



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 AM GMT

PDB ID : 3QHR  
Title : Structure of a pCDK2/CyclinA transition-state mimic  
Authors : Young, M.A.; Jacobsen, D.M.; Bao, Z.Q.  
Deposited on : 2011-01-26  
Resolution : 2.17 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

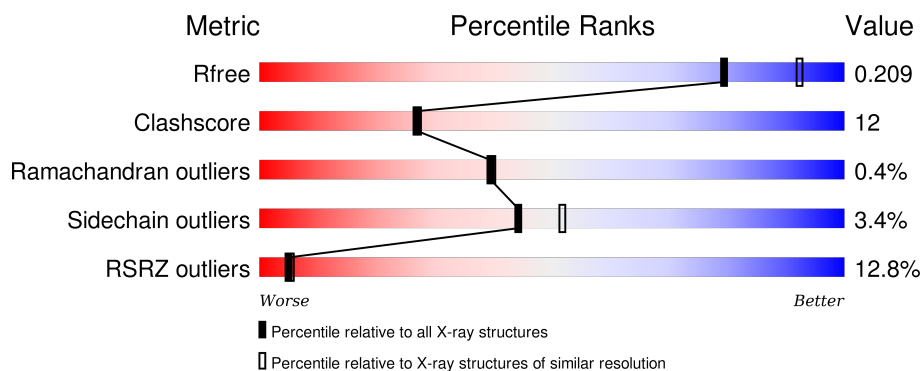
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	298	<div> <div>15%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	C	298	<div> <div>10%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	B	261	<div> <div>10%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	D	261	<div> <div>11%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
3	J	10	<div> <div>70%</div> <div>20%</div> <div>80%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	K	10	
3	L	10	
3	M	10	

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
8	GOL	A	303	-	-	X	-
8	GOL	A	305	-	-	X	-
8	GOL	B	3	-	-	-	X
8	GOL	B	8	-	-	-	X
8	GOL	C	302	-	-	X	X
8	GOL	C	303	-	-	-	X
8	GOL	D	5	-	-	-	X
8	GOL	D	7	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10077 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	298	Total	C	N	O	P	S	0	0	0
			2396	1555	407	425	1	8			
1	C	298	Total	C	N	O	P	S	0	0	0
			2396	1555	407	425	1	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	HIS	-	EXPRESSION TAG	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	HIS	-	EXPRESSION TAG	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S		0	0	0
			2099	1357	341	391	10				
2	D	261	Total	C	N	O	S		0	0	0
			2099	1357	341	391	10				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	172	SER	-	EXPRESSION TAG	UNP P51943
D	172	SER	-	EXPRESSION TAG	UNP P51943

- Molecule 3 is a protein called CDK2 substrate peptide: PKTPKKAKKL.

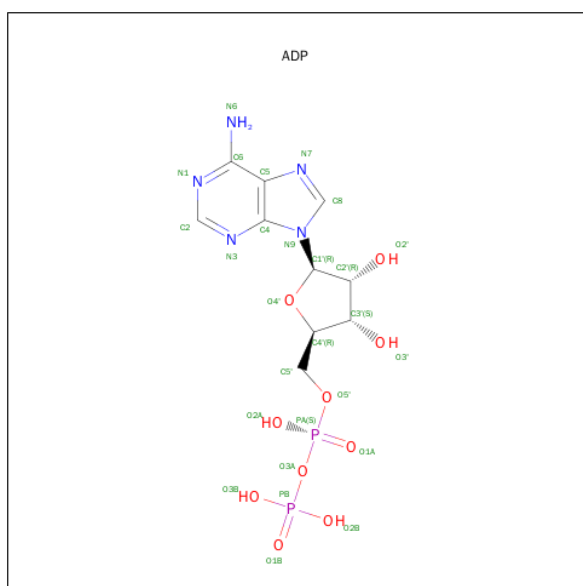
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	10	Total	C	N	O	0	0	0
			79	53	15	11			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	10	Total	C	N	O	0	0	0
			79	53	15	11			
3	L	10	Total	C	N	O	48	0	0
			79	53	15	11			
3	M	10	Total	C	N	O	48	0	0
			79	53	15	11			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

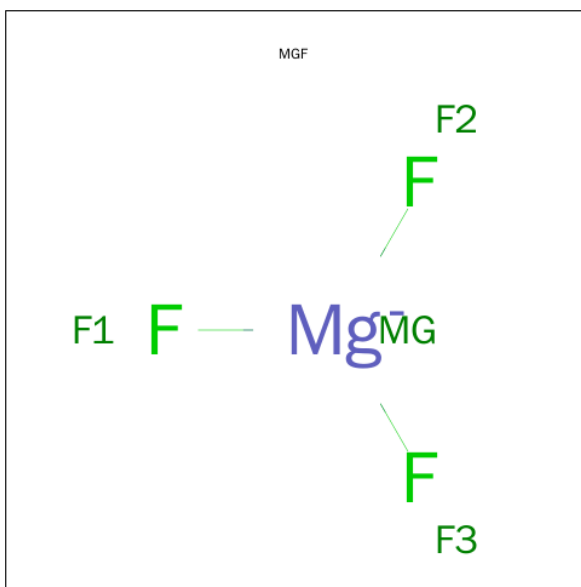


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula:  $F_3Mg$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	F	Mg	0	0
			4	3	1		
6	C	1	Total	F	Mg	0	0
			4	3	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 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
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	K	1	Total	C	O	0	0
			6	3	3		

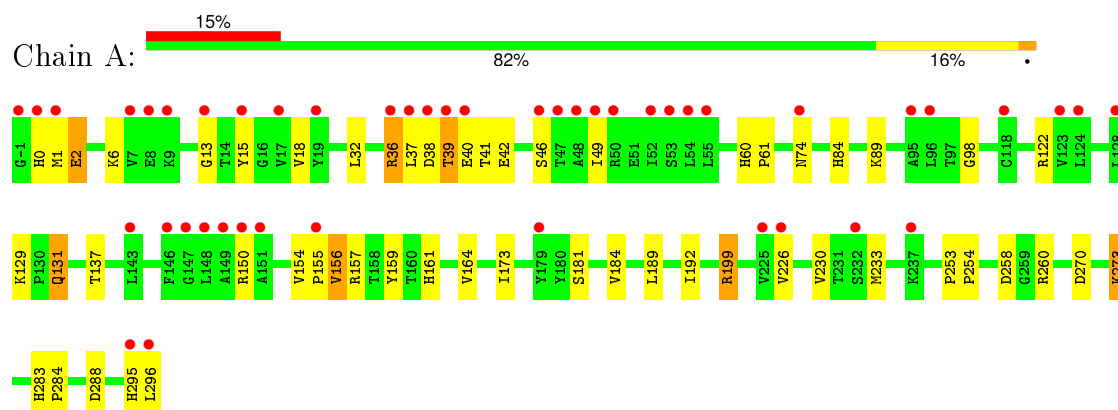
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	146	Total	O	0	0
			146	146		
9	B	156	Total	O	0	0
			156	156		
9	C	183	Total	O	0	0
			183	183		
9	D	104	Total	O	0	0
			104	104		
9	J	1	Total	O	0	0
			1	1		
9	K	5	Total	O	0	0
			5	5		
9	L	4	Total	O	0	0
			4	4		
9	M	2	Total	O	0	0
			2	2		

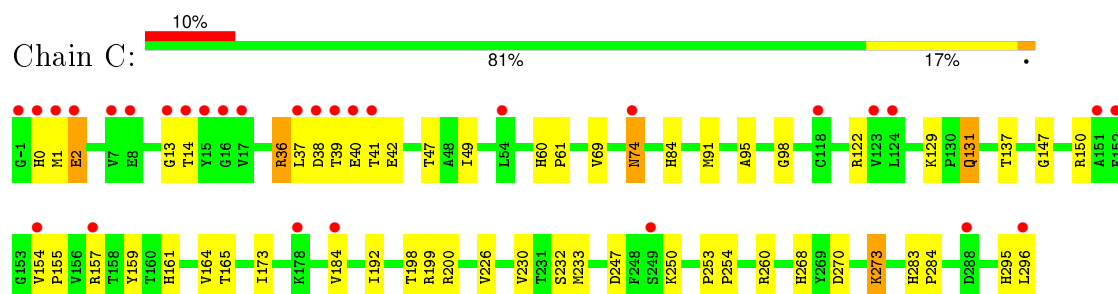
### 3 Residue-property plots [i](#)

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.

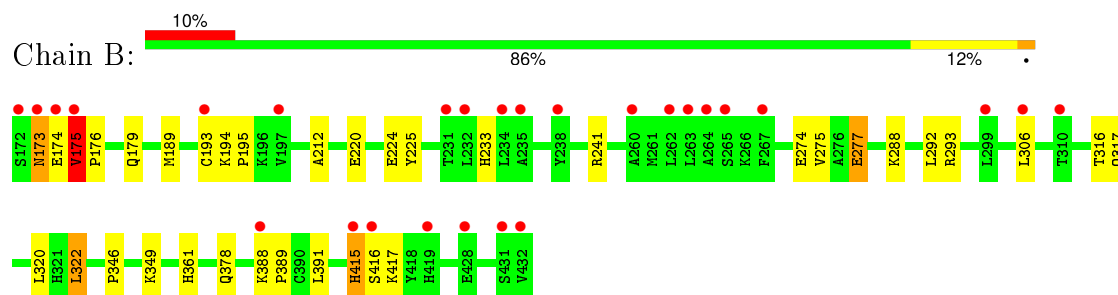
- Molecule 1: Cell division protein kinase 2



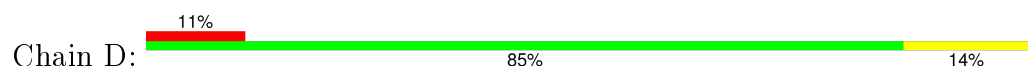
- Molecule 1: Cell division protein kinase 2

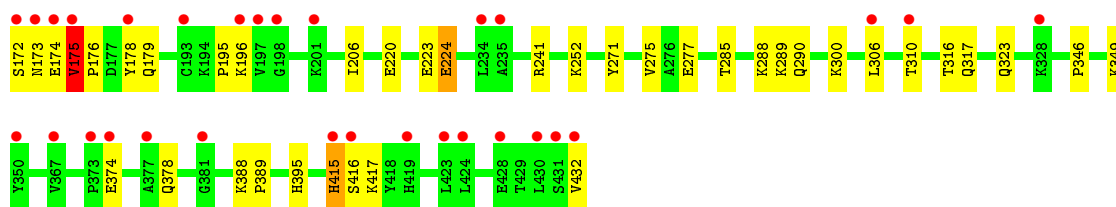


- Molecule 2: Cyclin-A2



- Molecule 2: Cyclin-A2

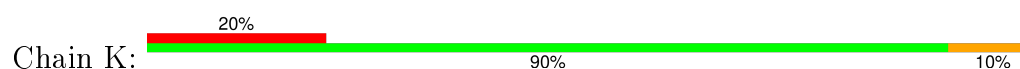




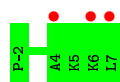
- Molecule 3: CDK2 substrate peptide: PKTPKKAKKL



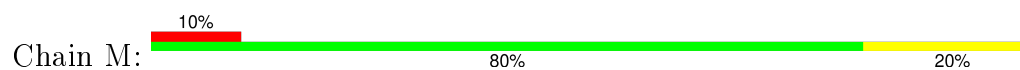
- Molecule 3: CDK2 substrate peptide: PKTPKKAKKL



- Molecule 3: CDK2 substrate peptide: PKTPKKAKKL



- Molecule 3: CDK2 substrate peptide: PKTPKKAKKL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.69Å 163.91Å 73.28Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	37.80 – 2.17 37.80 – 2.17	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.80-2.17) 99.9 (37.80-2.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.179 , 0.210 0.175 , 0.209	Depositor DCC
$R_{free}$ test set	4193 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.0	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83863 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.44% 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: GOL, MG, MGF, ADP, CL, TPO

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	0.49	0/2447	0.56	0/3320
1	C	0.51	0/2447	0.56	0/3320
2	B	0.50	0/2149	0.54	0/2921
2	D	0.45	0/2149	0.54	0/2921
3	J	0.88	0/80	0.98	0/103
3	K	1.27	0/80	0.98	0/103
3	L	0.92	0/80	0.94	0/103
3	M	1.19	0/80	0.91	0/103
All	All	0.52	0/9512	0.57	0/12894

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	2396	0	2435	66	0
1	C	2396	0	2435	73	0
2	B	2099	0	2110	52	0
2	D	2099	0	2110	49	0
3	J	79	0	104	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	79	0	104	4	0
3	L	79	0	104	0	0
3	M	79	0	104	1	0
4	A	27	0	12	2	0
4	C	27	0	12	2	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
7	A	1	0	0	1	0
7	C	1	0	0	1	0
8	A	24	0	32	10	0
8	B	30	0	40	4	0
8	C	12	0	16	7	0
8	D	30	0	40	4	0
8	K	6	0	8	0	0
9	A	146	0	0	9	0
9	B	156	0	0	8	0
9	C	183	0	0	11	0
9	D	104	0	0	3	0
9	J	1	0	0	5	0
9	K	5	0	0	0	0
9	L	4	0	0	0	0
9	M	2	0	0	0	0
All	All	10077	0	9666	229	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 12.

All (229) 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:37:LEU:O	1:A:40:GLU:HB2	1.45	1.16
2:B:175:VAL:H	2:B:176:PRO:HD3	1.09	1.15
1:A:161:HIS:H	8:A:303:GOL:H12	1.12	1.14
1:C:37:LEU:O	1:C:40:GLU:HB2	1.50	1.10
1:C:41:THR:HG22	2:D:288:LYS:HE3	1.32	1.06
1:A:36:ARG:N	1:A:36:ARG:HD3	1.69	1.06
1:C:41:THR:CG2	2:D:288:LYS:HE3	1.84	1.05
1:A:154:VAL:O	2:B:316:THR:HG22	1.58	1.03
1:A:38:ASP:O	1:A:39:THR:HG23	1.59	1.03

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:H	1:A:36:ARG:CD	1.69	1.02
1:C:36:ARG:N	1:C:36:ARG:HD3	1.69	1.01
1:C:36:ARG:CD	1:C:36:ARG:H	1.69	1.00
1:A:36:ARG:HD3	1:A:36:ARG:H	0.83	0.99
1:C:41:THR:HG22	2:D:288:LYS:CE	1.92	0.98
2:D:175:VAL:H	2:D:176:PRO:HD3	1.30	0.95
1:C:36:ARG:HD3	1:C:36:ARG:H	0.83	0.95
2:B:175:VAL:N	2:B:176:PRO:CD	2.30	0.94
2:B:175:VAL:N	2:B:176:PRO:HD3	1.80	0.94
1:A:41:THR:HG22	2:B:288:LYS:CE	1.98	0.94
1:C:38:ASP:O	1:C:39:THR:HG23	1.69	0.91
1:A:41:THR:HG22	2:B:288:LYS:HE3	1.52	0.90
3:K:7:LEU:O	3:K:7:LEU:HD12	1.72	0.89
1:A:38:ASP:C	1:A:39:THR:HG23	1.88	0.89
2:D:175:VAL:H	2:D:176:PRO:CD	1.85	0.89
1:C:154:VAL:O	2:D:316:THR:HG22	1.72	0.88
2:D:174:GLU:OE1	2:D:174:GLU:HA	1.73	0.87
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.56	0.86
1:C:38:ASP:C	1:C:39:THR:HG23	1.96	0.86
2:B:175:VAL:H	2:B:176:PRO:CD	1.85	0.86
1:A:37:LEU:C	1:A:40:GLU:HB2	1.97	0.84
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.60	0.83
1:C:41:THR:CG2	2:D:288:LYS:CE	2.52	0.83
8:B:16:GOL:H31	9:B:483:HOH:O	1.80	0.82
3:J:6:LYS:O	3:J:7:LEU:CB	2.29	0.81
2:D:175:VAL:N	2:D:176:PRO:CD	2.42	0.81
2:D:175:VAL:O	2:D:175:VAL:CG2	2.30	0.80
1:A:154:VAL:HG11	2:B:179:GLN:OE1	1.83	0.79
3:K:7:LEU:O	3:K:7:LEU:CD1	2.30	0.79
1:C:37:LEU:O	1:C:40:GLU:CB	2.30	0.78
3:K:7:LEU:O	3:K:7:LEU:CG	2.30	0.78
1:A:38:ASP:O	1:A:39:THR:CG2	2.30	0.78
1:A:154:VAL:O	2:B:316:THR:CG2	2.31	0.77
2:B:293:ARG:HH22	1:C:2:GLU:HG2	1.51	0.76
3:J:-1:LYS:HD3	9:J:655:HOH:O	1.85	0.76
1:A:37:LEU:O	1:A:40:GLU:CB	2.30	0.75
1:A:0:HIS:ND1	1:A:1:MET:HG2	2.01	0.75
2:B:378:GLN:HG2	9:B:481:HOH:O	1.85	0.75
1:C:98:GLY:HA3	1:C:199:ARG:NH1	2.00	0.75
1:A:41:THR:HG22	2:B:288:LYS:NZ	2.00	0.75
1:C:161:HIS:HD2	9:C:380:HOH:O	1.70	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:0:HIS:ND1	1:C:1:MET:HG2	2.02	0.75
1:A:181:SER:HB3	9:A:342:HOH:O	1.87	0.74
1:C:154:VAL:CG2	2:D:317:GLN:HG2	2.18	0.73
2:D:196:LYS:HE3	9:D:626:HOH:O	1.88	0.73
2:B:415:HIS:ND1	2:B:416:SER:N	2.37	0.72
3:K:7:LEU:O	3:K:7:LEU:HG	1.87	0.72
2:D:415:HIS:ND1	2:D:416:SER:N	2.38	0.72
1:C:41:THR:HG23	2:D:288:LYS:NZ	2.05	0.71
9:A:509:HOH:O	2:B:193:CYS:SG	2.47	0.71
1:A:41:THR:CG2	2:B:288:LYS:NZ	2.54	0.71
3:J:6:LYS:O	3:J:7:LEU:HB2	1.92	0.70
2:B:173:ASN:OD1	2:B:173:ASN:C	2.30	0.69
8:A:303:GOL:H2	9:A:559:HOH:O	1.92	0.69
1:C:38:ASP:O	1:C:39:THR:CG2	2.39	0.69
2:B:220:GLU:O	2:B:224:GLU:HG2	1.93	0.69
1:A:260:ARG:HD3	9:A:569:HOH:O	1.91	0.69
1:C:260:ARG:HD3	9:C:395:HOH:O	1.93	0.68
1:A:161:HIS:N	8:A:303:GOL:H12	1.97	0.67
2:B:175:VAL:HG23	2:B:175:VAL:O	1.92	0.67
2:D:220:GLU:O	2:D:224:GLU:HG2	1.95	0.67
8:A:304:GOL:H31	8:A:305:GOL:H31	1.77	0.67
1:C:230:VAL:O	1:C:233:MET:HG3	1.95	0.66
1:C:154:VAL:HG23	2:D:317:GLN:HG2	1.76	0.66
1:A:157:ARG:HB3	1:A:159:TYR:CE1	2.31	0.65
1:C:69:VAL:HG23	8:C:303:GOL:H31	1.79	0.65
1:A:38:ASP:O	1:A:39:THR:CB	2.46	0.64
2:B:173:ASN:OD1	2:B:174:GLU:N	2.31	0.64
2:D:175:VAL:N	2:D:176:PRO:HD3	2.05	0.63
8:A:305:GOL:H11	2:D:300:LYS:NZ	2.14	0.63
1:C:38:ASP:C	1:C:39:THR:CG2	2.67	0.63
1:A:288:ASP:OD1	8:A:302:GOL:H12	2.00	0.62
1:A:36:ARG:NH2	9:A:370:HOH:O	2.32	0.62
3:J:0:THR:HG23	3:J:1:PRO:HD2	1.82	0.62
2:D:220:GLU:O	2:D:224:GLU:CG	2.48	0.61
2:D:388:LYS:HB2	2:D:389:PRO:HD3	1.82	0.61
2:D:395:HIS:ND1	9:D:589:HOH:O	2.31	0.61
2:D:346:PRO:HB2	2:D:349:LYS:HE2	1.81	0.61
2:D:175:VAL:O	2:D:175:VAL:HG23	1.98	0.61
2:D:175:VAL:O	2:D:175:VAL:HG22	2.02	0.60
1:C:36:ARG:NH2	9:C:480:HOH:O	2.34	0.60
1:A:230:VAL:O	1:A:233:MET:HG3	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:C	1:A:39:THR:CG2	2.59	0.59
2:B:415:HIS:HB2	9:B:562:HOH:O	2.02	0.59
1:C:154:VAL:O	1:C:154:VAL:HG23	2.01	0.58
2:B:388:LYS:HB2	2:B:389:PRO:HD3	1.84	0.58
1:C:98:GLY:CA	1:C:199:ARG:NH1	2.67	0.58
1:C:38:ASP:O	1:C:39:THR:CB	2.51	0.58
2:D:172:SER:O	2:D:173:ASN:OD1	2.22	0.57
2:B:322:LEU:HD23	9:B:494:HOH:O	2.03	0.57
1:A:98:GLY:HA2	1:A:199:ARG:HD3	1.87	0.56
3:J:6:LYS:O	3:J:7:LEU:HB3	2.03	0.56
1:C:41:THR:CG2	2:D:288:LYS:NZ	2.68	0.56
2:B:388:LYS:NZ	2:B:388:LYS:HB3	2.20	0.56
2:D:223:GLU:HA	2:D:223:GLU:OE1	2.05	0.56
2:B:293:ARG:NH2	1:C:2:GLU:HG2	2.19	0.56
1:A:38:ASP:C	1:A:40:GLU:H	2.09	0.56
1:C:154:VAL:O	2:D:316:THR:CG2	2.49	0.55
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.06	0.55
1:A:137:THR:HG22	1:A:296:LEU:HD12	1.88	0.55
2:D:388:LYS:NZ	2:D:388:LYS:HB3	2.21	0.55
1:A:154:VAL:CG1	2:B:179:GLN:OE1	2.53	0.55
1:C:37:LEU:HB2	1:C:74:ASN:O	2.08	0.54
1:C:1:MET:HG3	1:C:2:GLU:N	2.23	0.54
8:A:305:GOL:H11	2:D:300:LYS:HZ2	1.71	0.54
1:C:295:HIS:CE1	9:C:643:HOH:O	2.60	0.54
2:B:346:PRO:HB2	2:B:349:LYS:HE2	1.89	0.54
2:D:175:VAL:N	2:D:176:PRO:HD2	2.22	0.54
9:C:358:HOH:O	3:J:-2:PRO:HD2	2.07	0.54
2:D:310:THR:HA	8:D:5:GOL:H12	1.89	0.54
1:C:137:THR:HG22	1:C:296:LEU:HD12	1.90	0.54
1:A:13:GLY:HA3	4:A:297:ADP:O1B	2.07	0.54
1:A:295:HIS:HD2	9:A:624:HOH:O	1.91	0.54
3:J:-1:LYS:CG	9:J:655:HOH:O	2.54	0.54
1:A:270:ASP:OD2	1:A:273:LYS:HE2	2.09	0.53
1:A:154:VAL:HG13	2:B:175:VAL:HG21	1.90	0.53
2:D:285:THR:OG1	3:M:6:LYS:HB2	2.09	0.52
2:B:317:GLN:NE2	9:B:471:HOH:O	2.42	0.52
1:A:283:HIS:ND1	1:A:284:PRO:HD2	2.25	0.52
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.90	0.52
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.25	0.52
1:A:41:THR:CG2	2:B:288:LYS:HZ2	2.23	0.51
1:A:1:MET:HG3	1:A:2:GLU:N	2.24	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASP:HB3	1:A:273:LYS:HE3	1.93	0.51
2:D:206:ILE:O	8:D:7:GOL:H32	2.10	0.51
1:A:41:THR:CG2	2:B:288:LYS:HE3	2.35	0.51
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.93	0.50
8:A:304:GOL:H31	8:A:305:GOL:C3	2.40	0.50
2:B:189:MET:CG	9:B:590:HOH:O	2.59	0.50
1:C:95:ALA:O	1:C:199:ARG:HD2	2.11	0.50
1:A:156:VAL:HG22	1:A:159:TYR:HE2	1.76	0.50
1:C:198:THR:O	1:C:199:ARG:HB2	2.11	0.50
1:A:15:TYR:CD2	9:A:333:HOH:O	2.53	0.50
1:A:6:LYS:NZ	9:A:503:HOH:O	2.41	0.50
1:C:98:GLY:CA	1:C:199:ARG:HH11	2.25	0.50
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.94	0.50
1:C:270:ASP:HB3	1:C:273:LYS:HE3	1.93	0.49
2:D:252:LYS:HE3	8:D:13:GOL:H32	1.94	0.49
1:A:258:ASP:OD2	8:A:302:GOL:H32	2.12	0.49
1:A:38:ASP:O	1:A:39:THR:OG1	2.30	0.49
1:A:42:GLU:OE2	2:B:274:GLU:HB2	2.12	0.49
1:C:14:THR:HG23	3:J:2:LYS:NZ	2.27	0.49
1:C:200:ARG:CA	8:C:302:GOL:O1	2.61	0.49
1:A:38:ASP:C	1:A:40:GLU:N	2.64	0.49
1:A:156:VAL:HG22	1:A:159:TYR:CE2	2.47	0.49
1:C:270:ASP:OD2	1:C:273:LYS:HE2	2.12	0.49
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.94	0.49
3:J:-1:LYS:HB3	9:J:655:HOH:O	2.13	0.48
1:C:37:LEU:C	1:C:40:GLU:HB2	2.30	0.48
2:D:346:PRO:O	2:D:349:LYS:HG2	2.12	0.48
3:J:0:THR:CG2	3:J:1:PRO:HD2	2.44	0.48
1:A:131:GLN:HB3	7:A:301:CL:CL	2.50	0.48
1:C:157:ARG:HB2	1:C:159:TYR:CE1	2.48	0.48
2:B:212:ALA:HB2	8:B:6:GOL:H32	1.95	0.48
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.49	0.48
1:C:154:VAL:CG2	1:C:154:VAL:O	2.62	0.47
1:A:41:THR:HG23	2:B:288:LYS:NZ	2.27	0.47
1:C:268:HIS:CD2	9:C:582:HOH:O	2.66	0.47
2:B:175:VAL:N	2:B:176:PRO:HD2	2.25	0.47
2:B:225:TYR:OH	2:B:277:GLU:HG2	2.14	0.47
9:C:457:HOH:O	3:J:3:LYS:HE3	2.14	0.47
1:C:232:SER:HB2	9:C:647:HOH:O	2.13	0.47
1:C:38:ASP:O	1:C:39:THR:OG1	2.30	0.47
1:C:199:ARG:O	8:C:302:GOL:H12	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:HIS:CE1	2:B:417:LYS:H	2.32	0.46
2:D:289:LYS:HE3	9:D:606:HOH:O	2.15	0.46
1:A:161:HIS:HB2	8:A:303:GOL:H31	1.98	0.46
1:C:199:ARG:C	8:C:302:GOL:O1	2.55	0.46
2:B:275:VAL:HG21	2:B:292:LEU:HD21	1.98	0.46
8:B:1:GOL:H12	9:B:452:HOH:O	2.15	0.46
1:A:41:THR:HG23	2:B:288:LYS:HZ2	1.81	0.45
2:D:172:SER:C	2:D:173:ASN:OD1	2.54	0.45
2:D:415:HIS:CE1	2:D:417:LYS:H	2.34	0.45
1:C:91:MET:HB3	8:C:302:GOL:H31	1.99	0.45
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.52	0.45
3:J:-1:LYS:CB	9:J:655:HOH:O	2.65	0.45
1:A:84:HIS:ND1	1:A:296:LEU:HD13	2.32	0.45
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.99	0.45
1:C:147:GLY:HA3	9:C:551:HOH:O	2.16	0.45
2:B:179:GLN:HE22	2:B:320:LEU:HD12	1.82	0.44
2:D:290:GLN:HE22	8:D:13:GOL:C3	2.30	0.44
2:B:233:HIS:ND1	8:B:1:GOL:O1	2.50	0.44
1:C:129:LYS:HE3	1:C:131:GLN:HG2	2.00	0.44
1:A:157:ARG:HB3	1:A:159:TYR:HE1	1.82	0.44
1:C:41:THR:O	2:D:288:LYS:HE2	2.18	0.44
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.99	0.44
1:C:47:THR:HG23	9:C:604:HOH:O	2.17	0.44
1:A:18:VAL:HA	1:A:32:LEU:O	2.19	0.43
1:C:199:ARG:O	8:C:302:GOL:C1	2.66	0.43
2:D:220:GLU:O	2:D:224:GLU:HG3	2.18	0.43
1:A:41:THR:CG2	2:B:288:LYS:CE	2.85	0.43
2:B:179:GLN:HE22	2:B:320:LEU:CD1	2.30	0.43
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.78	0.43
3:J:-1:LYS:CD	9:J:655:HOH:O	2.51	0.43
1:C:13:GLY:HA3	4:C:297:ADP:O1B	2.18	0.43
2:D:174:GLU:OE1	2:D:174:GLU:CA	2.50	0.43
1:C:273:LYS:HB2	1:C:273:LYS:HE3	1.88	0.43
2:B:194:LYS:HD2	2:B:195:PRO:HD2	2.00	0.42
1:C:131:GLN:HB3	7:C:301:CL:CL	2.57	0.42
1:C:173:ILE:HD11	1:C:184:VAL:HG11	2.01	0.42
2:D:271:TYR:CD1	3:J:6:LYS:HB2	2.55	0.42
2:B:346:PRO:O	2:B:349:LYS:HG2	2.19	0.42
1:C:84:HIS:ND1	1:C:296:LEU:HD13	2.35	0.42
1:C:268:HIS:HD2	9:C:582:HOH:O	2.01	0.42
2:D:374:GLU:O	2:D:378:GLN:HG3	2.20	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:MET:HG3	9:B:590:HOH:O	2.17	0.42
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.81	0.42
1:C:129:LYS:HD3	1:C:165:THR:OG1	2.20	0.41
2:D:195:PRO:HG3	2:D:241:ARG:HG3	2.01	0.41
1:C:42:GLU:OE1	2:D:275:VAL:HG23	2.20	0.41
1:A:173:ILE:HD11	1:A:184:VAL:HG11	2.01	0.41
4:A:297:ADP:O5'	4:A:297:ADP:H8	2.04	0.41
1:A:273:LYS:HE3	1:A:273:LYS:HB2	1.89	0.41
1:C:247:ASP:O	1:C:250:LYS:HB3	2.21	0.41
1:A:89:LYS:HE3	9:A:366:HOH:O	2.20	0.41
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.56	0.41
2:B:195:PRO:HG3	2:B:241:ARG:HG3	2.03	0.40
4:C:297:ADP:O5'	4:C:297:ADP:H8	2.04	0.40
1:C:98:GLY:HA2	1:C:199:ARG:HH11	1.85	0.40
1:C:200:ARG:HA	8:C:302:GOL:O1	2.21	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	295/298 (99%)	286 (97%)	8 (3%)	1 (0%)	46	48
1	C	295/298 (99%)	283 (96%)	11 (4%)	1 (0%)	46	48
2	B	259/261 (99%)	253 (98%)	5 (2%)	1 (0%)	39	40
2	D	259/261 (99%)	255 (98%)	3 (1%)	1 (0%)	39	40
3	J	8/10 (80%)	8 (100%)	0	0	100	100
3	K	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	L	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
3	M	8/10 (80%)	7 (88%)	1 (12%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1140/1158 (98%)	1106 (97%)	30 (3%)	4 (0%)	39	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL
2	D	175	VAL
2	B	175	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	261/261 (100%)	249 (95%)	12 (5%)	33	37
1	C	261/261 (100%)	253 (97%)	8 (3%)	47	56
2	B	234/234 (100%)	229 (98%)	5 (2%)	61	72
2	D	234/234 (100%)	226 (97%)	8 (3%)	44	52
3	J	9/9 (100%)	9 (100%)	0	100	100
3	K	9/9 (100%)	8 (89%)	1 (11%)	8	6
3	L	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	8 (89%)	1 (11%)	8	6
All	All	1026/1026 (100%)	991 (97%)	35 (3%)	44	52

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	36	ARG
1	A	39	THR
1	A	46	SER
1	A	74	ASN
1	A	122	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	131	GLN
1	A	150	ARG
1	A	156	VAL
1	A	199	ARG
1	A	226	VAL
1	A	273	LYS
2	B	173	ASN
2	B	175	VAL
2	B	277	GLU
2	B	322	LEU
2	B	415	HIS
1	C	2	GLU
1	C	36	ARG
1	C	74	ASN
1	C	122	ARG
1	C	131	GLN
1	C	150	ARG
1	C	226	VAL
1	C	273	LYS
2	D	175	VAL
2	D	178	TYR
2	D	179	GLN
2	D	224	GLU
2	D	277	GLU
2	D	323	GLN
2	D	415	HIS
2	D	432	VAL
3	K	7	LEU
3	M	-1	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
2	B	296	HIS

### 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	8,10,11	1.06	0	7,14,16	1.15	0
1	TPO	C	160	1	8,10,11	1.03	0	7,14,16	1.02	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

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.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 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	$\# Z  > 2$
4	ADP	A	297	5,6	22,29,29	1.00	1 (4%)	27,45,45	2.03	5 (18%)
6	MGF	A	300	3,4	0,3,3	0.00	-	0,3,3	0.00	-
8	GOL	A	302	-	5,5,5	0.32	0	5,5,5	0.60	0
8	GOL	A	303	-	5,5,5	0.35	0	5,5,5	0.44	0
8	GOL	A	304	-	5,5,5	0.38	0	5,5,5	0.81	0
8	GOL	A	305	-	5,5,5	0.24	0	5,5,5	0.56	0
8	GOL	B	1	-	5,5,5	0.63	0	5,5,5	0.93	0
8	GOL	B	16	-	5,5,5	0.75	0	5,5,5	0.47	0
8	GOL	B	3	-	5,5,5	0.40	0	5,5,5	0.46	0
8	GOL	B	6	-	5,5,5	0.53	0	5,5,5	0.37	0
8	GOL	B	8	-	5,5,5	0.53	0	5,5,5	0.74	0
4	ADP	C	297	5,6	22,29,29	1.03	1 (4%)	27,45,45	1.98	4 (14%)
6	MGF	C	300	3,4	0,3,3	0.00	-	0,3,3	0.00	-
8	GOL	C	302	-	5,5,5	0.44	0	5,5,5	0.62	0
8	GOL	C	303	-	5,5,5	0.50	0	5,5,5	0.83	0
8	GOL	D	13	-	5,5,5	0.35	0	5,5,5	0.59	0
8	GOL	D	15	-	5,5,5	0.28	0	5,5,5	0.55	0
8	GOL	D	2	-	5,5,5	0.31	0	5,5,5	0.50	0
8	GOL	D	5	-	5,5,5	0.56	0	5,5,5	0.69	0
8	GOL	D	7	-	5,5,5	0.45	0	5,5,5	0.50	0
8	GOL	K	12	-	5,5,5	0.11	0	5,5,5	0.56	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
4	ADP	A	297	5,6	-	0/12/32/32	0/3/3/3
6	MGF	A	300	3,4	-	0/0/0/0	0/0/0/0
8	GOL	A	302	-	-	0/4/4/4	0/0/0/0
8	GOL	A	303	-	-	0/4/4/4	0/0/0/0
8	GOL	A	304	-	-	0/4/4/4	0/0/0/0
8	GOL	A	305	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	16	-	-	0/4/4/4	0/0/0/0
8	GOL	B	3	-	-	0/4/4/4	0/0/0/0
8	GOL	B	6	-	-	0/4/4/4	0/0/0/0
8	GOL	B	8	-	-	0/4/4/4	0/0/0/0
4	ADP	C	297	5,6	-	0/12/32/32	0/3/3/3
6	MGF	C	300	3,4	-	0/0/0/0	0/0/0/0
8	GOL	C	302	-	-	0/4/4/4	0/0/0/0
8	GOL	C	303	-	-	0/4/4/4	0/0/0/0
8	GOL	D	13	-	-	0/4/4/4	0/0/0/0
8	GOL	D	15	-	-	0/4/4/4	0/0/0/0
8	GOL	D	2	-	-	0/4/4/4	0/0/0/0
8	GOL	D	5	-	-	0/4/4/4	0/0/0/0
8	GOL	D	7	-	-	0/4/4/4	0/0/0/0
8	GOL	K	12	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	297	ADP	C5-C4	3.00	1.47	1.40
4	A	297	ADP	C5-C4	3.03	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	297	ADP	N3-C2-N1	-7.54	123.12	128.89
4	C	297	ADP	N3-C2-N1	-6.86	123.64	128.89
4	C	297	ADP	C2'-C1'-N9	-5.00	106.65	114.29
4	A	297	ADP	C2'-C1'-N9	-4.87	106.85	114.29
4	C	297	ADP	C4-C5-N7	-2.86	106.85	109.48
4	A	297	ADP	C4-C5-N7	-2.53	107.16	109.48
4	A	297	ADP	O3A-PA-O5'	-2.25	96.98	102.94
4	A	297	ADP	O3B-PB-O2B	2.02	115.08	107.38
4	C	297	ADP	O3B-PB-O2B	2.27	116.04	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	297	ADP	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	302	GOL	2	0
8	A	303	GOL	4	0
8	A	304	GOL	2	0
8	A	305	GOL	4	0
8	B	1	GOL	2	0
8	B	16	GOL	1	0
8	B	6	GOL	1	0
4	C	297	ADP	2	0
8	C	302	GOL	6	0
8	C	303	GOL	1	0
8	D	13	GOL	2	0
8	D	5	GOL	1	0
8	D	7	GOL	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	297/298 (99%)	0.70	46 (15%) 3 3	25, 45, 106, 163	0
1	C	297/298 (99%)	0.53	30 (10%) 9 10	25, 45, 106, 163	0
2	B	261/261 (100%)	0.55	27 (10%) 9 9	24, 43, 95, 163	0
2	D	261/261 (100%)	0.63	30 (11%) 6 7	27, 48, 96, 163	0
3	J	10/10 (100%)	2.80	7 (70%) 0 0	72, 92, 119, 132	0
3	K	10/10 (100%)	1.25	2 (20%) 1 1	71, 93, 113, 140	0
3	L	4/10 (40%)	2.40	3 (75%) 0 0	65, 71, 75, 82	0
3	M	4/10 (40%)	1.18	1 (25%) 1 1	64, 72, 78, 83	0
All	All	1144/1158 (98%)	0.64	146 (12%) 5 5	24, 46, 106, 163	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	ASP	10.3
2	B	173	ASN	10.2
2	D	173	ASN	9.3
2	B	431	SER	9.0
2	D	172	SER	8.9
2	D	174	GLU	8.1
1	C	38	ASP	7.6
1	C	39	THR	7.5
2	D	175	VAL	7.3
1	A	39	THR	7.1
3	J	7	LEU	6.8
2	B	432	VAL	6.5
2	D	193	CYS	6.3
2	B	193	CYS	5.9
2	D	197	VAL	5.6
3	K	7	LEU	5.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	174	GLU	5.3
1	A	0	HIS	5.1
2	D	432	VAL	5.1
2	B	172	SER	5.0
1	C	14	THR	4.8
2	B	175	VAL	4.5
1	A	295	HIS	4.5
1	C	-1	GLY	4.5
1	C	0	HIS	4.3
2	D	431	SER	4.3
1	A	40	GLU	4.3
1	A	-1	GLY	4.2
2	B	306	LEU	4.0
1	A	8	GLU	4.0
2	D	196	LYS	4.0
1	C	13	GLY	3.9
3	L	4	ALA	3.9
1	C	296	LEU	3.9
1	C	17	VAL	3.8
1	A	17	VAL	3.8
1	A	74	ASN	3.7
2	D	428	GLU	3.7
3	J	-2	PRO	3.7
1	A	225	VAL	3.6
1	A	149	ALA	3.6
2	B	263	LEU	3.6
1	C	15	TYR	3.5
1	A	13	GLY	3.5
1	C	249	SER	3.5
2	D	423	LEU	3.5
3	J	4	ALA	3.4
3	K	-2	PRO	3.4
1	C	16	GLY	3.4
2	D	419	HIS	3.4
1	A	124	LEU	3.3
1	A	49	ILE	3.2
2	D	416	SER	3.2
1	A	296	LEU	3.2
1	A	123	VAL	3.2
3	J	0	THR	3.2
1	A	128	LEU	3.2
1	C	40	GLU	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	52	ILE	3.1
3	L	7	LEU	3.1
2	D	374	GLU	3.1
2	D	415	HIS	3.0
1	A	151	ALA	3.0
1	C	74	ASN	3.0
1	A	47	THR	3.0
1	A	54	LEU	3.0
1	A	143	LEU	3.0
1	A	48	ALA	3.0
1	C	152	PHE	2.9
1	C	288	ASP	2.9
1	A	148	LEU	2.9
2	B	234	LEU	2.9
2	D	424	LEU	2.9
1	A	232	SER	2.9
1	C	37	LEU	2.9
2	D	235	ALA	2.9
1	A	1	MET	2.8
2	B	267	PHE	2.8
1	A	96	LEU	2.8
3	J	2	LYS	2.8
1	A	37	LEU	2.8
2	B	419	HIS	2.8
1	C	151	ALA	2.8
1	A	50	ARG	2.8
1	C	124	LEU	2.7
2	D	328	LYS	2.7
1	A	147	GLY	2.7
1	C	8	GLU	2.7
1	A	53	SER	2.5
3	J	5	LYS	2.5
2	B	262	LEU	2.5
2	D	430	LEU	2.5
2	B	264	ALA	2.5
1	A	15	TYR	2.5
1	A	7	VAL	2.4
1	A	95	ALA	2.4
2	B	299	LEU	2.4
2	D	234	LEU	2.4
2	B	388	LYS	2.4
1	A	150	ARG	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	201	LYS	2.4
1	A	118	CYS	2.4
1	A	55	LEU	2.4
1	A	226	VAL	2.3
2	B	416	SER	2.3
2	B	428	GLU	2.3
1	C	184	VAL	2.3
2	B	310	THR	2.3
1	A	146	PHE	2.3
2	D	310	THR	2.3
2	B	232	LEU	2.3
1	A	19	TYR	2.3
3	J	6	LYS	2.3
1	A	179	TYR	2.3
1	C	41	THR	2.2
1	A	155	PRO	2.2
1	C	118	CYS	2.2
2	D	198	GLY	2.2
2	D	373	PRO	2.2
2	B	197	VAL	2.2
1	C	157	ARG	2.2
2	B	235	ALA	2.2
2	D	350	TYR	2.2
1	A	36	ARG	2.2
2	B	231	THR	2.2
2	D	178	TYR	2.2
1	C	54	LEU	2.1
2	B	265	SER	2.1
2	B	238	TYR	2.1
3	M	7	LEU	2.1
2	D	377	ALA	2.1
1	C	2	GLU	2.1
2	D	381	GLY	2.1
1	C	7	VAL	2.1
1	C	154	VAL	2.1
1	A	9	LYS	2.1
2	B	260	ALA	2.1
1	C	1	MET	2.1
1	A	237	LYS	2.0
2	D	306	LEU	2.0
1	C	178	LYS	2.0
3	L	6	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	415	HIS	2.0
1	C	123	VAL	2.0
2	D	367	VAL	2.0
1	A	46	SER	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	0.94	0.16	-	32,47,65,75	4
1	TPO	A	160	11/12	0.95	0.14	-	32,45,62,73	4

## 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
8	GOL	C	302	6/6	0.71	0.34	10.47	93,99,114,131	0
8	GOL	C	303	6/6	0.87	0.21	6.08	78,87,101,105	0
8	GOL	B	3	6/6	0.91	0.30	3.04	66,75,85,90	0
8	GOL	B	8	6/6	0.94	0.23	2.52	71,72,84,84	0
8	GOL	D	7	6/6	0.81	0.35	2.31	78,85,94,99	0
8	GOL	D	5	6/6	0.91	0.26	2.03	40,69,77,82	0
8	GOL	D	13	6/6	0.95	0.19	1.48	71,81,89,89	0
8	GOL	B	16	6/6	0.96	0.21	1.00	50,75,84,95	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	GOL	D	15	6/6	0.93	0.18	0.86	64,70,77,85	0
8	GOL	B	6	6/6	0.92	0.15	0.41	58,80,93,98	0
8	GOL	K	12	6/6	0.93	0.18	0.30	65,77,85,96	0
8	GOL	A	304	6/6	0.95	0.15	0.28	37,62,73,79	0
8	GOL	D	2	6/6	0.82	0.16	0.14	81,92,100,109	0
8	GOL	A	305	6/6	0.81	0.15	-0.00	78,83,87,91	0
6	MGF	C	300	4/4	0.97	0.22	-0.07	61,64,70,171	0
4	ADP	C	297	27/27	0.93	0.15	-0.18	45,60,78,106	0
4	ADP	A	297	27/27	0.94	0.13	-0.46	53,60,73,104	0
8	GOL	B	1	6/6	0.93	0.18	-0.53	27,63,71,81	0
8	GOL	A	303	6/6	0.94	0.13	-0.73	56,76,86,92	0
8	GOL	A	302	6/6	0.91	0.12	-0.94	69,77,79,86	0
6	MGF	A	300	4/4	0.94	0.13	-1.05	56,67,80,97	0
5	MG	C	299	1/1	0.89	0.08	-1.17	41,41,41,41	0
5	MG	C	298	1/1	0.77	0.08	-1.28	71,71,71,71	0
5	MG	A	298	1/1	0.91	0.04	-2.35	58,58,58,58	0
5	MG	A	299	1/1	0.99	0.05	-4.34	36,36,36,36	0
7	CL	A	301	1/1	0.96	0.07	-	60,60,60,60	0
7	CL	C	301	1/1	0.97	0.09	-	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.