



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:15 pm BST

PDB ID : 2PK9  
Title : Structure of the Pho85-Pho80 CDK-cyclin Complex of the Phosphate-responsive Signal Transduction Pathway  
Authors : Huang, K.; Ferrin-O'Connell, I.; Zhang, W.; Leonard, G.A.; O'Shea, E.K.; Quioco, F.A.  
Deposited on : 2007-04-17  
Resolution : 2.91 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

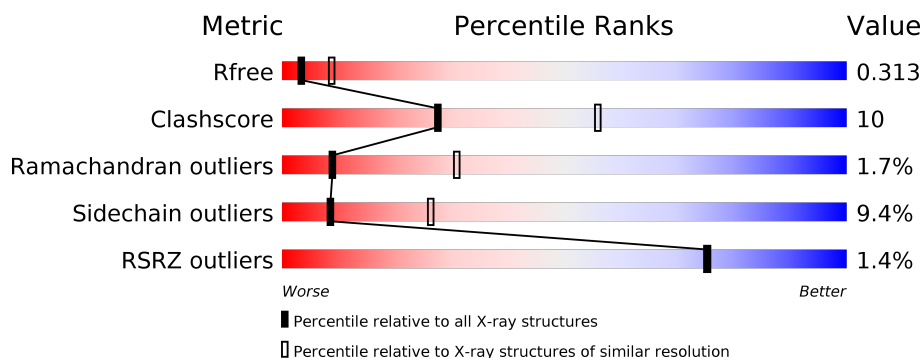
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 respectively. 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	317	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>24%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	317	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>
2	B	293	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>21%</div> <div>•</div> <div>27%</div> </div> </div>
2	D	293	<div> <div>%</div> <div> <div></div> <div>50%</div> <div>21%</div> <div>•</div> <div>25%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8018 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 Cyclin-dependent protein kinase PHO85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	63	0	0
			2329	1501	398	419	11			
1	C	266	Total	C	N	O	S	44	0	0
			2159	1396	368	384	11			

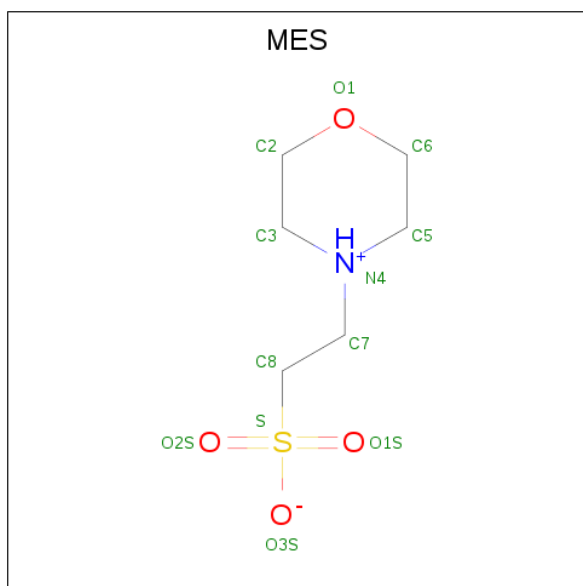
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	MET	-	EXPRESSION TAG	UNP P17157
A	307	GLY	-	EXPRESSION TAG	UNP P17157
A	308	GLY	-	EXPRESSION TAG	UNP P17157
A	309	SER	-	EXPRESSION TAG	UNP P17157
A	310	ARG	-	EXPRESSION TAG	UNP P17157
A	311	SER	-	EXPRESSION TAG	UNP P17157
A	312	HIS	-	EXPRESSION TAG	UNP P17157
A	313	HIS	-	EXPRESSION TAG	UNP P17157
A	314	HIS	-	EXPRESSION TAG	UNP P17157
A	315	HIS	-	EXPRESSION TAG	UNP P17157
A	316	HIS	-	EXPRESSION TAG	UNP P17157
A	317	HIS	-	EXPRESSION TAG	UNP P17157
C	306	MET	-	EXPRESSION TAG	UNP P17157
C	307	GLY	-	EXPRESSION TAG	UNP P17157
C	308	GLY	-	EXPRESSION TAG	UNP P17157
C	309	SER	-	EXPRESSION TAG	UNP P17157
C	310	ARG	-	EXPRESSION TAG	UNP P17157
C	311	SER	-	EXPRESSION TAG	UNP P17157
C	312	HIS	-	EXPRESSION TAG	UNP P17157
C	313	HIS	-	EXPRESSION TAG	UNP P17157
C	314	HIS	-	EXPRESSION TAG	UNP P17157
C	315	HIS	-	EXPRESSION TAG	UNP P17157
C	316	HIS	-	EXPRESSION TAG	UNP P17157
C	317	HIS	-	EXPRESSION TAG	UNP P17157

- Molecule 2 is a protein called PHO85 cyclin PHO80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	7	0	0
			1730	1113	300	310	7			
2	D	219	Total	C	N	O	S	21	0	0
			1776	1142	307	320	7			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).

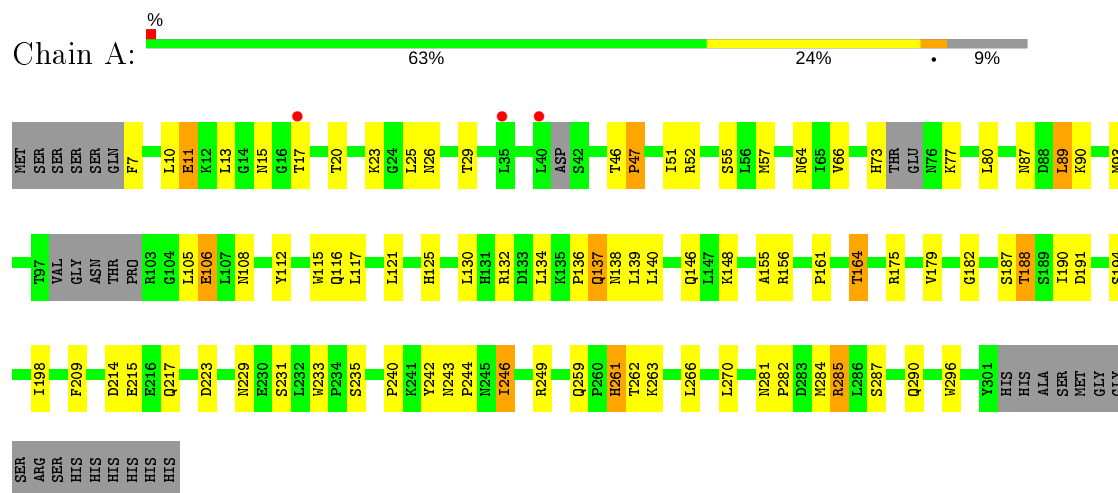


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

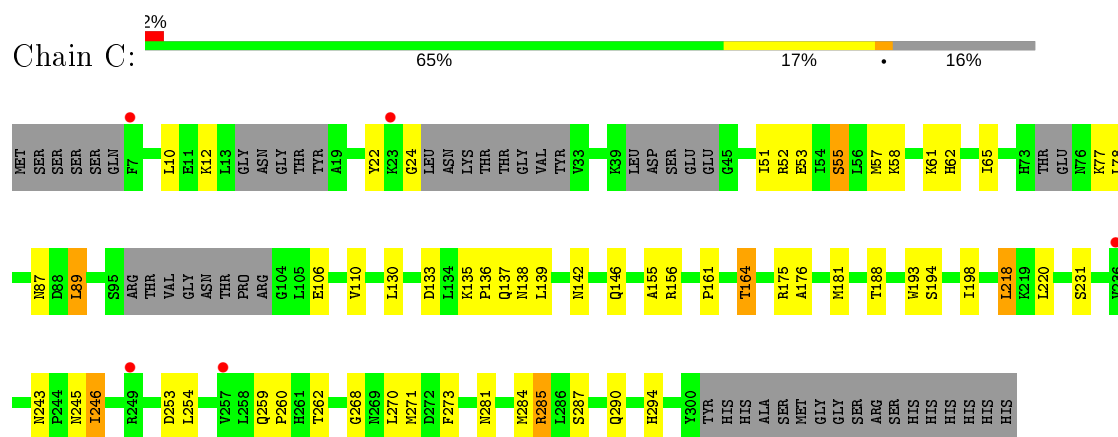
### 3 Residue-property plots [i](#)

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.

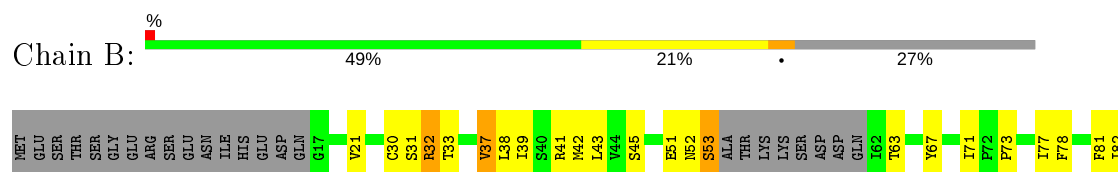
#### • Molecule 1: Cyclin-dependent protein kinase PHO85

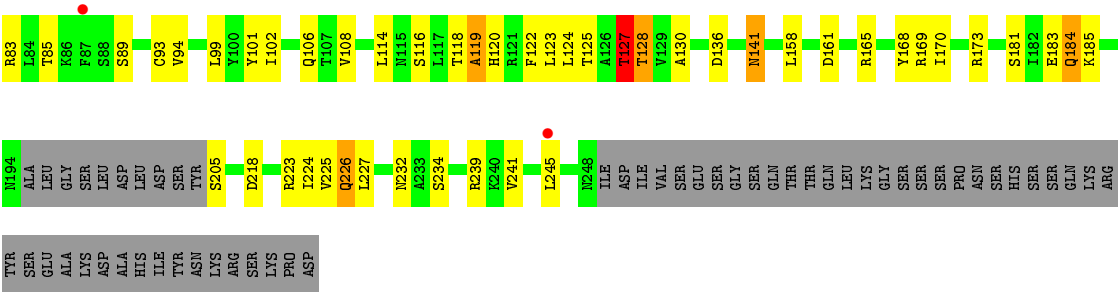


#### • Molecule 1: Cyclin-dependent protein kinase PHO85

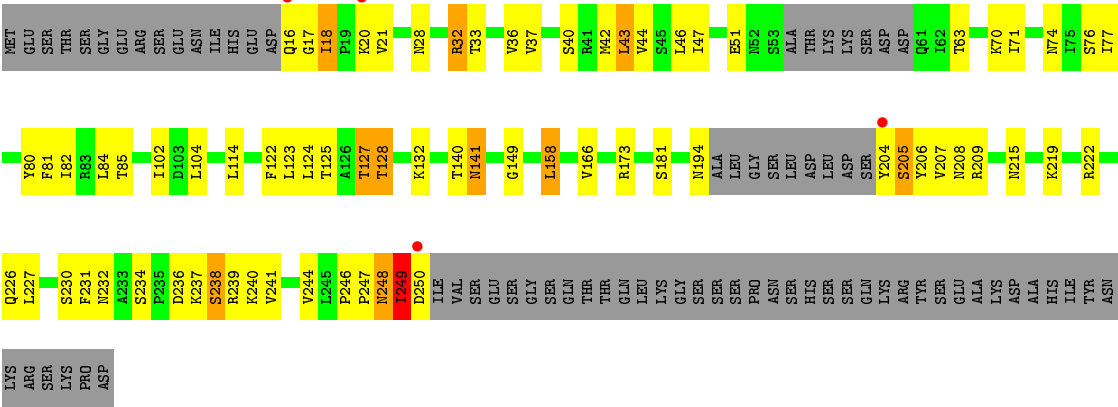


#### • Molecule 2: PHO85 cyclin PHO80





● Molecule 2: PHO85 cyclin PHO80



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.78Å 147.78Å 211.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.03 – 2.91 15.03 – 2.91	Depositor EDS
% Data completeness (in resolution range)	88.5 (15.03-2.91) 88.5 (15.03-2.91)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2, CNS 1.1	Depositor
R, $R_{free}$	0.281 , 0.315 0.278 , 0.313	Depositor DCC
$R_{free}$ test set	2622 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 20.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	8018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: MES

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	0.48	1/2382 (0.0%)	0.62	1/3220 (0.0%)
1	C	0.43	1/2207 (0.0%)	0.59	2/2980 (0.1%)
2	B	0.44	0/1765	0.58	0/2391
2	D	0.46	1/1811 (0.1%)	0.70	3/2452 (0.1%)
All	All	0.45	3/8165 (0.0%)	0.62	6/11043 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	261	HIS	CB-CG	-7.93	1.35	1.50
2	D	250	ASP	CB-CG	-5.66	1.39	1.51
1	C	24	GLY	C-O	5.18	1.31	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	250	ASP	CB-CG-OD2	12.03	129.13	118.30
2	D	250	ASP	CB-CG-OD1	-12.02	107.49	118.30
1	C	22	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	C	22	TYR	CB-CG-CD1	7.03	125.22	121.00
1	A	263	LYS	CA-CB-CG	-5.47	101.36	113.40
2	D	248	ASN	CB-CA-C	5.06	120.52	110.40

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	2329	0	2356	54	1
1	C	2159	0	2191	32	0
2	B	1730	0	1777	35	0
2	D	1776	0	1816	45	1
3	B	12	0	12	1	0
3	D	12	0	12	1	0
All	All	8018	0	8164	159	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 10.

All (159) 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:16:GLN:C	2:D:17:GLY:HA2	1.84	0.97
2:B:106:GLN:HE21	2:B:114:LEU:H	1.20	0.88
2:B:73:PRO:HG2	2:B:120:HIS:HD2	1.42	0.85
2:D:222:ARG:HG3	2:D:222:ARG:HH21	1.45	0.82
2:B:73:PRO:HG2	2:B:120:HIS:CD2	2.15	0.81
2:D:104:LEU:HD21	2:D:166:VAL:HG11	1.62	0.80
2:D:16:GLN:C	2:D:17:GLY:CA	2.49	0.80
2:B:38:LEU:HB3	2:B:224:ILE:HD12	1.65	0.77
1:C:176:ALA:HB1	1:C:285:ARG:HH22	1.50	0.77
2:D:124:LEU:O	2:D:128:THR:HG23	1.84	0.77
1:C:287:SER:H	1:C:290:GLN:HE21	1.35	0.75
2:D:44:VAL:HG12	2:D:77:ILE:HG21	1.67	0.75
1:A:194:SER:O	1:A:198:ILE:HG12	1.87	0.74
1:A:51:ILE:O	1:A:55:SER:HB2	1.89	0.72
2:B:106:GLN:NE2	2:B:114:LEU:H	1.90	0.69
2:B:102:ILE:HG13	2:B:122:PHE:CE2	2.28	0.69
2:D:16:GLN:C	2:D:17:GLY:N	2.46	0.69
1:A:57:MET:HA	1:A:57:MET:CE	2.24	0.68
2:D:44:VAL:CG1	2:D:77:ILE:HG21	2.24	0.68
1:A:121:LEU:HD13	1:A:134:LEU:HD11	1.74	0.67
2:B:124:LEU:O	2:B:128:THR:HG23	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:LEU:O	2:D:127:THR:HB	1.94	0.67
1:A:130:LEU:HD22	1:A:188:THR:HA	1.78	0.66
1:A:259:GLN:HE22	1:A:266:LEU:H	1.42	0.65
2:B:94:VAL:HG13	2:B:130:ALA:HB3	1.79	0.65
1:A:10:LEU:O	1:A:11:GLU:CB	2.43	0.65
1:C:193:TRP:HB2	1:C:285:ARG:HH21	1.62	0.64
1:A:287:SER:H	1:A:290:GLN:HE21	1.44	0.64
1:A:52:ARG:HD3	1:A:155:ALA:O	1.97	0.63
1:A:10:LEU:O	1:A:11:GLU:HB2	1.98	0.63
1:A:90:LYS:HB2	1:A:136:PRO:HB2	1.80	0.62
1:A:116:GLN:HE22	1:A:146:GLN:HA	1.64	0.62
1:A:243:ASN:HB2	2:D:71:ILE:HD12	1.83	0.61
1:C:89:LEU:HD12	1:C:139:LEU:HD12	1.82	0.60
1:A:64:ASN:HA	1:A:148:LYS:HG2	1.84	0.60
1:C:89:LEU:HB3	1:C:136:PRO:HB3	1.83	0.60
2:B:101:TYR:OH	2:B:170:ILE:HB	2.02	0.59
1:C:281:ASN:HD22	1:C:284:MET:HG2	1.68	0.59
2:D:149:GLY:HA3	3:D:294:MES:O1S	2.04	0.57
1:A:209:PHE:HB2	1:A:217:GLN:HE22	1.69	0.57
1:A:26:ASN:HB3	1:A:29:THR:O	2.04	0.57
1:C:176:ALA:HB1	1:C:285:ARG:NH2	2.17	0.57
2:D:207:VAL:O	2:D:208:ASN:HB2	2.05	0.57
1:A:242:TYR:HB3	2:D:74:ASN:HD22	1.69	0.56
1:C:51:ILE:O	1:C:55:SER:HB3	2.06	0.56
1:C:53:GLU:O	1:C:57:MET:HG2	2.06	0.56
2:B:225:VAL:HG11	2:B:245:LEU:HB2	1.87	0.56
2:D:104:LEU:HD21	2:D:166:VAL:CG1	2.32	0.56
1:A:229:ASN:OD1	1:A:231:SER:HB3	2.05	0.56
1:C:194:SER:O	1:C:198:ILE:HG12	2.06	0.56
2:B:33:THR:O	2:B:37:VAL:HG13	2.06	0.55
1:A:161:PRO:HG2	2:B:93:CYS:SG	2.46	0.55
1:C:52:ARG:HD3	1:C:155:ALA:O	2.07	0.55
2:D:18:ILE:HG22	2:D:240:LYS:HG2	1.87	0.55
2:D:36:VAL:HG12	2:D:36:VAL:O	2.07	0.55
2:B:73:PRO:CG	2:B:120:HIS:HD2	2.19	0.54
1:A:209:PHE:HB2	1:A:217:GLN:NE2	2.22	0.53
1:A:243:ASN:HD22	1:A:246:ILE:HG23	1.74	0.53
1:C:52:ARG:NH1	1:C:156:ARG:HG3	2.24	0.53
1:C:243:ASN:HB3	1:C:246:ILE:HG23	1.90	0.53
2:D:219:LYS:HA	2:D:222:ARG:HH22	1.72	0.53
1:A:282:PRO:HA	1:A:285:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLY:HA2	1:C:271:MET:HB2	1.91	0.51
1:A:57:MET:HA	1:A:57:MET:HE3	1.92	0.51
2:D:102:ILE:HG13	2:D:122:PHE:CE2	2.45	0.51
2:D:219:LYS:HA	2:D:222:ARG:NH2	2.26	0.51
1:A:243:ASN:O	1:A:246:ILE:HG12	2.11	0.50
1:A:73:HIS:CE1	2:B:168:TYR:HH	2.29	0.50
1:A:93:MET:HG2	1:A:105:LEU:HD21	1.94	0.50
1:A:187:SER:OG	1:A:188:THR:N	2.44	0.50
2:D:20:LYS:HE2	2:D:244:VAL:HG21	1.94	0.50
2:B:141:ASN:HD22	2:B:141:ASN:N	2.08	0.50
2:B:169:ARG:NH1	2:B:183:GLU:OE2	2.44	0.50
2:D:222:ARG:HG3	2:D:222:ARG:NH2	2.20	0.50
1:A:287:SER:OG	1:A:290:GLN:HG3	2.12	0.49
1:C:243:ASN:O	1:C:246:ILE:HG12	2.12	0.49
2:B:39:ILE:HG23	2:B:99:LEU:HD13	1.94	0.49
2:D:33:THR:O	2:D:37:VAL:HG23	2.13	0.49
2:B:42:MET:HE1	2:B:227:LEU:HB2	1.95	0.49
1:C:181:MET:HG2	1:C:218:LEU:HD11	1.95	0.49
1:C:62:HIS:HB3	1:C:65:ILE:HD12	1.95	0.49
1:A:106:GLU:OE2	1:A:108:ASN:HB2	2.13	0.48
2:B:43:LEU:HD11	2:B:102:ILE:CD1	2.43	0.48
2:B:108:VAL:HB	2:B:184:GLN:HE22	1.77	0.48
2:B:125:THR:OG1	2:B:158:LEU:HG	2.13	0.48
2:B:51:GLU:O	2:B:53:SER:N	2.45	0.48
1:C:57:MET:HE2	1:C:57:MET:HA	1.96	0.48
1:C:135:LYS:HG3	1:C:137:GLN:HG2	1.95	0.48
1:C:273:PHE:HB2	1:C:294:HIS:CE1	2.49	0.47
1:A:270:LEU:HD13	1:A:296:TRP:CZ2	2.49	0.47
2:B:223:ARG:NH1	2:B:226:GLN:OE1	2.47	0.47
1:C:287:SER:H	1:C:290:GLN:NE2	2.07	0.47
2:D:206:TYR:O	2:D:209:ARG:HB3	2.13	0.47
1:A:89:LEU:HD12	1:A:139:LEU:HD12	1.96	0.47
2:D:236:ASP:O	2:D:238:SER:N	2.47	0.47
1:A:223:ASP:OD1	1:A:249:ARG:NH1	2.46	0.47
1:A:132:ARG:HH22	2:B:136:ASP:CG	2.16	0.47
1:A:156:ARG:HH12	1:A:164:THR:HB	1.79	0.47
2:D:166:VAL:O	2:D:166:VAL:HG12	2.15	0.47
2:B:127:THR:HG22	2:B:128:THR:HG22	1.96	0.47
1:A:73:HIS:CE1	2:B:168:TYR:OH	2.68	0.47
1:A:89:LEU:HB3	1:A:136:PRO:HB3	1.95	0.47
1:A:112:TYR:O	1:A:115:TRP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:LEU:HB2	2:D:114:LEU:HD23	1.96	0.47
1:A:281:ASN:HB3	1:A:284:MET:HG3	1.98	0.46
1:A:66:VAL:HG21	1:A:140:LEU:HD13	1.97	0.46
2:D:125:THR:OG1	2:D:158:LEU:HG	2.17	0.45
1:A:46:THR:O	1:A:47:PRO:C	2.54	0.45
2:D:246:PRO:HB2	2:D:247:PRO:HD3	1.98	0.45
2:D:36:VAL:O	2:D:36:VAL:CG1	2.64	0.45
2:D:32:ARG:HD2	2:D:85:THR:HG22	1.99	0.45
1:C:142:ASN:HD21	1:C:146:GLN:HB2	1.81	0.45
1:A:7:PHE:HA	1:A:25:LEU:O	2.17	0.45
1:A:182:GLY:HA3	1:A:240:PRO:HG2	1.99	0.45
1:C:259:GLN:N	1:C:260:PRO:HD2	2.31	0.45
2:D:84:LEU:HD13	2:D:127:THR:HG21	1.99	0.44
1:C:161:PRO:HG2	2:D:28:ASN:HD21	1.81	0.44
2:D:102:ILE:HG13	2:D:122:PHE:CZ	2.53	0.44
1:A:121:LEU:CD1	1:A:134:LEU:HD11	2.46	0.43
1:A:13:LEU:HD11	1:A:23:LYS:HB2	1.99	0.43
2:B:127:THR:HG22	2:B:128:THR:N	2.32	0.43
2:D:132:LYS:NZ	2:D:141:ASN:HD21	2.15	0.43
1:A:179:VAL:HG21	1:A:190:ILE:HG13	2.00	0.43
3:B:294:MES:H81	3:B:294:MES:H32	1.51	0.43
2:D:42:MET:HE1	2:D:227:LEU:HB2	2.00	0.43
1:A:57:MET:HA	1:A:57:MET:HE2	2.00	0.43
2:D:132:LYS:HZ1	2:D:141:ASN:HD21	1.67	0.43
2:B:37:VAL:HG12	2:B:78:PHE:CE1	2.54	0.43
1:C:156:ARG:HH12	1:C:164:THR:HB	1.83	0.43
1:C:78:LEU:HG	1:C:78:LEU:O	2.19	0.43
1:C:52:ARG:HH12	1:C:156:ARG:HG3	1.84	0.42
2:B:77:ILE:HD13	2:B:119:ALA:HB1	2.02	0.42
1:C:57:MET:HA	1:C:57:MET:CE	2.50	0.42
2:D:47:ILE:O	2:D:51:GLU:HG3	2.18	0.42
2:D:43:LEU:HD11	2:D:102:ILE:CD1	2.50	0.42
2:B:67:TYR:O	2:B:118:THR:HA	2.19	0.42
2:B:82:ILE:HG13	2:B:83:ARG:N	2.35	0.42
1:A:243:ASN:HB2	2:D:71:ILE:CD1	2.48	0.41
2:B:32:ARG:HH21	2:B:85:THR:HG22	1.85	0.41
2:B:161:ASP:O	2:B:165:ARG:HG3	2.19	0.41
2:B:37:VAL:O	2:B:41:ARG:HG3	2.20	0.41
1:C:281:ASN:ND2	1:C:284:MET:HG2	2.35	0.41
1:A:52:ARG:HH12	1:A:156:ARG:HG3	1.85	0.41
2:D:141:ASN:N	2:D:141:ASN:HD22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:204:TYR:O	2:D:205:SER:HB2	2.21	0.41
1:A:130:LEU:CD2	1:A:188:THR:HA	2.49	0.41
1:A:209:PHE:CB	1:A:217:GLN:NE2	2.83	0.41
1:C:106:GLU:O	1:C:110:VAL:HG23	2.21	0.41
1:C:133:ASP:O	1:C:138:ASN:ND2	2.54	0.41
2:D:40:SER:O	2:D:44:VAL:HG13	2.20	0.41
2:D:43:LEU:HD12	2:D:43:LEU:HA	1.92	0.41
1:A:137:GLN:HG3	1:A:138:ASN:N	2.35	0.41
2:D:80:TYR:O	2:D:84:LEU:HG	2.21	0.41
1:A:125:HIS:CG	1:A:188:THR:HG1	2.38	0.40
1:A:243:ASN:HA	1:A:244:PRO:HD3	1.85	0.40
1:C:58:LYS:HA	1:C:61:LYS:HE3	2.03	0.40
2:B:77:ILE:HD11	2:B:123:LEU:HD22	2.04	0.40
2:D:230:SER:C	2:D:232:ASN:H	2.24	0.40
1:A:125:HIS:CE1	1:A:191:ASP:HB2	2.56	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)
1:A:112:TYR:OH	2:D:249:ILE:CG1[4_655]	1.85	0.35

## 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	279/317 (88%)	252 (90%)	24 (9%)	3 (1%)	14	42
1	C	254/317 (80%)	234 (92%)	18 (7%)	2 (1%)	19	51
2	B	208/293 (71%)	184 (88%)	19 (9%)	5 (2%)	6	22
2	D	212/293 (72%)	185 (87%)	21 (10%)	6 (3%)	5	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	953/1220 (78%)	855 (90%)	82 (9%)	16 (2%)	9	31

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
2	B	234	SER
2	D	234	SER
2	D	249	ILE
1	C	188	THR
2	D	231	PHE
2	D	237	LYS
1	A	233	TRP
2	B	116	SER
2	B	127	THR
2	D	238	SER
1	A	47	PRO
2	B	52	ASN
2	D	205	SER
2	B	119	ALA
1	C	253	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/284 (91%)	238 (92%)	20 (8%)	12	34
1	C	240/284 (84%)	222 (92%)	18 (8%)	13	37
2	B	200/271 (74%)	176 (88%)	24 (12%)	5	15
2	D	205/271 (76%)	182 (89%)	23 (11%)	6	18
All	All	903/1110 (81%)	818 (91%)	85 (9%)	8	26

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	17	THR
1	A	20	THR
1	A	77	LYS
1	A	80	LEU
1	A	87	ASN
1	A	89	LEU
1	A	106	GLU
1	A	117	LEU
1	A	137	GLN
1	A	164	THR
1	A	175	ARG
1	A	188	THR
1	A	214	ASP
1	A	215	GLU
1	A	235	SER
1	A	246	ILE
1	A	261	HIS
1	A	262	THR
1	A	285	ARG
2	B	21	VAL
2	B	30	CYS
2	B	31	SER
2	B	32	ARG
2	B	37	VAL
2	B	45	SER
2	B	53	SER
2	B	63	THR
2	B	71	ILE
2	B	81	PHE
2	B	89	SER
2	B	127	THR
2	B	128	THR
2	B	141	ASN
2	B	173	ARG
2	B	181	SER
2	B	184	GLN
2	B	185	LYS
2	B	205	SER
2	B	218	ASP
2	B	226	GLN
2	B	232	ASN
2	B	239	ARG

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Mol	Chain	Res	Type
2	B	241	VAL
1	C	10	LEU
1	C	12	LYS
1	C	55	SER
1	C	77	LYS
1	C	87	ASN
1	C	89	LEU
1	C	130	LEU
1	C	164	THR
1	C	175	ARG
1	C	218	LEU
1	C	220	LEU
1	C	231	SER
1	C	245	ASN
1	C	246	ILE
1	C	254	LEU
1	C	262	THR
1	C	270	LEU
1	C	285	ARG
2	D	18	ILE
2	D	21	VAL
2	D	32	ARG
2	D	43	LEU
2	D	63	THR
2	D	70	LYS
2	D	76	SER
2	D	81	PHE
2	D	82	ILE
2	D	127	THR
2	D	128	THR
2	D	140	THR
2	D	141	ASN
2	D	158	LEU
2	D	173	ARG
2	D	181	SER
2	D	194	ASN
2	D	215	ASN
2	D	226	GLN
2	D	239	ARG
2	D	241	VAL
2	D	248	ASN
2	D	249	ILE



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	87	ASN
1	A	116	GLN
1	A	243	ASN
1	A	245	ASN
1	A	259	GLN
1	A	290	GLN
1	A	293	HIS
2	B	74	ASN
2	B	79	ASN
2	B	92	HIS
2	B	106	GLN
2	B	120	HIS
2	B	141	ASN
2	B	194	ASN
1	C	87	ASN
1	C	138	ASN
1	C	163	ASN
1	C	217	GLN
1	C	245	ASN
1	C	279	GLN
1	C	290	GLN
2	D	28	ASN
2	D	50	ASN
2	D	74	ASN
2	D	79	ASN
2	D	92	HIS
2	D	141	ASN
2	D	156	ASN
2	D	186	GLN
2	D	215	ASN
2	D	226	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	MES	D	294	-	12,12,12	2.14	1 (8%)	14,16,16	7.71	10 (71%)
3	MES	B	294	-	12,12,12	1.89	1 (8%)	14,16,16	7.60	8 (57%)

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	MES	D	294	-	-	4/6/14/14	0/1/1/1
3	MES	B	294	-	-	2/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	294	MES	C8-S	-6.92	1.67	1.77
3	B	294	MES	C8-S	-6.11	1.68	1.77

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	294	MES	O2S-S-C8	-19.50	83.43	106.92
3	B	294	MES	O2S-S-C8	-19.29	83.69	106.92
3	B	294	MES	O1S-S-C8	-16.43	87.13	106.92
3	D	294	MES	O1S-S-C8	-15.60	88.13	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	294	MES	O3S-S-C8	-10.60	88.62	105.77
3	B	294	MES	O3S-S-C8	-9.23	90.84	105.77
3	B	294	MES	C5-N4-C3	5.39	120.97	108.83
3	D	294	MES	C5-N4-C3	5.32	120.81	108.83
3	D	294	MES	O3S-S-O2S	4.80	123.00	111.27
3	B	294	MES	C7-N4-C3	4.01	121.50	111.23
3	B	294	MES	O3S-S-O1S	3.98	121.00	111.27
3	D	294	MES	C7-N4-C3	3.45	120.07	111.23
3	D	294	MES	C7-N4-C5	3.08	119.12	111.23
3	B	294	MES	O3S-S-O2S	2.89	118.34	111.27
3	D	294	MES	C2-C3-N4	-2.82	105.83	110.10
3	D	294	MES	O3S-S-O1S	2.79	118.10	111.27
3	B	294	MES	C7-N4-C5	2.45	117.51	111.23
3	D	294	MES	C6-C5-N4	-2.15	106.85	110.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	294	MES	C8-C7-N4-C3
3	B	294	MES	N4-C7-C8-S
3	D	294	MES	C7-C8-S-O3S
3	D	294	MES	C7-C8-S-O1S
3	D	294	MES	C8-C7-N4-C5
3	D	294	MES	C7-C8-S-O2S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	294	MES	1	0
3	B	294	MES	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	16:GLN	C	17:GLY	N	2.46

## 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	287/317 (90%)	0.16	3 (1%) 82 82	48, 66, 110, 133	17 (5%)
1	C	266/317 (83%)	0.30	5 (1%) 66 65	60, 92, 130, 154	13 (4%)
2	B	214/293 (73%)	0.17	2 (0%) 84 84	45, 63, 96, 115	4 (1%)
2	D	219/293 (74%)	0.35	4 (1%) 68 67	44, 60, 98, 137	6 (2%)
All	All	986/1220 (80%)	0.24	14 (1%) 75 75	44, 69, 118, 154	40 (4%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	16	GLN	20.9
1	A	17	THR	3.2
2	D	204	TYR	3.0
2	D	20	LYS	2.7
1	C	23	LYS	2.6
1	C	7	PHE	2.5
1	C	257	VAL	2.4
1	C	236	VAL	2.3
2	B	87	PHE	2.2
2	B	245	LEU	2.2
1	A	40	LEU	2.2
2	D	250	ASP	2.1
1	C	249	ARG	2.0
1	A	35	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MES	B	294	12/12	0.96	0.26	84,85,86,87	0
3	MES	D	294	12/12	0.97	0.20	62,63,65,66	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.