



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:27 PM UTC

PDB ID : 4QG9 / pdb_00004qg9
Title : crystal structure of PKM2-R399E mutant
Authors : Wang, P.; Sun, C.; Zhu, T.; Xu, Y.
Deposited on : 2014-05-22
Resolution : 2.38 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

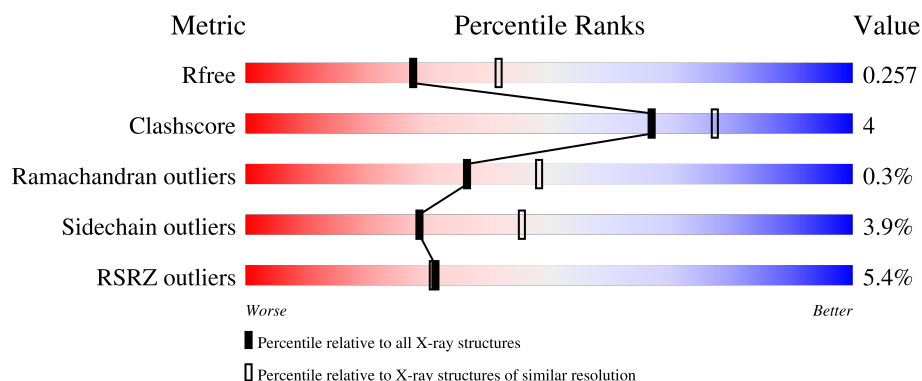
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	11% 83% 10% 7%
1	B	535	2% 83% 10% 6%
1	C	535	2% 68% 10% 22%
1	D	535	3% 67% 8% 24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14467 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	499	Total	C	N	O	S	0	0	0
			3829	2410	677	718	24			
1	B	503	Total	C	N	O	S	0	0	0
			3852	2422	681	725	24			
1	C	417	Total	C	N	O	S	0	0	0
			3202	2010	577	594	21			
1	D	405	Total	C	N	O	S	0	0	0
			3117	1959	560	577	21			

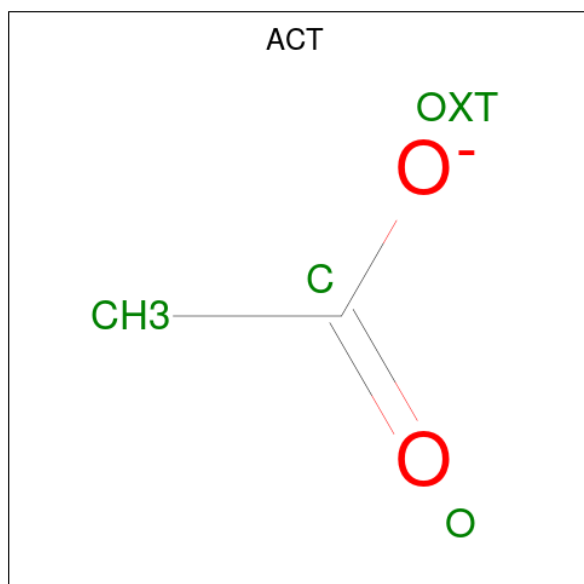
There are 20 discrepancies between the modelled and reference sequences:

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	399	GLU	ARG	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	399	GLU	ARG	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	399	GLU	ARG	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	399	GLU	ARG	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 ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		
4	B	136	Total	O	0	0
			136	136		

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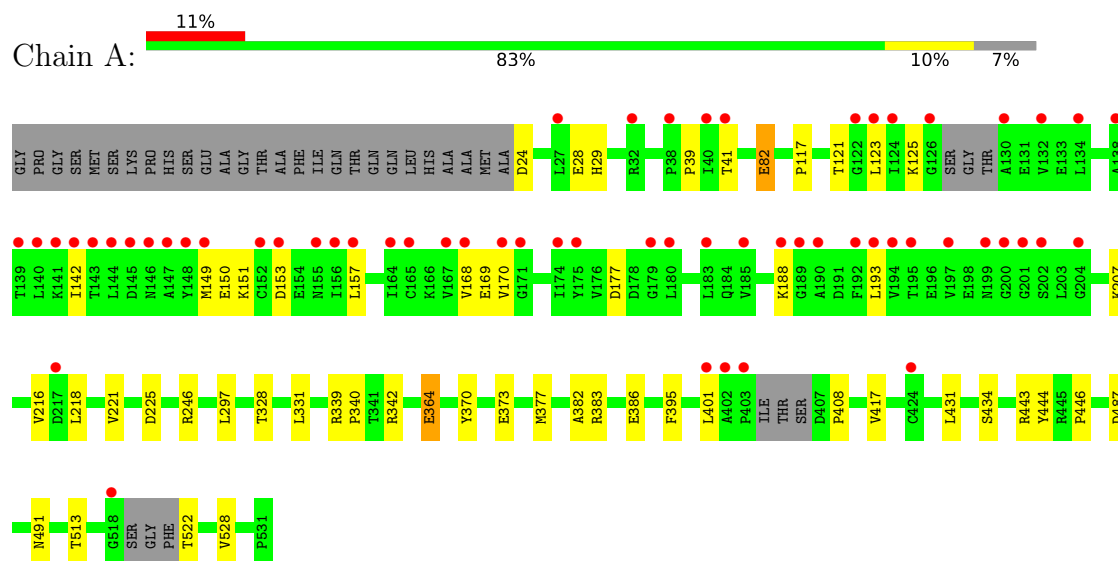
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	122	Total 122	O 122	0	0
4	D	95	Total 95	O 95	0	0

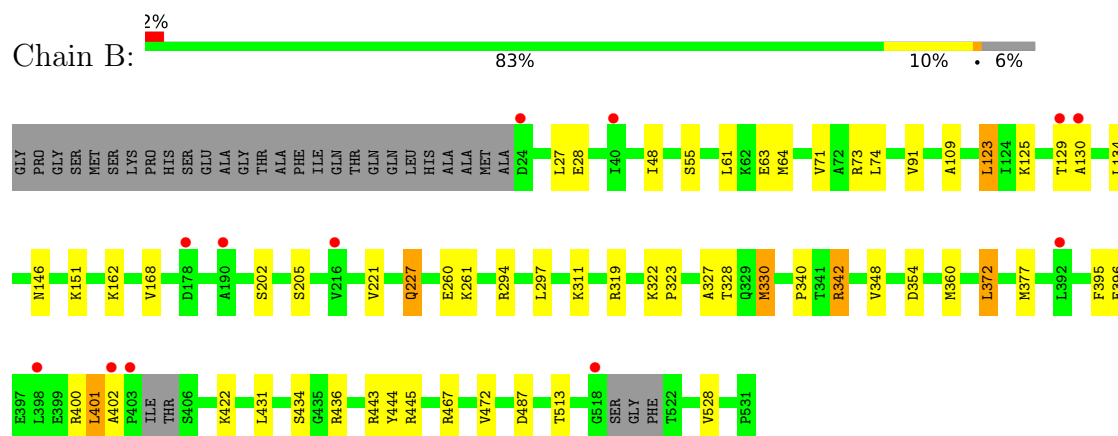
3 Residue-property plots [i](#)

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

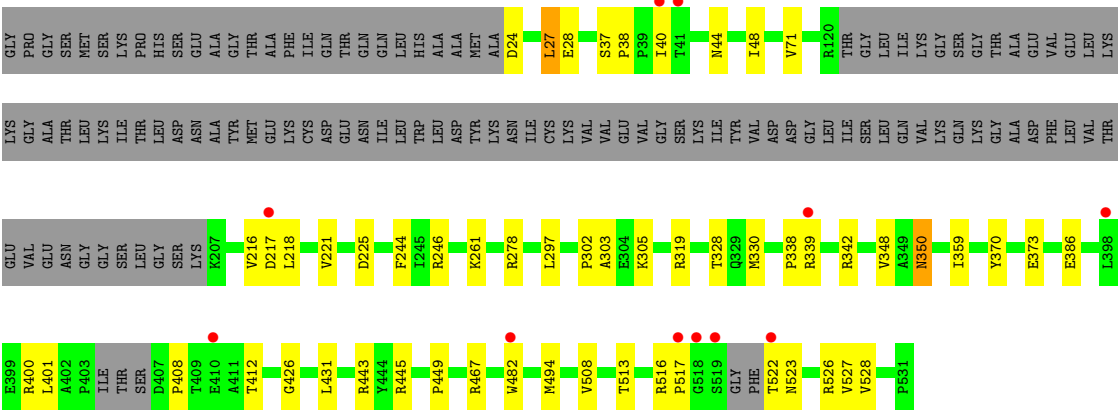


• Molecule 1: Pyruvate kinase PKM

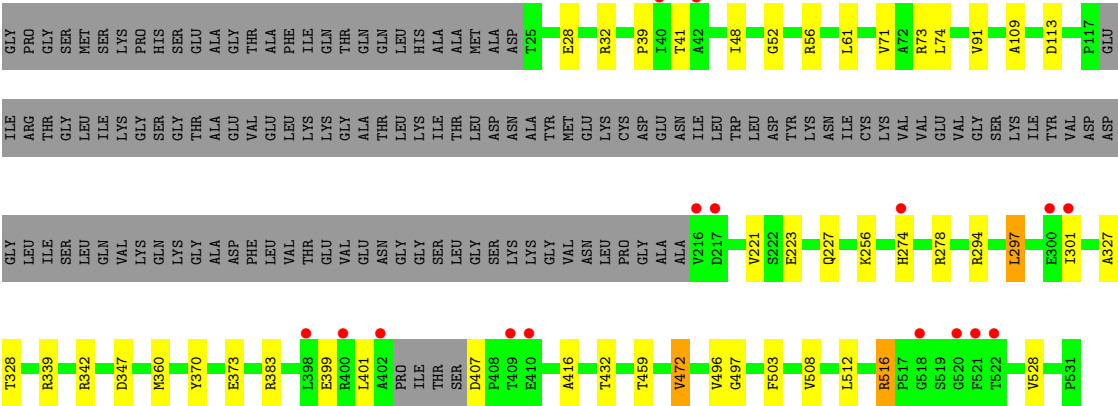


• Molecule 1: Pyruvate kinase PKM





● 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	95.63Å 71.18Å 170.29Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	43.65 – 2.38 43.65 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.65-2.38) 94.0 (43.65-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.210 , 0.256 0.211 , 0.257	Depositor DCC
R_{free} test set	4387 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14467	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: ACT, 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	0.26	0/3888	0.72	0/5246
1	B	0.28	0/3912	0.74	0/5280
1	C	0.27	0/3255	0.72	0/4395
1	D	0.27	0/3170	0.72	2/4280 (0.0%)
All	All	0.27	0/14225	0.73	2/19201 (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	D	407	ASP	CA-C-N	5.36	124.55	118.97
1	D	407	ASP	C-N-CA	5.36	124.55	118.97

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	3829	0	3911	29	0
1	B	3852	0	3932	33	0
1	C	3202	0	3259	31	0
1	D	3117	0	3169	23	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	4	0	3	1	0
3	B	4	0	3	1	0
3	C	4	0	3	0	0
3	D	4	0	3	1	0
4	A	95	0	0	3	0
4	B	136	0	0	1	0
4	C	122	0	0	4	0
4	D	95	0	0	1	0
All	All	14467	0	14283	104	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 (104) 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:338:PRO:HG2	1:C:339:ARG:HD2	1.68	0.73
1:D:28:GLU:OE1	1:D:32:ARG:NH2	2.28	0.67
1:B:146:ASN:OD1	1:B:162:LYS:NZ	2.27	0.67
1:B:487:ASP:OD2	1:D:516:ARG:NH1	2.30	0.63
1:B:63:GLU:HB3	1:B:372:LEU:HD21	1.80	0.63
1:A:28:GLU:HG3	1:D:401:LEU:HD11	1.82	0.62
1:C:526:ARG:NH2	4:C:1153:HOH:O	2.30	0.61
1:D:472:VAL:HG21	1:D:496:VAL:HG21	1.82	0.61
1:B:402:ALA:HB1	1:B:443:ARG:HH22	1.65	0.60
1:C:330:MET:HE3	1:C:348:VAL:HG22	1.86	0.58
1:A:487:ASP:OD2	1:C:516:ARG:NH2	2.32	0.58
1:D:383:ARG:NH1	4:D:787:HOH:O	2.38	0.57
1:B:319:ARG:HB2	1:C:27:LEU:HD11	1.87	0.56
1:A:434:SER:H	3:A:1002:ACT:H3	1.69	0.56
1:B:401:LEU:HD11	1:C:28:GLU:HG3	1.86	0.56
1:B:330:MET:HE2	1:B:348:VAL:HG22	1.86	0.56
1:C:350:ASN:ND2	4:C:1106:HOH:O	2.36	0.55
1:A:142:ILE:HB	1:A:193:LEU:HB2	1.88	0.55
1:C:319:ARG:O	1:C:443:ARG:NH1	2.40	0.55
1:B:445:ARG:NH1	4:B:1119:HOH:O	2.39	0.55
1:C:302:PRO:HG2	1:C:305:LYS:HD2	1.88	0.53
1:A:370:TYR:HB3	1:A:373:GLU:HB2	1.90	0.53
1:A:39:PRO:O	1:A:383:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:TRP:HB2	1:C:517:PRO:HG3	1.92	0.52
1:D:71:VAL:HG22	1:D:109:ALA:HB3	1.93	0.51
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.93	0.51
1:B:125:LYS:HB3	1:B:151:LYS:HA	1.93	0.50
1:B:401:LEU:HD12	1:C:27:LEU:HD12	1.93	0.50
1:A:177:ASP:HB2	1:A:207:LYS:HB3	1.93	0.50
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.93	0.50
1:B:294:ARG:NH2	1:B:330:MET:HE3	2.25	0.50
1:B:443:ARG:NH2	1:B:444:TYR:OH	2.43	0.50
4:A:1165:HOH:O	1:D:339:ARG:NH2	2.41	0.50
1:D:370:TYR:HB3	1:D:373:GLU:HB2	1.94	0.50
1:A:149:MET:HG3	1:A:150:GLU:HG3	1.93	0.50
1:B:27:LEU:HD23	1:C:401:LEU:HD12	1.94	0.49
1:A:221:VAL:HG13	1:A:225:ASP:HB2	1.94	0.49
1:C:431:LEU:HD22	1:C:513:THR:HG22	1.95	0.49
1:D:274:HIS:CE1	1:D:278:ARG:HE	2.30	0.49
1:A:401:LEU:HD11	1:D:28:GLU:HB2	1.95	0.49
1:B:422:LYS:NZ	1:D:399:GLU:OE2	2.38	0.49
1:C:408:PRO:O	1:C:412:THR:OG1	2.30	0.48
1:D:73:ARG:NH1	1:D:113:ASP:OD1	2.43	0.48
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.96	0.48
1:C:216:VAL:HG12	1:C:218:LEU:H	1.77	0.48
1:C:244:PHE:O	1:C:246:ARG:NH1	2.47	0.48
1:B:48:ILE:HG12	1:B:71:VAL:HB	1.96	0.47
1:C:278:ARG:NH2	4:C:1120:HOH:O	2.35	0.47
1:A:331:LEU:O	1:A:364:GLU:HG2	2.14	0.47
1:B:71:VAL:HG22	1:B:109:ALA:HB3	1.96	0.47
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.95	0.47
1:D:432:THR:OG1	3:D:601:ACT:OXT	2.23	0.47
1:A:125:LYS:HB3	1:A:151:LYS:HA	1.97	0.47
1:B:73:ARG:HD3	1:B:360:MET:SD	2.55	0.47
1:C:339:ARG:NH1	4:C:1180:HOH:O	2.49	0.46
1:A:117:PRO:HB2	1:A:218:LEU:HD13	1.97	0.46
1:A:216:VAL:HG12	1:A:218:LEU:H	1.80	0.46
1:D:52:GLY:O	1:D:56:ARG:HG3	2.16	0.46
1:B:342:ARG:HA	1:C:303:ALA:HB1	1.97	0.46
1:C:523:ASN:N	1:C:523:ASN:OD1	2.49	0.45
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.99	0.45
1:C:370:TYR:HB3	1:C:373:GLU:HB2	1.98	0.45
1:B:327:ALA:HB1	1:B:360:MET:HE2	2.00	0.44
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LYS:NZ	1:B:354:ASP:OD1	2.50	0.44
1:A:39:PRO:HB2	1:A:383:ARG:HG2	2.00	0.44
1:B:395:PHE:CD2	1:B:444:TYR:HB3	2.53	0.44
1:B:123:LEU:HD12	1:B:205:SER:HB3	2.00	0.43
1:B:395:PHE:HD2	1:B:444:TYR:HB3	1.83	0.43
1:C:44:ASN:ND2	1:C:386:GLU:OE2	2.49	0.43
1:C:445:ARG:NE	1:C:467:ARG:HD3	2.32	0.43
1:D:61:LEU:HD13	1:D:91:VAL:HA	2.00	0.43
1:A:382:ALA:O	1:A:386:GLU:HG2	2.18	0.43
1:B:227:GLN:H	1:B:227:GLN:HG2	1.47	0.43
1:C:221:VAL:HG13	1:C:225:ASP:HB2	2.00	0.43
1:C:24:ASP:OD1	1:C:24:ASP:N	2.52	0.43
1:B:445:ARG:NE	1:B:467:ARG:HD3	2.34	0.43
1:A:408:PRO:HB3	1:C:527:VAL:O	2.19	0.43
1:C:386:GLU:OE2	1:C:467:ARG:NH2	2.48	0.43
1:D:297:LEU:HD12	1:D:297:LEU:HA	1.88	0.43
1:B:28:GLU:OE1	1:C:319:ARG:NH2	2.51	0.42
1:D:223:GLU:O	1:D:227:GLN:HG2	2.19	0.42
1:B:322:LYS:HA	1:B:323:PRO:HD3	1.93	0.42
1:C:426:GLY:O	1:C:449:PRO:HD2	2.20	0.42
1:A:24:ASP:N	4:A:1102:HOH:O	2.53	0.42
1:B:431:LEU:HD22	1:B:513:THR:HG22	2.00	0.42
1:A:82:GLU:H	1:A:82:GLU:CD	2.28	0.42
1:A:169:GLU:HG3	1:A:188:LYS:HD2	2.02	0.42
1:A:395:PHE:HD2	1:A:444:TYR:HB3	1.85	0.42
1:B:61:LEU:HD13	1:B:91:VAL:HA	2.01	0.41
1:B:434:SER:H	3:B:1002:ACT:H3	1.84	0.41
1:D:327:ALA:HB1	1:D:360:MET:HE2	2.01	0.41
1:A:417:VAL:HG13	1:A:446:PRO:HB3	2.02	0.41
1:A:443:ARG:NH1	4:A:1169:HOH:O	2.52	0.41
1:B:129:THR:N	1:B:130:ALA:HB3	2.35	0.41
1:A:153:ASP:OD2	1:A:153:ASP:N	2.54	0.41
1:A:218:LEU:O	1:A:246:ARG:NH2	2.36	0.41
1:D:39:PRO:HB2	1:D:383:ARG:HG2	2.03	0.40
1:A:340:PRO:HG3	1:A:377:MET:HG2	2.02	0.40
1:D:294:ARG:NH2	1:D:347:ASP:OD2	2.50	0.40
1:B:55:SER:HB2	1:B:64:MET:SD	2.62	0.40
1:C:37:SER:HA	1:C:38:PRO:HD3	1.91	0.40
1:A:125:LYS:HB3	1:A:151:LYS:HG2	2.03	0.40
1:A:395:PHE:CD2	1:A:444:TYR:HB3	2.57	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	491/535 (92%)	477 (97%)	12 (2%)	2 (0%)	30	40
1	B	497/535 (93%)	484 (97%)	12 (2%)	1 (0%)	43	56
1	C	409/535 (76%)	405 (99%)	3 (1%)	1 (0%)	43	56
1	D	399/535 (75%)	393 (98%)	5 (1%)	1 (0%)	36	48
All	All	1796/2140 (84%)	1759 (98%)	32 (2%)	5 (0%)	36	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	B	328	THR
1	A	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	412/438 (94%)	398 (97%)	14 (3%)	32	51
1	B	415/438 (95%)	396 (95%)	19 (5%)	24	38
1	C	343/438 (78%)	330 (96%)	13 (4%)	29	46
1	D	334/438 (76%)	322 (96%)	12 (4%)	31	49
All	All	1504/1752 (86%)	1446 (96%)	58 (4%)	28	45

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

Mol	Chain	Res	Type
1	A	29	HIS
1	A	41	THR
1	A	82	GLU
1	A	123	LEU
1	A	157	LEU
1	A	168	VAL
1	A	170	VAL
1	A	297	LEU
1	A	339	ARG
1	A	342	ARG
1	A	364	GLU
1	A	491	ASN
1	A	522	THR
1	A	528	VAL
1	B	74	LEU
1	B	123	LEU
1	B	134	LEU
1	B	168	VAL
1	B	202	SER
1	B	221	VAL
1	B	227	GLN
1	B	260	GLU
1	B	261	LYS
1	B	297	LEU
1	B	330	MET
1	B	342	ARG
1	B	372	LEU
1	B	396	GLU
1	B	400	ARG
1	B	401	LEU
1	B	436	ARG
1	B	472	VAL
1	B	528	VAL
1	C	27	LEU
1	C	40	ILE
1	C	217	ASP
1	C	261	LYS
1	C	297	LEU
1	C	342	ARG
1	C	350	ASN
1	C	359	ILE
1	C	400	ARG

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Mol	Chain	Res	Type
1	C	494	MET
1	C	508	VAL
1	C	522	THR
1	C	528	VAL
1	D	41	THR
1	D	74	LEU
1	D	221	VAL
1	D	256	LYS
1	D	297	LEU
1	D	301	ILE
1	D	342	ARG
1	D	459	THR
1	D	472	VAL
1	D	508	VAL
1	D	516	ARG
1	D	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	HIS
1	A	440	GLN
1	A	458	GLN
1	B	391	HIS
1	B	458	GLN
1	C	318	ASN
1	D	252	HIS
1	D	458	GLN

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 [i](#)

Of 7 ligands modelled in this entry, 3 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	$\# Z > 2$
3	ACT	D	601	-	3,3,3	0.82	0	3,3,3	1.32	0
3	ACT	C	1002	-	3,3,3	0.81	0	3,3,3	1.34	0
3	ACT	A	1002	-	3,3,3	0.79	0	3,3,3	1.27	0
3	ACT	B	1002	-	3,3,3	0.81	0	3,3,3	1.30	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	ACT	1	0
3	A	1002	ACT	1	0
3	B	1002	ACT	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	499/535 (93%)	0.50	60 (12%) 9 8	13, 30, 86, 95	0
1	B	503/535 (94%)	0.12	12 (2%) 59 59	15, 27, 48, 76	0
1	C	417/535 (77%)	0.09	11 (2%) 57 56	12, 25, 48, 82	0
1	D	405/535 (75%)	0.15	16 (3%) 42 42	15, 26, 52, 78	0
All	All	1824/2140 (85%)	0.22	99 (5%) 31 31	12, 27, 67, 95	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	521	PHE	6.2
1	B	129	THR	5.2
1	A	130	ALA	4.8
1	B	403	PRO	4.7
1	A	190	ALA	4.7
1	A	157	LEU	4.6
1	A	140	LEU	4.5
1	A	194	VAL	4.4
1	A	142	ILE	4.1
1	A	126	GLY	4.1
1	A	403	PRO	4.1
1	A	168	VAL	3.8
1	A	156	ILE	3.8
1	A	518	GLY	3.7
1	A	40	ILE	3.7
1	A	180	LEU	3.7
1	A	193	LEU	3.6
1	A	402	ALA	3.6
1	C	519	SER	3.6
1	A	170	VAL	3.4
1	A	27	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	200	GLY	3.3
1	A	189	GLY	3.3
1	A	424	CYS	3.3
1	A	188	LYS	3.3
1	B	402	ALA	3.2
1	D	409	THR	3.2
1	B	518	GLY	3.2
1	D	216	VAL	3.1
1	B	130	ALA	3.1
1	A	132	VAL	3.1
1	A	153	ASP	3.0
1	D	402	ALA	3.0
1	A	134	LEU	3.0
1	A	164	ILE	3.0
1	A	124	ILE	2.9
1	C	518	GLY	2.9
1	A	167	VAL	2.9
1	A	139	THR	2.9
1	A	401	LEU	2.8
1	A	143	THR	2.8
1	D	522	THR	2.7
1	C	398	LEU	2.7
1	A	175	TYR	2.7
1	D	40	ILE	2.7
1	D	520	GLY	2.7
1	A	148	TYR	2.6
1	A	195	THR	2.6
1	D	410	GLU	2.6
1	C	40	ILE	2.6
1	A	217	ASP	2.6
1	B	392	LEU	2.5
1	A	41	THR	2.5
1	B	40	ILE	2.5
1	A	146	ASN	2.5
1	B	24	ASP	2.5
1	D	518	GLY	2.5
1	A	202	SER	2.4
1	A	185	VAL	2.4
1	C	482	TRP	2.4
1	D	274	HIS	2.4
1	A	165	CYS	2.4
1	A	171	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	41	THR	2.4
1	A	152	CYS	2.4
1	A	197	VAL	2.4
1	A	122	GLY	2.3
1	A	138	ALA	2.3
1	D	398	LEU	2.3
1	A	199	ASN	2.3
1	D	42	ALA	2.3
1	C	522	THR	2.3
1	A	141	LYS	2.3
1	A	201	GLY	2.3
1	A	145	ASP	2.3
1	A	155	ASN	2.3
1	A	32	ARG	2.3
1	B	190	ALA	2.3
1	C	410	GLU	2.3
1	A	123	LEU	2.2
1	A	179	GLY	2.2
1	D	400	ARG	2.2
1	B	216	VAL	2.2
1	A	204	GLY	2.2
1	D	300	GLU	2.2
1	D	301	ILE	2.2
1	A	192	PHE	2.2
1	D	217	ASP	2.2
1	A	149	MET	2.1
1	B	178	ASP	2.1
1	B	398	LEU	2.1
1	A	38	PRO	2.1
1	C	517	PRO	2.1
1	A	147	ALA	2.1
1	A	183	LEU	2.1
1	A	174	ILE	2.1
1	C	217	ASP	2.0
1	A	144	LEU	2.0
1	C	339	ARG	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 [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	C	1001	1/1	0.67	0.40	60,60,60,60	0
3	ACT	A	1002	4/4	0.73	0.20	23,28,30,30	0
2	MG	A	1001	1/1	0.86	0.30	50,50,50,50	0
3	ACT	B	1002	4/4	0.86	0.15	30,32,36,38	0
2	MG	B	1001	1/1	0.88	0.11	32,32,32,32	0
3	ACT	C	1002	4/4	0.93	0.12	22,24,26,27	0
3	ACT	D	601	4/4	0.94	0.10	29,33,36,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.