



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 AM GMT

PDB ID : 2IW8  
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2-CYCLIN A F82H-L83V-H84D MUTANT WITH AN O6-CYCLOHEXYLMETHYLGUANINE INHIBITOR  
Authors : Pratt, D.J.; Bentley, J.; Jewsbury, P.; Boyle, F.T.; Endicott, J.A.; Noble, M.E.M.  
Deposited on : 2006-06-27  
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

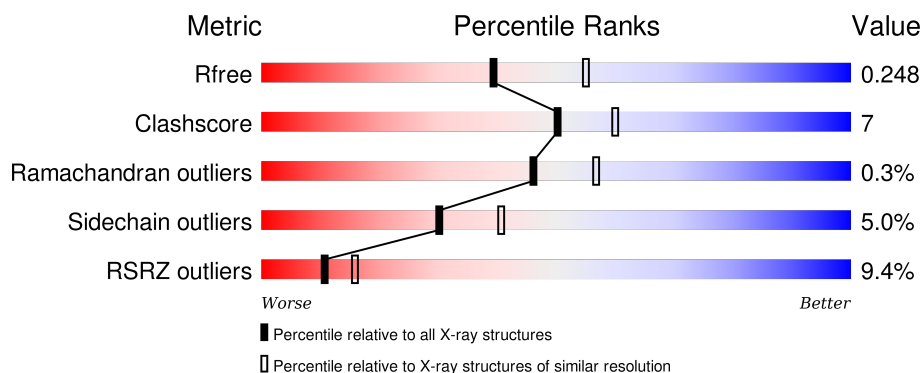
# 1 Overall quality at a glance

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	302	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	C	302	<div> <div>13%</div> <div>71%</div> <div>16%</div> <div>•</div> <div>12%</div> </div>
2	B	260	<div> <div>4%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>
2	D	260	<div> <div>17%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9027 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	1	0
			2399	1552	409	429	1	8			
1	C	266	Total	C	N	O	P	S	0	0	0
			2130	1377	364	381	1	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P24941
A	-2	PRO	-	EXPRESSION TAG	UNP P24941
A	-1	GLY	-	EXPRESSION TAG	UNP P24941
A	0	SER	-	EXPRESSION TAG	UNP P24941
A	82	HIS	PHE	ENGINEERED MUTATION	UNP P24941
A	83	VAL	LEU	ENGINEERED MUTATION	UNP P24941
A	84	ASP	HIS	ENGINEERED MUTATION	UNP P24941
C	-3	GLY	-	EXPRESSION TAG	UNP P24941
C	-2	PRO	-	EXPRESSION TAG	UNP P24941
C	-1	GLY	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941
C	82	HIS	PHE	ENGINEERED MUTATION	UNP P24941
C	83	VAL	LEU	ENGINEERED MUTATION	UNP P24941
C	84	ASP	HIS	ENGINEERED MUTATION	UNP P24941

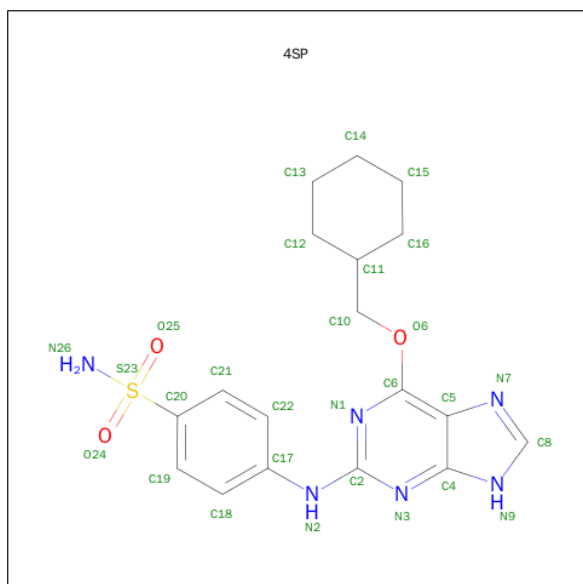
- Molecule 2 is a protein called CYCLIN-A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S		0	0	0
			2060	1337	336	376	11				
2	D	255	Total	C	N	O	S		0	0	0
			2061	1336	336	378	11				

There are 2 discrepancies between the modelled and reference sequences:

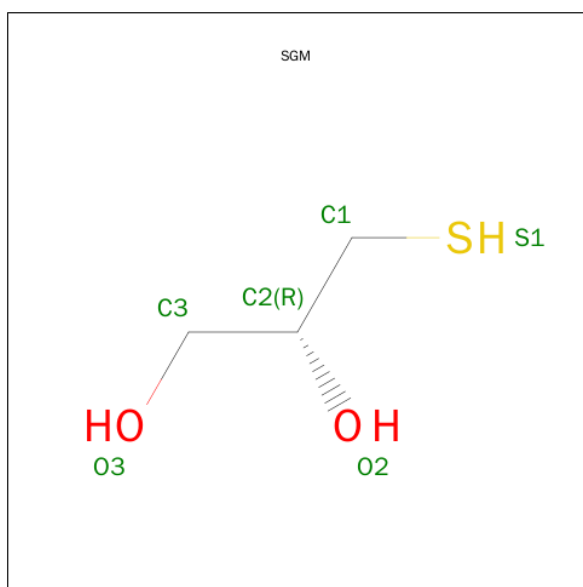
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	EXPRESSION TAG	UNP P20248
D	173	MET	-	EXPRESSION TAG	UNP P20248

- Molecule 3 is O6-CYCLOHEXYLMETHOXY-2-(4'-SULPHAMOYLANILINO) PURINE (three-letter code: 4SP) (formula:  $C_{18}H_{22}N_6O_3S$ ).



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

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



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

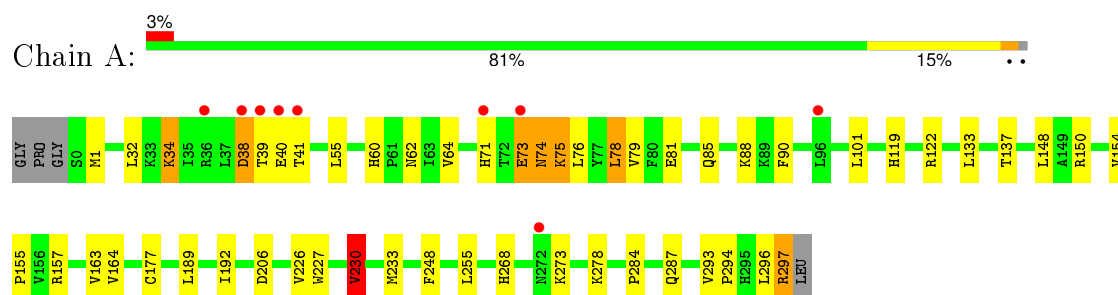
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		
5	B	96	Total	O	0	0
			96	96		
5	C	54	Total	O	0	0
			54	54		
5	D	35	Total	O	0	0
			35	35		

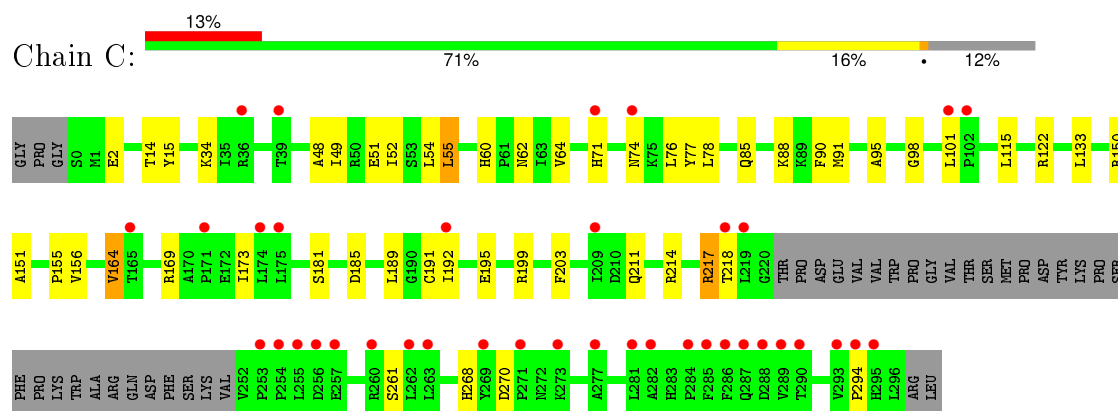
### 3 Residue-property plots

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.

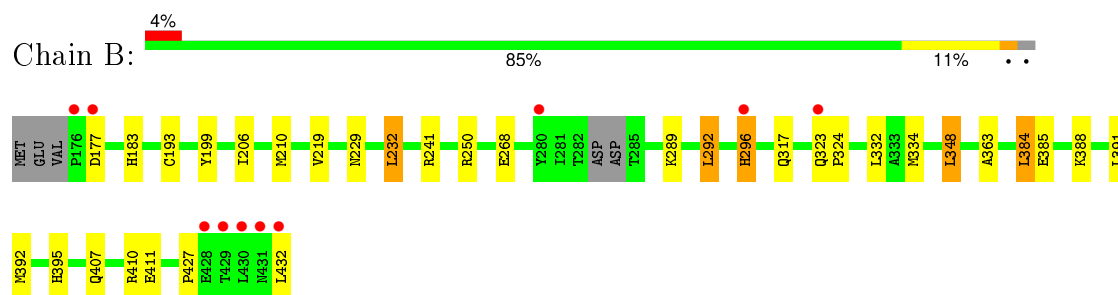
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



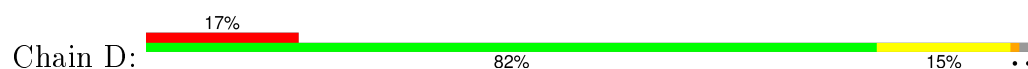
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

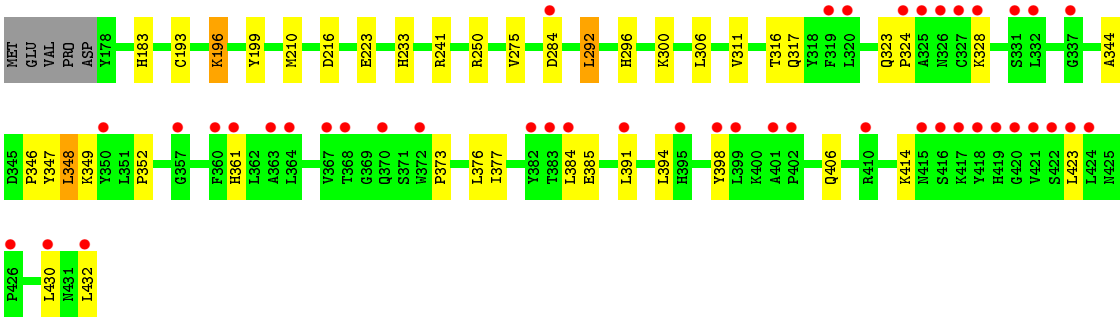


#### • Molecule 2: CYCLIN-A2



#### • Molecule 2: CYCLIN-A2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.89Å 135.32Å 148.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 48.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (100.00-2.30) 96.6 (48.82-2.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.212 , 0.255 0.208 , 0.248	Depositor DCC
$R_{free}$ test set	3271 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 64505 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SGM, 4SP

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	0.70	0/2452	0.74	2/3327 (0.1%)
1	C	0.55	0/2166	0.63	0/2933
2	B	0.62	0/2109	0.70	0/2861
2	D	0.50	0/2110	0.64	1/2864 (0.0%)
All	All	0.60	0/8837	0.68	3/11985 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CB-CA-C	-5.61	100.74	111.40
1	A	297	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	D	241	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2399	0	2438	42	0
1	C	2130	0	2180	36	0
2	B	2060	0	2089	28	0
2	D	2061	0	2087	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	22	1	0
3	C	28	0	22	3	0
4	B	6	0	7	0	0
4	D	6	0	8	1	0
5	A	124	0	0	3	0
5	B	96	0	0	4	0
5	C	54	0	0	3	0
5	D	35	0	0	1	0
All	All	9027	0	8853	123	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 7.

All (123) 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:155:PRO:HD2	2:D:316:THR:HG22	1.38	1.04
1:A:296:LEU:O	1:A:297:ARG:HB2	1.77	0.83
1:A:137:THR:O	1:A:293:VAL:HG13	1.77	0.83
1:A:284:PRO:O	1:A:287:GLN:HG2	1.79	0.82
1:A:268:HIS:CD2	5:A:2094:HOH:O	2.34	0.81
1:A:177:CYS:HB2	1:A:233:MET:CE	2.09	0.81
1:A:39:THR:HG21	2:B:289:LYS:CD	2.10	0.80
1:C:88:LYS:HA	1:C:91:MET:HE2	1.63	0.78
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.57	0.73
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.70	0.72
1:C:64:VAL:HG21	3:C:1297:4SP:H8	1.72	0.71
1:C:191:CYS:HB3	5:C:2044:HOH:O	1.91	0.71
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.19	0.70
2:D:361:HIS:HD2	2:D:391:LEU:HD11	1.56	0.70
1:A:39:THR:HG21	2:B:289:LYS:HD3	1.73	0.69
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.74	0.69
1:C:64:VAL:HG21	3:C:1297:4SP:C8	2.24	0.68
1:A:39:THR:HG21	2:B:289:LYS:HD2	1.75	0.67
2:B:317:GLN:NE2	5:B:2057:HOH:O	2.05	0.67
1:C:98:GLY:HA2	1:C:199:ARG:HD3	1.78	0.65
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.80	0.64
2:B:229:ASN:HD22	2:B:334:MET:CE	2.13	0.62
2:D:196:LYS:HG3	2:D:199:TYR:HB3	1.81	0.62
2:B:210:MET:HE1	2:B:250:ARG:CB	2.29	0.62
1:C:51:GLU:O	1:C:55:LEU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:CD2	1:A:62:ASN:H	2.19	0.60
1:A:227:TRP:HB3	1:A:230:VAL:CG2	2.31	0.60
1:A:60:HIS:HD2	1:A:62:ASN:H	1.50	0.59
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.93	0.57
2:B:210:MET:CE	2:B:250:ARG:HB2	2.35	0.57
1:C:217:ARG:HG2	1:C:218:THR:N	2.19	0.57
2:D:361:HIS:CD2	2:D:391:LEU:HD11	2.38	0.57
2:B:229:ASN:HD22	2:B:334:MET:HE2	1.69	0.55
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.72	0.55
2:B:206:ILE:HG22	2:B:210:MET:HE1	1.90	0.54
1:A:39:THR:HG22	1:A:40:GLU:N	2.22	0.54
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.90	0.53
2:D:193:CYS:SG	4:D:1433:SGM:S1	2.40	0.52
1:C:88:LYS:HA	1:C:91:MET:CE	2.35	0.52
1:A:85:GLN:HE21	1:A:90:PHE:HB2	1.73	0.52
2:B:395:HIS:HE1	2:B:427:PRO:O	1.92	0.52
2:B:384:LEU:HG	2:B:432:LEU:HD22	1.91	0.52
2:D:373:PRO:HD2	2:D:376:LEU:HD12	1.91	0.51
1:A:227:TRP:O	1:A:230:VAL:CG2	2.58	0.51
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.92	0.51
2:D:275:VAL:HG11	2:D:292:LEU:CD1	2.42	0.50
1:C:115:LEU:HD21	1:C:185:ASP:HB3	1.93	0.50
1:A:34:LYS:HD3	1:A:75:LYS:HE2	1.93	0.49
2:D:233:HIS:HD2	5:D:2027:HOH:O	1.95	0.49
1:A:81:GLU:HG3	1:A:81:GLU:O	2.11	0.49
1:C:156:VAL:HG11	1:C:181:SER:OG	2.12	0.49
2:D:384:LEU:HG	2:D:432:LEU:HD11	1.94	0.49
1:C:195:GLU:HB2	5:C:2049:HOH:O	2.12	0.49
1:A:39:THR:HA	2:B:292:LEU:HD23	1.95	0.49
1:A:227:TRP:O	1:A:230:VAL:HG23	2.13	0.49
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.95	0.49
1:A:71:HIS:CE1	2:B:296:HIS:CG	3.01	0.49
2:D:210:MET:HE1	2:D:250:ARG:NH1	2.27	0.49
1:A:1:MET:HE1	1:A:32:LEU:HD13	1.95	0.49
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.49	0.48
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.02	0.47
1:A:227:TRP:CB	1:A:230:VAL:HG22	2.44	0.47
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.44	0.47
1:A:268:HIS:HD2	5:A:2094:HOH:O	1.83	0.47
1:A:73:GLU:HG2	1:A:74:ASN:HD22	1.79	0.46
1:A:157:ARG:NH1	2:B:268:GLU:OE2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:GLN:HA	2:D:324:PRO:HA	1.74	0.46
1:A:293:VAL:HG13	1:A:294:PRO:HD2	1.98	0.46
1:C:217:ARG:HG2	1:C:218:THR:H	1.80	0.46
2:D:210:MET:CE	2:D:250:ARG:NH1	2.79	0.46
1:C:268:HIS:HD2	1:C:270:ASP:H	1.62	0.46
1:C:203:PHE:HB2	1:C:211:GLN:HE22	1.81	0.45
2:D:430:LEU:HB3	2:D:432:LEU:HD23	1.98	0.45
2:B:183:HIS:HE1	5:B:2059:HOH:O	1.99	0.45
1:A:119:HIS:HD2	5:B:2015:HOH:O	1.99	0.45
2:B:210:MET:HE1	2:B:250:ARG:HB3	1.99	0.44
1:C:34:LYS:HG3	1:C:77:TYR:CE1	2.52	0.44
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.98	0.44
2:B:323:GLN:HA	2:B:324:PRO:HA	1.78	0.44
1:A:133:LEU:HD11	1:A:192:ILE:HD13	1.99	0.44
3:A:1298:4SP:N1	3:A:1298:4SP:H18	2.33	0.44
1:C:95:ALA:O	1:C:199:ARG:NH1	2.50	0.44
1:A:71:HIS:CE1	2:B:296:HIS:CD2	3.06	0.44
1:C:85:GLN:HE21	1:C:90:PHE:HB2	1.83	0.44
2:D:373:PRO:O	2:D:377:ILE:HD12	2.18	0.43
2:B:407:GLN:OE1	2:B:410:ARG:HD3	2.18	0.43
1:A:39:THR:O	1:A:40:GLU:HB2	2.19	0.43
2:D:414:LYS:HG2	2:D:423:LEU:HG	2.00	0.43
2:D:346:PRO:O	2:D:349:LYS:HG2	2.18	0.43
1:C:169:ARG:HG2	1:C:173:ILE:HB	2.01	0.43
1:A:38:ASP:O	1:A:39:THR:HB	2.19	0.43
1:C:60:HIS:CD2	1:C:62:ASN:H	2.37	0.43
1:C:15:TYR:OH	1:C:48:ALA:HA	2.19	0.43
2:D:196:LYS:CG	2:D:199:TYR:HB3	2.49	0.42
2:B:407:GLN:O	2:B:411:GLU:HG2	2.19	0.42
1:C:133:LEU:HD11	1:C:192:ILE:HD13	2.00	0.42
2:D:275:VAL:HG11	2:D:292:LEU:HD11	2.01	0.42
2:D:347:TYR:OH	2:D:394:LEU:HA	2.19	0.42
1:A:154:VAL:HA	1:A:155:PRO:HA	1.91	0.42
1:C:52:ILE:CD1	1:C:78:LEU:HD21	2.49	0.42
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.77	0.42
1:A:60:HIS:HE1	5:A:2044:HOH:O	2.02	0.42
1:C:214:ARG:HA	1:C:217:ARG:CD	2.50	0.42
2:B:332:LEU:HD23	2:B:363:ALA:HA	2.01	0.42
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.55	0.42
1:C:71:HIS:HA	1:C:76:LEU:HD12	2.02	0.42
2:B:388:LYS:O	2:B:392:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:VAL:HG22	2:D:352:PRO:HA	2.02	0.41
1:A:39:THR:HG22	1:A:40:GLU:H	1.85	0.41
3:C:1297:4SP:H18	3:C:1297:4SP:N1	2.36	0.41
1:C:217:ARG:CG	1:C:218:THR:N	2.84	0.41
2:D:344:ALA:O	2:D:348:LEU:HB2	2.21	0.41
1:C:54:LEU:HD21	1:C:151:ALA:HB2	2.02	0.41
1:A:39:THR:CG2	1:A:40:GLU:N	2.84	0.41
1:C:214:ARG:HA	1:C:217:ARG:HD2	2.02	0.40
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.56	0.40
1:C:294:PRO:HG3	5:C:2034:HOH:O	2.20	0.40
2:D:216:ASP:HB2	2:D:406:GLN:HG2	2.02	0.40
1:A:227:TRP:O	1:A:230:VAL:HG22	2.22	0.40
1:A:78:LEU:N	1:A:78:LEU:HD23	2.36	0.40
1:C:71:HIS:NE2	2:D:296:HIS:NE2	2.68	0.40
2:B:183:HIS:CE1	5:B:2059:HOH:O	2.73	0.40
2:B:193:CYS:O	2:B:241:ARG:HD2	2.22	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	296/302 (98%)	286 (97%)	8 (3%)	2 (1%)	26	31
1	C	261/302 (86%)	245 (94%)	15 (6%)	1 (0%)	39	48
2	B	251/260 (96%)	249 (99%)	2 (1%)	0	100	100
2	D	253/260 (97%)	248 (98%)	5 (2%)	0	100	100
All	All	1061/1124 (94%)	1028 (97%)	30 (3%)	3 (0%)	46	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	164	VAL
1	C	164	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/264 (100%)	242 (92%)	21 (8%)	15	18
1	C	232/264 (88%)	222 (96%)	10 (4%)	35	47
2	B	229/234 (98%)	221 (96%)	8 (4%)	43	58
2	D	229/234 (98%)	220 (96%)	9 (4%)	39	53
All	All	953/996 (96%)	905 (95%)	48 (5%)	30	41

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	41	THR
1	A	55	LEU
1	A	64	VAL
1	A	73	GLU
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	88	LYS
1	A	101	LEU
1	A	122	ARG
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	189	LEU
1	A	206	ASP
1	A	226	VAL
1	A	230	VAL
1	A	248	PHE

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Mol	Chain	Res	Type
1	A	255	LEU
1	A	278	LYS
2	B	177	ASP
2	B	232	LEU
2	B	292	LEU
2	B	296	HIS
2	B	348	LEU
2	B	384	LEU
2	B	385	GLU
2	B	391	LEU
1	C	2	GLU
1	C	14	THR
1	C	55	LEU
1	C	74	ASN
1	C	101	LEU
1	C	122	ARG
1	C	150	ARG
1	C	164	VAL
1	C	217	ARG
1	C	261	SER
2	D	196	LYS
2	D	223	GLU
2	D	284	ASP
2	D	292	LEU
2	D	300	LYS
2	D	328	LYS
2	D	348	LEU
2	D	385	GLU
2	D	398	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	74	ASN
1	A	85	GLN
1	A	119	HIS
1	A	268	HIS
2	B	179	HIS
2	B	183	HIS
2	B	254	GLN

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Mol	Chain	Res	Type
2	B	296	HIS
2	B	395	HIS
2	B	396	GLN
1	C	59	ASN
1	C	60	HIS
1	C	62	ASN
1	C	85	GLN
1	C	119	HIS
1	C	268	HIS
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	361	HIS
2	D	395	HIS
2	D	403	GLN

### 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	0.78	0	7,14,16	1.47	1 (14%)
1	TPO	C	160	1	8,10,11	0.73	0	7,14,16	1.05	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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	160	TPO	O-C-CA	-2.25	119.50	125.44

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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	4SP	A	1298	-	28,31,31	2.18	5 (17%)	35,44,44	2.42	12 (34%)
4	SGM	B	1433	-	5,5,5	0.65	0	5,5,5	0.61	0
3	4SP	C	1297	-	28,31,31	1.98	5 (17%)	35,44,44	2.36	8 (22%)
4	SGM	D	1433	-	5,5,5	0.35	0	5,5,5	0.71	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	4SP	A	1298	-	-	0/15/23/23	0/4/4/4
4	SGM	B	1433	-	-	0/4/4/4	0/0/0/0
3	4SP	C	1297	-	-	0/15/23/23	0/4/4/4
4	SGM	D	1433	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	4SP	C20-S23	-9.17	1.63	1.77
3	C	1297	4SP	C20-S23	-8.13	1.64	1.77
3	A	1298	4SP	S23-N26	-3.73	1.52	1.60
3	C	1297	4SP	S23-N26	-3.05	1.53	1.60
3	C	1297	4SP	O24-S23	2.09	1.47	1.43
3	A	1298	4SP	C6-N1	2.42	1.36	1.31
3	C	1297	4SP	C6-N1	2.53	1.36	1.31
3	A	1298	4SP	O25-S23	2.54	1.48	1.43
3	C	1297	4SP	O25-S23	2.64	1.48	1.43
3	A	1298	4SP	O24-S23	2.85	1.48	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	4SP	O25-S23-O24	-7.32	108.52	118.80
3	C	1297	4SP	O25-S23-O24	-7.25	108.61	118.80
3	C	1297	4SP	N3-C2-N1	-4.55	119.24	126.22
3	A	1298	4SP	N3-C2-N1	-4.37	119.52	126.22
3	A	1298	4SP	C5-C6-N1	-2.88	118.72	123.81
3	C	1297	4SP	C15-C16-C11	-2.85	107.62	112.22
3	A	1298	4SP	C15-C16-C11	-2.53	108.14	112.22
3	C	1297	4SP	C5-C6-N1	-2.33	119.69	123.81
3	A	1298	4SP	C12-C11-C10	-2.22	106.78	111.47
3	A	1298	4SP	C21-C20-C19	-2.12	117.58	120.42
3	A	1298	4SP	O24-S23-C20	2.43	110.39	107.39
3	A	1298	4SP	O25-S23-N26	3.08	111.27	107.28
3	C	1297	4SP	O6-C6-C5	3.37	120.34	115.07
3	A	1298	4SP	O6-C6-C5	3.81	121.02	115.07
3	A	1298	4SP	C20-S23-N26	3.90	113.62	108.45
3	A	1298	4SP	C2-N3-C4	4.21	120.16	115.09
3	C	1297	4SP	C2-N1-C6	4.72	122.05	115.32
3	C	1297	4SP	O25-S23-N26	4.89	113.62	107.28
3	C	1297	4SP	C2-N3-C4	4.96	121.06	115.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	4SP	C2-N1-C6	5.24	122.79	115.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	4SP	1	0
3	C	1297	4SP	3	0
4	D	1433	SGM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	297/302 (98%)	0.19	9 (3%) 54 63	5, 11, 28, 34	1 (0%)
1	C	265/302 (87%)	0.74	38 (14%) 4 6	4, 12, 26, 33	0
2	B	255/260 (98%)	0.14	10 (3%) 43 52	6, 13, 25, 44	0
2	D	255/260 (98%)	0.91	44 (17%) 2 3	7, 14, 25, 44	0
All	All	1072/1124 (95%)	0.49	101 (9%) 11 16	4, 13, 26, 44	1 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	LEU	11.4
1	A	39	THR	5.9
1	A	40	GLU	5.9
2	D	423	LEU	5.6
2	D	419	HIS	5.2
1	C	295	HIS	5.0
2	D	391	LEU	4.8
2	D	367	VAL	4.7
1	C	287	GLN	4.6
1	C	293	VAL	4.6
1	A	96	LEU	4.5
1	A	38	ASP	4.5
1	C	256	ASP	4.4
2	B	431	ASN	4.4
2	D	418	TYR	4.4
2	D	415	ASN	4.3
2	D	368	THR	4.0
2	D	372	TRP	3.9
2	D	417	LYS	3.9
1	C	262	LEU	3.9
1	C	288	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	3.8
2	D	424	LEU	3.7
1	C	218	THR	3.6
2	D	364	LEU	3.6
2	D	422	SER	3.6
1	C	273	LYS	3.5
2	D	360	PHE	3.5
1	C	253	PRO	3.5
2	D	421	VAL	3.5
2	D	328	LYS	3.5
2	D	384	LEU	3.5
1	C	285	PHE	3.2
2	D	363	ALA	3.2
1	C	269	TYR	3.1
2	D	357	GLY	3.1
1	C	271	PRO	3.1
2	D	426	PRO	3.1
1	C	102	PRO	3.1
1	C	286	PHE	3.1
2	D	327	CYS	3.0
2	D	326	ASN	2.9
1	C	101	LEU	2.9
1	C	284	PRO	2.9
2	B	432	LEU	2.9
1	C	254	PRO	2.9
1	A	36	ARG	2.8
1	C	39	THR	2.8
2	D	325	ALA	2.8
2	D	324	PRO	2.8
1	C	277	ALA	2.8
1	C	219	LEU	2.8
2	D	401	ALA	2.7
1	C	289	VAL	2.7
2	D	332	LEU	2.7
1	C	257	GLU	2.7
1	A	272[A]	ASN	2.7
2	D	383	THR	2.6
1	A	71	HIS	2.6
1	C	175	LEU	2.6
1	C	282	ALA	2.6
2	D	284	ASP	2.6
2	D	416	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	319	PHE	2.5
2	D	320	LEU	2.5
2	D	410	ARG	2.5
2	D	331	SER	2.5
1	C	255	LEU	2.5
1	C	174	LEU	2.4
1	C	294	PRO	2.4
1	A	73	GLU	2.4
2	B	176	PRO	2.4
2	D	382	TYR	2.4
2	B	296	HIS	2.3
1	C	260	ARG	2.3
2	D	361	HIS	2.3
1	C	192	ILE	2.3
2	D	430	LEU	2.3
1	C	36	ARG	2.3
1	C	209	ILE	2.3
2	D	398	TYR	2.3
2	D	395	HIS	2.2
2	B	280	TYR	2.2
1	C	165	THR	2.2
2	B	428	GLU	2.2
2	D	402	PRO	2.2
2	D	420	GLY	2.2
2	D	399	LEU	2.2
2	D	370	GLN	2.2
1	C	290	THR	2.2
2	B	429	THR	2.2
2	D	350	TYR	2.1
1	C	71	HIS	2.1
2	D	337	GLY	2.1
1	C	171	PRO	2.1
2	B	177	ASP	2.1
1	C	74	ASN	2.1
1	C	281	LEU	2.0
2	B	323	GLN	2.0
1	C	263	LEU	2.0
2	B	430	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	C	160	11/12	0.96	0.12	-	7,10,13,13	0
1	TPO	A	160	11/12	0.99	0.14	-	7,10,11,12	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SGM	B	1433	6/6	0.90	0.18	1.67	28,31,32,33	0
3	4SP	C	1297	28/28	0.94	0.14	-0.03	13,15,18,19	0
4	SGM	D	1433	6/6	0.92	0.14	-0.57	41,42,42,43	0
3	4SP	A	1298	28/28	0.98	0.09	-2.40	2,2,6,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.