



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:42 pm GMT

PDB ID : 1OIU  
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2/CYCLIN A COM-  
PLEXED WITH A 6-CYCLOHEXYLMETHYLOXY-2-ANILINO-PURINE  
INHIBITOR  
Authors : Pratt, D.J.; Endicott, J.A.; Noble, M.E.M.  
Deposited on : 2003-06-26  
Resolution : 2.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

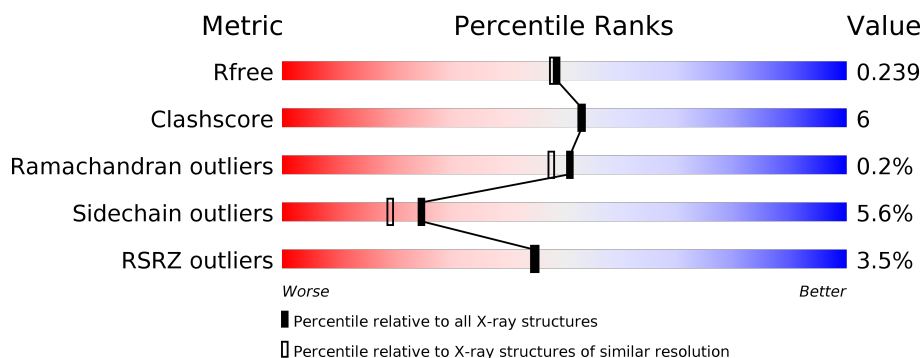
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	302	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	302	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>15%</div> <div>• 12%</div> </div> </div>
2	B	260	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>• •</div> </div> </div>
2	D	260	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>• •</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SGM	B	1193	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9399 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.

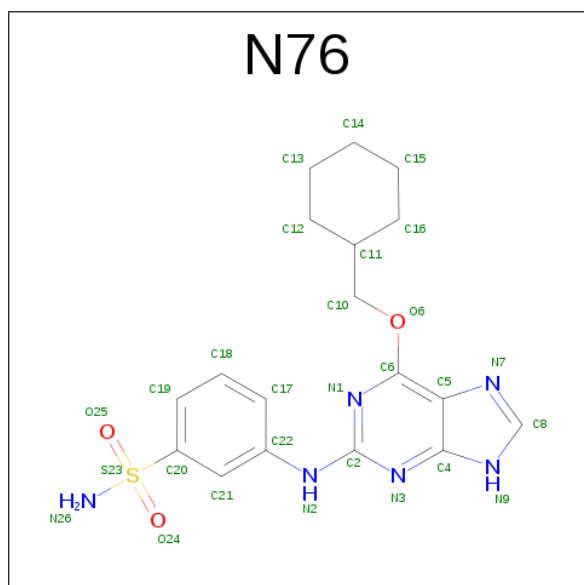
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	8	0
			2413	1567	414	423	1	8			
1	C	266	Total	C	N	O	P	S	0	1	0
			2136	1384	364	380	1	7			

- Molecule 2 is a protein called CYCLIN A2.

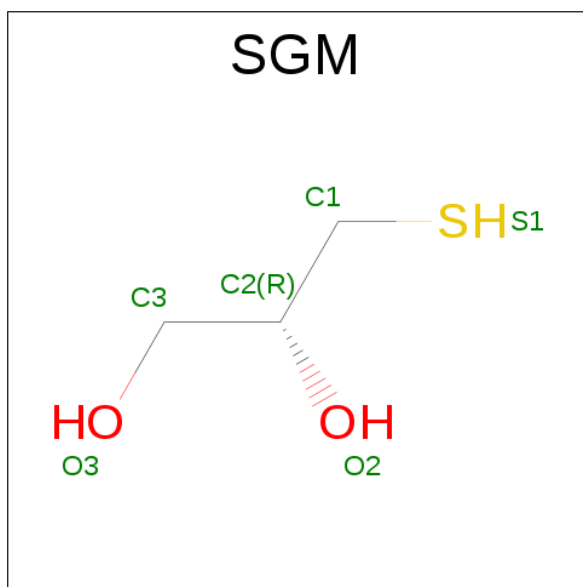
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	256	Total	C	N	O	S		0	2	0
			2066	1339	338	378	11				
2	D	256	Total	C	N	O	S		0	0	0
			2069	1340	337	381	11				

- Molecule 3 is 3-(6-CYCLOHEXYLMETHOXY-9H-PURIN-2-YLAMINO)-BENZENESULFONAMIDE (three-letter code: N76) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	18	6	3	1		
3	C	1	Total	C	N	O	S	0	0
			28	18	6	3	1		

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula:  $C_3H_8O_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			6	3	2	1		
4	D	1	Total	C	O	S	0	0
			6	3	2	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	219	Total	O	0	0
			219	219		
6	B	187	Total	O	0	0
			187	187		

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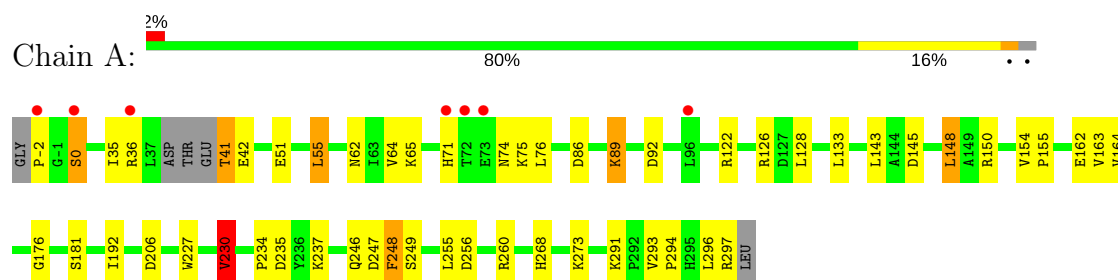
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	128	Total 128	O 128	0	0
6	D	112	Total 112	O 112	0	0

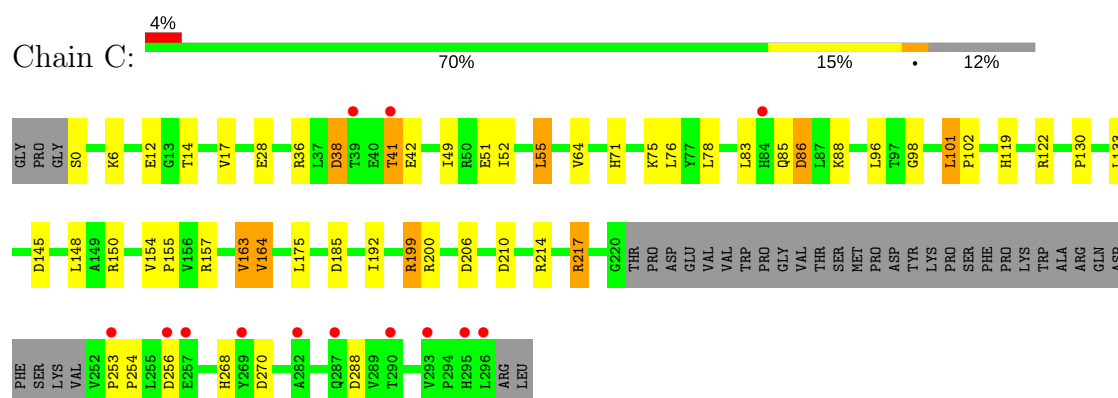
### 3 Residue-property plots [i](#)

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

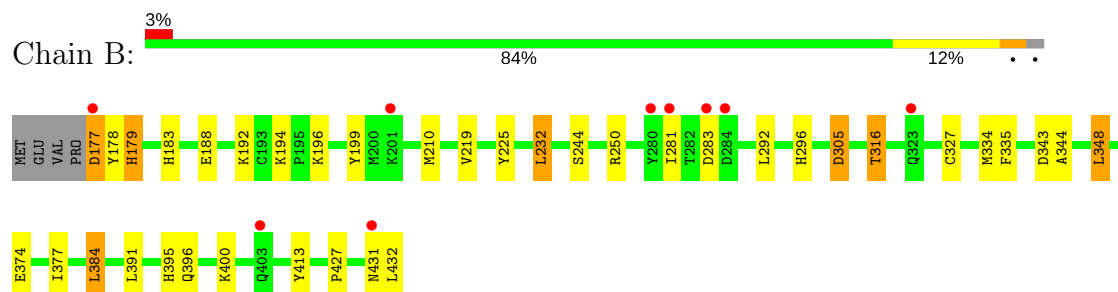
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



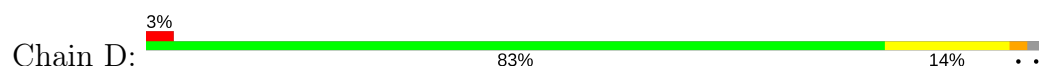
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

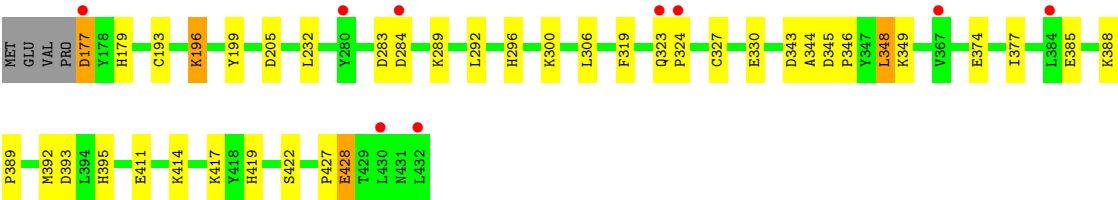


#### • Molecule 2: CYCLIN A2



#### • Molecule 2: CYCLIN A2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.65Å 133.78Å 148.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.00 65.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (100.00-2.00) 98.9 (65.96-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.253 0.205 , 0.239	Depositor DCC
$R_{free}$ test set	4923 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: TPO, MG, SGM, N76

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.51	0/2497	0.75	7/3384 (0.2%)
1	C	0.43	0/2178	0.71	7/2949 (0.2%)
2	B	0.50	0/2127	0.69	2/2886 (0.1%)
2	D	0.40	0/2118	0.69	6/2875 (0.2%)
All	All	0.46	0/8920	0.71	22/12094 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ASP	CB-CG-OD2	6.70	124.33	118.30
1	C	256	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	235	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	247	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	86	ASP	CB-CG-OD2	6.05	123.75	118.30
2	D	205	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C	38	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	145	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	288	ASP	CB-CG-OD2	5.82	123.54	118.30
2	D	343	ASP	CB-CG-OD2	5.65	123.38	118.30
2	D	393	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	86	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	210	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	92	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	145	ASP	CB-CG-OD2	5.33	123.09	118.30
2	B	343	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	230	VAL	CB-CA-C	-5.25	101.43	111.40
2	B	305	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	206	ASP	CB-CG-OD2	5.17	122.95	118.30
2	D	177	ASP	CB-CG-OD2	5.16	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	283	ASP	CB-CG-OD2	5.16	122.95	118.30
2	D	284	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2413	0	2459	40	0
1	C	2136	0	2190	29	0
2	B	2066	0	2084	28	0
2	D	2069	0	2091	21	0
3	A	28	0	22	1	0
3	C	28	0	22	1	0
4	B	6	0	7	2	0
4	D	6	0	8	1	0
5	B	1	0	0	0	0
6	A	219	0	0	11	1
6	B	187	0	0	6	1
6	C	128	0	0	5	0
6	D	112	0	0	0	0
All	All	9399	0	8883	110	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (110) 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)
2:D:193:CYS:SG	4:D:1193:SGM:S1	2.35	1.22
1:A:246:GLN:O	6:A:2180:HOH:O	1.76	1.01
1:A:0:SER:O	6:A:2001:HOH:O	1.78	1.00
1:C:28:GLU:OE2	6:C:2021:HOH:O	1.84	0.94
1:C:71:HIS:HD2	2:D:296:HIS:NE2	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ASP:HB3	1:C:41:THR:HB	1.50	0.92
1:A:296:LEU:O	1:A:297:ARG:HB2	1.82	0.80
1:C:71:HIS:CD2	2:D:296:HIS:NE2	2.49	0.79
2:B:210:MET:CE	2:B:250:ARG:HB2	2.12	0.78
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.65	0.77
1:A:273:LYS:HE3	6:A:2202:HOH:O	1.85	0.76
1:A:227:TRP:O	1:A:230:VAL:HG22	1.87	0.75
1:A:248:PHE:HB2	6:A:2183:HOH:O	1.87	0.73
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.70	0.72
1:A:154:VAL:O	2:B:316:THR:HG23	1.92	0.69
1:A:154:VAL:O	2:B:316:THR:CG2	2.40	0.69
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.28	0.68
1:A:248:PHE:O	6:A:2182:HOH:O	2.12	0.67
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.77	0.66
2:B:316:THR:HG21	6:B:2020:HOH:O	1.95	0.66
1:A:181[A]:SER:OG	6:A:2123:HOH:O	2.15	0.63
2:B:305:ASP:HB3	4:B:1193:SGM:H2	1.79	0.63
2:B:395:HIS:HE1	2:B:427:PRO:O	1.82	0.63
2:D:428:GLU:CD	2:D:428:GLU:H	2.02	0.63
1:A:62:ASN:O	1:A:143[B]:LEU:HD23	1.99	0.62
2:D:346:PRO:O	2:D:349:LYS:HG2	1.99	0.62
2:B:327:CYS:SG	6:B:2131:HOH:O	2.56	0.61
2:B:183:HIS:HD2	6:B:2040:HOH:O	1.83	0.61
1:A:126:ARG:HB3	1:A:163:VAL:HG22	1.83	0.59
1:C:12:GLU:HG2	1:C:17:VAL:HG22	1.83	0.59
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.86	0.58
1:C:14:THR:HG21	6:C:2082:HOH:O	2.02	0.58
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.68	0.57
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.87	0.57
1:C:253:PRO:HD2	1:C:254:PRO:HD3	1.85	0.56
1:C:268:HIS:HD2	1:C:270:ASP:H	1.52	0.56
1:A:126:ARG:HB3	1:A:163:VAL:CG2	2.36	0.56
2:D:196:LYS:HB3	2:D:199:TYR:HB3	1.88	0.56
1:A:268[A]:HIS:CD2	1:A:273:LYS:HB2	2.41	0.56
1:A:293:VAL:HG13	1:A:294:PRO:HD2	1.87	0.55
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.90	0.54
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.90	0.53
1:A:64:VAL:HG21	3:A:1298:N76:C8	2.39	0.53
1:C:214:ARG:HG2	1:C:217:ARG:HH11	1.74	0.53
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.92	0.52
1:C:38:ASP:HB3	1:C:41:THR:CB	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268[A]:HIS:CD2	6:A:2157:HOH:O	2.63	0.51
1:A:-2:PRO:O	2:D:300:LYS:HD3	2.10	0.51
1:A:128:LEU:HD21	1:A:143[B]:LEU:HD12	1.92	0.51
2:B:177:ASP:O	2:B:178:TYR:HB2	2.11	0.51
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.94	0.49
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.47	0.49
1:C:98:GLY:HA2	1:C:199:ARG:HD3	1.94	0.48
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.48	0.48
1:C:214:ARG:HG2	1:C:217:ARG:NH1	2.29	0.48
2:D:346:PRO:HB2	2:D:349:LYS:HE2	1.96	0.48
1:A:273:LYS:CE	6:A:2202:HOH:O	2.54	0.47
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.49	0.47
1:C:133:LEU:HD11	1:C:192:ILE:HD13	1.97	0.47
1:A:148:LEU:HD23	1:A:163:VAL:HG23	1.95	0.47
1:A:128:LEU:CD2	1:A:143[B]:LEU:HD12	2.45	0.46
1:A:260:ARG:HD3	6:A:2187:HOH:O	2.16	0.46
1:A:35:ILE:HB	1:A:76:LEU:HB3	1.98	0.46
1:A:51:GLU:O	1:A:55:LEU:HB2	2.15	0.46
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.98	0.46
1:C:14:THR:CG2	6:C:2082:HOH:O	2.64	0.46
1:A:162:GLU:CG	6:A:2111:HOH:O	2.64	0.45
2:D:388:LYS:O	2:D:392:MET:HG2	2.17	0.45
2:B:396:GLN:HE21	2:B:400:LYS:HE3	1.80	0.45
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.98	0.45
1:C:253:PRO:CD	1:C:254:PRO:HD3	2.47	0.45
1:C:51:GLU:O	1:C:55:LEU:HB2	2.16	0.44
2:B:384:LEU:HG	2:B:432:LEU:HD22	1.99	0.44
1:C:41:THR:HB	1:C:42:GLU:H	1.48	0.44
1:A:71:HIS:CD2	2:B:296:HIS:CE1	3.06	0.44
2:D:327:CYS:HB3	2:D:419:HIS:CE1	2.52	0.44
1:A:89:LYS:HA	1:A:89:LYS:HD2	1.78	0.44
1:C:64:VAL:HG21	3:C:1298:N76:C8	2.48	0.43
1:A:293:VAL:HG12	1:A:294:PRO:O	2.18	0.43
1:A:176:GLY:O	1:A:234:PRO:HG2	2.19	0.43
1:A:291:LYS:HG2	1:A:291:LYS:O	2.18	0.43
1:C:88:LYS:HB2	1:C:130:PRO:HB2	2.00	0.43
1:C:85:GLN:CG	1:C:86:ASP:N	2.82	0.43
1:C:119:HIS:HD2	6:C:2124:HOH:O	2.02	0.43
2:D:395:HIS:HE1	2:D:427:PRO:O	2.01	0.43
1:C:49:ILE:HG23	2:D:306:LEU:HD12	2.01	0.42
2:B:177:ASP:HB2	6:B:2031:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:GLU:HB3	6:C:2035:HOH:O	2.18	0.42
2:B:305:ASP:CB	4:B:1193:SGM:H2	2.46	0.42
2:B:334:MET:HE3	6:B:2115:HOH:O	2.20	0.42
2:B:225:TYR:CE1	2:B:281:ILE:HG21	2.50	0.42
1:C:154:VAL:HA	1:C:155:PRO:HA	1.94	0.42
2:D:319:PHE:CG	2:D:330:GLU:HG2	2.54	0.42
1:A:65:LYS:HG3	6:A:2052:HOH:O	2.20	0.42
1:A:41:THR:HB	1:A:42:GLU:H	1.60	0.41
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.55	0.41
2:D:345:ASP:HA	2:D:346:PRO:HA	1.75	0.41
1:A:249:SER:HA	1:A:260:ARG:HD3	2.02	0.41
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.56	0.41
2:D:323:GLN:HA	2:D:324:PRO:HA	1.83	0.41
1:C:36:ARG:HD3	1:C:36:ARG:HA	1.89	0.41
2:D:374:GLU:HA	2:D:377:ILE:HD12	2.02	0.41
2:B:194:LYS:NZ	6:B:2047:HOH:O	2.54	0.40
1:A:154:VAL:HA	1:A:155:PRO:HA	1.90	0.40
2:B:196:LYS:HG3	2:B:244:SER:HB3	2.03	0.40
2:B:335:PHE:HB2	2:B:413:TYR:CD2	2.57	0.40
2:B:188:GLU:HG2	2:B:192:LYS:HE2	2.04	0.40
1:C:101:LEU:N	1:C:102:PRO:CD	2.84	0.40
2:D:411:GLU:HA	2:D:414:LYS:HD2	2.02	0.40
2:D:414:LYS:HG3	2:D:422:SER:OG	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2185:HOH:O	6:B:2032:HOH:O[4_456]	1.74	0.46

## 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	300/302 (99%)	293 (98%)	6 (2%)	1 (0%)	44	40
1	C	262/302 (87%)	253 (97%)	8 (3%)	1 (0%)	38	33
2	B	256/260 (98%)	254 (99%)	2 (1%)	0	100	100
2	D	254/260 (98%)	252 (99%)	2 (1%)	0	100	100
All	All	1072/1124 (95%)	1052 (98%)	18 (2%)	2 (0%)	51	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL

### 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	267/264 (101%)	252 (94%)	15 (6%)	25	19
1	C	233/264 (88%)	215 (92%)	18 (8%)	15	9
2	B	230/234 (98%)	220 (96%)	10 (4%)	33	29
2	D	230/234 (98%)	220 (96%)	10 (4%)	33	29
All	All	960/996 (96%)	907 (94%)	53 (6%)	25	20

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	36	ARG
1	A	41	THR
1	A	55	LEU
1	A	74	ASN
1	A	75	LYS
1	A	89	LYS
1	A	122	ARG
1	A	148	LEU

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Mol	Chain	Res	Type
1	A	150	ARG
1	A	206	ASP
1	A	230	VAL
1	A	237	LYS
1	A	248	PHE
1	A	255	LEU
2	B	177	ASP
2	B	179	HIS
2	B	232	LEU
2	B	283	ASP
2	B	292	LEU
2	B	316	THR
2	B	348	LEU
2	B	384	LEU
2	B	391	LEU
2	B	431	ASN
1	C	0	SER
1	C	6	LYS
1	C	41	THR
1	C	55	LEU
1	C	75	LYS
1	C	76	LEU
1	C	83	LEU
1	C	96	LEU
1	C	101	LEU
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG
1	C	157	ARG
1	C	163	VAL
1	C	175	LEU
1	C	199	ARG
1	C	200	ARG
1	C	217	ARG
2	D	177	ASP
2	D	179	HIS
2	D	196	LYS
2	D	232	LEU
2	D	289	LYS
2	D	292	LEU
2	D	348	LEU
2	D	385	GLU

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Mol	Chain	Res	Type
2	D	417	LYS
2	D	428	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	84	HIS
2	B	179	HIS
2	B	183	HIS
2	B	254	GLN
2	B	296	HIS
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
1	C	71	HIS
1	C	84	HIS
1	C	119	HIS
1	C	268	HIS
2	D	183	HIS
2	D	233	HIS
2	D	254	GLN
2	D	317	GLN
2	D	395	HIS
2	D	403	GLN
2	D	406	GLN
2	D	431	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TPO	A	160	1	9,10,11	1.17	1 (11%)	10,14,16	0.85	0
1	TPO	C	160	1	9,10,11	1.22	1 (11%)	10,14,16	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
1	TPO	A	160	1	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O1P	2.30	1.58	1.50
1	C	160	TPO	P-O1P	2.37	1.58	1.50

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.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	N76	A	1298	-	28,31,31	1.87	3 (10%)	35,44,44	1.88	8 (22%)
4	SGM	B	1193	-	5,5,5	0.34	0	5,5,5	0.74	0
3	N76	C	1298	-	28,31,31	2.12	3 (10%)	35,44,44	1.96	8 (22%)
4	SGM	D	1193	-	5,5,5	0.33	0	5,5,5	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N76	A	1298	-	-	0/15/23/23	0/4/4/4
4	SGM	B	1193	-	-	0/4/4/4	0/0/0/0
3	N76	C	1298	-	-	0/15/23/23	0/4/4/4
4	SGM	D	1193	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	N76	C20-S23	-9.54	1.61	1.77
3	A	1298	N76	C20-S23	-8.92	1.62	1.77
3	A	1298	N76	C22-N2	-2.27	1.35	1.40
3	A	1298	N76	C6-N1	2.37	1.36	1.31
3	C	1298	N76	C6-N1	2.37	1.36	1.31
3	C	1298	N76	O6-C6	4.03	1.37	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	N76	O25-S23-O24	-5.72	108.22	118.70
3	A	1298	N76	O25-S23-O24	-4.64	110.19	118.70
3	C	1298	N76	N3-C2-N1	-3.47	120.98	126.23
3	A	1298	N76	N3-C2-N1	-3.33	121.19	126.23
3	A	1298	N76	C6-C5-C4	-2.55	114.79	117.26
3	C	1298	N76	O25-S23-N26	2.13	110.69	107.34
3	C	1298	N76	O24-S23-C20	2.44	110.24	107.39
3	A	1298	N76	O24-S23-C20	2.89	110.77	107.39
3	A	1298	N76	C22-C21-C20	2.92	120.75	118.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	N76	C22-C21-C20	2.98	120.79	118.79
3	C	1298	N76	O6-C6-C5	3.10	119.95	115.14
3	A	1298	N76	O6-C6-C5	3.17	120.05	115.14
3	C	1298	N76	C2-N3-C4	3.87	119.53	115.11
3	A	1298	N76	C2-N1-C6	3.89	122.05	115.18
3	C	1298	N76	C2-N1-C6	4.54	123.20	115.18
3	A	1298	N76	C2-N3-C4	4.75	120.53	115.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	N76	1	0
4	B	1193	SGM	2	0
3	C	1298	N76	1	0
4	D	1193	SGM	1	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 ⓘ

### 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	296/302 (98%)	0.14	7 (2%) 59 59	11, 20, 39, 49	0
1	C	265/302 (87%)	0.24	13 (4%) 30 30	19, 29, 48, 57	0
2	B	256/260 (98%)	0.02	9 (3%) 44 45	13, 22, 37, 48	0
2	D	256/260 (98%)	0.32	9 (3%) 44 45	15, 31, 48, 65	0
All	All	1073/1124 (95%)	0.18	38 (3%) 44 45	11, 26, 46, 65	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	284	ASP	6.0
2	D	284	ASP	5.8
1	C	295	HIS	5.5
2	D	432	LEU	4.8
1	C	293	VAL	4.6
2	B	283	ASP	4.3
1	A	0	SER	4.0
1	A	71	HIS	3.9
1	C	253	PRO	3.7
2	D	324	PRO	3.7
2	D	177	ASP	3.6
1	C	282	ALA	3.6
2	B	177	ASP	3.4
1	A	73	GLU	3.4
2	B	323	GLN	3.3
1	C	287	GLN	3.2
1	A	96	LEU	3.0
1	C	39	THR	2.9
2	B	280	TYR	2.9
1	A	72	THR	2.7
1	C	269	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	281	ILE	2.5
1	A	-2	PRO	2.5
2	B	201	LYS	2.5
2	D	280	TYR	2.5
2	D	384	LEU	2.4
1	C	84	HIS	2.4
1	C	290	THR	2.3
2	D	367	VAL	2.2
2	D	430	LEU	2.2
2	D	323	GLN	2.2
1	C	256	ASP	2.1
2	B	403	GLN	2.1
1	A	36	ARG	2.1
2	B	431	ASN	2.0
1	C	41	THR	2.0
1	C	257	GLU	2.0
1	C	296	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	C	160	11/12	0.98	0.11	-	20,23,26,26	0
1	TPO	A	160	11/12	0.99	0.11	-	14,18,20,20	0

## 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( $\text{\AA}^2$ )	Q<0.9
4	SGM	B	1193	6/6	0.91	0.21	5.86	38,43,44,46	0
4	SGM	D	1193	6/6	0.93	0.17	1.90	46,50,50,52	0
3	N76	A	1298	28/28	0.96	0.13	-0.26	19,26,30,31	0
3	N76	C	1298	28/28	0.95	0.10	-0.58	26,28,33,34	0
5	MG	B	1433	1/1	0.98	0.10	-0.98	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.