



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:35 PM GMT

PDB ID : 3U2Z  
Title : Activator-Bound Structure of Human Pyruvate Kinase M2  
Authors : Hong, B.; Dimov, S.; Tempel, W.; Auld, D.; Thomas, C.; Boxer, M.; Jianq, J.-K.; Skoumbourdis, A.; Min, S.; Southall, N.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Inglese, J.; Park, H.; Structural Genomics Consortium (SGC)  
Deposited on : 2011-10-04  
Resolution : 2.10 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

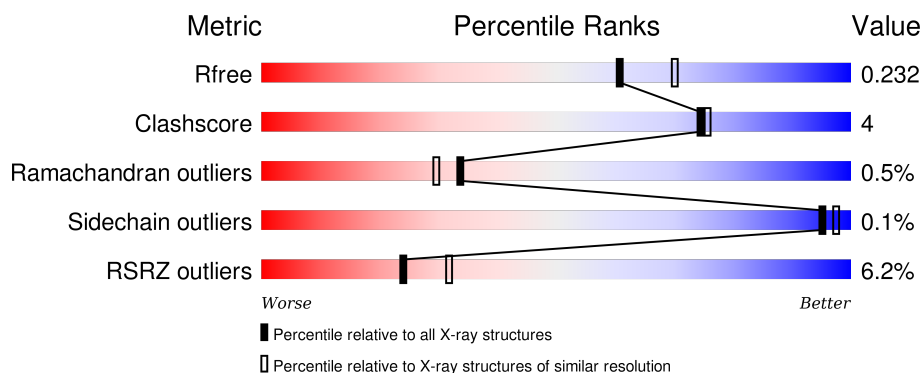
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	533	<div> <div>5%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	B	533	<div> <div>8%</div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	C	533	<div> <div>6%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	D	533	<div> <div>5%</div> <div>86%</div> <div>10%</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	UNX	A	532	-	-	-	X
3	UNX	A	535	-	-	-	X
3	UNX	B	533	-	-	-	X
3	UNX	B	534	-	-	-	X
3	UNX	B	535	-	-	-	X
3	UNX	B	536	-	-	-	X
3	UNX	C	533	-	-	-	X
3	UNX	C	534	-	-	-	X
3	UNX	C	535	-	-	-	X
3	UNX	D	532	-	-	-	X
3	UNX	D	535	-	-	-	X
3	UNX	D	536	-	-	-	X
3	UNX	D	537	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15896 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.

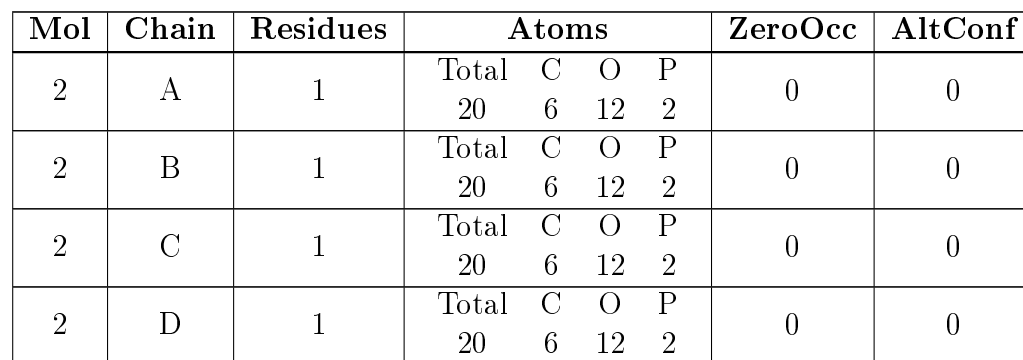
- Molecule 1 is a protein called Pyruvate kinase isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	5	1
			3826	2419	668	714	25			
1	B	514	Total	C	N	O	S	0	6	0
			3804	2407	671	699	27			
1	C	517	Total	C	N	O	S	0	6	0
			3835	2422	669	718	26			
1	D	513	Total	C	N	O	S	0	9	0
			3861	2441	681	713	26			

There are 8 discrepancies between the modelled and reference sequences:

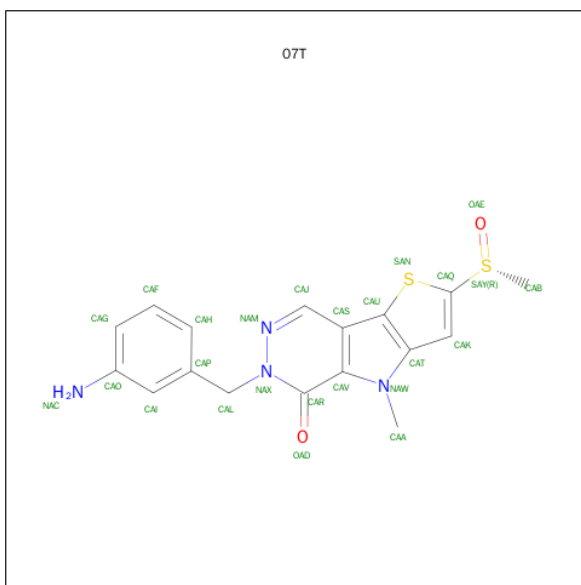
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P14618
A	0	SER	-	EXPRESSION TAG	UNP P14618
B	-1	GLY	-	EXPRESSION TAG	UNP P14618
B	0	SER	-	EXPRESSION TAG	UNP P14618
C	-1	GLY	-	EXPRESSION TAG	UNP P14618
C	0	SER	-	EXPRESSION TAG	UNP P14618
D	-1	GLY	-	EXPRESSION TAG	UNP P14618
D	0	SER	-	EXPRESSION TAG	UNP P14618

- Molecule 2 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>12</sub>P<sub>2</sub>).



- | Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 3   | B     | 5        | Total X<br>5 5 | 0       | 0       |
| 3   | A     | 6        | Total X<br>6 6 | 0       | 0       |
| 3   | D     | 6        | Total X<br>6 6 | 0       | 0       |
| 3   | C     | 4        | Total X<br>4 4 | 0       | 0       |

- 



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 50	C 34	N 8	O 4	S 4	0	1
4	C	1	Total 50	C 34	N 8	O 4	S 4	0	1

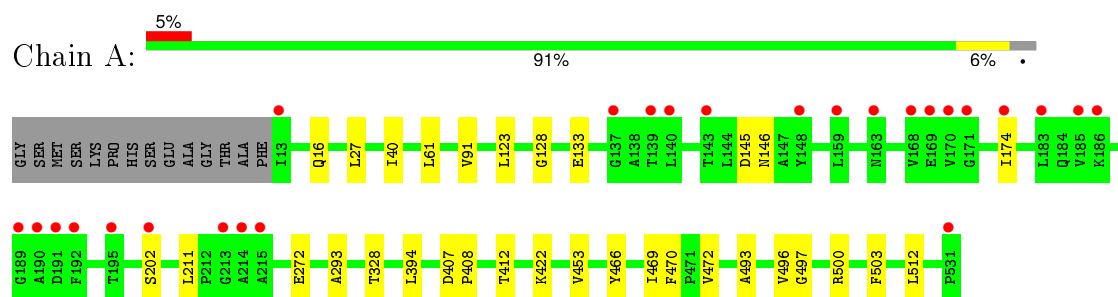
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	98	Total O 98 98	0	0
5	B	90	Total O 91 91	0	1
5	C	80	Total O 81 81	0	1
5	D	99	Total O 99 99	0	0

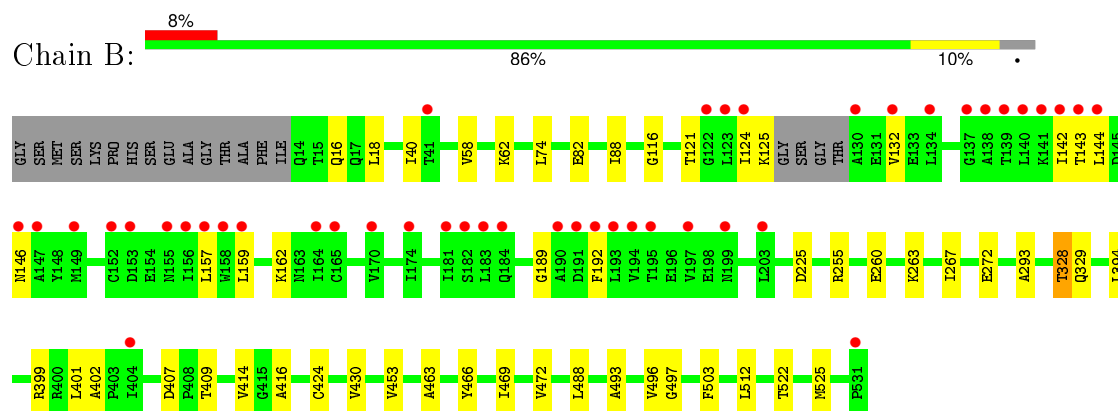
### 3 Residue-property plots

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.

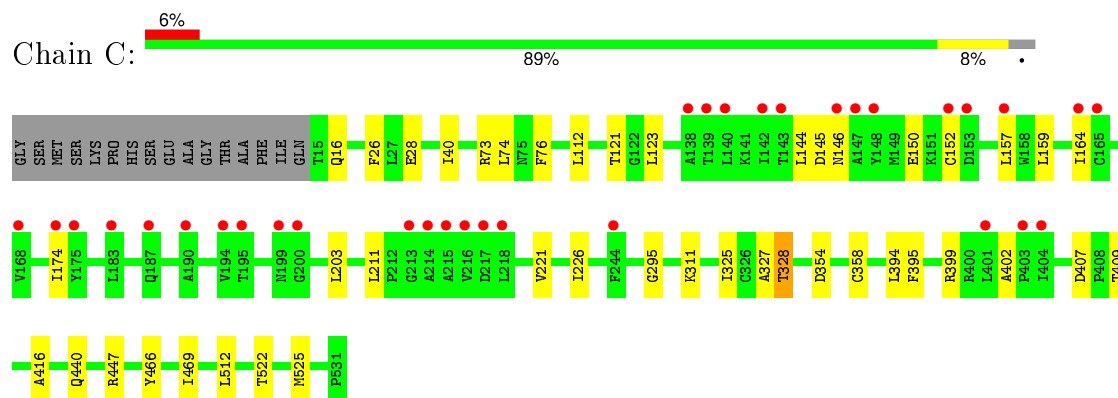
- Molecule 1: Pyruvate kinase isozymes M1/M2



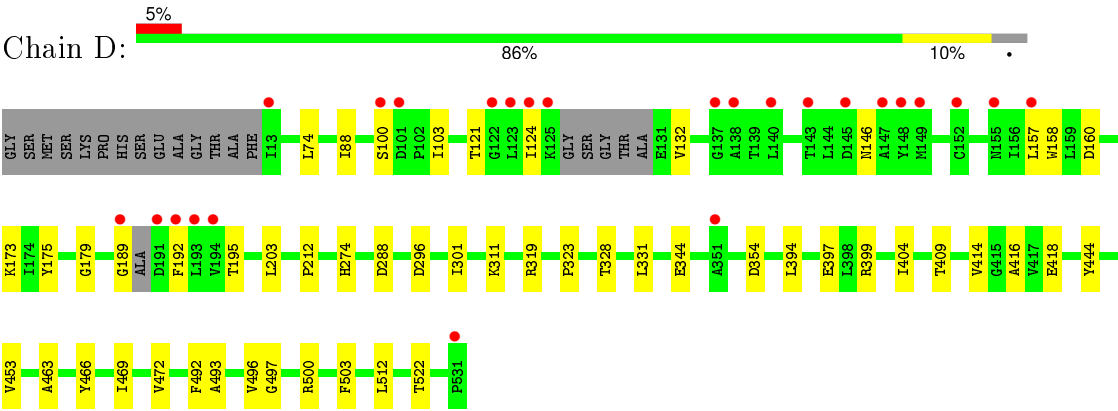
- Molecule 1: Pyruvate kinase isozymes M1/M2



- Molecule 1: Pyruvate kinase isozymes M1/M2



- Molecule 1: Pyruvate kinase isozymes M1/M2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.76 Å 151.16 Å 93.21 Å 90.00° 102.94° 90.00°	Depositor
Resolution (Å)	44.45 – 2.10 43.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.45-2.10) 98.6 (43.50-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.190 , 0.231 0.197 , 0.232	Depositor DCC
$R_{free}$ test set	1545 reflections (1.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 124988 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: UNX, 07T, FBP

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	0.67	0/3900	0.66	0/5288
1	B	0.65	0/3881	0.68	1/5264 (0.0%)
1	C	0.63	0/3911	0.67	1/5308 (0.0%)
1	D	0.67	0/3957	0.69	0/5361
All	All	0.66	0/15649	0.67	2/21221 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	525	MET	CG-SD-CE	6.39	110.42	100.20
1	B	407	ASP	CB-CG-OD1	6.00	123.70	118.30

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	3826	0	3730	22	0
1	B	3804	0	3754	42	0
1	C	3835	0	3770	33	0
1	D	3861	0	3809	37	0
2	A	20	0	10	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	A	6	0	0	0	0
3	B	5	0	0	0	0
3	C	4	0	0	0	0
3	D	6	0	0	1	0
4	B	50	0	32	3	0
4	C	50	0	32	5	0
5	A	98	0	0	0	0
5	B	91	0	0	0	0
5	C	81	0	0	0	0
5	D	99	0	0	0	0
All	All	15896	0	15167	122	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 4.

All (122) 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:B:399[A]:ARG:NH1	1:D:399[A]:ARG:CD	2.04	1.07
1:B:399[A]:ARG:HH12	1:D:399[A]:ARG:CD	1.62	1.00
1:B:399[A]:ARG:NH1	1:D:399[A]:ARG:HD3	1.87	0.86
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.63	0.81
1:B:424[B]:CYS:SG	1:D:404:ILE:HG21	2.22	0.79
1:B:399[A]:ARG:HH12	1:D:399[A]:ARG:HD3	1.47	0.74
1:C:407:ASP:OD1	1:C:409[B]:THR:HG22	1.88	0.72
1:C:395:PHE:CZ	1:C:399:ARG:HD2	2.26	0.70
1:A:422:LYS:NZ	1:C:402:ALA:HB1	2.07	0.69
1:D:296:ASP:OD2	3:D:534:UNX:UNK	1.74	0.68
1:B:399[A]:ARG:HH12	1:D:399[A]:ARG:HD2	1.57	0.65
1:C:409[B]:THR:HG23	1:C:440:GLN:OE1	1.96	0.65
1:C:157:LEU:CD1	1:C:203:LEU:HD21	2.30	0.62
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.82	0.61
1:A:272:GLU:HG2	1:A:293:ALA:HB3	1.83	0.61
1:D:311:LYS:NZ	1:D:354:ASP:OD1	2.33	0.60
1:D:414:VAL:HG12	1:D:444:TYR:CE2	2.38	0.59
1:B:124:ILE:HD12	1:B:132:VAL:HG22	1.85	0.58
1:A:412:THR:HG22	1:A:512:LEU:CD2	2.33	0.58
1:A:16:GLN:HG2	1:A:40:ILE:HG23	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:LEU:HD23	1:B:488:LEU:C	2.24	0.58
1:B:394:LEU:HD13	4:B:551[B]:07T:H7	1.84	0.58
1:B:260:GLU:OE2	1:B:263:LYS:HE2	2.04	0.58
4:C:551[B]:07T:H7	1:D:394:LEU:HD13	1.84	0.57
1:B:142:ILE:HG21	1:B:159:LEU:HD12	1.85	0.57
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.86	0.57
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.86	0.56
1:A:422:LYS:HZ1	1:C:402:ALA:HB1	1.71	0.56
1:C:416:ALA:CB	1:C:512:LEU:HD21	2.35	0.56
1:C:394:LEU:HD13	4:C:551[A]:07T:H7	1.88	0.55
1:A:123:LEU:HD22	1:A:128:GLY:HA2	1.89	0.55
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.88	0.55
1:B:144:LEU:HD13	1:B:162:LYS:HA	1.89	0.54
1:D:274[B]:HIS:CD2	1:D:301:ILE:HG22	2.43	0.54
1:B:463:ALA:HB1	1:B:469:ILE:HG21	1.89	0.53
1:C:221:VAL:HG12	1:C:226:ILE:HG13	1.91	0.53
1:B:409[B]:THR:HG22	1:B:522:THR:O	2.08	0.53
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.91	0.52
1:B:121:THR:CG2	1:B:157:LEU:HD11	2.41	0.51
1:A:61:LEU:HD13	1:A:91:VAL:HA	1.91	0.51
1:C:26:PHE:CZ	4:C:551[B]:07T:H3	2.46	0.51
1:B:424[B]:CYS:SG	1:D:404:ILE:CG2	2.97	0.51
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.41	0.50
1:D:463:ALA:HB1	1:D:469:ILE:HG21	1.94	0.50
1:D:414:VAL:HG12	1:D:444:TYR:CZ	2.46	0.50
1:D:103:ILE:HD13	1:D:492:PHE:CE1	2.47	0.50
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.47	0.50
1:C:123:LEU:HD12	1:C:150:GLU:HG2	1.94	0.49
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.93	0.49
1:B:16:GLN:CD	1:B:40:ILE:HG23	2.32	0.49
1:C:144:LEU:HD21	1:C:164:ILE:HG22	1.93	0.49
1:C:16:GLN:HG2	1:C:40:ILE:HG23	1.95	0.49
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.48	0.48
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.94	0.48
1:A:27:LEU:HD23	1:B:401:LEU:HD12	1.94	0.48
1:D:189:GLY:HA3	1:D:192:PHE:CE1	2.48	0.48
1:A:412:THR:HG22	1:A:512:LEU:HD22	1.95	0.48
1:B:116:GLY:HA2	1:B:225:ASP:OD2	2.14	0.48
1:B:189:GLY:HA3	1:B:192:PHE:CE2	2.49	0.48
4:C:551[A]:07T:H14	1:D:397:GLU:OE1	2.14	0.47
1:D:175:TYR:HB3	1:D:179:GLY:HA2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:HD23	1:B:525:MET:HA	1.97	0.47
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.97	0.47
1:C:174:ILE:HG12	1:C:211:LEU:CD2	2.45	0.47
1:D:331:LEU:HD23	1:D:344:GLU:HB3	1.98	0.46
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.97	0.46
1:D:496:VAL:HG13	1:D:500[B]:ARG:NE	2.31	0.46
1:C:73:ARG:C	1:C:74:LEU:HD23	2.35	0.46
1:B:16:GLN:CG	1:B:40:ILE:HG23	2.46	0.45
1:C:74:LEU:HD23	1:C:74:LEU:N	2.32	0.45
1:D:414:VAL:CG1	1:D:444:TYR:CZ	3.00	0.45
1:A:412:THR:HG22	1:A:512:LEU:HD21	1.98	0.45
1:A:174:ILE:HG12	1:A:211:LEU:HD21	1.99	0.45
1:B:82:GLU:H	1:B:82:GLU:CD	2.20	0.45
1:C:28:GLU:OE2	1:D:319:ARG:NH1	2.50	0.44
1:C:409[A]:THR:HG22	1:C:522:THR:O	2.17	0.44
1:B:74:LEU:HD11	1:B:88:ILE:HG13	1.99	0.44
1:C:123:LEU:HD12	1:C:150:GLU:CG	2.47	0.44
1:C:16:GLN:O	1:C:447[A]:ARG:NH2	2.50	0.44
1:C:311:LYS:NZ	1:C:354:ASP:OD1	2.41	0.44
1:D:124:ILE:HD11	1:D:203:LEU:HG	2.00	0.44
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.48	0.43
1:C:144:LEU:HD21	1:C:164:ILE:CG2	2.48	0.43
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.99	0.43
1:C:395:PHE:CE1	1:C:399:ARG:HD2	2.53	0.43
1:D:414:VAL:CG1	1:D:444:TYR:CE2	3.00	0.43
1:B:272:GLU:HG2	1:B:293:ALA:HB3	2.01	0.43
1:C:152:CYS:HB3	1:C:157:LEU:HD12	2.01	0.43
1:B:58:VAL:HG12	1:B:62:LYS:HE3	2.01	0.43
1:D:472:VAL:HG11	1:D:496:VAL:HG11	2.00	0.43
1:D:409:THR:HG23	1:D:522:THR:HB	2.00	0.43
1:C:76:PHE:CE1	1:C:112:LEU:HG	2.55	0.42
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.54	0.42
1:B:255:ARG:CZ	1:B:267:ILE:HD12	2.48	0.42
1:D:288:ASP:O	1:D:323:PRO:HD2	2.19	0.42
1:D:74:LEU:HD11	1:D:88:ILE:HG13	2.00	0.42
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.49	0.42
1:A:133:GLU:HA	1:A:202:SER:HA	2.02	0.42
1:C:466:TYR:HB2	1:C:469:ILE:HD12	2.01	0.42
1:A:394:LEU:HA	4:B:551[A]:07T:H7	2.02	0.42
1:B:143:THR:C	1:B:144:LEU:HD23	2.39	0.42
1:D:132:VAL:HG23	1:D:203:LEU:HB3	2.01	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD23	1:B:18:LEU:HA	1.86	0.41
1:C:295:GLY:CA	1:C:328:THR:HG21	2.50	0.41
1:C:327:ALA:O	1:C:328:THR:HB	2.20	0.41
1:A:174:ILE:HG12	1:A:211:LEU:CD2	2.50	0.41
1:D:158:TRP:CH2	1:D:160:ASP:HB3	2.54	0.41
1:B:414:VAL:HG13	1:D:418:GLU:HG3	2.02	0.41
1:D:121:THR:HB	1:D:157:LEU:HD11	2.02	0.41
1:C:121:THR:HG22	1:C:159:LEU:CD2	2.51	0.41
1:B:328:THR:HG22	1:B:329:GLN:HG3	2.03	0.41
1:C:325:ILE:HG12	1:C:358:CYS:HB2	2.03	0.41
1:B:430:VAL:HG22	1:B:512:LEU:HD12	2.02	0.41
1:B:74:LEU:HD11	1:B:88:ILE:CG1	2.50	0.41
1:A:407:ASP:HA	1:A:408:PRO:HD3	1.97	0.41
1:A:470[B]:PHE:CZ	1:A:500:ARG:CD	3.04	0.41
1:B:394:LEU:CD1	4:B:551[B]:07T:H7	2.51	0.41
1:C:394:LEU:HA	4:C:551[A]:07T:H6	2.03	0.41
1:D:173:LYS:O	1:D:212:PRO:HD2	2.20	0.41
1:A:412:THR:CG2	1:A:512:LEU:HD22	2.50	0.40
1:B:124:ILE:O	1:B:125:LYS:O	2.39	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	520/533 (98%)	509 (98%)	8 (2%)	3 (1%)	30	24
1	B	515/533 (97%)	503 (98%)	10 (2%)	2 (0%)	39	37
1	C	521/533 (98%)	504 (97%)	14 (3%)	3 (1%)	30	24
1	D	515/533 (97%)	502 (98%)	11 (2%)	2 (0%)	39	37
All	All	2071/2132 (97%)	2018 (97%)	43 (2%)	10 (0%)	34	30

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	B	328	THR
1	C	146	ASN
1	C	328	THR
1	D	146	ASN
1	D	328	THR
1	A	146	ASN
1	B	146	ASN
1	A	145	ASP
1	C	145	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	376/437 (86%)	376 (100%)	0	100	100
1	B	379/437 (87%)	379 (100%)	0	100	100
1	C	385/437 (88%)	385 (100%)	0	100	100
1	D	391/437 (90%)	389 (100%)	2 (0%)	92	95
All	All	1531/1748 (88%)	1529 (100%)	2 (0%)	95	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	100	SER
1	D	195	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	491	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 ⓘ

Of 29 ligands modelled in this entry, 21 are unknown - leaving 8 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$
2	FBP	A	541	-	18,20,20	1.02	1 (5%)	21,32,32	0.71	1 (4%)
2	FBP	B	541	-	18,20,20	1.14	1 (5%)	21,32,32	0.75	0
4	07T	B	551[A]	-	20,28,28	1.75	4 (20%)	17,42,42	1.56	4 (23%)
4	07T	B	551[B]	-	20,28,28	1.66	3 (15%)	17,42,42	1.71	2 (11%)
2	FBP	C	541	-	18,20,20	0.98	1 (5%)	21,32,32	0.80	0
4	07T	C	551[A]	-	20,28,28	1.73	3 (15%)	17,42,42	2.66	5 (29%)
4	07T	C	551[B]	-	20,28,28	1.81	4 (20%)	17,42,42	1.77	3 (17%)
2	FBP	D	541	-	18,20,20	0.90	1 (5%)	21,32,32	1.02	1 (4%)

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
2	FBP	A	541	-	-	0/13/32/32	0/1/1/1
2	FBP	B	541	-	-	0/13/32/32	0/1/1/1
4	07T	B	551[A]	-	-	0/3/8/8	0/4/4/4
4	07T	B	551[B]	-	-	0/3/8/8	0/4/4/4
2	FBP	C	541	-	-	0/13/32/32	0/1/1/1
4	07T	C	551[A]	-	-	0/3/8/8	0/4/4/4
4	07T	C	551[B]	-	-	0/3/8/8	0/4/4/4
2	FBP	D	541	-	-	0/13/32/32	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	551[B]	07T	CAQ-SAY	-4.89	1.71	1.79
4	B	551[B]	07T	CAQ-SAY	-4.54	1.72	1.79
4	B	551[A]	07T	CAQ-SAY	-4.45	1.72	1.79
4	C	551[A]	07T	CAQ-SAY	-4.21	1.72	1.79
4	C	551[A]	07T	CAQ-SAN	-4.02	1.65	1.72
4	B	551[A]	07T	CAQ-SAN	-3.96	1.65	1.72
4	C	551[B]	07T	CAQ-SAN	-3.60	1.66	1.72
4	C	551[A]	07T	CAJ-CAS	-3.18	1.38	1.41
4	B	551[B]	07T	CAQ-SAN	-2.88	1.67	1.72
4	C	551[B]	07T	CAJ-CAS	-2.75	1.38	1.41
4	B	551[A]	07T	CAJ-CAS	-2.15	1.39	1.41
4	B	551[A]	07T	CAJ-NAM	2.05	1.32	1.30
4	B	551[B]	07T	CAA-NAW	2.22	1.52	1.49
4	C	551[B]	07T	CAJ-NAM	2.56	1.33	1.30
2	C	541	FBP	O2-C2	2.58	1.45	1.41
2	A	541	FBP	O2-C2	2.96	1.45	1.41
2	D	541	FBP	O2-C2	2.99	1.45	1.41
2	B	541	FBP	O2-C2	3.58	1.46	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	551[B]	07T	CAS-CAJ-NAM	-4.98	119.08	124.83
4	C	551[B]	07T	CAS-CAJ-NAM	-3.57	120.70	124.83
4	C	551[A]	07T	CAS-CAJ-NAM	-3.07	121.28	124.83
4	B	551[A]	07T	CAS-CAJ-NAM	-2.86	121.52	124.83
4	C	551[A]	07T	CAO-CAI-CAP	-2.63	118.75	120.84
4	B	551[A]	07T	CAR-CAV-CAS	-2.40	115.58	121.03
4	B	551[A]	07T	CAO-CAI-CAP	-2.28	119.03	120.84
2	D	541	FBP	O6P-P2-O5P	2.08	115.30	107.38
2	A	541	FBP	O6P-P2-O5P	2.10	115.36	107.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	551[A]	07T	OAE-SAY-CAB	2.31	108.67	105.62
4	C	551[B]	07T	OAE-SAY-CAB	2.66	109.14	105.62
4	B	551[A]	07T	CAB-SAY-CAQ	3.50	101.20	97.52
4	B	551[B]	07T	CAB-SAY-CAQ	3.76	101.47	97.52
4	C	551[A]	07T	OAE-SAY-CAQ	4.03	109.69	105.44
4	C	551[B]	07T	CAB-SAY-CAQ	4.78	102.54	97.52
4	C	551[A]	07T	CAB-SAY-CAQ	8.29	106.24	97.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	551[A]	07T	1	0
4	B	551[B]	07T	2	0
4	C	551[A]	07T	3	0
4	C	551[B]	07T	2	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	519/533 (97%)	0.04	26 (5%)	32	41	18, 30, 68, 83	0
1	B	514/533 (96%)	0.21	44 (8%)	13	18	17, 33, 75, 93	1 (0%)
1	C	517/533 (96%)	0.20	33 (6%)	23	30	19, 34, 59, 72	0
1	D	513/533 (96%)	0.14	25 (4%)	33	42	17, 30, 63, 81	3 (0%)
All	All	2063/2132 (96%)	0.15	128 (6%)	24	32	17, 32, 67, 93	4 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	ILE	6.4
1	C	215	ALA	6.3
1	B	190	ALA	6.2
1	C	140	LEU	6.2
1	B	138	ALA	6.1
1	C	165	CYS	5.9
1	B	144	LEU	5.6
1	B	142	ILE	5.4
1	A	192	PHE	5.4
1	B	123	LEU	5.1
1	B	203	LEU	5.0
1	B	156	ILE	5.0
1	D	192	PHE	4.9
1	D	152	CYS	4.9
1	D	148	TYR	4.9
1	C	195	THR	4.9
1	B	170	VAL	4.5
1	B	197	VAL	4.5
1	C	214	ALA	4.5
1	C	216	VAL	4.5
1	B	194	VAL	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	183	LEU	4.3
1	B	134	LEU	4.3
1	C	164	ILE	4.3
1	B	137	GLY	4.3
1	B	152	CYS	4.2
1	A	185	VAL	4.2
1	B	193	LEU	4.2
1	B	192	PHE	4.2
1	A	190	ALA	4.2
1	C	139	THR	4.1
1	B	158	TRP	4.1
1	C	190	ALA	4.1
1	B	140	LEU	4.1
1	D	123	LEU	4.1
1	D	191	ASP	4.0
1	A	170	VAL	4.0
1	C	404	ILE	4.0
1	A	214	ALA	3.9
1	B	147	ALA	3.9
1	A	163	ASN	3.9
1	A	213[A]	GLY	3.9
1	C	142	ILE	3.8
1	D	193	LEU	3.7
1	B	143	THR	3.7
1	B	165	CYS	3.5
1	B	181	ILE	3.5
1	B	139	THR	3.4
1	B	183	LEU	3.4
1	B	41	THR	3.4
1	D	189	GLY	3.4
1	D	147	ALA	3.4
1	B	195	THR	3.4
1	D	124	ILE	3.3
1	A	159	LEU	3.3
1	D	140	LEU	3.3
1	B	122	GLY	3.2
1	D	125	LYS	3.2
1	A	13	ILE	3.2
1	A	168	VAL	3.1
1	A	148	TYR	3.1
1	B	153	ASP	3.1
1	A	140	LEU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	213[A]	GLY	3.0
1	A	143	THR	3.0
1	C	244	PHE	3.0
1	B	149	MET	3.0
1	D	138	ALA	3.0
1	A	531	PRO	3.0
1	C	157	LEU	3.0
1	B	141	LYS	3.0
1	B	191	ASP	2.9
1	C	143	THR	2.9
1	A	186	LYS	2.9
1	B	159	LEU	2.9
1	A	191	ASP	2.9
1	C	174	ILE	2.9
1	B	531	PRO	2.9
1	B	184	GLN	2.9
1	D	155	ASN	2.8
1	A	139	THR	2.8
1	B	164	ILE	2.7
1	B	199	ASN	2.7
1	D	157	LEU	2.7
1	A	171	GLY	2.6
1	C	200	GLY	2.6
1	C	152	CYS	2.6
1	A	174	ILE	2.6
1	D	137	GLY	2.6
1	D	100	SER	2.6
1	B	157	LEU	2.6
1	C	168	VAL	2.5
1	C	194	VAL	2.5
1	B	182	SER	2.5
1	B	146	ASN	2.4
1	B	155	ASN	2.4
1	A	169	GLU	2.4
1	B	130	ALA	2.4
1	B	404	ILE	2.3
1	C	401	LEU	2.3
1	C	187	GLN	2.3
1	A	189	GLY	2.3
1	C	183	LEU	2.3
1	D	149	MET	2.2
1	D	194	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	2.2
1	D	122	GLY	2.2
1	C	175	TYR	2.2
1	D	351	ALA	2.2
1	C	218	LEU	2.2
1	D	143	THR	2.2
1	C	217	ASP	2.2
1	A	215	ALA	2.2
1	A	137	GLY	2.1
1	A	195	THR	2.1
1	B	132	VAL	2.1
1	D	531	PRO	2.1
1	B	174	ILE	2.1
1	C	146	ASN	2.1
1	D	101	ASP	2.1
1	D	145	ASP	2.1
1	C	153	ASP	2.1
1	C	403	PRO	2.1
1	C	148	TYR	2.1
1	C	138	ALA	2.0
1	C	147	ALA	2.0
1	C	199	ASN	2.0
1	A	202	SER	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( $\text{\AA}^2$ )	Q<0.9
3	UNX	A	532	1/1	0.98	0.49	22.19	30,30,30,30	0
3	UNX	D	535	1/1	0.99	0.35	13.18	30,30,30,30	0
3	UNX	C	535	1/1	0.80	0.42	12.81	30,30,30,30	0
3	UNX	A	535	1/1	0.86	0.43	11.45	30,30,30,30	0
3	UNX	B	534	1/1	0.92	0.27	10.05	30,30,30,30	0
3	UNX	C	533	1/1	0.93	0.32	10.02	30,30,30,30	0
3	UNX	B	533	1/1	0.83	0.40	9.64	30,30,30,30	0
3	UNX	D	536	1/1	0.99	0.23	8.84	30,30,30,30	0
3	UNX	B	535	1/1	0.94	0.28	8.77	30,30,30,30	0
3	UNX	D	532	1/1	0.91	0.30	5.69	30,30,30,30	0
3	UNX	D	537	1/1	0.88	0.22	3.99	30,30,30,30	0
3	UNX	B	536	1/1	0.86	0.20	3.44	30,30,30,30	0
3	UNX	C	534	1/1	0.78	0.26	2.23	30,30,30,30	0
4	07T	B	551[B]	25/25	0.94	0.15	1.83	17,21,33,36	25
4	07T	B	551[A]	25/25	0.94	0.15	1.52	14,22,28,31	25
4	07T	C	551[B]	25/25	0.95	0.13	0.74	14,22,33,36	25
3	UNX	A	537	1/1	0.69	0.15	0.52	30,30,30,30	0
4	07T	C	551[A]	25/25	0.95	0.13	0.47	14,23,29,32	25
2	FBP	D	541	20/20	0.98	0.09	-0.82	19,24,27,28	0
2	FBP	B	541	20/20	0.98	0.09	-0.90	21,26,30,32	0
2	FBP	A	541	20/20	0.98	0.07	-1.87	21,31,33,34	0
2	FBP	C	541	20/20	0.98	0.09	-2.16	27,38,43,45	0
3	UNX	D	534	1/1	0.86	0.10	-	30,30,30,30	0
3	UNX	A	533	1/1	0.86	0.10	-	30,30,30,30	0
3	UNX	A	536	1/1	0.86	0.17	-	30,30,30,30	0
3	UNX	D	533	1/1	0.82	0.61	-	30,30,30,30	0
3	UNX	B	532	1/1	0.70	0.16	-	30,30,30,30	0
3	UNX	A	534	1/1	0.83	0.23	-	30,30,30,30	0
3	UNX	C	532	1/1	0.92	0.17	-	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.