
1:C:122:VAL:HB	1:C:164:VAL:HG22	1.86	0.57
1:A:166:SER:O	1:A:170:LYS:HD2	2.04	0.57
1:C:122:VAL:CB	1:C:164:VAL:HG22	2.35	0.57
1:C:138:PHE:HE1	3:C:528:HOH:O	1.88	0.56
1:C:73:VAL:HG21	1:C:291:VAL:CG1	2.36	0.56
1:A:73:VAL:CG2	1:A:291:VAL:CG1	2.83	0.56
1:A:20:LEU:HD21	1:A:88:VAL:HA	1.89	0.55
1:B:247:ARG:NH1	3:B:512:HOH:O	2.40	0.55
1:A:190:ARG:NH1	3:A:516:HOH:O	2.40	0.55
1:C:99:PRO:HB3	3:C:709:HOH:O	2.07	0.53
1:C:20:LEU:HD21	1:C:88:VAL:HA	1.90	0.53
1:D:120:VAL:CG2	1:D:282:TRP:CD1	2.88	0.53
1:D:69:LYS:HE2	3:D:559:HOH:O	2.09	0.53
1:C:13:SER:HA	3:C:504:HOH:O	2.08	0.52
3:C:510:HOH:O	1:D:137:PHE:HB2	2.10	0.52
1:B:20:LEU:HD11	1:B:88:VAL:HA	1.92	0.52
1:B:218:GLU:CD	1:B:218:GLU:H	2.14	0.51
1:A:8:ALA:O	1:A:10:PRO:HD3	2.11	0.50
1:A:218:GLU:H	1:A:218:GLU:CD	2.14	0.50
1:D:219:LYS:HG3	1:D:223:ASP:OD2	2.11	0.50
1:C:13:SER:O	3:C:504:HOH:O	2.18	0.50
1:A:271:GLU:OE2	1:A:272:SER:N	2.46	0.49
1:B:288:GLN:CB	3:B:514:HOH:O	2.62	0.48
1:C:73:VAL:CG2	1:C:291:VAL:CG1	2.91	0.48
1:A:51:HIS:ND1	1:C:53:GLU:OE1	2.42	0.48
1:D:269:ILE:CG2	3:D:501:HOH:O	2.61	0.48
1:C:289:THR:O	1:C:293:THR:HG23	2.13	0.48
1:D:168:GLU:HG2	3:D:773:HOH:O	2.14	0.48
1:D:82:VAL:HG13	1:D:240:HIS:CG	2.49	0.48
1:B:43:LEU:HB3	1:B:75:ILE:HD13	1.96	0.47
1:D:193:ASP:N	3:D:517:HOH:O	2.47	0.47
1:B:50:GLY:HA3	1:D:26:GLN:HE21	1.76	0.47
1:A:73:VAL:CG2	1:A:291:VAL:HG12	2.44	0.47
1:B:9:MET:HG2	1:B:94:ALA:CB	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:THR:HG23	1:B:88:VAL:HG21	1.98	0.46
1:C:174:LEU:HB2	1:C:281:PHE:CE2	2.50	0.46
1:B:219:LYS:HD2	3:B:502:HOH:O	2.15	0.46
1:B:82:VAL:HG13	1:B:240:HIS:CG	2.50	0.46
1:D:112:ARG:NE	1:D:114:GLU:OE1	2.46	0.46
1:A:120:VAL:CG1	1:A:282:TRP:CD1	2.90	0.45
1:C:217:ASN:HA	3:C:579:HOH:O	2.15	0.45
1:B:101:THR:HG22	1:B:253:GLN:OE1	2.17	0.45
1:A:10:PRO:HB2	1:A:18:LEU:HG	1.98	0.45
1:B:68:VAL:HG23	1:B:73:VAL:HG11	1.98	0.45
1:B:113:GLU:CD	1:B:113:GLU:H	2.19	0.45
1:A:1:MET:N	3:A:520:HOH:O	2.44	0.44
1:D:269:ILE:HG23	3:D:501:HOH:O	2.17	0.44
1:C:247:ARG:HA	1:C:247:ARG:HD3	1.82	0.44
1:B:185:ASP:O	1:B:189:LEU:HG	2.18	0.44
1:C:218:GLU:HG2	1:C:219:LYS:HG2	2.00	0.44
1:D:190:ARG:NH1	3:D:504:HOH:O	2.09	0.44
1:A:13:SER:CA	3:A:503:HOH:O	2.66	0.43
1:A:268:GLN:HG2	1:A:269:ILE:N	2.33	0.43
1:C:20:LEU:HD22	1:C:91:GLU:HB2	2.00	0.43
1:A:82:VAL:HG13	1:A:240:HIS:CG	2.53	0.43
1:D:262:ALA:HB2	1:D:269:ILE:HD13	2.00	0.42
1:B:210:ASP:O	3:B:505:HOH:O	2.22	0.42
1:A:102:ILE:O	1:A:254:ALA:HA	2.20	0.42
1:A:43:LEU:HB3	1:A:75:ILE:HD13	2.02	0.42
1:B:50:GLY:CA	1:D:26:GLN:HE21	2.33	0.42
1:C:218:GLU:CD	1:C:218:GLU:H	2.23	0.41
1:C:73:VAL:CG2	1:C:291:VAL:HG12	2.50	0.41
1:B:13:SER:OG	3:B:504:HOH:O	2.21	0.41
1:C:116:PRO:HA	3:C:700:HOH:O	2.19	0.41
1:B:69:LYS:CE	3:B:514:HOH:O	2.67	0.41
1:B:247:ARG:HD3	1:B:247:ARG:HA	1.89	0.41
1:D:69:LYS:HD3	1:D:288:GLN:OE1	2.21	0.41
1:B:201:SER:O	1:B:206:GLN:HG3	2.21	0.41
1:B:288:GLN:CG	3:B:514:HOH:O	2.56	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:541:HOH:O	3:D:737:HOH:O[2_444]	1.85	0.35

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:731:HOH:O	3:B:735:HOH:O[1_556]	1.98	0.22
3:B:796:HOH:O	3:C:795:HOH:O[1_454]	1.99	0.21
3:A:766:HOH:O	3:C:708:HOH:O[2_545]	2.02	0.18
3:A:810:HOH:O	3:D:809:HOH:O[2_545]	2.05	0.15
3:A:739:HOH:O	3:B:575:HOH:O[1_556]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	300/309 (97%)	290 (97%)	10 (3%)	0	100	100
1	B	287/309 (93%)	280 (98%)	7 (2%)	0	100	100
1	C	286/309 (93%)	278 (97%)	8 (3%)	0	100	100
1	D	298/309 (96%)	285 (96%)	10 (3%)	3 (1%)	17	3
All	All	1171/1236 (95%)	1133 (97%)	35 (3%)	3 (0%)	43	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	185	ASP
1	D	186	CYS
1	D	14	ASP

### 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	247/253 (98%)	244 (99%)	3 (1%)	74	54
1	B	238/253 (94%)	236 (99%)	2 (1%)	83	71
1	C	238/253 (94%)	233 (98%)	5 (2%)	56	29
1	D	245/253 (97%)	242 (99%)	3 (1%)	74	54
All	All	968/1012 (96%)	955 (99%)	13 (1%)	71	51

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	LEU
1	A	235	GLU
1	A	242	LEU
1	B	13	SER
1	B	235	GLU
1	C	9	MET
1	C	157	SER
1	C	190	ARG
1	C	235	GLU
1	C	247	ARG
1	D	184	SER
1	D	235	GLU
1	D	266	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	97	ASN

### 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

6 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	GOL	A	401	-	5,5,5	0.54	0	5,5,5	0.77	0
2	GOL	A	402	-	5,5,5	0.63	0	5,5,5	0.96	0
2	GOL	B	401	-	5,5,5	0.39	0	5,5,5	0.72	0
2	GOL	C	401	-	5,5,5	0.29	0	5,5,5	0.56	0
2	GOL	D	401	-	5,5,5	0.34	0	5,5,5	0.59	0
2	GOL	D	402	-	5,5,5	0.66	0	5,5,5	0.86	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
2	GOL	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	B	401	-	-	0/4/4/4	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	401	-	-	0/4/4/4	0/0/0/0
2	GOL	D	402	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	302/309 (97%)	-0.37	3 (0%) 82 84	8, 15, 32, 40	0
1	B	289/309 (93%)	-0.40	6 (2%) 63 65	8, 15, 36, 52	0
1	C	288/309 (93%)	-0.36	8 (2%) 53 54	8, 15, 37, 53	0
1	D	300/309 (97%)	-0.38	3 (1%) 82 84	8, 15, 33, 43	0
All	All	1179/1236 (95%)	-0.38	20 (1%) 70 71	8, 15, 34, 53	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	VAL	4.2
1	D	270	VAL	4.1
1	C	188	ALA	3.9
1	D	267	GLY	3.5
1	C	179	VAL	3.3
1	A	267	GLY	3.2
1	B	181	ALA	3.1
1	C	185	ASP	2.9
1	C	178	PRO	2.8
1	C	186	CYS	2.8
1	B	176	ALA	2.8
1	B	183	SER	2.6
1	B	185	ASP	2.5
1	D	269	ILE	2.4
1	A	265	LEU	2.2
1	B	179	VAL	2.1
1	C	176	ALA	2.1
1	C	184	SER	2.1
1	B	209	LEU	2.0
1	C	183	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	402	6/6	0.97	0.10	14,20,25,25	0
2	GOL	D	402	6/6	0.97	0.12	16,19,25,25	0
2	GOL	A	401	6/6	0.98	0.06	10,13,18,18	0
2	GOL	B	401	6/6	0.98	0.05	8,11,12,13	0
2	GOL	D	401	6/6	0.98	0.06	10,12,16,16	0
2	GOL	C	401	6/6	0.98	0.05	9,12,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.