



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:57 PM GMT

PDB ID : 1VYW  
Title : STRUCTURE OF CDK2/CYCLIN A WITH PNU-292137  
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Deposited on : 2004-05-07  
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 (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

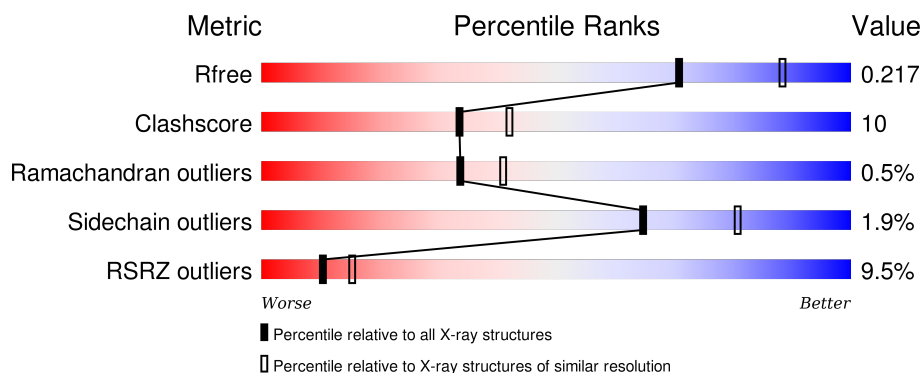
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	309	<div> <div>7%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	C	309	<div> <div>10%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>
2	B	265	<div> <div>11%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>
2	D	265	<div> <div>9%</div> <div>79%</div> <div>16%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	D	1433	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9442 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	302	Total	C	N	O	S	0	0	0
			2427	1579	412	428	8			
1	C	299	Total	C	N	O	S	0	0	0
			2405	1563	409	425	8			

- Molecule 2 is a protein called CYCLIN A2.

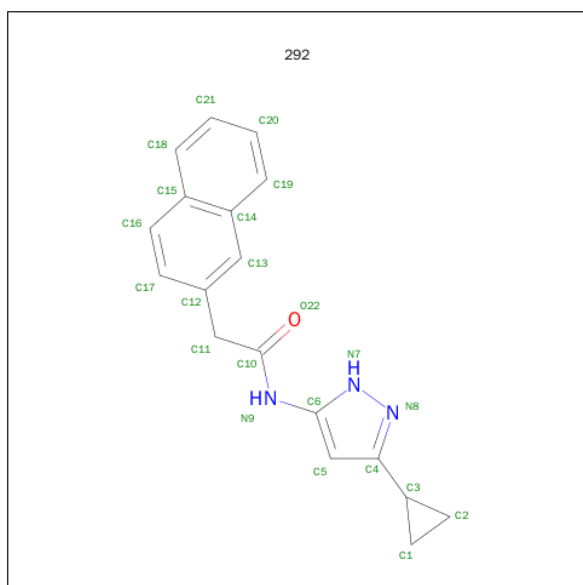
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			
2	D	255	Total	C	N	O	S	0	0	0
			2062	1336	336	379	11			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is N-(3-CYCLOPROPYL-1H-PYRAZOL-5-YL)-2-(2-NAPHTHYL)ACETAMIDE (three-letter code: 292) (formula: C<sub>18</sub>H<sub>17</sub>N<sub>3</sub>O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 22 18 3 1	0	0
4	C	1	Total C N O 22 18 3 1	0	0

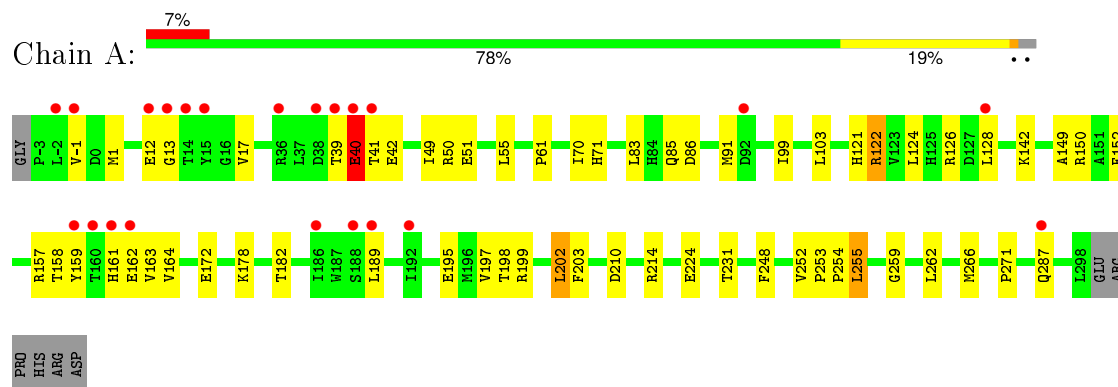
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	153	Total O 153 153	0	0
5	B	66	Total O 66 66	0	0
5	C	55	Total O 55 55	0	0
5	D	136	Total O 136 136	0	0

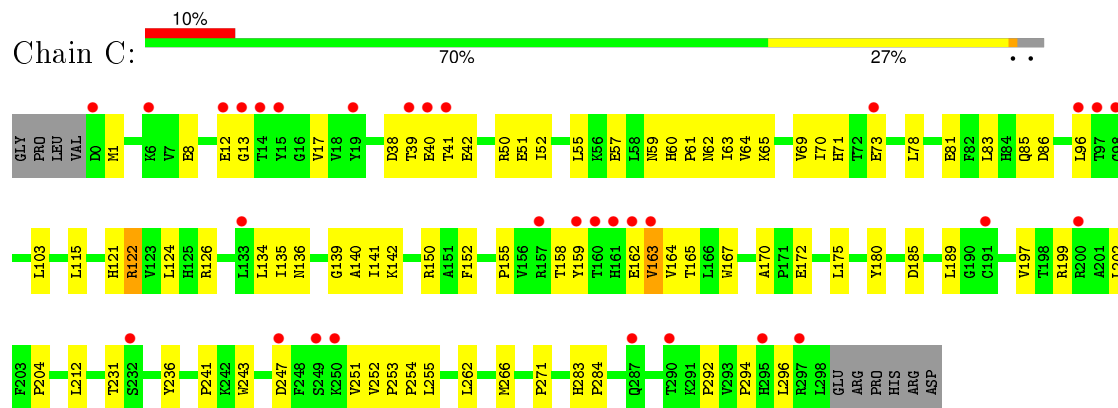
### 3 Residue-property plots [i](#)

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

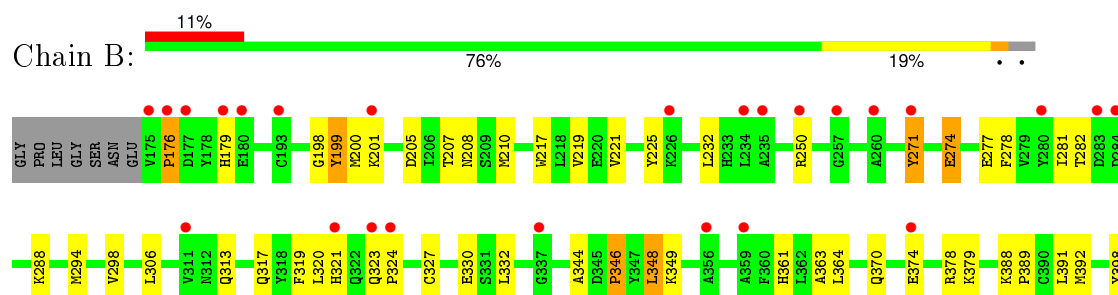
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

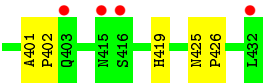


#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

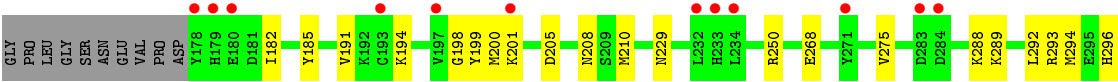
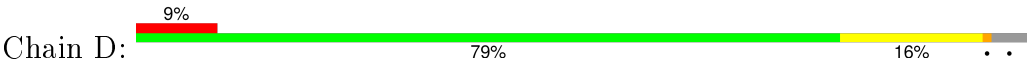


#### • Molecule 2: CYCLIN A2





● Molecule 2: CYCLIN A2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.22Å 184.22Å 214.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.86 – 2.30 29.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.86-2.30) 99.1 (29.86-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.31Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.229 , 0.258 0.231 , 0.217	Depositor DCC
$R_{free}$ test set	1869 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 179325 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: 292, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.37	0/2490	0.62	0/3381
1	C	0.33	0/2467	0.59	0/3349
2	B	0.33	0/2134	0.55	0/2897
2	D	0.38	0/2111	0.58	0/2864
All	All	0.35	0/9202	0.59	0/12491

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	2427	0	2481	53	0
1	C	2405	0	2454	61	0
2	B	2084	0	2107	42	0
2	D	2062	0	2087	41	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	22	0	17	1	0
4	C	22	0	17	2	0
5	A	153	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	66	0	0	2	0
5	C	55	0	0	1	0
5	D	136	0	0	3	0
All	All	9442	0	9163	185	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 10.

All (185) 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:C:163:VAL:HG23	1:C:164:VAL:H	1.33	0.92
2:D:323:GLN:HB2	2:D:324:PRO:HD3	1.54	0.86
1:C:83:LEU:H	4:C:2300:292:H7	1.23	0.84
1:C:163:VAL:HG21	1:C:180:TYR:OH	1.82	0.80
2:D:323:GLN:HE21	2:D:324:PRO:HD3	1.47	0.79
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.64	0.78
2:D:323:GLN:NE2	2:D:323:GLN:H	1.82	0.77
1:A:83:LEU:H	4:A:2300:292:H7	1.31	0.77
1:A:126:ARG:O	1:A:164:VAL:HG22	1.85	0.77
1:A:262:LEU:HG	1:A:266:MET:CE	2.17	0.73
2:B:346:PRO:HB2	2:B:349:LYS:HE2	1.70	0.72
1:A:262:LEU:HG	1:A:266:MET:HE1	1.69	0.72
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.53	0.72
1:A:172:GLU:HG2	1:A:271:PRO:HG3	1.75	0.68
1:A:158:THR:HG21	5:A:2092:HOH:O	1.91	0.68
1:C:51:GLU:O	1:C:55:LEU:HB2	1.94	0.68
1:C:61:PRO:O	1:C:142:LYS:HE2	1.96	0.66
2:D:275:VAL:HG21	2:D:292:LEU:HD21	1.77	0.66
2:B:321:HIS:NE2	2:B:379:LYS:HD2	2.10	0.66
2:D:321:HIS:NE2	2:D:379:LYS:HD2	2.12	0.65
2:D:346:PRO:O	2:D:349:LYS:HG2	1.97	0.65
2:B:205:ASP:OD2	2:B:250:ARG:HG3	1.97	0.65
2:D:374:GLU:HG3	2:D:378:ARG:NH1	2.11	0.65
1:A:-1:VAL:HG11	2:D:296:HIS:CE1	2.34	0.63
2:D:344:ALA:O	2:D:348:LEU:HB2	1.99	0.62
2:D:198:GLY:O	2:D:201:LYS:HG2	1.99	0.62
1:C:126:ARG:O	1:C:164:VAL:HG22	2.00	0.62
1:C:262:LEU:HG	1:C:266:MET:HE2	1.81	0.62
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.36	0.61
1:C:262:LEU:HG	1:C:266:MET:CE	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:LYS:O	2:D:293:ARG:HG3	2.01	0.60
2:B:278:PHE:O	2:B:282:THR:HG23	2.01	0.60
1:C:12:GLU:HG2	1:C:17:VAL:HG13	1.82	0.60
1:A:51:GLU:O	1:A:55:LEU:HB2	2.01	0.60
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.36	0.60
1:A:121:HIS:O	1:A:122:ARG:HG3	2.01	0.60
1:A:210:ASP:O	1:A:214:ARG:HG2	2.02	0.60
1:C:163:VAL:HG23	1:C:164:VAL:N	2.12	0.60
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.18	0.58
2:B:346:PRO:O	2:B:349:LYS:HG2	2.04	0.58
1:C:158:THR:HA	1:C:180:TYR:CE2	2.38	0.58
2:D:210:MET:HE1	2:D:250:ARG:HG2	1.86	0.57
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.86	0.57
1:A:41:THR:HB	2:B:288:LYS:NZ	2.19	0.57
1:A:126:ARG:NH2	1:A:150:ARG:HD2	2.20	0.57
1:C:170:ALA:HB1	1:C:172:GLU:OE2	2.05	0.56
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.40	0.56
1:C:155:PRO:HD3	2:D:316:THR:HG21	1.86	0.56
2:B:176:PRO:HD2	2:B:179:HIS:HD2	1.70	0.56
2:D:194:LYS:HE2	5:D:2093:HOH:O	2.06	0.56
2:B:198:GLY:O	2:B:201:LYS:HG2	2.06	0.55
1:A:50:ARG:NH1	1:A:150:ARG:NH2	2.54	0.55
1:A:197:VAL:CG1	1:A:254:PRO:HG2	2.37	0.55
2:B:200:MET:HG2	2:B:208:ASN:ND2	2.21	0.55
1:C:163:VAL:CG2	1:C:164:VAL:H	2.09	0.54
2:B:294:MET:O	2:B:298:VAL:HG23	2.07	0.54
1:C:70:ILE:N	1:C:70:ILE:HD12	2.22	0.54
2:B:179:HIS:NE2	2:B:320:LEU:HD12	2.22	0.54
1:A:126:ARG:CZ	1:A:150:ARG:HD2	2.37	0.54
1:C:1:MET:HE2	1:C:70:ILE:HG12	1.91	0.54
2:B:207:THR:OG1	2:B:210:MET:HG3	2.08	0.53
1:A:149:ALA:O	1:A:150:ARG:HG3	2.08	0.53
2:D:414:LYS:HE2	2:D:423:LEU:HD21	1.90	0.53
2:D:388:LYS:O	2:D:392:MET:HG2	2.08	0.53
1:C:165:THR:HG22	5:C:2037:HOH:O	2.09	0.53
2:D:289:LYS:HD3	5:D:2073:HOH:O	2.08	0.52
1:C:62:ASN:HA	1:C:142:LYS:HG2	1.92	0.52
2:D:205:ASP:OD1	2:D:250:ARG:NH1	2.43	0.52
1:C:134:LEU:O	1:C:141:ILE:HA	2.10	0.52
1:A:159:TYR:HH	2:B:271:TYR:HD2	1.57	0.52
1:C:139:GLY:HA2	1:C:294:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:GLU:HG3	2:B:378:ARG:NH1	2.25	0.52
2:D:323:GLN:HB2	2:D:324:PRO:CD	2.35	0.52
1:A:262:LEU:HG	1:A:266:MET:HE2	1.92	0.51
2:B:205:ASP:OD1	2:B:250:ARG:NH1	2.44	0.51
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.92	0.51
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.91	0.51
2:D:205:ASP:OD2	2:D:250:ARG:HG3	2.10	0.51
1:A:159:TYR:CE2	1:A:162:GLU:HG3	2.45	0.51
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.93	0.51
1:C:39:THR:O	1:C:39:THR:HG22	2.12	0.50
1:C:38:ASP:HB3	1:C:42:GLU:HB3	1.94	0.50
1:A:12:GLU:OE2	1:A:17:VAL:HG22	2.12	0.49
1:C:69:VAL:C	1:C:70:ILE:HD12	2.33	0.49
1:A:159:TYR:CD2	1:A:162:GLU:HG3	2.47	0.49
1:A:157:ARG:HH12	1:A:178:LYS:HE2	1.78	0.49
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.94	0.49
1:C:57:GLU:HG2	2:D:185:TYR:OH	2.13	0.48
1:A:40:GLU:OE1	1:A:40:GLU:N	2.46	0.48
1:A:202:LEU:HD13	1:A:203:PHE:CZ	2.48	0.48
1:A:39:THR:HG22	1:A:39:THR:O	2.13	0.48
1:C:241:PRO:HB2	1:C:243:TRP:CZ3	2.49	0.47
1:C:197:VAL:CG1	1:C:254:PRO:HG2	2.44	0.47
1:A:-1:VAL:HG13	1:C:73:GLU:OE2	2.15	0.47
1:C:8:GLU:OE2	4:C:2300:292:H20	2.15	0.47
1:C:167:TRP:CD1	1:C:204:PRO:HA	2.50	0.47
1:A:85:GLN:HG3	1:A:86:ASP:N	2.29	0.47
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.50	0.47
1:A:12:GLU:HG3	1:A:13:GLY:H	1.79	0.46
2:D:200:MET:HG2	2:D:208:ASN:ND2	2.30	0.46
1:C:1:MET:CE	1:C:70:ILE:HG12	2.46	0.46
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.50	0.46
1:A:287:GLN:HB3	5:A:2142:HOH:O	2.15	0.46
1:A:41:THR:HB	2:B:288:LYS:HZ1	1.81	0.46
1:C:197:VAL:HG11	1:C:255:LEU:HD13	1.98	0.46
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.97	0.46
2:B:313:GLN:O	2:B:317:GLN:HG2	2.16	0.46
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.97	0.46
2:D:191:VAL:O	2:D:191:VAL:HG12	2.16	0.46
1:A:1:MET:HE2	1:A:70:ILE:HG12	1.98	0.46
1:A:50:ARG:HH12	1:A:150:ARG:NH2	2.14	0.45
2:B:319:PHE:CE2	2:B:330:GLU:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.98	0.45
2:D:229:ASN:HD22	2:D:334:MET:CE	2.30	0.45
1:C:40:GLU:HG3	1:C:41:THR:HG23	1.96	0.45
1:A:121:HIS:C	1:A:122:ARG:HG3	2.37	0.45
2:D:371:SER:O	2:D:372:TRP:C	2.54	0.45
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.52	0.45
2:D:346:PRO:HB2	2:D:349:LYS:HE2	1.98	0.45
2:B:217:TRP:O	2:B:221:VAL:HG23	2.16	0.45
2:B:210:MET:CE	2:B:250:ARG:HG2	2.47	0.45
2:B:327:CYS:HB3	2:B:419:HIS:NE2	2.32	0.44
2:B:274:GLU:HG2	2:B:277:GLU:HG2	1.99	0.44
2:D:319:PHE:CE2	2:D:330:GLU:HG2	2.53	0.44
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.82	0.44
1:C:121:HIS:O	1:C:122:ARG:HG3	2.18	0.44
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.53	0.44
1:C:175:LEU:HD21	1:C:212:LEU:HD21	2.00	0.44
2:D:334:MET:HE2	5:D:2082:HOH:O	2.18	0.44
1:A:71:HIS:CD2	5:B:2038:HOH:O	2.69	0.44
1:C:12:GLU:HB3	1:C:13:GLY:H	1.64	0.43
1:A:124:LEU:HD21	1:A:182:THR:HA	2.00	0.43
1:A:40:GLU:HG2	1:A:42:GLU:H	1.83	0.43
2:B:219:VAL:HG22	2:B:232:LEU:HD21	2.00	0.43
2:D:191:VAL:O	2:D:191:VAL:CG1	2.65	0.43
2:B:199:TYR:CD1	2:B:199:TYR:C	2.91	0.43
2:B:398:TYR:CE1	2:B:426:PRO:HG3	2.54	0.43
1:A:128:LEU:HD13	1:A:189:LEU:HD13	2.00	0.43
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.53	0.43
2:B:348:LEU:HD12	2:B:348:LEU:HA	1.81	0.43
1:C:40:GLU:O	2:D:288:LYS:HD2	2.19	0.43
1:C:121:HIS:C	1:C:122:ARG:HG3	2.39	0.43
2:D:323:GLN:HE21	2:D:324:PRO:CD	2.25	0.43
1:A:159:TYR:CE2	1:A:161:HIS:HB2	2.54	0.43
1:A:159:TYR:CZ	1:A:161:HIS:HB2	2.54	0.42
2:D:199:TYR:CD1	2:D:199:TYR:C	2.93	0.42
1:A:252:VAL:N	1:A:253:PRO:HD3	2.35	0.42
2:D:323:GLN:H	2:D:323:GLN:CD	2.23	0.42
1:C:60:HIS:ND1	1:C:61:PRO:HD2	2.35	0.42
1:A:124:LEU:CD2	1:A:182:THR:HA	2.49	0.42
2:B:425:ASN:HA	2:B:426:PRO:HD3	1.89	0.42
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.49	0.42
2:D:388:LYS:HB3	2:D:389:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:THR:O	1:A:199:ARG:HB2	2.19	0.42
2:B:364:LEU:HG	2:B:370:GLN:HB2	2.02	0.42
1:A:159:TYR:HD2	1:A:162:GLU:HB2	1.85	0.42
1:A:71:HIS:HD2	5:B:2038:HOH:O	2.01	0.42
1:C:65:LYS:H	1:C:81:GLU:HG2	1.84	0.42
1:C:85:GLN:HG3	1:C:86:ASP:N	2.35	0.42
1:C:50:ARG:NH1	1:C:150:ARG:NH2	2.68	0.42
1:A:91:MET:HE1	1:A:195:GLU:HG2	2.01	0.41
1:A:61:PRO:O	1:A:142:LYS:HE2	2.19	0.41
2:B:323:GLN:HB2	2:B:324:PRO:HD3	2.01	0.41
2:B:323:GLN:N	2:B:324:PRO:HD2	2.35	0.41
1:C:63:ILE:O	1:C:64:VAL:C	2.59	0.41
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.55	0.41
1:C:150:ARG:HH22	2:D:268:GLU:C	2.24	0.41
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.82	0.41
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.29	0.41
1:C:159:TYR:HB2	1:C:163:VAL:HG13	2.03	0.41
2:D:330:GLU:O	2:D:334:MET:HG2	2.21	0.41
1:C:135:ILE:HD12	1:C:296:LEU:HD21	2.01	0.41
1:C:247:ASP:O	1:C:251:VAL:HG23	2.21	0.41
2:B:281:ILE:HD12	2:B:281:ILE:C	2.41	0.41
2:D:294:MET:O	2:D:298:VAL:HG23	2.21	0.41
1:C:103:LEU:HD13	1:C:292:PRO:HB2	2.03	0.41
1:C:172:GLU:HG2	1:C:271:PRO:HG3	2.02	0.40
2:B:374:GLU:HG3	2:B:378:ARG:HH11	1.85	0.40
1:A:159:TYR:CE1	2:B:271:TYR:CE2	3.09	0.40
1:C:189:LEU:HA	1:C:189:LEU:HD12	1.92	0.40
1:C:164:VAL:O	1:C:165:THR:C	2.59	0.40
1:C:152:PHE:CE2	2:D:182:ILE:HD11	2.55	0.40
2:B:388:LYS:O	2:B:392:MET:HG2	2.22	0.40
1:A:99:ILE:HG23	1:A:103:LEU:HD23	2.04	0.40
1:C:115:LEU:HD21	1:C:185:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

## 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%)	292 (97%)	7 (2%)	1 (0%)	46	57
1	C	297/309 (96%)	283 (95%)	11 (4%)	3 (1%)	19	21
2	B	256/265 (97%)	247 (96%)	8 (3%)	1 (0%)	39	48
2	D	253/265 (96%)	247 (98%)	6 (2%)	0	100	100
All	All	1106/1148 (96%)	1069 (97%)	32 (3%)	5 (0%)	34	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	GLU
1	A	40	GLU
1	C	96	LEU
1	C	163	VAL
2	B	176	PRO

### 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	267/273 (98%)	261 (98%)	6 (2%)	60	77
1	C	264/273 (97%)	258 (98%)	6 (2%)	58	75
2	B	232/237 (98%)	227 (98%)	5 (2%)	60	77
2	D	229/237 (97%)	227 (99%)	2 (1%)	84	93
All	All	992/1020 (97%)	973 (98%)	19 (2%)	65	81

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

Mol	Chain	Res	Type
1	A	40	GLU

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Mol	Chain	Res	Type
1	A	122	ARG
1	A	163	VAL
1	A	202	LEU
1	A	248	PHE
1	A	255	LEU
2	B	199	TYR
2	B	271	TYR
2	B	274	GLU
2	B	346	PRO
2	B	348	LEU
1	C	59	ASN
1	C	71	HIS
1	C	122	ARG
1	C	199	ARG
1	C	202	LEU
1	C	252	VAL
2	D	323	GLN
2	D	346	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	295	HIS
2	B	208	ASN
2	B	322	GLN
2	B	425	ASN
1	C	59	ASN
2	D	208	ASN
2	D	229	ASN
2	D	296	HIS
2	D	322	GLN
2	D	323	GLN
2	D	396	GLN
2	D	425	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 ⓘ

4 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	$\# Z  > 2$
3	SO4	A	1300	-	4,4,4	1.47	0	6,6,6	0.23	0
4	292	A	2300	-	24,25,25	1.80	9 (37%)	31,35,35	1.12	4 (12%)
4	292	C	2300	-	24,25,25	1.85	8 (33%)	31,35,35	1.17	4 (12%)
3	SO4	D	1433	-	4,4,4	1.12	0	6,6,6	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	SO4	A	1300	-	-	0/0/0/0	0/0/0/0
4	292	A	2300	-	-	0/10/14/14	0/3/4/4
4	292	C	2300	-	-	0/10/14/14	0/3/4/4
3	SO4	D	1433	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2300	292	C17-C12	2.13	1.43	1.38
4	A	2300	292	C6-N7	2.15	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2300	292	C17-C12	2.18	1.43	1.38
4	A	2300	292	C13-C12	2.19	1.42	1.37
4	C	2300	292	C21-C18	2.34	1.42	1.36
4	C	2300	292	C20-C19	2.40	1.42	1.36
4	C	2300	292	C16-C17	2.40	1.41	1.36
4	A	2300	292	C16-C17	2.43	1.41	1.36
4	A	2300	292	C21-C18	2.58	1.42	1.36
4	A	2300	292	C20-C19	2.67	1.42	1.36
4	C	2300	292	C6-N9	2.88	1.46	1.40
4	A	2300	292	C6-N9	2.97	1.46	1.40
4	C	2300	292	C15-C14	2.98	1.49	1.42
4	C	2300	292	C6-N7	3.03	1.39	1.34
4	A	2300	292	C4-N8	3.17	1.38	1.33
4	A	2300	292	C15-C14	3.32	1.50	1.42
4	C	2300	292	C4-N8	3.85	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2300	292	C2-C3-C4	-2.98	116.79	120.09
4	C	2300	292	C2-C3-C4	-2.87	116.91	120.09
4	A	2300	292	C5-C4-N8	-2.23	107.42	110.34
4	C	2300	292	C5-C4-N8	-2.10	107.59	110.34
4	A	2300	292	C3-C4-N8	2.16	123.77	120.24
4	C	2300	292	C3-C4-N8	2.37	124.10	120.24
4	A	2300	292	C6-N9-C10	2.62	132.39	128.09
4	C	2300	292	C6-N9-C10	3.01	133.03	128.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2300	292	1	0
4	C	2300	292	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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%)	0.33	22 (7%) 18 25	28, 39, 71, 85	0
1	C	299/309 (96%)	0.65	31 (10%) 8 12	34, 54, 74, 86	0
2	B	258/265 (97%)	0.57	29 (11%) 7 10	34, 49, 71, 86	0
2	D	255/265 (96%)	0.31	24 (9%) 11 16	28, 37, 64, 86	0
All	All	1114/1148 (97%)	0.47	106 (9%) 10 15	28, 45, 72, 86	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	323	GLN	11.0
1	A	161	HIS	8.5
2	B	323	GLN	8.0
1	C	96	LEU	7.6
1	C	15	TYR	7.3
1	C	161	HIS	7.2
2	B	175	VAL	7.2
2	B	324	PRO	6.8
1	C	159	TYR	6.4
1	A	15	TYR	6.4
1	A	159	TYR	6.2
1	C	13	GLY	6.0
2	D	193	CYS	5.9
1	C	160	THR	5.6
1	A	39	THR	5.6
1	C	162	GLU	5.6
2	B	271	TYR	5.4
1	A	13	GLY	5.4
1	A	40	GLU	5.3
1	A	162	GLU	5.3
2	D	324	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	14	THR	5.2
1	C	14	THR	5.2
2	B	432	LEU	5.1
1	C	297	ARG	4.8
1	A	38	ASP	4.7
2	B	177	ASP	4.7
1	C	40	GLU	4.6
1	C	163	VAL	4.5
1	A	-2	LEU	4.4
1	A	41	THR	4.3
1	C	250	LYS	4.2
1	C	287	GLN	4.1
2	D	178	TYR	3.9
2	D	311	VAL	3.9
1	C	97	THR	3.9
2	B	283	ASP	3.9
1	C	295	HIS	3.8
2	B	284	ASP	3.7
1	A	189	LEU	3.5
1	A	36	ARG	3.4
2	B	235	ALA	3.4
2	B	179	HIS	3.3
2	D	179	HIS	3.3
2	B	176	PRO	3.2
1	C	39	THR	3.1
1	C	19	TYR	3.1
2	B	180	GLU	3.0
2	B	311	VAL	3.0
1	C	247	ASP	2.9
1	A	287	GLN	2.9
1	A	-1	VAL	2.9
2	D	271	TYR	2.9
1	C	249	SER	2.9
2	B	280	TYR	2.9
1	A	12	GLU	2.8
1	A	188	SER	2.8
1	C	133	LEU	2.7
1	C	0	ASP	2.7
1	C	73	GLU	2.7
2	B	260	ALA	2.6
2	D	325	ALA	2.6
2	B	403	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	200	ARG	2.5
2	B	201	LYS	2.5
2	B	226	LYS	2.5
1	C	41	THR	2.5
2	D	180	GLU	2.5
1	C	290	THR	2.5
1	C	12	GLU	2.5
2	D	201	LYS	2.4
1	A	186	ILE	2.4
2	B	415	ASN	2.4
2	D	283	ASP	2.4
1	A	192	ILE	2.4
2	B	193	CYS	2.4
2	D	284	ASP	2.3
2	D	233	HIS	2.3
2	D	359	ALA	2.3
2	D	232	LEU	2.3
2	D	327	CYS	2.3
1	C	98	GLY	2.3
2	B	416	SER	2.3
2	D	356	ALA	2.2
1	C	232	SER	2.2
2	B	257	GLY	2.2
2	B	250	ARG	2.2
2	D	197	VAL	2.2
2	D	340	SER	2.2
1	C	157	ARG	2.1
2	B	374	GLU	2.1
2	D	431	ASN	2.1
1	A	128	LEU	2.1
2	B	321	HIS	2.1
2	B	359	ALA	2.1
2	D	337	GLY	2.1
1	C	6	LYS	2.1
2	D	341	LEU	2.1
1	C	191	CYS	2.1
2	B	356	ALA	2.1
1	A	92	ASP	2.1
2	B	234	LEU	2.0
2	D	234	LEU	2.0
2	B	337	GLY	2.0
1	A	160	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	428	GLU	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. 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	SO4	D	1433	5/5	0.95	0.20	5.82	82,82,83,83	0
4	292	C	2300	22/22	0.89	0.16	-0.19	43,52,56,57	0
4	292	A	2300	22/22	0.97	0.12	-0.38	30,35,41,41	0
3	SO4	A	1300	5/5	0.93	0.23	-	83,83,84,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.