



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 PM GMT

PDB ID : 4QG8  
Title : crystal structure of PKM2-K305Q mutant  
Authors : Wang, P.; Sun, C.; Zhu, T.; Xu, Y.  
Deposited on : 2014-05-22  
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

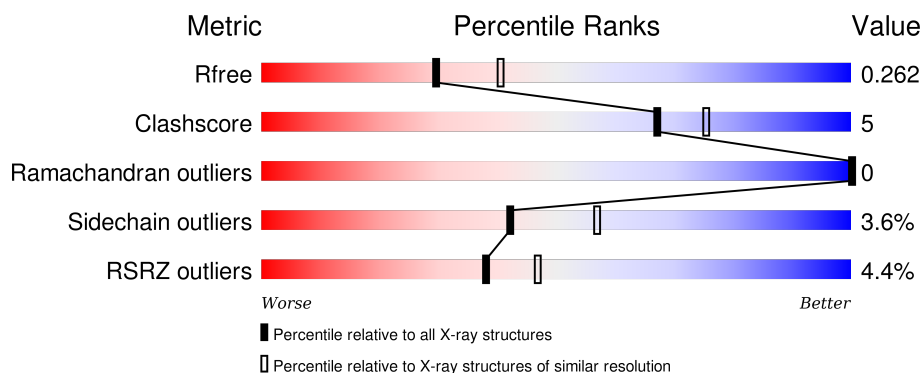
# 1 Overall quality at a glance

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	535	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>6%</div> </div> </div>
1	B	535	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	C	535	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	D	535	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>11%</div> <div>24%</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
5	MLI	A	1004	-	-	X	X
5	MLI	B	1003	-	-	-	X
5	MLI	C	1003	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15432 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	505	Total	C	N	O	S	0	0	0
			3873	2437	686	726	24			
1	B	504	Total	C	N	O	S	0	0	0
			3868	2435	685	724	24			
1	C	505	Total	C	N	O	S	0	0	0
			3876	2439	686	727	24			
1	D	406	Total	C	N	O	S	0	0	0
			3125	1961	564	579	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P14618
A	-2	PRO	-	EXPRESSION TAG	UNP P14618
A	-1	GLY	-	EXPRESSION TAG	UNP P14618
A	0	SER	-	EXPRESSION TAG	UNP P14618
A	305	GLN	LYS	ENGINEERED MUTATION	UNP P14618
B	-3	GLY	-	EXPRESSION TAG	UNP P14618
B	-2	PRO	-	EXPRESSION TAG	UNP P14618
B	-1	GLY	-	EXPRESSION TAG	UNP P14618
B	0	SER	-	EXPRESSION TAG	UNP P14618
B	305	GLN	LYS	ENGINEERED MUTATION	UNP P14618
C	-3	GLY	-	EXPRESSION TAG	UNP P14618
C	-2	PRO	-	EXPRESSION TAG	UNP P14618
C	-1	GLY	-	EXPRESSION TAG	UNP P14618
C	0	SER	-	EXPRESSION TAG	UNP P14618
C	305	GLN	LYS	ENGINEERED MUTATION	UNP P14618
D	-3	GLY	-	EXPRESSION TAG	UNP P14618
D	-2	PRO	-	EXPRESSION TAG	UNP P14618
D	-1	GLY	-	EXPRESSION TAG	UNP P14618
D	0	SER	-	EXPRESSION TAG	UNP P14618
D	305	GLN	LYS	ENGINEERED MUTATION	UNP P14618

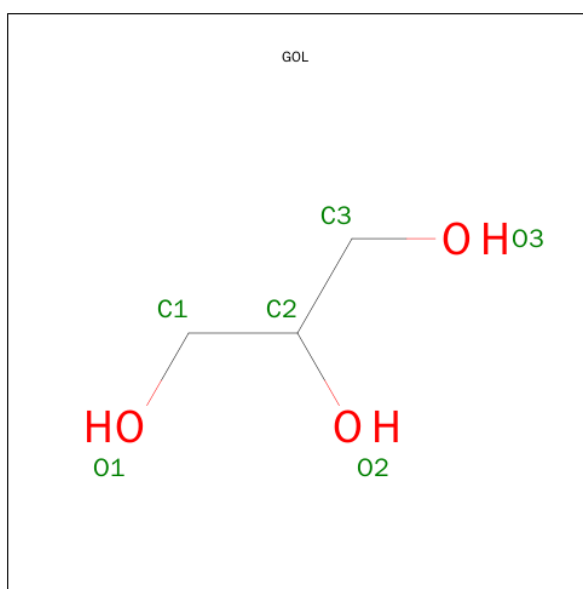
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

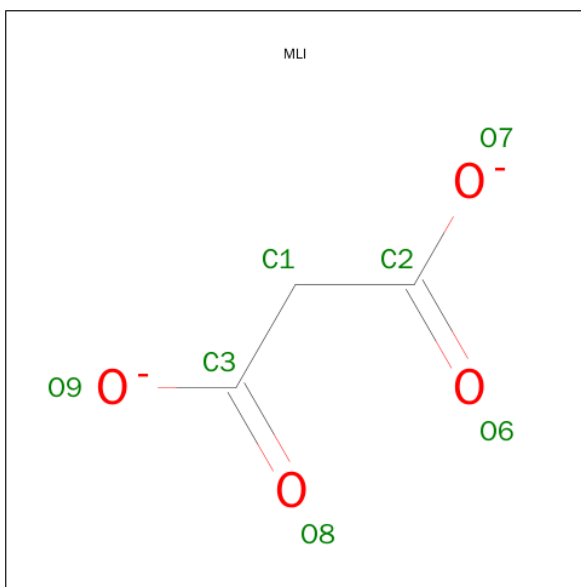
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: C<sub>3</sub>H<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	B	1	Total	C	O	0	0
			7	3	4		
5	C	1	Total	C	O	0	0
			7	3	4		

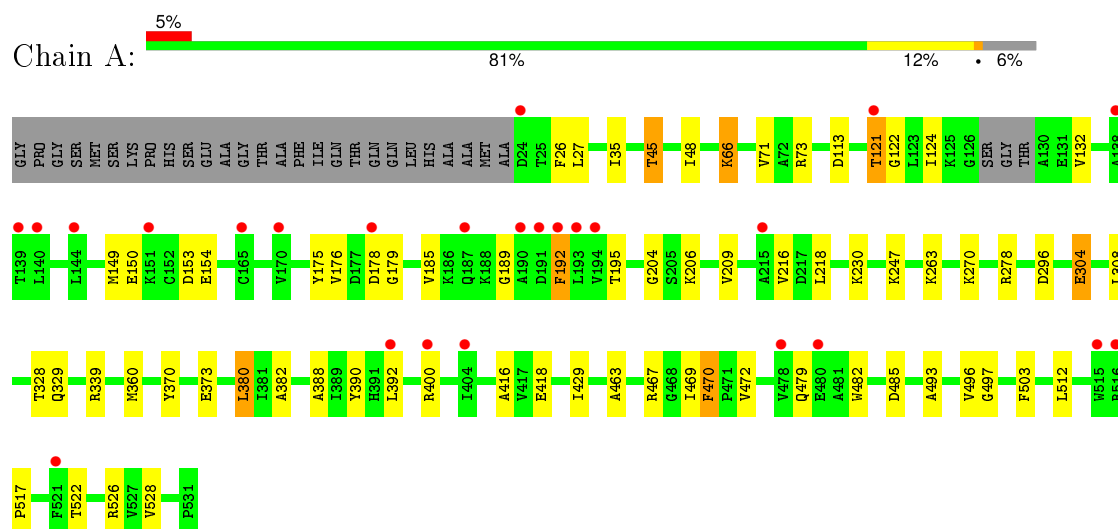
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	173	Total	O	0	0
			173	173		
6	B	214	Total	O	0	0
			214	214		
6	C	194	Total	O	0	0
			194	194		
6	D	76	Total	O	0	0
			76	76		

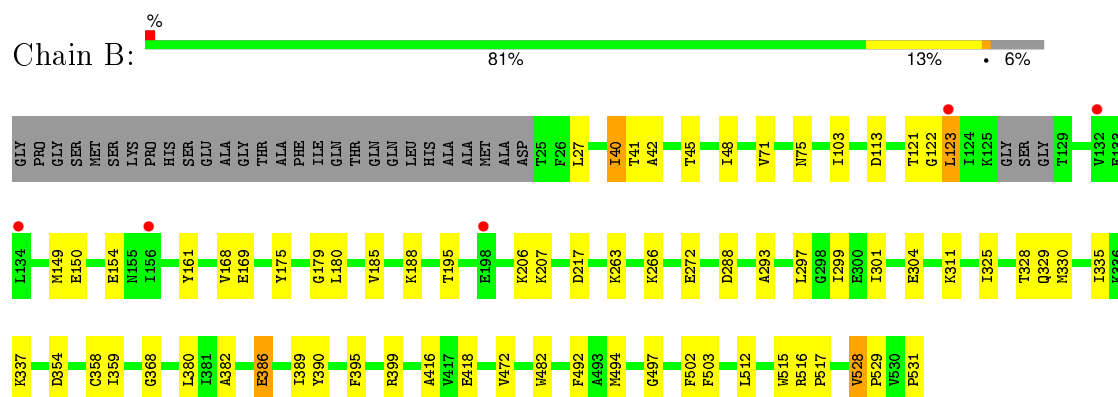
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

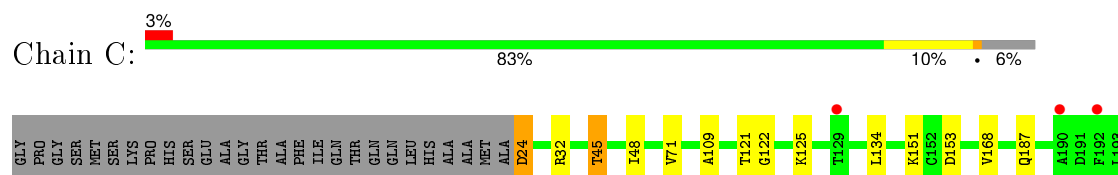
#### • Molecule 1: Pyruvate kinase PKM

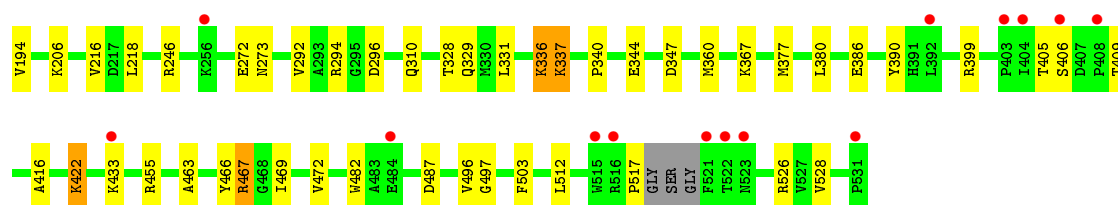


#### • Molecule 1: Pyruvate kinase PKM

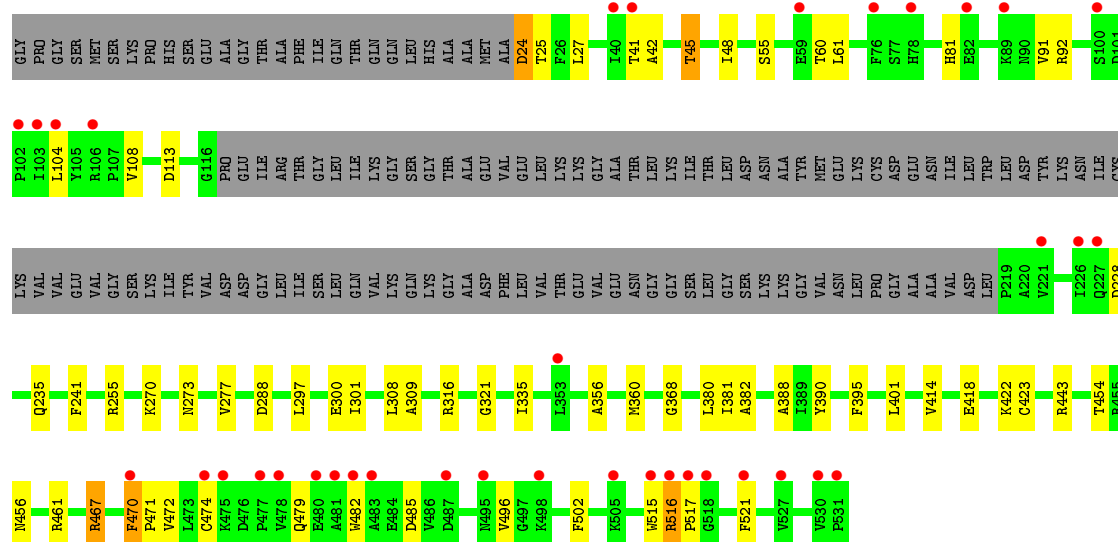


#### • Molecule 1: Pyruvate kinase PKM





● 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, $\alpha$ , $\beta$ , $\gamma$	94.81Å 117.38Å 110.33Å 90.00° 113.21° 90.00°	Depositor
Resolution (Å)	46.54 – 2.30 46.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.54-2.30) 99.5 (46.54-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.00 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.213 , 0.260 0.220 , 0.262	Depositor DCC
$R_{free}$ test set	4896 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.3	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 98003 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15432	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: GOL, K, MLI, MG

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	0.21	0/3935	0.40	0/5313
1	B	0.21	0/3930	0.40	0/5307
1	C	0.21	0/3938	0.41	0/5318
1	D	0.21	0/3179	0.39	0/4293
All	All	0.21	0/14982	0.40	0/20231

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	3873	0	3954	45	0
1	B	3868	0	3954	38	0
1	C	3876	0	3958	35	0
1	D	3125	0	3176	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	6	0	8	1	0
5	A	7	0	2	2	0
5	B	7	0	2	0	0
5	C	7	0	2	0	0
6	A	173	0	0	5	0
6	B	214	0	0	2	0
6	C	194	0	0	3	0
6	D	76	0	0	4	0
All	All	15432	0	15056	144	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 5.

All (144) 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:A:304:GLU:HG2	1:D:380:LEU:HB3	1.61	0.81
1:C:45:THR:HG22	1:C:467:ARG:HD2	1.69	0.74
1:C:422:LYS:HG3	1:D:414:VAL:HG11	1.77	0.66
1:D:474:CYS:SG	6:D:603:HOH:O	2.55	0.65
1:C:399:ARG:NH1	1:D:418:GLU:OE1	2.30	0.64
1:D:24:ASP:N	6:D:657:HOH:O	2.31	0.64
1:C:472:VAL:HG11	1:C:496:VAL:HG21	1.79	0.64
1:C:467:ARG:NH2	6:C:2162:HOH:O	2.32	0.62
1:A:472:VAL:HG21	1:A:496:VAL:HG21	1.81	0.62
1:C:405:THR:HA	1:C:406:SER:HB2	1.82	0.61
1:A:247:LYS:NZ	6:A:1148:HOH:O	2.33	0.61
1:A:132:VAL:HG11	1:A:153:ASP:HA	1.83	0.61
1:A:35:ILE:HD12	1:D:277:VAL:HG11	1.84	0.60
1:C:433:LYS:HE2	1:C:455:ARG:HB2	1.83	0.60
1:A:176:VAL:HG12	1:A:209:VAL:HG22	1.83	0.59
1:A:467:ARG:NH2	6:A:1166:HOH:O	2.25	0.59
1:C:187:GLN:HB2	1:C:194:VAL:HB	1.83	0.58
1:A:526:ARG:HD3	1:B:515:TRP:CD2	2.38	0.58
1:A:121:THR:HG22	1:A:122:GLY:HA3	1.86	0.58
1:A:35:ILE:HD11	1:D:309:ALA:HB2	1.86	0.57
1:B:399:ARG:NH1	6:B:1175:HOH:O	2.33	0.57
1:C:294:ARG:NH2	1:C:347:ASP:OD1	2.35	0.56
1:A:230:LYS:NZ	6:A:1259:HOH:O	2.37	0.56
1:D:316:ARG:NH2	6:D:625:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:GLY:HA3	1:B:299:ILE:HD12	1.89	0.55
1:D:81:HIS:NE2	1:D:228:ASP:OD1	2.35	0.55
1:D:92:ARG:NH1	1:D:235:GLN:O	2.32	0.55
1:D:456:ASN:O	6:D:602:HOH:O	2.18	0.54
1:C:526:ARG:HD3	1:D:515:TRP:CD2	2.42	0.54
1:A:216:VAL:HG12	1:A:218:LEU:H	1.73	0.53
1:D:479:GLN:HB2	1:D:485:ASP:HB2	1.90	0.53
1:B:123:LEU:HB3	1:B:150:GLU:HA	1.91	0.52
1:A:370:TYR:HB3	1:A:373:GLU:HB2	1.90	0.52
1:B:482:TRP:CG	1:B:517:PRO:HG3	2.45	0.52
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.92	0.52
1:B:121:THR:HB	1:B:122:GLY:HA3	1.90	0.52
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.91	0.52
1:B:42:ALA:HB2	1:B:502:PHE:CE1	2.46	0.51
1:A:328:THR:OG1	5:A:1004:MLI:O8	2.21	0.51
1:B:40:ILE:HG12	1:B:41:THR:O	2.11	0.51
1:C:328:THR:HG22	1:C:329:GLN:HG3	1.92	0.51
1:A:304:GLU:HB3	1:D:381:ILE:HG12	1.93	0.50
1:A:185:VAL:HA	1:A:195:THR:HG22	1.94	0.50
1:B:149:MET:HG3	1:B:150:GLU:HG3	1.94	0.50
1:C:121:THR:HB	1:C:122:GLY:HA3	1.94	0.50
1:C:482:TRP:CE3	1:C:517:PRO:HG3	2.47	0.50
1:A:388:ALA:HB2	1:D:308:LEU:HD21	1.94	0.49
1:C:331:LEU:HD23	1:C:344:GLU:HB3	1.94	0.49
1:C:125:LYS:HA	1:C:151:LYS:HA	1.95	0.49
1:A:512:LEU:HB3	1:A:522:THR:HG21	1.96	0.48
1:A:328:THR:HG22	1:A:329:GLN:HG3	1.94	0.48
1:A:45:THR:HG23	1:A:382:ALA:HB1	1.95	0.48
1:A:124:ILE:HD11	1:A:204:GLY:HA2	1.95	0.48
1:C:48:ILE:HB	1:C:360:MET:HG3	1.95	0.48
1:C:125:LYS:HE3	1:C:153:ASP:HB3	1.95	0.47
1:D:482:TRP:CG	1:D:517:PRO:HB3	2.49	0.47
1:B:395:PHE:HZ	1:B:418:GLU:HG2	1.78	0.47
1:D:255:ARG:NH2	1:D:288:ASP:OD1	2.32	0.47
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.48	0.47
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.96	0.47
1:A:48:ILE:HB	1:A:360:MET:HG3	1.96	0.47
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.96	0.47
1:D:48:ILE:HB	1:D:360:MET:HG3	1.97	0.47
1:C:405:THR:O	1:D:423:CYS:HA	2.14	0.47
1:A:418:GLU:HG3	1:B:418:GLU:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ALA:HB2	1:D:502:PHE:CE1	2.50	0.46
1:B:121:THR:O	1:B:206:LYS:HA	2.16	0.46
1:C:336:LYS:HB2	1:C:337:LYS:HD2	1.98	0.46
1:C:455:ARG:NH1	6:C:2152:HOH:O	2.33	0.46
1:A:121:THR:O	1:A:206:LYS:HA	2.15	0.46
1:B:45:THR:HG21	1:B:359:ILE:HG12	1.96	0.46
1:B:395:PHE:CZ	1:B:418:GLU:HG2	2.51	0.46
1:A:482:TRP:CG	1:A:517:PRO:HD3	2.51	0.46
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.98	0.45
1:A:308:LEU:HD21	1:D:388:ALA:HB2	1.99	0.45
1:A:429:ILE:HD12	1:A:493:ALA:HB1	1.97	0.45
1:D:45:THR:HG23	1:D:382:ALA:HB1	1.98	0.45
1:D:472:VAL:HG21	1:D:496:VAL:HG11	1.98	0.45
1:A:339:ARG:NH2	6:A:1247:HOH:O	2.45	0.45
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.97	0.45
1:C:246:ARG:HE	1:C:273:ASN:ND2	2.14	0.45
1:A:479:GLN:HB2	1:A:485:ASP:HB2	1.98	0.45
1:C:292:VAL:HG12	1:C:294:ARG:HG3	1.99	0.44
1:A:48:ILE:HG12	1:A:71:VAL:HB	2.00	0.44
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.52	0.44
1:B:169:GLU:HA	1:B:188:LYS:HD2	1.99	0.44
1:B:330:MET:SD	1:B:359:ILE:HG23	2.58	0.44
1:B:75:ASN:HA	1:B:113:ASP:HB3	2.00	0.44
1:D:241:PHE:HB3	1:D:270:LYS:HD2	1.98	0.44
1:D:321:GLY:HA3	1:D:443:ARG:HE	1.83	0.44
1:B:297:LEU:O	1:B:301:ILE:HG12	2.18	0.44
1:D:55:SER:HA	1:D:60:THR:HG21	2.00	0.44
1:D:297:LEU:O	1:D:301:ILE:HG12	2.17	0.44
1:B:121:THR:OG1	1:B:207:LYS:N	2.38	0.43
1:C:121:THR:O	1:C:206:LYS:HA	2.18	0.43
1:C:45:THR:HG23	1:C:386:GLU:OE2	2.18	0.43
1:C:294:ARG:NE	1:C:310:GLN:OE1	2.49	0.43
1:D:395:PHE:HZ	1:D:418:GLU:HG2	1.83	0.43
1:B:528:VAL:HA	1:B:529:PRO:HD3	1.83	0.43
1:D:516:ARG:HB3	1:D:516:ARG:HE	1.61	0.43
1:C:24:ASP:OD1	1:C:24:ASP:N	2.51	0.43
1:D:335:ILE:HG23	1:D:368:GLY:HA2	2.00	0.43
1:D:61:LEU:HD13	1:D:91:VAL:HA	2.00	0.43
1:D:273:ASN:HB2	1:D:300:GLU:HG2	2.01	0.43
1:C:206:LYS:NZ	6:C:2101:HOH:O	2.43	0.43
1:A:470:PHE:CD1	4:A:1003:GOL:H12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLY:HA3	1:A:192:PHE:CE1	2.54	0.43
1:C:340:PRO:HG3	1:C:377:MET:HG2	2.01	0.43
1:B:325:ILE:HG12	1:B:358:CYS:HB2	2.01	0.42
1:D:470:PHE:HD1	1:D:470:PHE:HA	1.76	0.42
1:D:24:ASP:HB3	1:D:25:THR:H	1.61	0.42
1:B:311:LYS:NZ	1:B:354:ASP:OD1	2.51	0.42
1:B:263:LYS:NZ	6:B:1220:HOH:O	2.49	0.42
1:A:416:ALA:HB2	1:A:512:LEU:HD21	2.02	0.42
1:A:132:VAL:HB	1:A:154:GLU:HG3	2.02	0.42
1:A:400:ARG:HD3	1:D:25:THR:HG21	2.01	0.42
1:B:161:TYR:OH	1:B:217:ASP:OD1	2.26	0.42
1:C:466:TYR:HB2	1:C:469:ILE:HD12	2.02	0.42
1:C:463:ALA:HB1	1:C:469:ILE:HG21	2.01	0.42
1:B:386:GLU:HA	1:B:389:ILE:HG13	2.02	0.42
1:A:149:MET:HG3	1:A:150:GLU:HG3	2.02	0.42
1:A:392:LEU:HD13	1:A:392:LEU:HA	1.93	0.42
1:D:113:ASP:HA	1:D:241:PHE:HB2	2.02	0.42
1:A:270:LYS:NZ	5:A:1004:MLI:O6	2.42	0.41
1:C:272:GLU:HB3	1:C:296:ASP:HB2	2.02	0.41
1:B:48:ILE:HG12	1:B:71:VAL:HB	2.02	0.41
1:A:73:ARG:NH1	1:A:113:ASP:OD2	2.43	0.41
1:B:328:THR:HG22	1:B:329:GLN:HG3	2.01	0.41
1:A:263:LYS:NZ	6:A:1235:HOH:O	2.34	0.41
1:B:335:ILE:HG23	1:B:368:GLY:HA2	2.02	0.41
1:B:266:LYS:HD2	1:B:288:ASP:HB3	2.02	0.41
1:B:416:ALA:HB2	1:B:512:LEU:HD21	2.03	0.41
1:B:185:VAL:HA	1:B:195:THR:HG22	2.03	0.41
1:C:216:VAL:HG12	1:C:218:LEU:H	1.86	0.41
1:A:66:LYS:HG2	1:A:66:LYS:H	1.65	0.41
1:D:356:ALA:O	1:D:467:ARG:NH1	2.54	0.41
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.56	0.41
1:D:108:VAL:O	1:D:461:ARG:HD2	2.20	0.41
1:B:272:GLU:HA	1:B:297:LEU:HB2	2.04	0.40
1:B:382:ALA:O	1:B:386:GLU:HG2	2.20	0.40
1:D:395:PHE:CZ	1:D:418:GLU:HG2	2.56	0.40
1:B:272:GLU:HB3	1:B:293:ALA:HB3	2.04	0.40
1:A:380:LEU:HA	1:A:380:LEU:HD12	1.93	0.40
1:B:103:ILE:HG12	1:B:492:PHE:HE1	1.87	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	501/535 (94%)	487 (97%)	14 (3%)	0	100	100
1	B	500/535 (94%)	486 (97%)	14 (3%)	0	100	100
1	C	501/535 (94%)	486 (97%)	15 (3%)	0	100	100
1	D	402/535 (75%)	385 (96%)	17 (4%)	0	100	100
All	All	1904/2140 (89%)	1844 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	417/438 (95%)	403 (97%)	14 (3%)	44	59
1	B	417/438 (95%)	403 (97%)	14 (3%)	44	59
1	C	418/438 (95%)	403 (96%)	15 (4%)	42	57
1	D	335/438 (76%)	321 (96%)	14 (4%)	36	49
All	All	1587/1752 (91%)	1530 (96%)	57 (4%)	42	57

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	45	THR
1	A	66	LYS
1	A	121	THR
1	A	178	ASP
1	A	192	PHE
1	A	278	ARG
1	A	296	ASP
1	A	304	GLU
1	A	380	LEU
1	A	390	TYR
1	A	470	PHE
1	A	528	VAL
1	B	27	LEU
1	B	40	ILE
1	B	123	LEU
1	B	154	GLU
1	B	168	VAL
1	B	180	LEU
1	B	304	GLU
1	B	337	LYS
1	B	380	LEU
1	B	386	GLU
1	B	390	TYR
1	B	472	VAL
1	B	516	ARG
1	B	528	VAL
1	C	24	ASP
1	C	32	ARG
1	C	45	THR
1	C	134	LEU
1	C	168	VAL
1	C	336	LYS
1	C	337	LYS
1	C	367	LYS
1	C	380	LEU
1	C	390	TYR
1	C	409	THR
1	C	422	LYS
1	C	467	ARG
1	C	487	ASP
1	C	528	VAL
1	D	24	ASP

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Mol	Chain	Res	Type
1	D	27	LEU
1	D	41	THR
1	D	45	THR
1	D	104	LEU
1	D	390	TYR
1	D	401	LEU
1	D	422	LYS
1	D	454	THR
1	D	467	ARG
1	D	470	PHE
1	D	471	PRO
1	D	516	ARG
1	D	521	PHE

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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
4	GOL	A	1003	-	5,5,5	0.34	0	5,5,5	0.28	0
5	MLI	A	1004	2	0,6,6	0.00	-	0,7,7	0.00	-
5	MLI	B	1003	2	0,6,6	0.00	-	0,7,7	0.00	-
5	MLI	C	1003	2	0,6,6	0.00	-	0,7,7	0.00	-

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
4	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
5	MLI	A	1004	2	-	0/0/4/4	0/0/0/0
5	MLI	B	1003	2	-	0/0/4/4	0/0/0/0
5	MLI	C	1003	2	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	GOL	1	0
5	A	1004	MLI	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	505/535 (94%)	0.19	25 (4%) 32 41	4, 19, 50, 76	0
1	B	504/535 (94%)	-0.07	5 (0%) 84 88	4, 17, 41, 64	0
1	C	505/535 (94%)	0.16	17 (3%) 49 58	6, 20, 47, 74	0
1	D	406/535 (75%)	0.65	37 (9%) 11 17	14, 32, 57, 80	0
All	All	1920/2140 (89%)	0.21	84 (4%) 38 47	4, 22, 50, 80	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	PHE	6.2
1	D	517	PRO	5.7
1	C	515	TRP	4.6
1	D	40	ILE	4.4
1	C	404	ILE	4.1
1	C	523	ASN	4.1
1	D	221	VAL	4.0
1	A	516	ARG	3.9
1	D	474	CYS	3.8
1	C	406	SER	3.6
1	D	530	VAL	3.5
1	A	190	ALA	3.5
1	A	121	THR	3.4
1	D	477	PRO	3.4
1	D	531	PRO	3.3
1	A	138	ALA	3.3
1	B	134	LEU	3.3
1	C	408	PRO	3.2
1	A	515	TRP	3.2
1	D	481	ALA	3.2
1	A	392	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	482	TRP	3.1
1	C	522	THR	3.1
1	D	76	PHE	3.1
1	C	392	LEU	3.1
1	D	226	ILE	3.0
1	C	531	PRO	3.0
1	C	521	PHE	3.0
1	D	475	LYS	3.0
1	C	516	ARG	3.0
1	D	521	PHE	3.0
1	C	256	LYS	3.0
1	A	215	ALA	2.8
1	D	227	GLN	2.8
1	D	470	PHE	2.8
1	A	400	ARG	2.8
1	D	515	TRP	2.7
1	B	123	LEU	2.7
1	A	480	GLU	2.6
1	D	495	ASN	2.6
1	D	104	LEU	2.6
1	A	187	GLN	2.6
1	A	24	ASP	2.6
1	C	190	ALA	2.6
1	A	151	LYS	2.6
1	A	139	THR	2.5
1	D	527	VAL	2.5
1	A	404	ILE	2.5
1	D	100	SER	2.5
1	A	194	VAL	2.5
1	A	170	VAL	2.5
1	D	78	HIS	2.5
1	A	165	CYS	2.4
1	D	478	VAL	2.4
1	D	82	GLU	2.4
1	D	102	PRO	2.4
1	B	156	ILE	2.4
1	A	521	PHE	2.4
1	D	498	LYS	2.4
1	C	403	PRO	2.3
1	A	144	LEU	2.3
1	A	193	LEU	2.3
1	D	103	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	483	ALA	2.3
1	D	505	LYS	2.3
1	C	433	LYS	2.3
1	D	89	LYS	2.3
1	C	129	THR	2.3
1	A	191	ASP	2.3
1	B	132	VAL	2.2
1	D	480	GLU	2.2
1	C	192	PHE	2.2
1	A	478	VAL	2.2
1	D	487	ASP	2.2
1	D	41	THR	2.1
1	D	518	GLY	2.1
1	A	140	LEU	2.1
1	C	484	GLU	2.0
1	D	106	ARG	2.0
1	D	516	ARG	2.0
1	A	178	ASP	2.0
1	B	198	GLU	2.0
1	D	59	GLU	2.0
1	D	353	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
5	MLI	A	1004	7/7	0.87	0.35	11.02	7,9,13,19	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MLI	C	1003	7/7	0.91	0.50	8.41	7,9,13,14	7
5	MLI	B	1003	7/7	0.93	0.32	6.76	3,7,13,13	7
4	GOL	A	1003	6/6	0.88	0.18	1.54	25,26,31,42	0
3	K	A	1002	1/1	0.92	0.15	0.97	31,31,31,31	0
3	K	B	1002	1/1	0.86	0.10	-0.82	37,37,37,37	0
3	K	C	1002	1/1	0.92	0.08	-2.25	39,39,39,39	0
2	MG	C	1001	1/1	0.96	0.20	-	25,25,25,25	0
2	MG	B	1001	1/1	0.92	0.10	-	17,17,17,17	0
2	MG	A	1001	1/1	0.70	0.11	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.