



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2020 – 08:12 PM EDT

PDB ID : 6WP4  
Title : Pyruvate Kinase M2 mutant-S37E  
Authors : Nandi, S.; Razzaghi, M.; Srivastava, D.; Dey, M.  
Deposited on : 2020-04-26  
Resolution : 1.90 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 : 2.14.6  
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) : 2.14.6

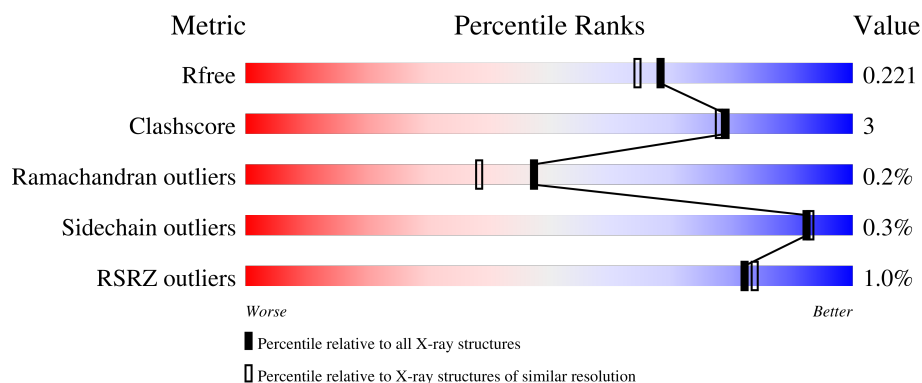
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	550	<div> <div>0%</div> <div>86% 7% 7%</div> </div>
1	B	550	<div> <div>0%</div> <div>85% 8% 7%</div> </div>
1	C	550	<div> <div>0%</div> <div>86% 6% 8%</div> </div>
1	D	550	<div> <div>2%</div> <div>86% 6% 8%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15950 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 PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			3849	2424	679	721	25			
1	B	511	Total	C	N	O	S	0	0	0
			3828	2420	671	712	25			
1	C	504	Total	C	N	O	S	0	0	0
			3773	2384	664	700	25			
1	D	506	Total	C	N	O	S	0	0	0
			3751	2364	656	706	25			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
A	37	GLU	SER	engineered mutation	UNP P14618
B	-18	MET	-	initiating methionine	UNP P14618

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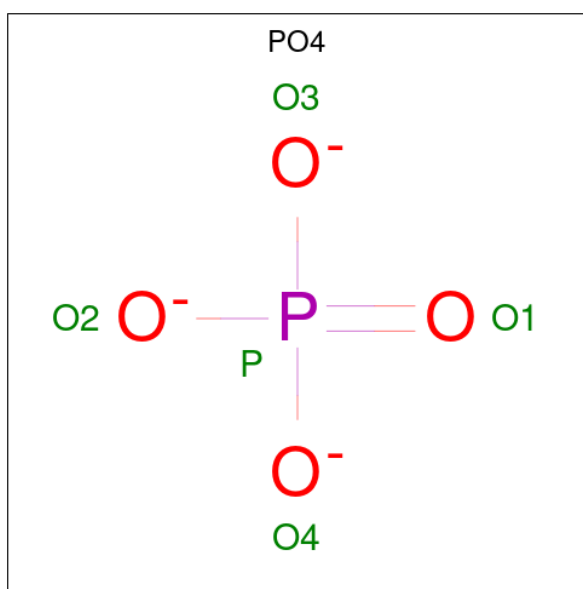
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
B	37	GLU	SER	engineered mutation	UNP P14618
C	-18	MET	-	initiating methionine	UNP P14618
C	-17	GLY	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	SER	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	HIS	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	SER	-	expression tag	UNP P14618
C	-6	GLY	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	VAL	-	expression tag	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	ARG	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
C	37	GLU	SER	engineered mutation	UNP P14618
D	-18	MET	-	initiating methionine	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
D	37	GLU	SER	engineered mutation	UNP P14618

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

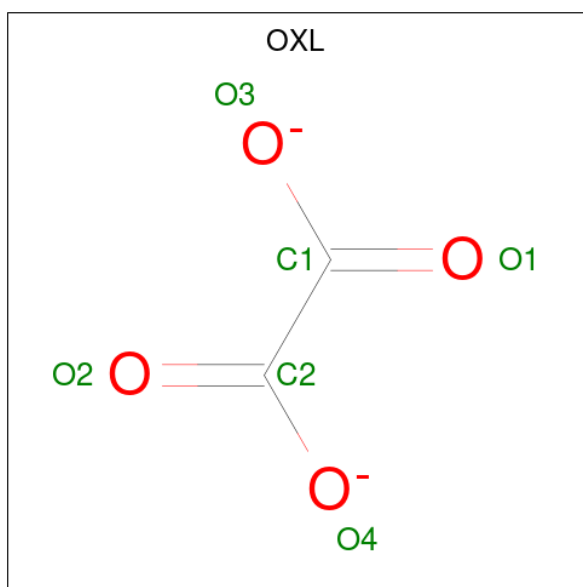
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

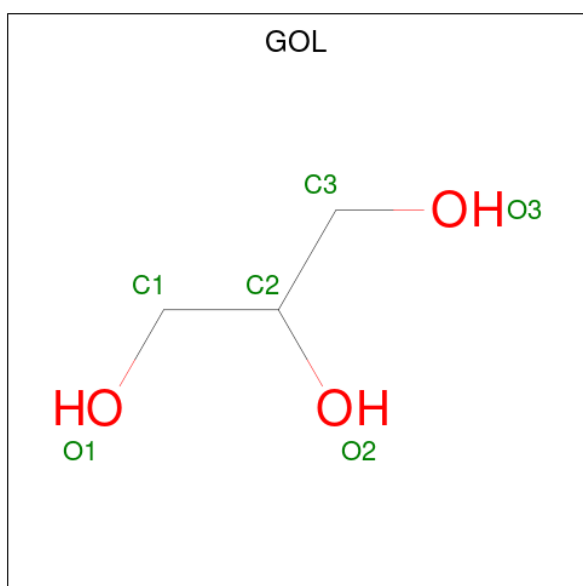
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	D	2	Total	K	0	0
			2	2		
4	C	1	Total	K	0	0
			1	1		

- Molecule 5 is OXALATE ION (three-letter code: OXL) (formula: C<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	2	4		
5	D	1	Total	C	O	0	0
			6	2	4		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	2	Total Cl 2 2	0	0

- Molecule 8 is water.

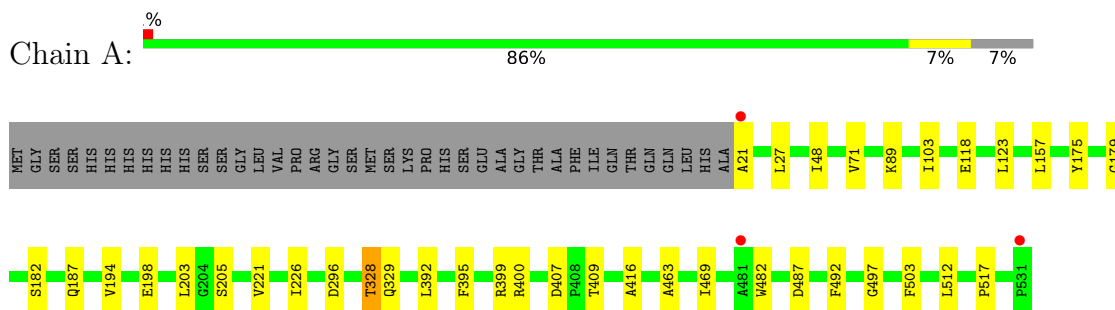


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	171	Total 171	O 171	0	0
8	B	149	Total 149	O 149	0	0
8	C	143	Total 143	O 143	0	0
8	D	100	Total 100	O 100	0	0

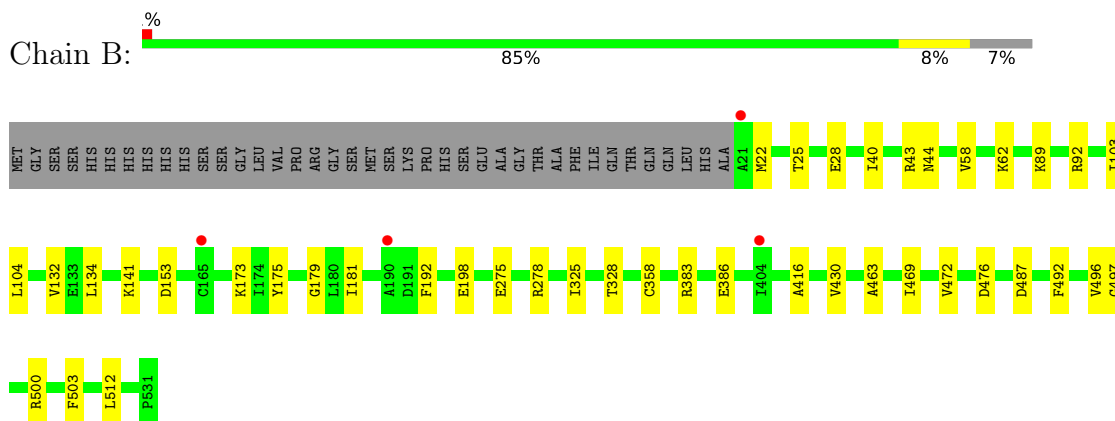
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

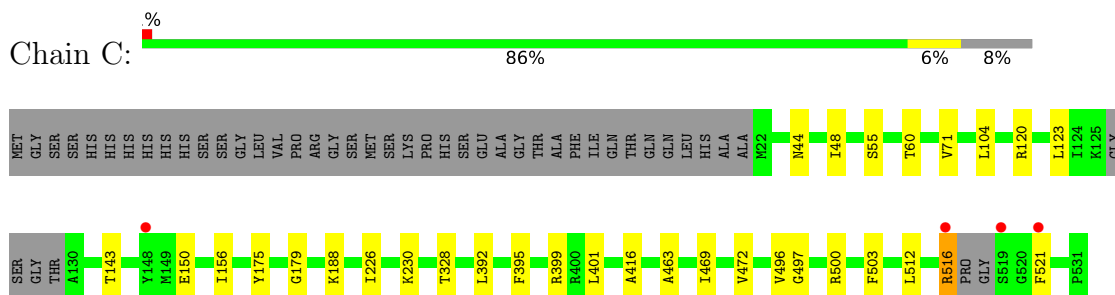
- Molecule 1: Pyruvate kinase PKM



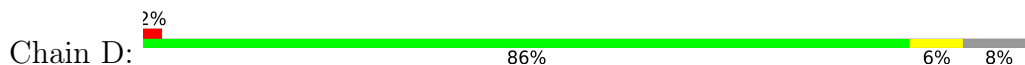
- Molecule 1: Pyruvate kinase PKM

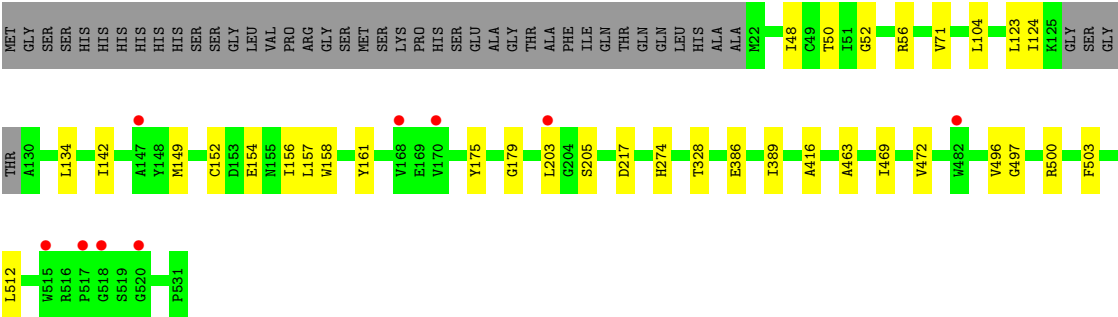


- Molecule 1: Pyruvate kinase PKM



- Molecule 1: Pyruvate kinase PKM





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.17Å 132.63Å 110.13Å 90.00° 112.74° 90.00°	Depositor
Resolution (Å)	55.53 – 1.90 55.53 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (55.53-1.90) 97.9 (55.53-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.189 , 0.221 0.189 , 0.221	Depositor DCC
$R_{free}$ test set	9566 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15950	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL, K, OXL, PO4

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	0.38	0/3909	0.53	0/5291
1	B	0.37	0/3891	0.53	0/5270
1	C	0.36	0/3831	0.52	0/5183
1	D	0.35	0/3811	0.52	0/5170
All	All	0.37	0/15442	0.52	0/20914

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	3849	0	3855	25	0
1	B	3828	0	3838	22	0
1	C	3773	0	3777	20	0
1	D	3751	0	3694	20	0
2	A	15	0	0	0	0
2	B	15	0	0	1	0
2	C	10	0	0	0	0
2	D	15	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	6	0	0	0	0
5	D	6	0	0	0	0
6	A	36	0	48	5	0
6	B	18	0	24	2	0
6	C	30	0	40	3	0
6	D	24	0	32	2	0
7	C	2	0	0	0	0
8	A	171	0	0	3	0
8	B	149	0	0	1	0
8	C	143	0	0	0	0
8	D	100	0	0	0	0
All	All	15950	0	15308	87	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 3.

All (87) 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:120:ARG:HH12	6:C:606:GOL:H2	1.34	0.92
6:B:606:GOL:O3	8:B:701:HOH:O	1.99	0.79
1:A:400:ARG:NE	8:A:701:HOH:O	2.26	0.69
6:A:609:GOL:H31	1:B:89:LYS:HA	1.75	0.68
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.83	0.61
1:A:407:ASP:OD1	1:A:409:THR:OG1	2.17	0.60
1:A:21:ALA:HB1	1:A:392:LEU:H	1.69	0.58
1:C:123:LEU:HD12	1:C:150:GLU:HG2	1.86	0.57
1:D:123:LEU:HA	1:D:205:SER:HB3	1.86	0.57
1:C:226:ILE:O	1:C:230:LYS:HG2	2.05	0.57
1:B:43:ARG:O	6:B:606:GOL:H32	2.05	0.56
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.87	0.56
1:A:27:LEU:HD23	1:C:401:LEU:HD12	1.88	0.55
1:C:104:LEU:O	1:C:500:ARG:NH1	2.39	0.55
1:B:430:VAL:HG22	1:B:512:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:HA	1:A:205:SER:HB3	1.89	0.53
1:D:175:TYR:HB3	1:D:179:GLY:HA2	1.90	0.53
1:B:134:LEU:HD12	1:B:181:ILE:HG21	1.91	0.52
1:A:400:ARG:NH1	8:A:701:HOH:O	2.43	0.52
1:C:395:PHE:CZ	1:C:399:ARG:HD2	2.44	0.52
1:A:395:PHE:CZ	1:A:399:ARG:HD3	2.46	0.51
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.92	0.51
1:C:123:LEU:HB2	1:C:150:GLU:HA	1.92	0.51
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.93	0.50
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.93	0.50
1:A:400:ARG:NH2	8:A:701:HOH:O	2.44	0.49
6:A:609:GOL:H32	1:B:92:ARG:HD2	1.93	0.49
1:D:274:HIS:HB3	6:D:611:GOL:H31	1.94	0.49
1:B:104:LEU:O	1:B:500:ARG:NH2	2.45	0.49
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.95	0.49
1:D:124:ILE:HA	1:D:152:CYS:HB2	1.94	0.48
1:A:182:SER:OG	1:A:198:GLU:HB3	2.14	0.48
1:A:416:ALA:CB	1:A:512:LEU:HD11	2.43	0.48
1:A:89:LYS:HA	6:A:608:GOL:H11	1.96	0.48
1:B:173:LYS:HE2	1:B:198:GLU:OE1	2.14	0.48
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.49	0.48
1:A:157:LEU:HD13	1:A:203:LEU:HD21	1.96	0.47
1:C:463:ALA:HB1	1:C:469:ILE:HG21	1.97	0.47
1:C:516:ARG:HD2	1:C:521:PHE:HB3	1.97	0.46
1:D:154:GLU:CD	1:D:154:GLU:H	2.17	0.46
1:D:142:ILE:HD13	1:D:157:LEU:HB3	1.97	0.46
1:A:118:GLU:HA	6:A:612:GOL:H32	1.96	0.46
1:B:40:ILE:O	1:B:383:ARG:HD2	2.16	0.46
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.96	0.46
1:D:124:ILE:HD13	1:D:152:CYS:HB2	1.97	0.46
1:D:149:MET:HG3	1:D:158:TRP:CH2	2.51	0.46
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.97	0.46
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.98	0.45
1:B:325:ILE:HG12	1:B:358:CYS:HB2	1.98	0.45
1:C:392:LEU:HA	6:C:609:GOL:H11	1.99	0.45
1:B:278:ARG:NH2	2:B:603:PO4:O3	2.48	0.44
1:B:275:GLU:HG3	1:B:278:ARG:NH2	2.32	0.44
1:D:156:ILE:HD12	1:D:156:ILE:HA	1.90	0.44
1:D:463:ALA:HB1	1:D:469:ILE:HG21	2.00	0.44
1:B:463:ALA:HB1	1:B:469:ILE:HG21	1.99	0.43
1:A:221:VAL:HG12	1:A:226:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ILE:HG12	1:D:71:VAL:HB	2.01	0.43
1:A:296:ASP:OD1	6:A:612:GOL:H12	2.19	0.43
1:B:58:VAL:HG12	1:B:62:LYS:HE3	2.00	0.43
1:D:50:THR:HG21	6:D:609:GOL:H2	2.01	0.43
1:D:104:LEU:O	1:D:500:ARG:NH1	2.52	0.43
1:A:103:ILE:HD13	1:A:492:PHE:CE1	2.54	0.43
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.54	0.43
1:C:44:ASN:O	6:C:605:GOL:H31	2.19	0.42
1:A:21:ALA:CB	1:A:392:LEU:H	2.31	0.42
1:D:386:GLU:HA	1:D:389:ILE:HD12	2.01	0.42
1:C:188:LYS:HB3	1:C:188:LYS:HE3	1.86	0.42
1:B:141:LYS:HE2	1:B:192:PHE:CD2	2.55	0.42
1:B:132:VAL:HG11	1:B:153:ASP:HA	2.02	0.42
1:D:472:VAL:HG11	1:D:496:VAL:HG11	2.01	0.42
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.54	0.42
1:D:52:GLY:O	1:D:56:ARG:HB2	2.19	0.42
1:C:143:THR:HB	1:C:156:ILE:HD11	2.01	0.42
1:D:134:LEU:HD11	1:D:203:LEU:HD22	2.01	0.42
1:B:44:ASN:H	1:B:386:GLU:CD	2.23	0.42
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.55	0.42
1:D:161:TYR:CE1	1:D:217:ASP:OD2	2.73	0.42
1:A:175:TYR:HB3	1:A:179:GLY:HA2	2.02	0.42
1:A:400:ARG:NE	1:A:400:ARG:HB3	2.35	0.42
1:A:328:THR:HG22	1:A:329:GLN:HG3	2.00	0.41
1:A:48:ILE:HG12	1:A:71:VAL:HB	2.03	0.41
1:B:103:ILE:HD13	1:B:492:PHE:CE1	2.56	0.41
1:A:482:TRP:CE3	1:A:517:PRO:HG3	2.56	0.41
1:B:25:THR:OG1	1:B:28:GLU:HG3	2.21	0.41
1:A:187:GLN:HB3	1:A:194:VAL:HB	2.03	0.40
1:C:516:ARG:HH11	1:C:521:PHE:HB3	1.86	0.40
1:C:55:SER:HA	1:C:60:THR:HG21	2.04	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	509/550 (92%)	501 (98%)	7 (1%)	1 (0%)	47	38
1	B	509/550 (92%)	498 (98%)	10 (2%)	1 (0%)	47	38
1	C	498/550 (90%)	488 (98%)	9 (2%)	1 (0%)	47	38
1	D	502/550 (91%)	493 (98%)	8 (2%)	1 (0%)	47	38
All	All	2018/2200 (92%)	1980 (98%)	34 (2%)	4 (0%)	47	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	B	328	THR
1	C	328	THR
1	D	328	THR

### 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	400/452 (88%)	399 (100%)	1 (0%)	92	93
1	B	395/452 (87%)	392 (99%)	3 (1%)	81	82
1	C	387/452 (86%)	386 (100%)	1 (0%)	92	93
1	D	381/452 (84%)	381 (100%)	0	100	100
All	All	1563/1808 (86%)	1558 (100%)	5 (0%)	92	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	487	ASP
1	B	22	MET
1	B	476	ASP
1	B	487	ASP

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Mol	Chain	Res	Type
1	C	516	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 11 are monoatomic - leaving 31 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	$\# Z  > 2$
6	GOL	B	607	-	5,5,5	0.67	0	5,5,5	1.10	0
6	GOL	A	610	-	5,5,5	0.63	0	5,5,5	1.44	1 (20%)
2	PO4	A	602	-	4,4,4	0.82	0	6,6,6	0.64	0
2	PO4	C	601	-	4,4,4	0.94	0	6,6,6	0.55	0
2	PO4	B	603	-	4,4,4	0.80	0	6,6,6	0.61	0
6	GOL	B	608	-	5,5,5	0.78	0	5,5,5	1.17	0
6	GOL	A	608	-	5,5,5	0.81	0	5,5,5	1.07	0
2	PO4	D	602	-	4,4,4	0.90	0	6,6,6	0.47	0
6	GOL	C	606	-	5,5,5	0.84	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	OXL	D	607	3	0,5,5	0.00	-	0,6,6	0.00	-
5	OXL	A	606	3	0,5,5	0.00	-	0,6,6	0.00	-
6	GOL	B	606	-	5,5,5	0.82	0	5,5,5	1.47	1 (20%)
6	GOL	A	609	-	5,5,5	0.81	0	5,5,5	0.81	0
6	GOL	D	610	-	5,5,5	0.83	0	5,5,5	1.05	0
2	PO4	D	603	-	4,4,4	0.88	0	6,6,6	0.44	0
6	GOL	C	608	-	5,5,5	0.97	0	5,5,5	0.93	0
2	PO4	B	602	-	4,4,4	0.99	0	6,6,6	0.79	0
6	GOL	A	611	-	5,5,5	0.47	0	5,5,5	1.05	0
6	GOL	D	611	-	5,5,5	1.09	0	5,5,5	0.86	0
2	PO4	C	602	-	4,4,4	0.91	0	6,6,6	0.59	0
6	GOL	A	607	-	5,5,5	0.86	0	5,5,5	1.10	0
6	GOL	C	605	-	5,5,5	1.54	2 (40%)	5,5,5	1.21	0
2	PO4	A	603	-	4,4,4	0.83	0	6,6,6	0.49	0
2	PO4	B	601	-	4,4,4	0.80	0	6,6,6	0.48	0
2	PO4	D	601	-	4,4,4	1.10	0	6,6,6	0.54	0
6	GOL	D	608	-	5,5,5	1.17	1 (20%)	5,5,5	0.86	0
2	PO4	A	601	-	4,4,4	0.91	0	6,6,6	0.86	0
6	GOL	A	612	-	5,5,5	0.82	0	5,5,5	1.01	0
6	GOL	D	609	-	5,5,5	0.87	0	5,5,5	0.96	0
6	GOL	C	609	-	5,5,5	1.03	0	5,5,5	0.97	0
6	GOL	C	607	-	5,5,5	0.77	0	5,5,5	1.11	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
6	GOL	A	607	-	-	3/4/4/4	-
6	GOL	B	607	-	-	0/4/4/4	-
6	GOL	B	608	-	-	4/4/4/4	-
6	GOL	A	608	-	-	2/4/4/4	-
6	GOL	C	608	-	-	2/4/4/4	-
6	GOL	A	610	-	-	0/4/4/4	-
6	GOL	C	606	-	-	1/4/4/4	-
5	OXL	D	607	3	-	0/0/4/4	-
6	GOL	C	605	-	-	2/4/4/4	-
5	OXL	A	606	3	-	0/0/4/4	-
6	GOL	A	611	-	-	0/4/4/4	-
6	GOL	D	611	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	608	-	-	2/4/4/4	-
6	GOL	A	612	-	-	4/4/4/4	-
6	GOL	B	606	-	-	2/4/4/4	-
6	GOL	D	609	-	-	4/4/4/4	-
6	GOL	A	609	-	-	4/4/4/4	-
6	GOL	C	609	-	-	2/4/4/4	-
6	GOL	C	607	-	-	2/4/4/4	-
6	GOL	D	610	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	605	GOL	C3-C2	2.36	1.61	1.51
6	C	605	GOL	O2-C2	-2.12	1.37	1.43
6	D	608	GOL	O2-C2	-2.02	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	606	GOL	C3-C2-C1	-3.00	100.04	111.70
6	A	610	GOL	C3-C2-C1	-2.71	101.17	111.70

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	608	GOL	C1-C2-C3-O3
6	B	608	GOL	O2-C2-C3-O3
6	A	609	GOL	C1-C2-C3-O3
6	A	612	GOL	O1-C1-C2-C3
6	A	612	GOL	C1-C2-C3-O3
6	D	609	GOL	O1-C1-C2-C3
6	D	609	GOL	C1-C2-C3-O3
6	D	610	GOL	C1-C2-C3-O3
6	B	606	GOL	O1-C1-C2-O2
6	A	609	GOL	O2-C2-C3-O3
6	B	608	GOL	O1-C1-C2-C3
6	A	608	GOL	O1-C1-C2-C3
6	B	606	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	609	GOL	O1-C1-C2-C3
6	C	608	GOL	O1-C1-C2-C3
6	D	611	GOL	C1-C2-C3-O3
6	A	607	GOL	O1-C1-C2-C3
6	C	605	GOL	O1-C1-C2-C3
6	D	608	GOL	C1-C2-C3-O3
6	C	607	GOL	O1-C1-C2-C3
6	B	608	GOL	O1-C1-C2-O2
6	D	611	GOL	O2-C2-C3-O3
6	A	607	GOL	O1-C1-C2-O2
6	C	605	GOL	O1-C1-C2-O2
6	D	608	GOL	O2-C2-C3-O3
6	D	609	GOL	O2-C2-C3-O3
6	A	612	GOL	O1-C1-C2-O2
6	D	610	GOL	O2-C2-C3-O3
6	A	608	GOL	O1-C1-C2-O2
6	C	608	GOL	O1-C1-C2-O2
6	A	612	GOL	O2-C2-C3-O3
6	D	609	GOL	O1-C1-C2-O2
6	C	609	GOL	O2-C2-C3-O3
6	C	607	GOL	O1-C1-C2-O2
6	A	609	GOL	O1-C1-C2-O2
6	C	606	GOL	O1-C1-C2-C3
6	D	611	GOL	O1-C1-C2-C3
6	A	607	GOL	C1-C2-C3-O3
6	C	609	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	PO4	1	0
6	A	608	GOL	1	0
6	C	606	GOL	1	0
6	B	606	GOL	2	0
6	A	609	GOL	2	0
6	D	611	GOL	1	0
6	C	605	GOL	1	0
6	A	612	GOL	2	0
6	D	609	GOL	1	0
6	C	609	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	511/550 (92%)	-0.20	3 (0%) 89 90	16, 25, 40, 52	0
1	B	511/550 (92%)	-0.29	4 (0%) 86 87	17, 26, 42, 56	0
1	C	504/550 (91%)	-0.19	4 (0%) 86 87	16, 28, 43, 55	0
1	D	506/550 (92%)	-0.15	9 (1%) 68 71	18, 30, 48, 63	0
All	All	2032/2200 (92%)	-0.21	20 (0%) 82 84	16, 27, 44, 63	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	482	TRP	3.9
1	A	21	ALA	3.2
1	B	190	ALA	3.2
1	D	147	ALA	3.0
1	C	148	TYR	2.6
1	C	516	ARG	2.5
1	B	21	ALA	2.5
1	D	168	VAL	2.5
1	D	517	PRO	2.4
1	C	519	SER	2.4
1	C	521	PHE	2.4
1	A	481	ALA	2.3
1	D	515	TRP	2.3
1	A	531	PRO	2.3
1	D	170	VAL	2.3
1	D	518	GLY	2.2
1	D	520	GLY	2.1
1	D	203	LEU	2.1
1	B	404	ILE	2.1
1	B	165	CYS	2.1

## 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 monosaccharides 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
6	GOL	D	611	6/6	0.58	0.23	41,47,50,53	0
4	K	D	606	1/1	0.75	0.10	73,73,73,73	0
6	GOL	B	606	6/6	0.81	0.17	24,28,32,38	0
6	GOL	C	608	6/6	0.84	0.20	32,37,40,40	0
6	GOL	C	606	6/6	0.85	0.15	32,39,41,45	0
6	GOL	D	608	6/6	0.86	0.14	30,32,36,36	0
6	GOL	A	610	6/6	0.88	0.12	24,33,36,36	0
6	GOL	B	607	6/6	0.89	0.13	28,35,36,38	0
6	GOL	A	612	6/6	0.89	0.14	24,28,34,40	0
6	GOL	A	607	6/6	0.90	0.18	32,35,38,48	0
7	CL	C	610	1/1	0.90	0.04	65,65,65,65	0
6	GOL	C	605	6/6	0.91	0.16	14,29,31,41	0
6	GOL	A	611	6/6	0.91	0.21	27,33,35,36	0
6	GOL	C	607	6/6	0.92	0.12	30,37,38,42	0
6	GOL	A	609	6/6	0.93	0.15	33,35,38,48	0
3	MG	B	604	1/1	0.93	0.07	27,27,27,27	0
6	GOL	C	609	6/6	0.93	0.09	32,36,39,43	0
6	GOL	A	608	6/6	0.93	0.11	31,37,42,49	0
6	GOL	D	609	6/6	0.94	0.10	36,39,44,45	0
7	CL	C	611	1/1	0.94	0.10	54,54,54,54	0
5	OXL	A	606	6/6	0.94	0.08	25,26,31,32	0
5	OXL	D	607	6/6	0.95	0.08	25,26,33,36	0
6	GOL	D	610	6/6	0.95	0.12	31,34,42,43	0
2	PO4	D	603	5/5	0.95	0.16	45,49,58,60	0
2	PO4	A	603	5/5	0.95	0.19	39,41,46,51	0
6	GOL	B	608	6/6	0.96	0.08	34,39,44,46	0
2	PO4	C	602	5/5	0.96	0.09	38,45,48,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	C	603	1/1	0.96	0.16	35,35,35,35	0
2	PO4	B	603	5/5	0.96	0.29	46,47,53,54	0
2	PO4	A	602	5/5	0.97	0.07	29,31,36,36	0
2	PO4	B	601	5/5	0.97	0.05	28,28,35,37	0
2	PO4	D	602	5/5	0.97	0.06	49,50,55,58	0
2	PO4	A	601	5/5	0.98	0.07	26,28,29,30	0
3	MG	D	604	1/1	0.98	0.02	31,31,31,31	0
4	K	A	605	1/1	0.99	0.06	21,21,21,21	0
2	PO4	C	601	5/5	0.99	0.09	27,29,31,33	0
4	K	B	605	1/1	0.99	0.06	23,23,23,23	0
2	PO4	B	602	5/5	0.99	0.07	25,27,29,29	0
3	MG	A	604	1/1	0.99	0.05	24,24,24,24	0
4	K	C	604	1/1	0.99	0.07	28,28,28,28	0
2	PO4	D	601	5/5	0.99	0.09	26,28,33,34	0
4	K	D	605	1/1	1.00	0.04	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.