



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 PM GMT

PDB ID : 4QG9
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

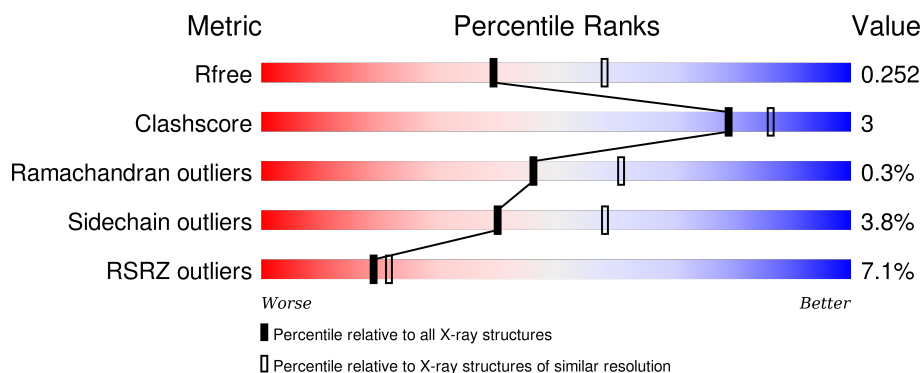
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>14%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
1	B	535	<div> <div>3%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
1	C	535	<div> <div>4%</div> <div>68%</div> <div>9%</div> <div>22%</div> </div>
1	D	535	<div> <div>4%</div> <div>68%</div> <div>7%</div> <div>24%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	1002	-	-	-	X

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			

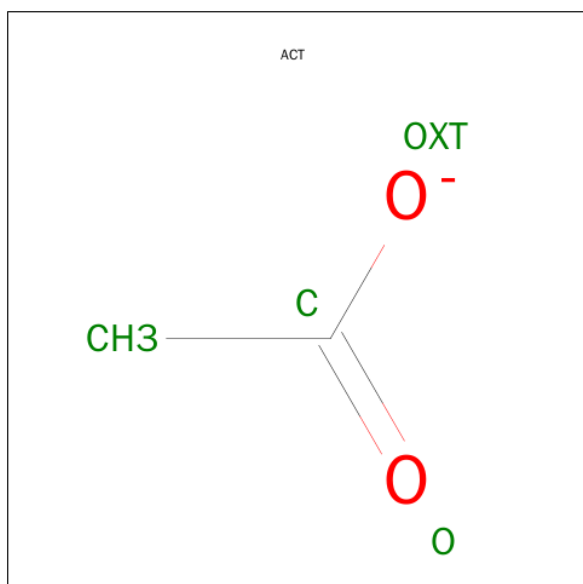
There are 20 discrepancies between the modelled and reference sequences:

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is water.

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

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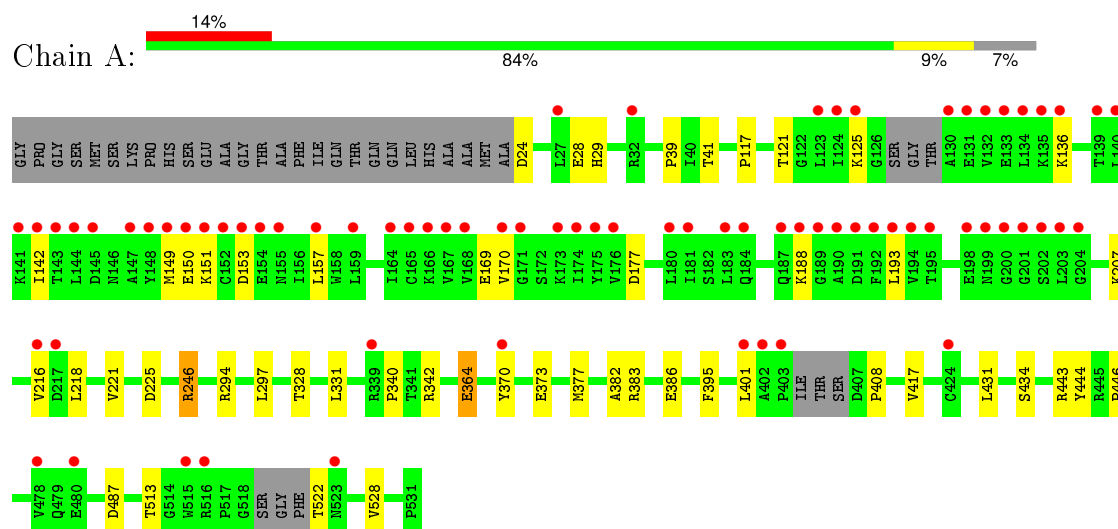
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	122	Total 122	O 122	0	0
4	D	95	Total 95	O 95	0	0

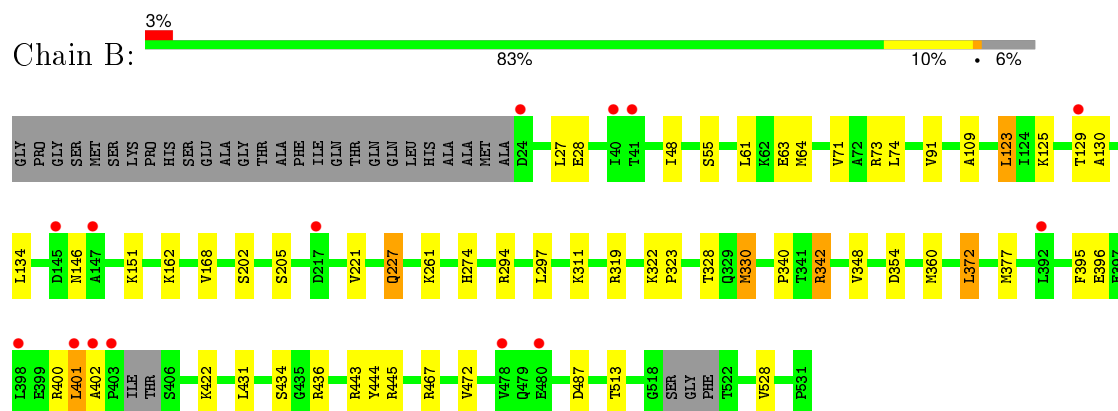
3 Residue-property plots

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.

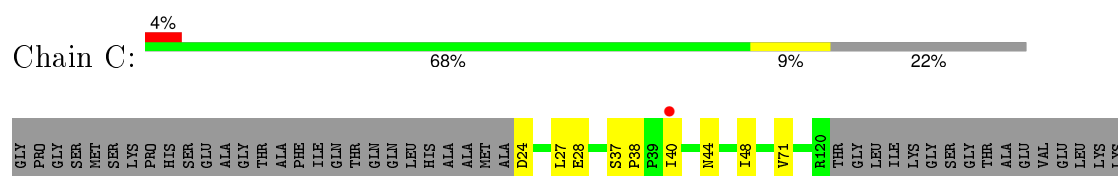
• Molecule 1: Pyruvate kinase PKM

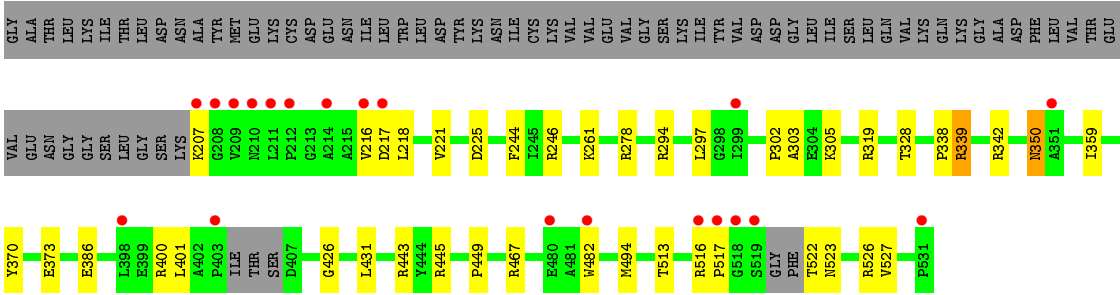


• Molecule 1: Pyruvate kinase PKM

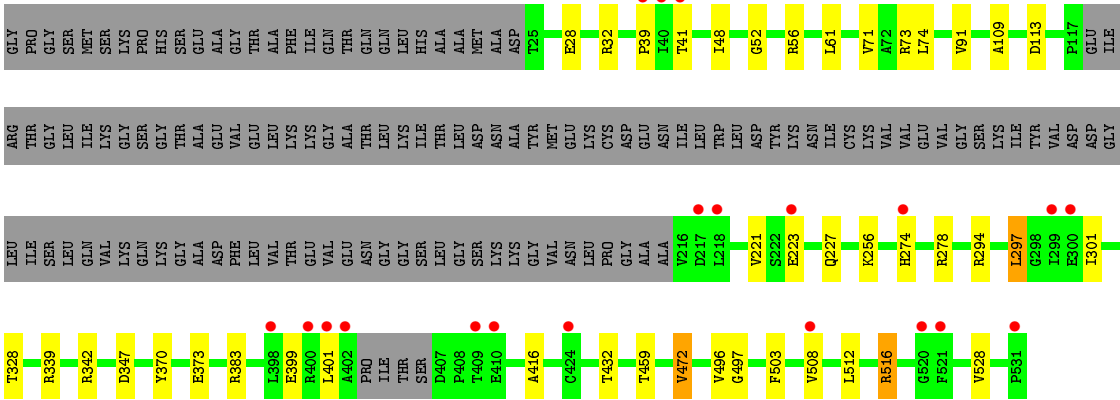


• Molecule 1: Pyruvate kinase PKM





● 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, 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	4.38 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.210 , 0.256 0.205 , 0.252	Depositor DCC
R_{free} test set	4212 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 87781 reflections	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 3.41% 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, 0.375 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: MG, ACT

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	0.20	0/3888	0.38	0/5246
1	B	0.20	0/3912	0.40	0/5280
1	C	0.20	0/3255	0.39	0/4395
1	D	0.20	0/3170	0.39	0/4280
All	All	0.20	0/14225	0.39	0/19201

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	3829	0	3911	28	0
1	B	3852	0	3932	31	0
1	C	3202	0	3259	29	0
1	D	3117	0	3169	22	0
2	A	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	98	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 (98) 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:B:330:MET:HE2	1:B:348:VAL:HG22	1.83	0.59
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:B:401:LEU:HD11	1:C:28:GLU:HG3	1.86	0.56
1:A:434:SER:H	3:A:1002:ACT:H3	1.69	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
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:401:LEU:HD12	1:C:27:LEU:HD12	1.93	0.50
1:B:125:LYS:HB3	1:B:151:LYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD22	1:A:513:THR:HG22	1.93	0.50
1:A:177:ASP:HB2	1:A:207:LYS:HB3	1.93	0.50
1:B:443:ARG:NH2	1:B:444:TYR:OH	2.43	0.50
1:D:370:TYR:HB3	1:D:373:GLU:HB2	1.94	0.50
4:A:1165:HOH:O	1:D:339:ARG:NH2	2.41	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: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:216:VAL:HG12	1:A:218:LEU:H	1.80	0.46
1:A:117:PRO:HB2	1:A:218:LEU:HD13	1.97	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:OD1	1:C:523:ASN:N	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:D:497:GLY:HA3	1:D:503:PHE:CZ	2.52	0.44
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: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:B:123:LEU:HD12	1:B:205:SER:HB3	2.00	0.43
1:D:61:LEU:HD13	1:D:91:VAL:HA	2.00	0.43
1:B:422:LYS:NZ	1:D:399:GLU:OE2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:D:297:LEU:HD12	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: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:434:SER:H	3:B:1002:ACT:H3	1.84	0.41
1:B:61:LEU:HD13	1:B:91:VAL:HA	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:218:LEU:O	1:A:246:ARG:NH2	2.36	0.41
1:A:153:ASP:N	1:A:153:ASP:OD2	2.54	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:C:37:SER:HA	1:C:38:PRO:HD3	1.91	0.40
1:B:55:SER:HB2	1:B:64:MET:SD	2.62	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%)	39	53
1	B	497/535 (93%)	484 (97%)	12 (2%)	1 (0%)	52	68
1	C	409/535 (76%)	405 (99%)	3 (1%)	1 (0%)	52	68
1	D	399/535 (75%)	393 (98%)	5 (1%)	1 (0%)	46	61
All	All	1796/2140 (84%)	1759 (98%)	32 (2%)	5 (0%)	46	61

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%)	400 (97%)	12 (3%)	50	69
1	B	415/438 (95%)	395 (95%)	20 (5%)	31	47
1	C	343/438 (78%)	330 (96%)	13 (4%)	40	58
1	D	334/438 (76%)	322 (96%)	12 (4%)	42	61
All	All	1504/1752 (86%)	1447 (96%)	57 (4%)	40	58

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

Mol	Chain	Res	Type
1	A	29	HIS
1	A	41	THR
1	A	136	LYS

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Mol	Chain	Res	Type
1	A	157	LEU
1	A	170	VAL
1	A	246	ARG
1	A	294	ARG
1	A	297	LEU
1	A	342	ARG
1	A	364	GLU
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	261	LYS
1	B	274	HIS
1	B	294	ARG
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	40	ILE
1	C	207	LYS
1	C	217	ASP
1	C	261	LYS
1	C	294	ARG
1	C	297	LEU
1	C	339	ARG
1	C	342	ARG
1	C	350	ASN
1	C	359	ILE
1	C	400	ARG
1	C	494	MET
1	C	522	THR

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	GLN
1	C	318	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	A	1002	-	1,3,3	0.95	0	0,3,3	0.00	-
3	ACT	B	1002	-	1,3,3	1.23	0	0,3,3	0.00	-
3	ACT	C	1002	-	1,3,3	1.17	0	0,3,3	0.00	-
3	ACT	D	601	-	1,3,3	1.20	0	0,3,3	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
3	ACT	A	1002	-	-	0/0/0/0	0/0/0/0
3	ACT	B	1002	-	-	0/0/0/0	0/0/0/0
3	ACT	C	1002	-	-	0/0/0/0	0/0/0/0
3	ACT	D	601	-	-	0/0/0/0	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	ACT	1	0
3	B	1002	ACT	1	0
3	D	601	ACT	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.68	74 (14%) 3 4	13, 30, 86, 95	0
1	B	503/535 (94%)	0.27	14 (2%) 56 59	15, 27, 48, 76	0
1	C	417/535 (77%)	0.32	21 (5%) 32 37	12, 25, 48, 82	0
1	D	405/535 (75%)	0.28	20 (4%) 33 38	15, 27, 52, 78	0
All	All	1824/2140 (85%)	0.40	129 (7%) 19 21	12, 27, 67, 95	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	LEU	8.0
1	A	190	ALA	7.3
1	A	193	LEU	6.7
1	A	168	VAL	6.6
1	A	402	ALA	6.4
1	B	402	ALA	5.9
1	A	157	LEU	5.9
1	A	142	ILE	5.7
1	A	188	LYS	5.6
1	D	521	PHE	5.4
1	A	167	VAL	5.4
1	A	403	PRO	5.4
1	C	519	SER	5.4
1	A	134	LEU	5.1
1	A	153	ASP	5.1
1	A	148	TYR	5.0
1	A	180	LEU	5.0
1	A	165	CYS	5.0
1	D	40	ILE	4.9
1	A	123	LEU	4.9
1	A	202	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	164	ILE	4.7
1	A	152	CYS	4.6
1	A	143	THR	4.4
1	B	403	PRO	4.4
1	A	189	GLY	4.4
1	A	132	VAL	4.4
1	A	149	MET	4.3
1	D	217	ASP	4.2
1	A	155	ASN	4.2
1	A	131	GLU	4.1
1	A	133	GLU	4.1
1	A	136	LYS	4.1
1	D	401	LEU	4.0
1	C	517	PRO	3.9
1	C	516	ARG	3.9
1	B	40	ILE	3.9
1	A	192	PHE	3.9
1	D	400	ARG	3.8
1	D	402	ALA	3.8
1	A	159	LEU	3.8
1	A	198	GLU	3.7
1	C	518	GLY	3.7
1	A	424	CYS	3.7
1	A	130	ALA	3.7
1	C	211	LEU	3.6
1	A	401	LEU	3.5
1	C	480	GLU	3.5
1	C	403	PRO	3.5
1	A	194	VAL	3.5
1	D	41	THR	3.5
1	A	201	GLY	3.4
1	A	478	VAL	3.3
1	A	145	ASP	3.3
1	A	135	LYS	3.2
1	A	187	GLN	3.1
1	A	154	GLU	3.1
1	C	531	PRO	3.1
1	B	478	VAL	3.1
1	A	173	LYS	3.0
1	D	218	LEU	3.0
1	A	183	LEU	3.0
1	A	199	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	392	LEU	2.9
1	A	125	LYS	2.9
1	C	214	ALA	2.9
1	B	480	GLU	2.9
1	C	40	ILE	2.9
1	A	170	VAL	2.8
1	A	195	THR	2.8
1	C	299	ILE	2.8
1	C	209	VAL	2.8
1	C	482	TRP	2.8
1	A	147	ALA	2.7
1	D	424	CYS	2.7
1	B	129	THR	2.7
1	A	184	GLN	2.7
1	D	410	GLU	2.7
1	B	147	ALA	2.7
1	A	139	THR	2.6
1	A	141	LYS	2.6
1	D	223	GLU	2.6
1	A	181	ILE	2.6
1	A	150	GLU	2.6
1	A	203	LEU	2.6
1	A	166	LYS	2.6
1	D	274	HIS	2.6
1	D	508	VAL	2.6
1	A	200	GLY	2.5
1	C	212	PRO	2.5
1	A	144	LEU	2.5
1	A	176	VAL	2.5
1	A	217	ASP	2.5
1	B	41	THR	2.4
1	C	217	ASP	2.4
1	A	516	ARG	2.4
1	D	398	LEU	2.4
1	B	145	ASP	2.4
1	A	32	ARG	2.4
1	A	151	LYS	2.4
1	A	339	ARG	2.4
1	B	398	LEU	2.3
1	D	520	GLY	2.3
1	A	216	VAL	2.3
1	D	299	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	175	TYR	2.3
1	D	531	PRO	2.3
1	A	171	GLY	2.3
1	C	207	LYS	2.3
1	B	401	LEU	2.3
1	A	27	LEU	2.3
1	C	398	LEU	2.3
1	C	208	GLY	2.2
1	C	210	ASN	2.2
1	D	409	THR	2.2
1	A	370	TYR	2.2
1	C	351	ALA	2.2
1	A	480	GLU	2.2
1	C	216	VAL	2.2
1	D	300	GLU	2.1
1	A	204	GLY	2.1
1	A	191	ASP	2.1
1	A	523	ASN	2.1
1	A	124	ILE	2.1
1	A	174	ILE	2.1
1	B	24	ASP	2.0
1	B	217	ASP	2.0
1	A	515	TRP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ACT	A	1002	4/4	0.85	0.30	3.93	23,28,30,30	0
3	ACT	B	1002	4/4	0.94	0.22	1.85	30,32,36,38	0
3	ACT	C	1002	4/4	0.97	0.20	1.74	22,24,26,27	0
3	ACT	D	601	4/4	0.94	0.16	-0.14	29,33,36,39	0
2	MG	A	1001	1/1	0.90	0.24	-	50,50,50,50	0
2	MG	C	1001	1/1	0.47	0.18	-	60,60,60,60	0
2	MG	B	1001	1/1	0.76	0.16	-	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.