



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:01 AM UTC

PDB ID : 4QG8 / pdb_00004qg8
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

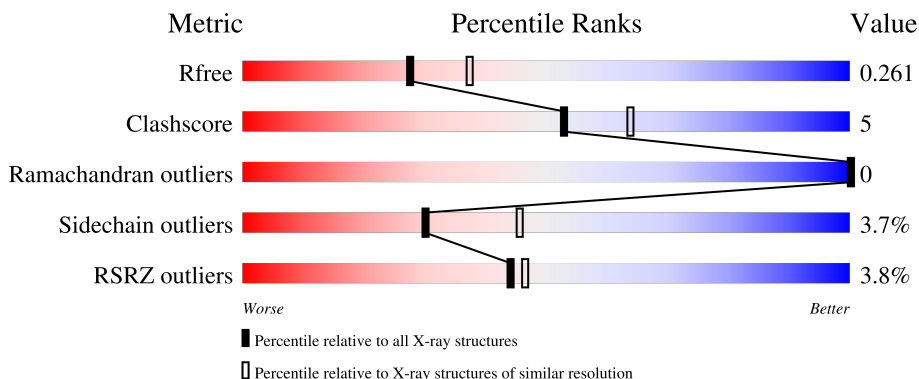
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	535	4% 81% 12% 6%
1	B	535	2% 81% 13% 6%
1	C	535	3% 83% 10% 6%
1	D	535	5% 63% 11% 24%

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

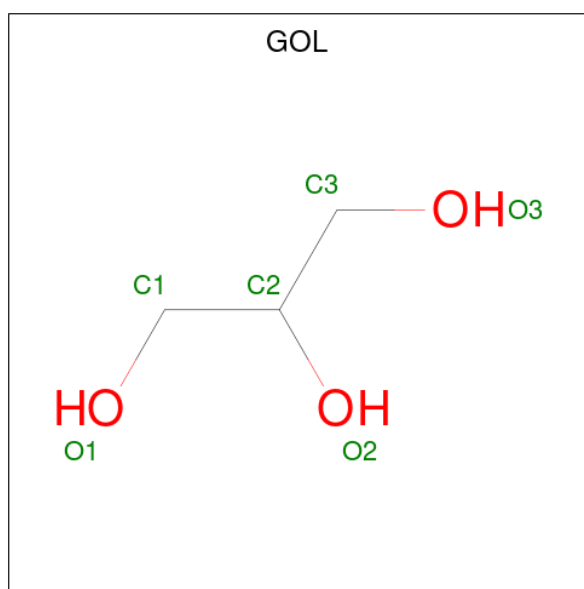
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).



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		

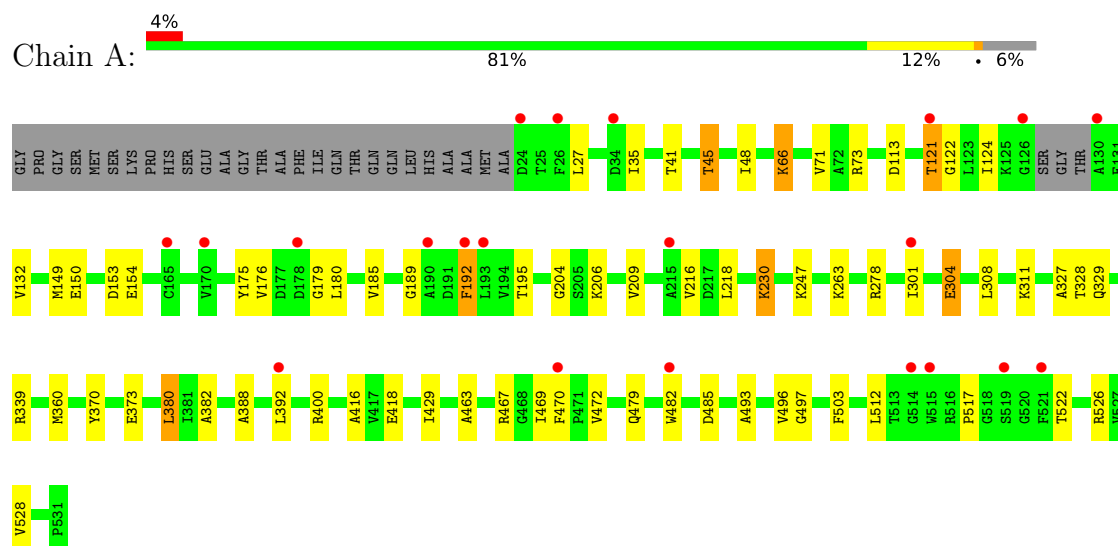
- Molecule 6 is water.

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		

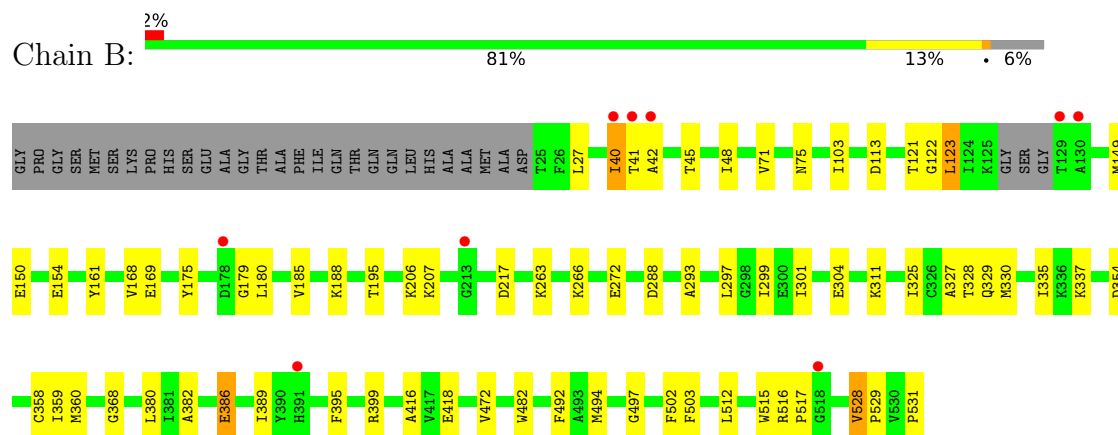
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

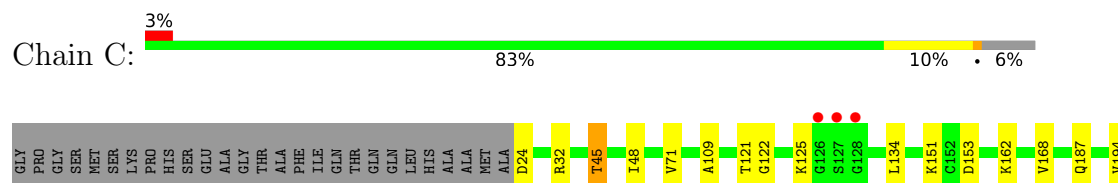
• Molecule 1: Pyruvate kinase PKM

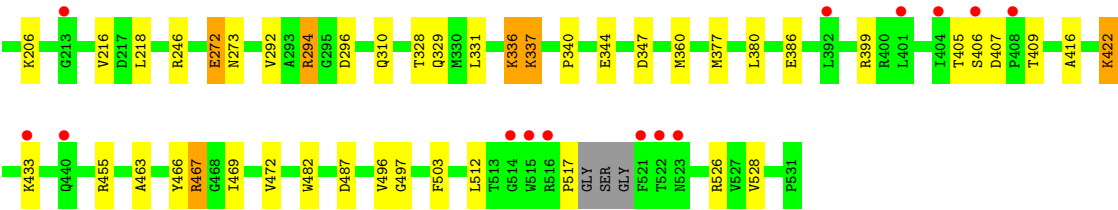


• Molecule 1: Pyruvate kinase PKM

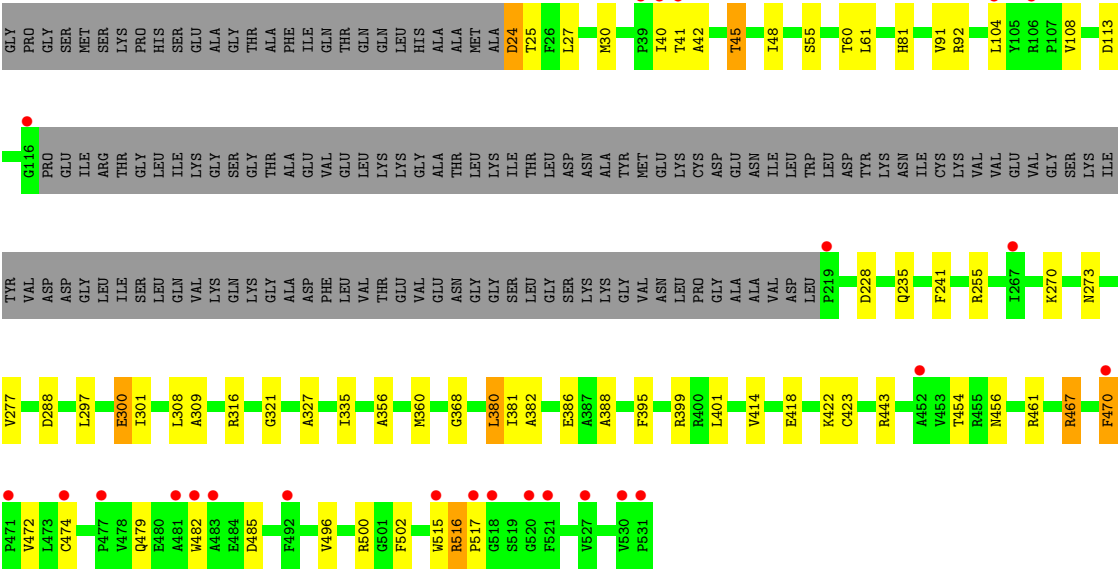


• Molecule 1: Pyruvate kinase PKM





● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.213 , 0.260 0.215 , 0.261	Depositor DCC
R_{free} test set	4896 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15432	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MLI, GOL, MG, K

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	0.28	0/3935	0.73	0/5313
1	B	0.28	0/3930	0.71	0/5307
1	C	0.28	0/3938	0.73	2/5318 (0.0%)
1	D	0.27	0/3179	0.74	0/4293
All	All	0.28	0/14982	0.73	2/20231 (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	407	ASP	CA-C-N	5.31	124.98	119.56
1	C	407	ASP	C-N-CA	5.31	124.98	119.56

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	46	0
1	B	3868	0	3954	39	0
1	C	3876	0	3958	36	0
1	D	3125	0	3176	41	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	C	1	0	0	0	0
4	A	6	0	8	1	0
5	A	7	0	2	1	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	148	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 (148) 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:C:472:VAL:HG11	1:C:496:VAL:HG21	1.79	0.64
1:D:24:ASP:N	6:D:657:HOH:O	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:121:THR:HB	1:B:122:GLY:HA3	1.90	0.52
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.92	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:A:263:LYS:NZ	6:A:1235:HOH:O	2.34	0.49
1:C:331:LEU:HD23	1:C:344:GLU:HB3	1.94	0.49
1:A:311:LYS:HB3	1:D:30:MET:HE2	1.95	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:A:48:ILE:HB	1:A:360:MET:HG3	1.96	0.47
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.48	0.47
1:D:255:ARG:NH2	1:D:288:ASP:OD1	2.32	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:A:418:GLU:HG3	1:B:418:GLU:HG3	1.95	0.47
1:C:405:THR:O	1:D:423:CYS:HA	2.14	0.47
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: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:C:455:ARG:NH1	6:C:2152:HOH:O	2.33	0.46
1:A:482:TRP:CG	1:A:517:PRO:HD3	2.51	0.46
1:B:395:PHE:CZ	1:B:418:GLU:HG2	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:D:327:ALA:HB1	1:D:360:MET:HE2	1.97	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:A:339:ARG:NH2	6:A:1247:HOH:O	2.45	0.45
1:D:472:VAL:HG21	1:D:496:VAL:HG11	1.98	0.45
1:B:494:MET:HG2	1:B:531:PRO:HD2	1.97	0.45
1:A:479:GLN:HB2	1:A:485:ASP:HB2	1.98	0.45
1:C:246:ARG:HE	1:C:273:ASN:ND2	2.14	0.45
1:A:48:ILE:HG12	1:A:71:VAL:HB	2.00	0.44
1:C:292:VAL:HG12	1:C:294:ARG:HG3	1.99	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:75:ASN:HA	1:B:113:ASP:HB3	2.00	0.44
1:B:330:MET:SD	1:B:359:ILE:HG23	2.58	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:A:327:ALA:HB1	1:A:360:MET:HE2	2.00	0.43
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:B:528:VAL:HA	1:B:529:PRO:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:PHE:HZ	1:D:418:GLU:HG2	1.83	0.43
1:C:24:ASP:N	1:C:24:ASP:OD1	2.51	0.43
1:D:335:ILE:HG23	1:D:368:GLY:HA2	2.00	0.43
1:D:516:ARG:HE	1:D:516:ARG:HB3	1.61	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:A:470:PHE:CD1	4:A:1003:GOL:H12	2.54	0.43
1:C:206:LYS:NZ	6:C:2101:HOH:O	2.43	0.43
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:B:263:LYS:NZ	6:B:1220:HOH:O	2.49	0.42
1:B:311:LYS:NZ	1:B:354:ASP:OD1	2.51	0.42
1:D:24:ASP:HB3	1:D:25:THR:H	1.61	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:B:327:ALA:HB1	1:B:360:MET:HE2	2.01	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:A:149:MET:HG3	1:A:150:GLU:HG3	2.02	0.42
1:B:386:GLU:HA	1:B:389:ILE:HG13	2.02	0.42
1:C:463:ALA:HB1	1:C:469:ILE:HG21	2.01	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:B:48:ILE:HG12	1:B:71:VAL:HB	2.02	0.41
1:C:272:GLU:HB3	1:C:296:ASP:HB2	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:C:405:THR:HB	1:C:406:SER:C	2.45	0.41
1:B:266:LYS:HD2	1:B:288:ASP:HB3	2.02	0.41
1:B:335:ILE:HG23	1:B:368:GLY:HA2	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:H	1:A:66:LYS:HG2	1.65	0.41
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.56	0.41
1:D:356:ALA:O	1:D:467:ARG:NH1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:380:LEU:HD12	1:A:380:LEU:HA	1.93	0.40
1:B:103:ILE:HG12	1:B:492:PHE:HE1	1.87	0.40
1:B:272:GLU:HB3	1:B:293:ALA:HB3	2.04	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	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 [i](#)

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%)	404 (97%)	13 (3%)	35	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	417/438 (95%)	404 (97%)	13 (3%)	35	52
1	C	418/438 (95%)	403 (96%)	15 (4%)	31	47
1	D	335/438 (76%)	318 (95%)	17 (5%)	21	32
All	All	1587/1752 (91%)	1529 (96%)	58 (4%)	30	45

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	41	THR
1	A	45	THR
1	A	66	LYS
1	A	121	THR
1	A	180	LEU
1	A	192	PHE
1	A	230	LYS
1	A	278	ARG
1	A	301	ILE
1	A	304	GLU
1	A	380	LEU
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	472	VAL
1	B	516	ARG
1	B	528	VAL
1	C	32	ARG
1	C	45	THR
1	C	134	LEU
1	C	162	LYS
1	C	168	VAL
1	C	272	GLU
1	C	294	ARG

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Mol	Chain	Res	Type
1	C	336	LYS
1	C	337	LYS
1	C	380	LEU
1	C	409	THR
1	C	422	LYS
1	C	467	ARG
1	C	487	ASP
1	C	528	VAL
1	D	24	ASP
1	D	27	LEU
1	D	40	ILE
1	D	41	THR
1	D	45	THR
1	D	104	LEU
1	D	300	GLU
1	D	380	LEU
1	D	386	GLU
1	D	399	ARG
1	D	401	LEU
1	D	422	LYS
1	D	454	THR
1	D	467	ARG
1	D	470	PHE
1	D	500	ARG
1	D	516	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	305	GLN
1	B	458	GLN
1	C	184	GLN
1	C	458	GLN
1	C	491	ASN
1	D	227	GLN
1	D	523	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	MLI	B	1003	2	6,6,6	1.21	0	7,7,7	1.34	0
5	MLI	C	1003	2	6,6,6	1.20	0	7,7,7	1.34	0
5	MLI	A	1004	2	6,6,6	1.20	0	7,7,7	1.24	0
4	GOL	A	1003	-	5,5,5	0.37	0	5,5,5	0.35	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
5	MLI	B	1003	2	-	4/4/4/4	-
5	MLI	C	1003	2	-	4/4/4/4	-
5	MLI	A	1004	2	-	0/4/4/4	-
4	GOL	A	1003	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	GOL	O1-C1-C2-C3
4	A	1003	GOL	O1-C1-C2-O2
5	B	1003	MLI	C2-C1-C3-O9
5	C	1003	MLI	C3-C1-C2-O7
5	C	1003	MLI	C2-C1-C3-O9
5	C	1003	MLI	C2-C1-C3-O8
5	B	1003	MLI	C2-C1-C3-O8
5	C	1003	MLI	C3-C1-C2-O6
5	B	1003	MLI	C3-C1-C2-O7
5	B	1003	MLI	C3-C1-C2-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1004	MLI	1	0
4	A	1003	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, 95th 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 ²)	Q<0.9
1	A	505/535 (94%)	0.05	21 (4%) 40 42	4, 19, 50, 76	0
1	B	504/535 (94%)	-0.20	9 (1%) 67 69	4, 17, 41, 64	0
1	C	505/535 (94%)	-0.03	17 (3%) 48 50	6, 20, 47, 74	0
1	D	406/535 (75%)	0.62	25 (6%) 26 28	14, 32, 57, 80	0
All	All	1920/2140 (89%)	0.09	72 (3%) 44 46	4, 22, 50, 80	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	4.7
1	A	121	THR	4.4
1	C	523	ASN	4.2
1	B	41	THR	4.0
1	D	518	GLY	3.8
1	D	40	ILE	3.6
1	D	470	PHE	3.6
1	D	116	GLY	3.6
1	A	392	LEU	3.6
1	C	392	LEU	3.5
1	D	517	PRO	3.3
1	D	520	GLY	3.3
1	A	215	ALA	3.1
1	A	192	PHE	3.1
1	C	515	TRP	3.0
1	D	474	CYS	3.0
1	B	129	THR	2.9
1	D	477	PRO	2.8
1	A	515	TRP	2.8
1	D	219	PRO	2.8
1	D	471	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	531	PRO	2.8
1	C	521	PHE	2.8
1	C	126	GLY	2.8
1	C	213	GLY	2.7
1	B	40	ILE	2.7
1	A	126	GLY	2.7
1	A	482	TRP	2.7
1	C	401	LEU	2.7
1	D	521	PHE	2.7
1	A	514	GLY	2.6
1	A	190	ALA	2.6
1	D	41	THR	2.6
1	D	515	TRP	2.5
1	A	170	VAL	2.5
1	C	440	GLN	2.5
1	C	516	ARG	2.4
1	A	521	PHE	2.4
1	C	128	GLY	2.4
1	A	519	SER	2.4
1	A	24	ASP	2.4
1	D	481	ALA	2.4
1	A	26	PHE	2.4
1	C	127	SER	2.3
1	A	178	ASP	2.3
1	C	433	LYS	2.3
1	B	518	GLY	2.3
1	C	522	THR	2.3
1	D	492	PHE	2.3
1	D	530	VAL	2.3
1	B	178	ASP	2.3
1	D	106	ARG	2.3
1	C	408	PRO	2.2
1	A	165	CYS	2.2
1	D	104	LEU	2.2
1	C	514	GLY	2.2
1	D	452	ALA	2.2
1	B	130	ALA	2.2
1	C	406	SER	2.2
1	C	404	ILE	2.1
1	A	34	ASP	2.1
1	D	527	VAL	2.1
1	A	470	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	42	ALA	2.1
1	D	483	ALA	2.1
1	A	193	LEU	2.1
1	D	267	ILE	2.1
1	B	391	HIS	2.1
1	B	213	GLY	2.0
1	D	482	TRP	2.0
1	A	301	ILE	2.0
1	D	39	PRO	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 oligosaccharides 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, 95th 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
2	MG	A	1001	1/1	0.80	0.09	27,27,27,27	0
5	MLI	A	1004	7/7	0.83	0.19	7,9,13,19	7
4	GOL	A	1003	6/6	0.86	0.13	25,26,31,42	0
5	MLI	C	1003	7/7	0.87	0.21	7,9,13,14	7
3	K	B	1002	1/1	0.89	0.11	37,37,37,37	0
5	MLI	B	1003	7/7	0.90	0.17	3,7,13,13	7
3	K	C	1002	1/1	0.90	0.10	39,39,39,39	0
3	K	A	1002	1/1	0.93	0.16	31,31,31,31	0
2	MG	C	1001	1/1	0.95	0.05	25,25,25,25	0
2	MG	B	1001	1/1	0.98	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.