



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:21 AM EDT

PDB ID : 7R6Y
Title : E117K mutant pyruvate kinase from rabbit muscle
Authors : Rodriguez-Romero, A.; Rodriguez-Hernandez, A.
Deposited on : 2021-06-24
Resolution : 2.25 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

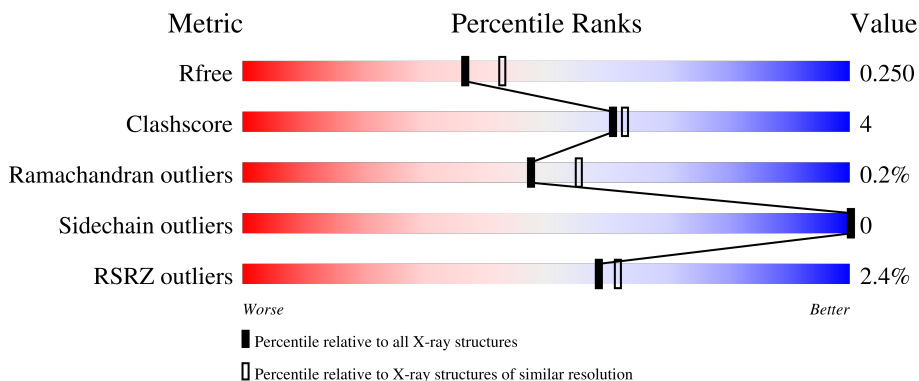
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	531	 85% 13% .
1	B	531	 86% 11% .
1	C	531	 74% 8% 18%
1	D	531	 71% 9% 21%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15009 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
			Total	C	N	O	S			
1	A	519	3944	2477	703	736	28	0	2	0
1	B	519	3883	2439	684	732	28	0	1	0
1	C	437	3290	2060	596	609	25	0	0	0
1	D	422	3190	1997	579	589	25	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

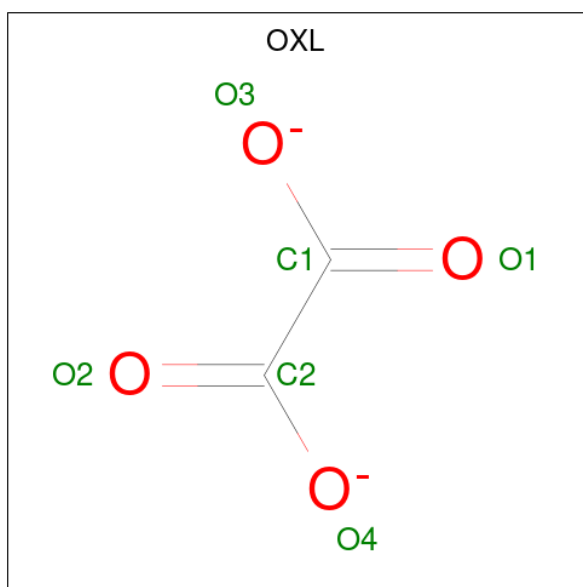
Chain	Residue	Modelled	Actual	Comment	Reference
A	117	LYS	GLU	engineered mutation	UNP P11974
B	117	LYS	GLU	engineered mutation	UNP P11974
C	117	LYS	GLU	engineered mutation	UNP P11974
D	117	LYS	GLU	engineered mutation	UNP P11974

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

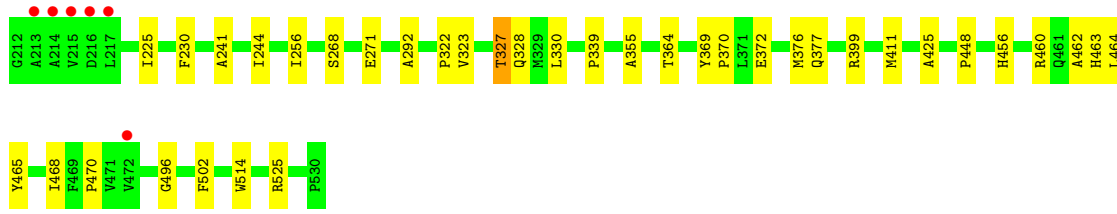
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	192	Total O 192 192	0	0

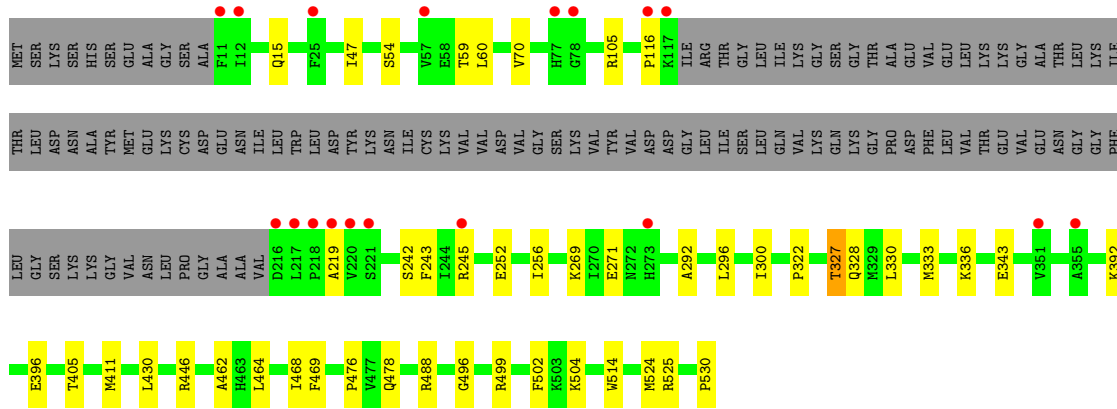
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	164	Total 164	O 164	0	0
5	C	148	Total 148	O 148	0	0
5	D	134	Total 134	O 134	0	0



● Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.34Å 121.83Å 161.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.97 – 2.25 47.32 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.97-2.25) 100.0 (47.32-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.201 , 0.250 0.201 , 0.250	Depositor DCC
R_{free} test set	4989 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtrriage
Anisotropy	0.139	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15009	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: OXL, 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	0.38	1/4010 (0.0%)	0.58	1/5416 (0.0%)
1	B	0.36	0/3948	0.57	0/5345
1	C	0.35	0/3344	0.54	0/4520
1	D	0.35	0/3241	0.55	0/4377
All	All	0.36	1/14543 (0.0%)	0.56	1/19658 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	GLU	CD-OE2	6.46	1.32	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	GLU	N-CA-CB	-5.36	100.94	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	GLU	Sidechain
1	B	389	PHE	Sidechain

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	3944	0	3982	41	0
1	B	3883	0	3860	39	0
1	C	3290	0	3288	31	0
1	D	3190	0	3210	29	0
2	A	8	0	6	1	0
2	B	8	0	6	0	0
2	C	8	0	6	0	0
2	D	12	0	9	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	192	0	0	1	0
5	B	164	0	0	1	0
5	C	148	0	0	0	0
5	D	134	0	0	0	0
All	All	15009	0	14367	128	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 (128) 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:B:167:VAL:HG21	1:B:192:LEU:HD11	1.67	0.75
1:A:219:ALA:HB3	1:A:252:GLU:OE1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:HH12	1:C:470:PRO:HD2	1.55	0.71
1:B:122:LEU:HD22	1:B:149:GLU:HG2	1.71	0.70
1:C:241:ALA:HB3	1:C:244:ILE:HD11	1.74	0.70
1:D:47:ILE:HG12	1:D:70:VAL:HB	1.76	0.67
1:D:327:THR:HG22	1:D:328:GLN:HG3	1.79	0.64
1:A:334:ILE:HG22	1:A:335:LYS:HE3	1.78	0.63
1:C:225:ILE:HG12	1:C:256:ILE:HD13	1.80	0.63
1:A:141:ILE:HB	1:A:192:LEU:HB2	1.81	0.62
1:B:327:THR:HG22	1:B:328:GLN:HG3	1.80	0.61
1:A:462:ALA:HB1	1:A:468:ILE:HG21	1.82	0.61
1:B:389:PHE:CE2	1:B:392:LYS:HG3	2.35	0.61
1:C:105:ARG:NH1	1:C:463:HIS:HE1	2.00	0.60
1:A:124:LYS:HD3	1:A:152:ASP:HB3	1.83	0.60
1:A:167:VAL:HG13	1:A:171:SER:HB2	1.84	0.58
1:D:504:LYS:HE2	1:D:530:PRO:O	2.03	0.58
1:B:525:ARG:HD3	1:C:514:TRP:CE3	2.39	0.58
1:A:220:VAL:HG12	1:A:225:ILE:HG13	1.87	0.56
1:A:189:PRO:HD2	1:A:191:PHE:CE2	2.41	0.56
1:D:252:GLU:O	1:D:256:ILE:HG12	2.05	0.56
1:A:514:TRP:CE3	1:D:525:ARG:HD3	2.41	0.56
1:C:496:GLY:HA3	1:C:502:PHE:CZ	2.40	0.55
1:B:15:GLN:HG2	1:B:39:ILE:HG23	1.89	0.55
1:B:381:ALA:O	1:B:385:GLU:HG3	2.08	0.54
1:D:496:GLY:HA3	1:D:502:PHE:CZ	2.43	0.54
1:A:455:ASN:HB3	1:A:458:THR:HB	1.89	0.54
1:D:462:ALA:HB1	1:D:468:ILE:HG21	1.89	0.54
1:A:269:LYS:HE2	1:A:271:GLU:OE2	2.08	0.53
1:B:514:TRP:CE3	1:C:525:ARG:HD3	2.44	0.53
1:A:318:ARG:HG3	1:A:400:SER:OG	2.10	0.52
1:A:465:TYR:HB2	1:A:468:ILE:HD12	1.92	0.52
1:C:47:ILE:HG12	1:C:70:VAL:HB	1.91	0.52
1:B:254:ARG:CZ	1:B:266:ILE:HD12	2.41	0.52
1:C:271:GLU:HB3	1:C:292:ALA:HB3	1.93	0.51
1:D:105:ARG:NH2	1:D:499:ARG:HH12	2.09	0.51
1:D:271:GLU:HG3	1:D:292:ALA:HB3	1.94	0.50
1:B:131:VAL:HG11	1:B:152:ASP:HA	1.92	0.50
1:B:242:SER:HA	1:B:269:LYS:HD3	1.95	0.49
1:C:70:VAL:HG22	1:C:108:ALA:HB3	1.94	0.49
1:B:406:ASP:HB3	1:B:409:GLU:HG3	1.95	0.49
1:C:99:SER:O	1:C:101:PRO:HD3	2.13	0.49
1:A:24:THR:HB	1:B:396:GLU:CD	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:ALA:CB	1:C:244:ILE:HD11	2.41	0.48
1:A:184:VAL:HA	1:A:194:THR:HG22	1.94	0.48
1:A:271:GLU:HG2	1:A:292:ALA:HB3	1.95	0.48
1:B:496:GLY:HA3	1:B:502:PHE:CZ	2.48	0.48
1:B:344:GLY:HA2	1:B:380:ILE:HD13	1.95	0.47
1:A:133:LEU:HD12	1:A:180:ILE:HD13	1.96	0.47
1:D:242:SER:HA	1:D:269:LYS:HD3	1.96	0.47
1:D:292:ALA:HB1	3:D:604:OXL:C1	2.44	0.46
1:A:310:LYS:HB3	1:B:29:MET:CG	2.46	0.46
1:A:139:LEU:HD21	1:A:156:LEU:CB	2.46	0.45
1:A:181:SER:HB3	1:A:198:ASN:HB2	1.98	0.45
1:C:100:ASP:OD2	1:C:103:LEU:HD12	2.16	0.45
1:D:322:PRO:HB3	1:D:464:LEU:O	2.15	0.45
1:A:520:PHE:HA	2:A:602:ACT:H1	1.99	0.45
1:D:296:LEU:O	1:D:300:ILE:HG12	2.16	0.45
1:B:164:CYS:O	1:B:187:LYS:HE3	2.17	0.45
1:C:244:ILE:HD13	1:C:268:SER:HA	1.99	0.45
1:A:435:ARG:NH1	5:A:705:HOH:O	2.46	0.45
1:B:478:GLN:HB2	1:B:484:ASP:HB2	1.99	0.45
1:A:327:THR:HG22	1:A:328:GLN:HG3	1.99	0.45
1:B:80:HIS:CE1	1:B:230:PHE:HB2	2.52	0.44
1:B:333:MET:HA	1:B:336:LYS:O	2.16	0.44
1:A:422:CYS:HA	1:D:405:THR:HB	1.99	0.44
1:C:330:LEU:HD11	1:C:377:GLN:HG3	1.98	0.44
1:C:465:TYR:HB2	1:C:468:ILE:HD12	1.98	0.44
1:A:139:LEU:HD21	1:A:156:LEU:HB3	2.00	0.44
1:A:47:ILE:HG12	1:A:70:VAL:HB	1.99	0.44
1:A:59:THR:O	1:A:63:MET:HG2	2.18	0.44
1:C:327:THR:HG22	1:C:328:GLN:HG3	2.00	0.44
1:D:54:SER:O	1:D:60:LEU:HG	2.18	0.44
1:B:481:TRP:HB2	1:B:516:PRO:HG3	2.00	0.44
1:A:215:VAL:O	1:A:245:ARG:NH2	2.51	0.44
1:B:376:MET:O	1:B:380:ILE:HG13	2.17	0.44
1:B:526:VAL:HG23	1:C:411:MET:SD	2.58	0.44
1:A:310:LYS:HB3	1:B:29:MET:HG3	2.00	0.43
1:B:27[B]:GLU:HG2	5:B:815:HOH:O	2.17	0.43
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.53	0.43
1:C:369:TYR:HB3	1:C:372:GLU:HB2	1.99	0.43
1:D:15:GLN:NE2	1:D:446:ARG:HD3	2.33	0.43
1:B:59:THR:O	1:B:63:MET:HG2	2.18	0.43
1:B:123:ILE:HD12	1:B:131:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLU:HG2	1:B:292:ALA:HB3	2.00	0.43
1:C:322:PRO:HB3	1:C:464:LEU:O	2.19	0.43
1:D:54:SER:HA	1:D:59:THR:HG21	2.01	0.43
1:D:116:PRO:HD2	1:D:243:PHE:HB2	2.01	0.43
1:A:324:ILE:HG12	1:A:357:CYS:HB2	2.01	0.43
1:C:292:ALA:HB1	3:C:603:OXL:C1	2.49	0.43
1:B:252:GLU:O	1:B:256:ILE:HG12	2.19	0.42
1:C:84:ALA:HB2	1:C:230:PHE:HZ	1.84	0.42
1:D:392:LYS:O	1:D:396:GLU:HG3	2.19	0.42
1:D:476:PRO:O	1:D:478:GLN:NE2	2.52	0.42
1:C:364:THR:HA	1:C:370:PRO:HB3	2.01	0.42
1:D:333:MET:HA	1:D:336:LYS:O	2.18	0.42
1:B:240:PHE:HD1	1:B:267:ILE:HB	1.84	0.42
1:B:322:PRO:HB3	1:B:464:LEU:O	2.20	0.42
1:D:411:MET:HE3	1:D:524:MET:HB2	2.01	0.42
1:A:287:ASP:O	1:A:322:PRO:HD2	2.20	0.42
1:A:391:ARG:HH11	1:A:391:ARG:HG2	1.85	0.42
1:D:219:ALA:HA	1:D:245:ARG:HH21	1.84	0.41
1:B:391:ARG:O	1:B:395:GLU:HG3	2.20	0.41
1:B:514:TRP:CD2	1:C:525:ARG:HD3	2.55	0.41
1:C:339:PRO:HG3	1:C:376:MET:HG2	2.02	0.41
1:D:271:GLU:CG	1:D:292:ALA:HB3	2.49	0.41
1:A:29:MET:CG	1:B:310:LYS:HB3	2.50	0.41
1:C:425:ALA:O	1:C:448:PRO:HD2	2.21	0.41
1:D:469:PHE:CZ	1:D:499:ARG:HD2	2.55	0.41
1:A:115:GLY:HA2	1:A:224:ASP:OD2	2.21	0.41
1:A:493:MET:HE2	1:A:508:VAL:HG21	2.03	0.41
1:B:169:VAL:HA	1:B:184:VAL:HG12	2.02	0.41
1:C:323:VAL:HG13	1:C:355:ALA:HA	2.01	0.41
1:C:399:ARG:HE	1:C:399:ARG:HB2	1.66	0.41
1:C:462:ALA:HB1	1:C:468:ILE:HG21	2.03	0.41
1:A:525:ARG:HD3	1:D:514:TRP:CD2	2.56	0.41
1:D:330:LEU:HD23	1:D:343:GLU:HB3	2.03	0.41
1:D:430:LEU:HD21	1:D:488:ARG:HB2	2.01	0.41
1:A:427:LEU:HG	1:A:509:ILE:HB	2.02	0.41
1:B:525:ARG:HD3	1:C:514:TRP:CD2	2.55	0.41
1:A:481:TRP:CG	1:A:516:PRO:HD3	2.56	0.41
1:A:452:VAL:CG2	1:A:492:ALA:HB2	2.51	0.40
1:B:54:SER:HA	1:B:59:THR:HG21	2.03	0.40
1:C:456:HIS:HB3	1:C:460:ARG:HH12	1.86	0.40
1:A:60:LEU:HD13	1:A:90:VAL:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:LEU:HD23	1:D:488:ARG:CZ	2.51	0.40
1:B:187:LYS:HA	1:B:192:LEU:HD23	2.03	0.40
1:B:318:ARG:HG3	1:B:400:SER:HB3	2.03	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	519/531 (98%)	513 (99%)	6 (1%)	0	100	100
1	B	518/531 (98%)	510 (98%)	7 (1%)	1 (0%)	47	55
1	C	433/531 (82%)	428 (99%)	4 (1%)	1 (0%)	47	55
1	D	418/531 (79%)	413 (99%)	4 (1%)	1 (0%)	47	55
All	All	1888/2124 (89%)	1864 (99%)	21 (1%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	THR
1	B	327	THR
1	C	327	THR

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	416/435 (96%)	416 (100%)	0	100	100
1	B	402/435 (92%)	402 (100%)	0	100	100
1	C	341/435 (78%)	341 (100%)	0	100	100
1	D	332/435 (76%)	332 (100%)	0	100	100
All	All	1491/1740 (86%)	1491 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z > 2$
2	ACT	B	602	-	3,3,3	1.20	0	3,3,3	1.46	0
2	ACT	D	603	-	3,3,3	1.25	0	3,3,3	1.52	0
2	ACT	C	602	-	3,3,3	1.08	0	3,3,3	1.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXL	A	603	4	5,5,5	1.77	1 (20%)	6,6,6	1.26	1 (16%)
2	ACT	D	601	-	3,3,3	1.17	0	3,3,3	1.54	0
3	OXL	B	603	4	5,5,5	1.81	1 (20%)	6,6,6	1.11	0
3	OXL	D	604	4	5,5,5	1.74	1 (20%)	6,6,6	1.30	1 (16%)
3	OXL	C	603	4	5,5,5	1.77	1 (20%)	6,6,6	1.06	0
2	ACT	A	601	-	3,3,3	1.46	1 (33%)	3,3,3	1.34	0
2	ACT	D	602	-	3,3,3	1.38	1 (33%)	3,3,3	1.41	0
2	ACT	A	602	-	3,3,3	1.16	0	3,3,3	1.40	0
2	ACT	B	601	-	3,3,3	1.39	0	3,3,3	1.30	0
2	ACT	C	601	-	3,3,3	1.37	0	3,3,3	1.35	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
3	OXL	D	604	4	-	0/4/4/4	-
3	OXL	B	603	4	-	4/4/4/4	-
3	OXL	A	603	4	-	0/4/4/4	-
3	OXL	C	603	4	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	OXL	C2-C1	-2.76	1.46	1.54
3	B	603	OXL	C2-C1	-2.76	1.46	1.54
3	C	603	OXL	C2-C1	-2.70	1.46	1.54
3	D	604	OXL	C2-C1	-2.62	1.47	1.54
2	A	601	ACT	CH3-C	2.31	1.58	1.49
2	D	602	ACT	CH3-C	2.02	1.57	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	604	OXL	O3-C1-C2	2.19	119.67	113.16
3	A	603	OXL	O4-C2-C1	2.07	119.31	113.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	603	OXL	O3-C1-C2-O4
3	B	603	OXL	O1-C1-C2-O2
3	B	603	OXL	O1-C1-C2-O4
3	B	603	OXL	O3-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	604	OXL	1	0
3	C	603	OXL	1	0
2	A	602	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	519/531 (97%)	-0.09	5 (0%) 82 84	19, 30, 52, 70	0
1	B	519/531 (97%)	-0.04	12 (2%) 60 63	20, 32, 57, 78	0
1	C	437/531 (82%)	-0.03	11 (2%) 57 60	21, 32, 50, 81	0
1	D	422/531 (79%)	0.20	18 (4%) 35 37	23, 33, 50, 78	0
All	All	1897/2124 (89%)	0.00	46 (2%) 59 62	19, 32, 54, 81	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	126	SER	5.9
1	C	214	ALA	5.6
1	B	125	GLY	5.1
1	A	147	TYR	4.4
1	D	217	LEU	4.2
1	D	220	VAL	4.0
1	B	147	TYR	3.8
1	C	213	ALA	3.6
1	D	218	PRO	3.6
1	D	351	VAL	3.5
1	D	216	ASP	3.5
1	D	11	PHE	3.4
1	D	219	ALA	3.1
1	B	122	LEU	3.1
1	D	77	HIS	3.0
1	C	217	LEU	3.0
1	C	120	THR	2.9
1	C	216	ASP	2.9
1	B	146	ALA	2.9
1	B	127	GLY	2.9
1	A	193	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	210	LEU	2.8
1	C	215	VAL	2.8
1	D	78	GLY	2.7
1	B	189	PRO	2.7
1	D	355	ALA	2.7
1	A	191	PHE	2.5
1	B	154	ASN	2.5
1	D	12	ILE	2.4
1	C	472	VAL	2.4
1	B	219	ALA	2.3
1	D	25	PHE	2.3
1	C	205	LYS	2.3
1	D	117	LYS	2.3
1	D	116	PRO	2.2
1	B	99	SER	2.2
1	A	164	CYS	2.2
1	D	245	ARG	2.2
1	D	221	SER	2.2
1	D	57	VAL	2.2
1	B	153	GLU	2.1
1	D	273	HIS	2.1
1	B	144	ASP	2.1
1	C	208	VAL	2.0
1	A	192	LEU	2.0
1	C	211	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	OXL	B	603	6/6	0.84	0.17	30,38,45,49	0
4	MG	C	604	1/1	0.84	0.07	38,38,38,38	0
2	ACT	A	601	4/4	0.87	0.21	28,29,36,38	0
2	ACT	D	601	4/4	0.88	0.30	33,36,37,40	0
4	MG	D	605	1/1	0.88	0.07	42,42,42,42	0
2	ACT	D	603	4/4	0.90	0.21	45,47,48,52	0
2	ACT	B	601	4/4	0.90	0.18	32,36,36,38	0
2	ACT	C	601	4/4	0.93	0.24	35,37,41,41	0
4	MG	A	604	1/1	0.93	0.10	39,39,39,39	0
2	ACT	D	602	4/4	0.94	0.15	30,31,35,37	0
2	ACT	C	602	4/4	0.94	0.19	21,27,32,33	0
3	OXL	A	603	6/6	0.95	0.12	25,30,34,41	0
4	MG	B	604	1/1	0.95	0.10	39,39,39,39	0
2	ACT	A	602	4/4	0.95	0.20	27,31,35,37	0
3	OXL	D	604	6/6	0.95	0.14	32,37,41,44	0
3	OXL	C	603	6/6	0.96	0.10	27,32,37,37	0
2	ACT	B	602	4/4	0.98	0.11	28,28,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.