



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:59 AM GMT

PDB ID : 3GR4
Title : Activator-Bound Structure of Human Pyruvate Kinase M2
Authors : Hong, B.; Dimov, S.; Tempel, W.; Auld, D.; Thomas, C.; Boxer, M.; Jianq, J.-K.; Skoumbourdis, A.; Min, S.; Southall, N.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Inglese, J.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-03-24
Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

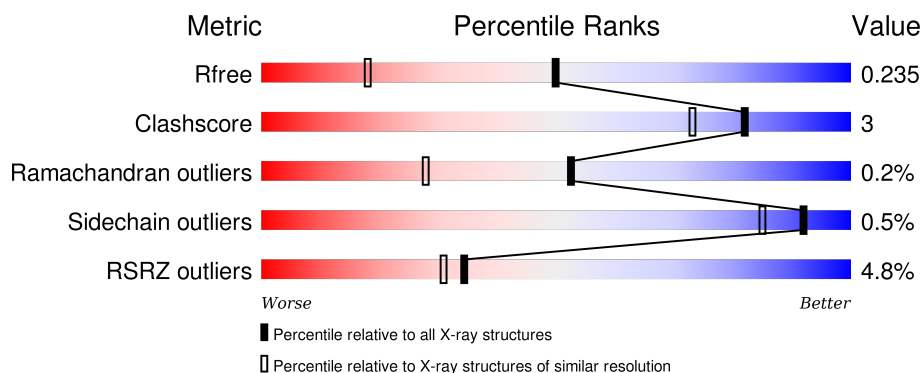
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	550	<div> <div>5%</div> <div>87%</div> <div>7%</div> <div>6%</div> </div>
1	B	550	<div> <div>7%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	C	550	<div> <div>2%</div> <div>89%</div> <div>•</div> <div>6%</div> </div>
1	D	550	<div> <div>4%</div> <div>87%</div> <div>6%</div> <div>7%</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
2	FBP	C	541	-	-	-	X
3	TLA	B	538	-	-	-	X
3	TLA	C	534	-	-	-	X
3	TLA	D	543	-	-	-	X
4	DYY	A	550[A]	-	-	-	X
4	DYY	A	550[B]	-	-	-	X
4	DYY	D	550[A]	-	-	-	X
4	DYY	D	550[B]	-	-	-	X
5	UNX	A	532	-	-	-	X
5	UNX	A	534	-	-	-	X
5	UNX	A	535	-	-	-	X
5	UNX	B	532	-	-	-	X
5	UNX	B	533	-	-	-	X
5	UNX	B	534	-	-	-	X
5	UNX	B	535	-	-	-	X
5	UNX	B	536	-	-	-	X
5	UNX	C	532	-	-	-	X
5	UNX	D	532	-	-	-	X
5	UNX	D	533	-	-	-	X
5	UNX	D	534	-	-	-	X
5	UNX	D	535	-	-	-	X
6	ADP	A	538	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16503 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 isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	2	0
			3885	2453	676	731	25			
1	B	505	Total	C	N	O	S	0	3	0
			3754	2361	663	706	24			
1	C	515	Total	C	N	O	S	0	4	0
			3847	2430	672	721	24			
1	D	509	Total	C	N	O	S	0	4	0
			3808	2398	679	706	25			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP P14618
A	-17	GLY	-	EXPRESSION TAG	UNP P14618
A	-16	SER	-	EXPRESSION TAG	UNP P14618
A	-15	SER	-	EXPRESSION TAG	UNP P14618
A	-14	HIS	-	EXPRESSION TAG	UNP P14618
A	-13	HIS	-	EXPRESSION TAG	UNP P14618
A	-12	HIS	-	EXPRESSION TAG	UNP P14618
A	-11	HIS	-	EXPRESSION TAG	UNP P14618
A	-10	HIS	-	EXPRESSION TAG	UNP P14618
A	-9	HIS	-	EXPRESSION TAG	UNP P14618
A	-8	SER	-	EXPRESSION TAG	UNP P14618
A	-7	SER	-	EXPRESSION TAG	UNP P14618
A	-6	GLY	-	EXPRESSION TAG	UNP P14618
A	-5	LEU	-	EXPRESSION TAG	UNP P14618
A	-4	VAL	-	EXPRESSION TAG	UNP P14618
A	-3	PRO	-	EXPRESSION TAG	UNP P14618
A	-2	ARG	-	EXPRESSION TAG	UNP P14618
A	-1	GLY	-	EXPRESSION TAG	UNP P14618
A	0	SER	-	EXPRESSION TAG	UNP P14618
B	-18	MET	-	EXPRESSION TAG	UNP P14618
B	-17	GLY	-	EXPRESSION TAG	UNP P14618

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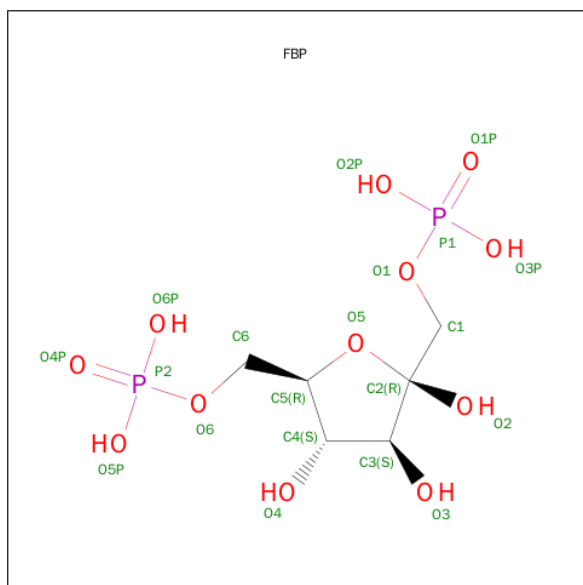
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP P14618
B	-15	SER	-	EXPRESSION TAG	UNP P14618
B	-14	HIS	-	EXPRESSION TAG	UNP P14618
B	-13	HIS	-	EXPRESSION TAG	UNP P14618
B	-12	HIS	-	EXPRESSION TAG	UNP P14618
B	-11	HIS	-	EXPRESSION TAG	UNP P14618
B	-10	HIS	-	EXPRESSION TAG	UNP P14618
B	-9	HIS	-	EXPRESSION TAG	UNP P14618
B	-8	SER	-	EXPRESSION TAG	UNP P14618
B	-7	SER	-	EXPRESSION TAG	UNP P14618
B	-6	GLY	-	EXPRESSION TAG	UNP P14618
B	-5	LEU	-	EXPRESSION TAG	UNP P14618
B	-4	VAL	-	EXPRESSION TAG	UNP P14618
B	-3	PRO	-	EXPRESSION TAG	UNP P14618
B	-2	ARG	-	EXPRESSION TAG	UNP P14618
B	-1	GLY	-	EXPRESSION TAG	UNP P14618
B	0	SER	-	EXPRESSION TAG	UNP P14618
C	-18	MET	-	EXPRESSION TAG	UNP P14618
C	-17	GLY	-	EXPRESSION TAG	UNP P14618
C	-16	SER	-	EXPRESSION TAG	UNP P14618
C	-15	SER	-	EXPRESSION TAG	UNP P14618
C	-14	HIS	-	EXPRESSION TAG	UNP P14618
C	-13	HIS	-	EXPRESSION TAG	UNP P14618
C	-12	HIS	-	EXPRESSION TAG	UNP P14618
C	-11	HIS	-	EXPRESSION TAG	UNP P14618
C	-10	HIS	-	EXPRESSION TAG	UNP P14618
C	-9	HIS	-	EXPRESSION TAG	UNP P14618
C	-8	SER	-	EXPRESSION TAG	UNP P14618
C	-7	SER	-	EXPRESSION TAG	UNP P14618
C	-6	GLY	-	EXPRESSION TAG	UNP P14618
C	-5	LEU	-	EXPRESSION TAG	UNP P14618
C	-4	VAL	-	EXPRESSION TAG	UNP P14618
C	-3	PRO	-	EXPRESSION TAG	UNP P14618
C	-2	ARG	-	EXPRESSION TAG	UNP P14618
C	-1	GLY	-	EXPRESSION TAG	UNP P14618
C	0	SER	-	EXPRESSION TAG	UNP P14618
D	-18	MET	-	EXPRESSION TAG	UNP P14618
D	-17	GLY	-	EXPRESSION TAG	UNP P14618
D	-16	SER	-	EXPRESSION TAG	UNP P14618
D	-15	SER	-	EXPRESSION TAG	UNP P14618
D	-14	HIS	-	EXPRESSION TAG	UNP P14618
D	-13	HIS	-	EXPRESSION TAG	UNP P14618

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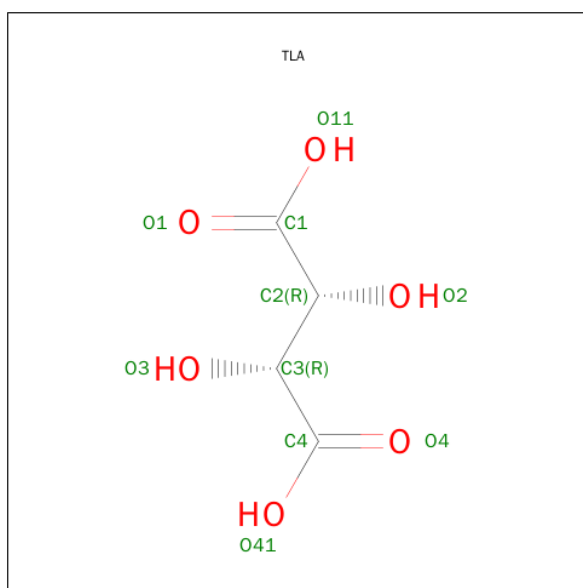
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	EXPRESSION TAG	UNP P14618
D	-11	HIS	-	EXPRESSION TAG	UNP P14618
D	-10	HIS	-	EXPRESSION TAG	UNP P14618
D	-9	HIS	-	EXPRESSION TAG	UNP P14618
D	-8	SER	-	EXPRESSION TAG	UNP P14618
D	-7	SER	-	EXPRESSION TAG	UNP P14618
D	-6	GLY	-	EXPRESSION TAG	UNP P14618
D	-5	LEU	-	EXPRESSION TAG	UNP P14618
D	-4	VAL	-	EXPRESSION TAG	UNP P14618
D	-3	PRO	-	EXPRESSION TAG	UNP P14618
D	-2	ARG	-	EXPRESSION TAG	UNP P14618
D	-1	GLY	-	EXPRESSION TAG	UNP P14618
D	0	SER	-	EXPRESSION TAG	UNP P14618

- Molecule 2 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



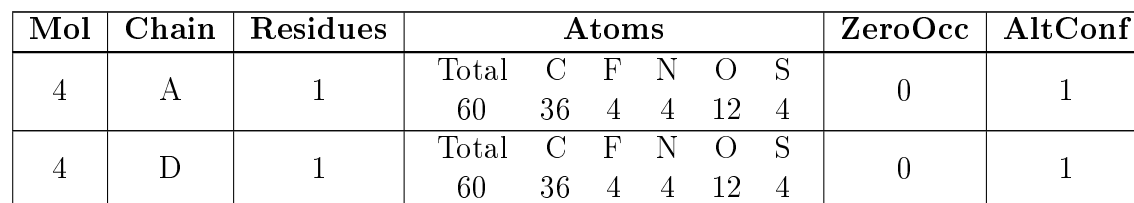
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			6	1	4	1		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



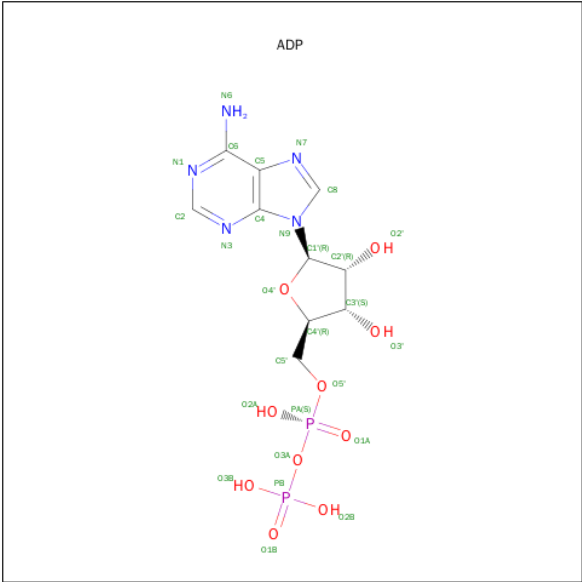
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is 1-[(2,6-DIFLUOROPHENYL)SULFONYL]-4-(2,3-DIHYDRO-1,4-BENZODIOXIN-6-YLSULFONYL)PIPERAZINE (three-letter code: DYY) (formula: $C_{18}H_{18}F_2N_2O_6S_2$).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 5 | B | 6 | Total X
6 6 | 0 | 0 |
| 5 | A | 6 | Total X
6 6 | 0 | 0 |
| 5 | D | 4 | Total X
4 4 | 0 | 0 |
| 5 | C | 2 | Total X
2 2 | 0 | 0 |

- 



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			18	5	1	10	2		

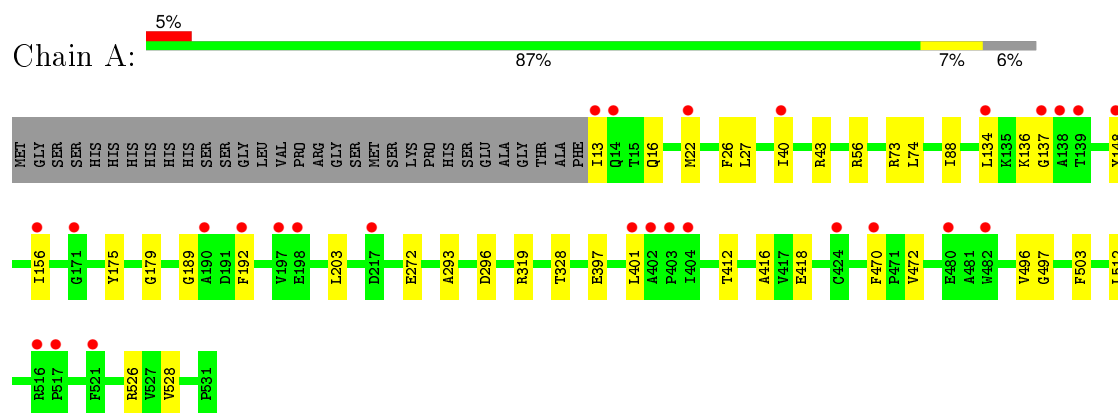
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	245	Total	O	0	0
			245	245		
7	B	237	Total	O	0	0
			237	237		
7	C	228	Total	O	0	0
			228	228		
7	D	207	Total	O	0	0
			207	207		

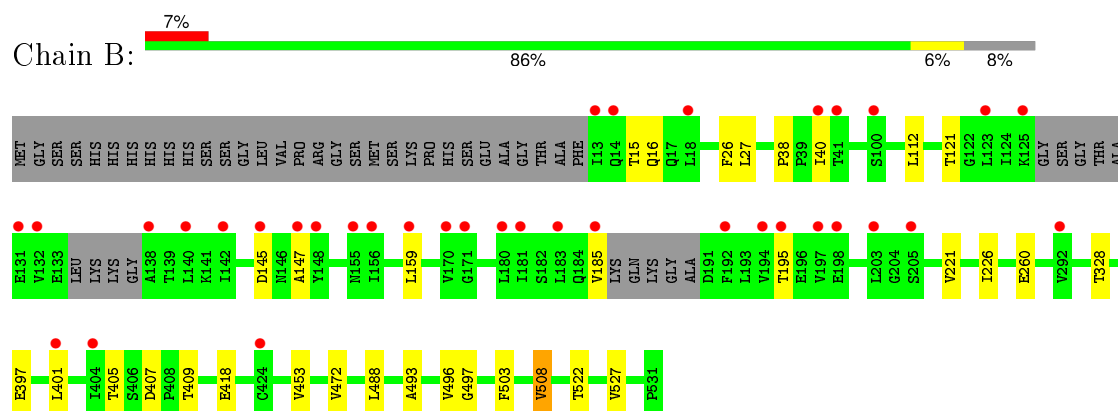
3 Residue-property plots [i](#)

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

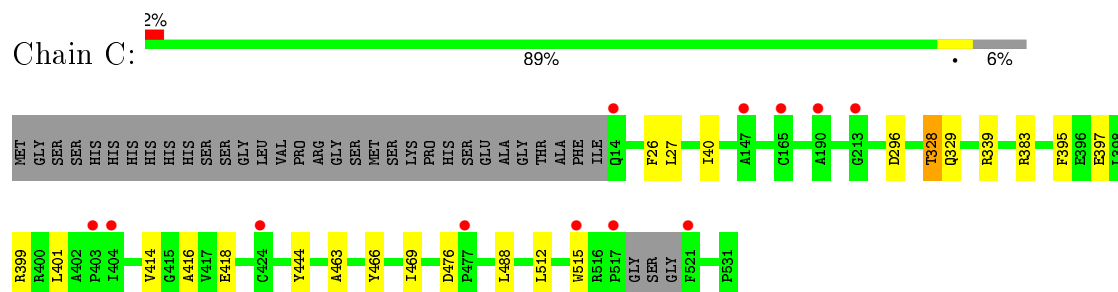
• Molecule 1: Pyruvate kinase isozymes M1/M2



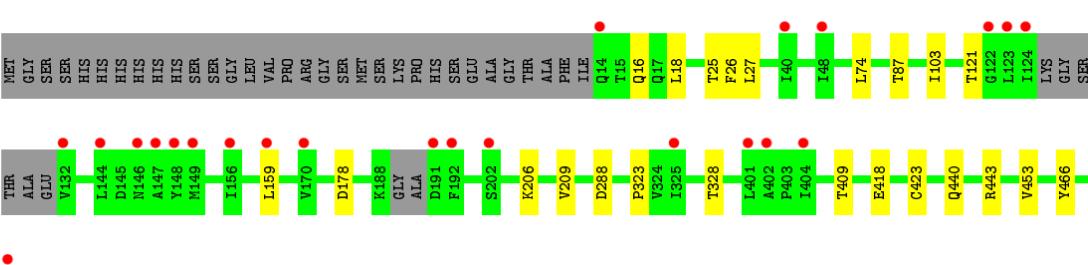
• Molecule 1: Pyruvate kinase isozymes M1/M2



• Molecule 1: Pyruvate kinase isozymes M1/M2



Chain D: 



Position	Amino Acid	Category
F470	F470	Green
P471	P471	Green
V472	V472	Green
L488	L488	Green
F492	F492	Green
A493	A493	Green
V496	V496	Green
G497	G497	Green
F503	F503	Green
V530	V530	Green
P531	P531	Green
T132	V132	Green
L144	L144	Green
D145	D145	Green
N146	N146	Green
A147	A147	Green
I148	I148	Green
M149	M149	Green
I156	I156	Green
L159	L159	Green
V170	V170	Green
D178	D178	Yellow
K188	K188	Green
G191	G191	Green
D191	D191	Green
F192	F192	Green
S202	S202	Green
K206	K206	Yellow
V209	V209	Yellow
D288	D288	Green
P323	P323	Green
V324	V324	Green
I325	I325	Green
T328	T328	Yellow
L401	L401	Green
A402	A402	Green
P403	P403	Green
L404	L404	Green
T409	T409	Yellow
E418	E418	Yellow
C423	C423	Yellow
Q440	Q440	Yellow
R443	R443	Yellow
V453	V453	Yellow
Y466	Y466	Yellow
V469	V469	Yellow
T121	T121	Green
G122	G122	Green
L123	L123	Green
I124	I124	Green
Lys	Lys	Green
Gly	Gly	Green
Ser	Ser	Green
Gly	Gly	Green
Met	Met	Grey
Gly	Gly	Grey
Ser	Ser	Grey
His	His	Grey
His	His	Grey
His	His	Grey
His	His	Grey
His	His	Grey
His	His	Grey
Ser	Ser	Grey
Gly	Gly	Grey
Leu	Leu	Grey
Val	Val	Grey
Pro	Pro	Grey
Arg	Arg	Grey
Gly	Gly	Grey
Ser	Ser	Grey
Met	Met	Grey
Ser	Ser	Grey
Lys	Lys	Grey
Pro	Pro	Grey
His	His	Grey
Ser	Ser	Grey
Gly	Gly	Grey
Ala	Ala	Grey
Gly	Gly	Grey
Thr	Thr	Grey
Ala	Ala	Grey
Phe	Phe	Grey
Ile	Ile	Grey
T15	T15	Green
Q16	Q16	Yellow
Q17	Q17	Yellow
L18	L18	Yellow
T25	T25	Yellow
F26	F26	Yellow
L27	L27	Yellow
I40	I40	Green
I48	I48	Green
L74	L74	Yellow
T87	T87	Yellow
I103	I103	Yellow

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.28Å 153.21Å 93.14Å 90.00° 102.91° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 29.27 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.3 (30.00-1.60) 96.3 (29.27-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0088, coot, molprobity, prodrgr	Depositor
R, R_{free}	0.208 , 0.231 0.212 , 0.235	Depositor DCC
R_{free} test set	2916 reflections (1.05%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 280370 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16503	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 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, TLA, FBP, DYY, ADP

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	0.71	1/3960 (0.0%)	0.67	2/5367 (0.0%)
1	B	0.68	0/3819	0.65	0/5177
1	C	0.68	0/3920	0.65	0/5315
1	D	0.66	0/3877	0.65	0/5255
All	All	0.68	1/15576 (0.0%)	0.65	2/21114 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	ARG	CB-CG	-5.28	1.38	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	73	ARG	NE-CZ-NH1	5.57	123.08	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3885	0	3853	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3754	0	3664	28	0
1	C	3847	0	3821	24	0
1	D	3808	0	3728	29	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	6	0	0	0	0
2	D	20	0	10	0	0
3	A	10	0	4	0	0
3	B	20	0	8	0	0
3	C	20	0	8	0	0
3	D	20	0	8	0	0
4	A	60	0	36	9	0
4	D	60	0	36	8	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	2	0	0	0	0
5	D	4	0	0	0	0
6	A	18	0	8	0	0
7	A	245	0	0	0	0
7	B	237	0	0	0	0
7	C	228	0	0	0	0
7	D	207	0	0	0	0
All	All	16503	0	15204	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.

The worst 5 of 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:B:418[B]:GLU:HG3	1:D:418:GLU:HG2	1.58	0.83
1:D:74:LEU:HD11	1:D:87:THR:HG21	1.69	0.73
1:A:526:ARG:HD3	1:C:515:TRP:CD2	2.24	0.72
1:C:27:LEU:HD13	4:D:550[A]:DYY:CAO	2.20	0.72
1:A:16:GLN:HG2	1:A:40:ILE:HG23	1.77	0.67

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	519/550 (94%)	510 (98%)	8 (2%)	1 (0%)	52	28
1	B	500/550 (91%)	492 (98%)	7 (1%)	1 (0%)	52	28
1	C	515/550 (94%)	505 (98%)	9 (2%)	1 (0%)	52	28
1	D	507/550 (92%)	496 (98%)	10 (2%)	1 (0%)	52	28
All	All	2041/2200 (93%)	2003 (98%)	34 (2%)	4 (0%)	52	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	C	328	THR
1	D	328	THR
1	B	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	399/452 (88%)	397 (100%)	2 (0%)	92	85
1	B	376/452 (83%)	374 (100%)	2 (0%)	92	85
1	C	391/452 (86%)	389 (100%)	2 (0%)	92	85
1	D	381/452 (84%)	380 (100%)	1 (0%)	94	90
All	All	1547/1808 (86%)	1540 (100%)	7 (0%)	92	85

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	508	VAL
1	D	178	ASP
1	C	296	ASP
1	A	528	VAL
1	C	339	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	19	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 18 are unknown - leaving 16 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	$\# Z > 2$
6	ADP	A	538	-	15,18,29	0.60	0	21,28,45	1.58	4 (19%)
2	FBP	A	541	-	18,20,20	0.91	1 (5%)	21,32,32	0.72	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TLA	A	542	-	3,9,9	0.53	0	6,12,12	1.29	1 (16%)
4	DYY	A	550[A]	-	31,33,33	2.21	6 (19%)	44,50,50	2.29	9 (20%)
4	DYY	A	550[B]	-	31,33,33	2.84	6 (19%)	44,50,50	2.58	12 (27%)
3	TLA	B	538	-	3,9,9	0.54	0	6,12,12	1.03	1 (16%)
2	FBP	B	541	-	18,20,20	0.86	1 (5%)	21,32,32	0.90	1 (4%)
3	TLA	B	542	-	3,9,9	0.91	0	6,12,12	1.71	2 (33%)
3	TLA	C	534	-	3,9,9	0.90	0	6,12,12	1.44	1 (16%)
2	FBP	C	541	-	5,5,20	0.80	0	5,7,32	0.84	0
3	TLA	C	542	-	3,9,9	0.72	0	6,12,12	1.52	1 (16%)
2	FBP	D	541	-	18,20,20	0.93	1 (5%)	21,32,32	0.91	1 (4%)
3	TLA	D	542	-	3,9,9	0.54	0	6,12,12	1.16	1 (16%)
3	TLA	D	543	-	3,9,9	0.74	0	6,12,12	1.05	1 (16%)
4	DYY	D	550[A]	-	31,33,33	2.41	6 (19%)	44,50,50	2.26	8 (18%)
4	DYY	D	550[B]	-	31,33,33	2.65	6 (19%)	44,50,50	2.58	12 (27%)

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
6	ADP	A	538	-	-	0/12/28/32	0/1/1/3
2	FBP	A	541	-	-	0/13/32/32	0/1/1/1
3	TLA	A	542	-	-	0/4/12/12	0/0/0/0
4	DYY	A	550[A]	-	-	0/24/41/41	0/4/4/4
4	DYY	A	550[B]	-	-	0/24/41/41	0/4/4/4
3	TLA	B	538	-	-	0/4/12/12	0/0/0/0
2	FBP	B	541	-	-	0/13/32/32	0/1/1/1
3	TLA	B	542	-	-	0/4/12/12	0/0/0/0
3	TLA	C	534	-	-	0/4/12/12	0/0/0/0
2	FBP	C	541	-	-	0/1/3/32	0/0/0/1
3	TLA	C	542	-	-	0/4/12/12	0/0/0/0
2	FBP	D	541	-	-	0/13/32/32	0/1/1/1
3	TLA	D	542	-	-	0/4/12/12	0/0/0/0
3	TLA	D	543	-	-	0/4/12/12	0/0/0/0
4	DYY	D	550[A]	-	-	0/24/41/41	0/4/4/4
4	DYY	D	550[B]	-	-	0/24/41/41	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	541	FBP	O2-C2	2.70	1.45	1.41
2	D	541	FBP	O2-C2	2.71	1.45	1.41
2	A	541	FBP	O2-C2	3.22	1.46	1.41
4	D	550[A]	DYY	SAF-NAG	4.00	1.69	1.63
4	A	550[A]	DYY	SAF-NAG	4.03	1.69	1.63

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	550[A]	DYY	OAJ-SAW-OB	-6.63	108.03	119.47
4	A	550[B]	DYY	OAJ-SAW-OB	-6.09	108.96	119.47
4	A	550[B]	DYY	OAS-SAF-OAB	-5.99	109.13	119.47
4	D	550[B]	DYY	OAJ-SAW-OB	-5.97	109.17	119.47
4	D	550[B]	DYY	OAS-SAF-OAB	-5.89	109.30	119.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	550[A]	DYY	4	0
4	A	550[B]	DYY	5	0
4	D	550[A]	DYY	4	0
4	D	550[B]	DYY	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	519/550 (94%)	0.14	27 (5%) 31 28	13, 23, 48, 60	0
1	B	505/550 (91%)	0.20	36 (7%) 19 17	13, 23, 59, 81	0
1	C	515/550 (93%)	-0.07	12 (2%) 64 62	13, 22, 40, 62	0
1	D	509/550 (92%)	0.07	23 (4%) 37 34	14, 23, 46, 65	0
All	All	2048/2200 (93%)	0.09	98 (4%) 34 31	13, 23, 49, 81	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	ILE	11.5
1	C	404	ILE	10.0
1	A	13	ILE	8.1
1	A	404	ILE	7.5
1	D	147	ALA	6.2

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
5	UNX	C	532	1/1	0.44	1.49	239.14	2,2,2,2	1
5	UNX	B	532	1/1	-0.34	1.83	182.83	3,3,3,3	1
5	UNX	D	535	1/1	0.24	1.79	176.60	2,2,2,2	1
5	UNX	A	532	1/1	0.07	2.12	170.03	2,2,2,2	1
5	UNX	B	535	1/1	0.48	2.99	169.76	2,2,2,2	1
5	UNX	D	534	1/1	0.13	3.02	140.71	2,2,2,2	1
5	UNX	D	532	1/1	0.33	2.35	130.40	2,2,2,2	1
5	UNX	B	533	1/1	0.55	2.51	120.06	2,2,2,2	1
5	UNX	B	534	1/1	0.04	2.91	110.47	2,2,2,2	1
5	UNX	A	535	1/1	0.35	2.35	109.72	2,2,2,2	1
5	UNX	A	534	1/1	0.05	1.42	90.73	2,2,2,2	1
5	UNX	D	533	1/1	-0.46	1.23	89.33	2,2,2,2	1
5	UNX	B	536	1/1	-0.27	2.74	87.94	2,2,2,2	1
6	ADP	A	538	18/27	0.80	0.26	10.04	19,25,26,28	18
3	TLA	B	538	10/10	0.91	0.18	7.60	34,35,36,36	0
3	TLA	D	543	10/10	0.82	0.22	5.96	46,48,51,52	0
4	DYY	D	550[B]	30/30	0.87	0.17	4.85	29,36,40,41	30
4	DYY	D	550[A]	30/30	0.87	0.17	4.54	30,38,44,45	30
4	DYY	A	550[B]	30/30	0.91	0.14	3.61	32,38,43,44	30
4	DYY	A	550[A]	30/30	0.91	0.14	3.55	24,35,38,39	30
3	TLA	C	534	10/10	0.90	0.10	2.82	22,24,28,29	0
2	FBP	C	541	6/20	0.80	0.18	2.44	42,45,47,48	0
3	TLA	D	542	10/10	0.85	0.14	1.72	32,34,36,36	0
3	TLA	C	542	10/10	0.88	0.13	1.61	23,32,37,39	0
2	FBP	A	541	20/20	0.95	0.15	0.56	21,29,33,35	0
3	TLA	B	542	10/10	0.89	0.10	-0.21	26,30,30,31	0
3	TLA	A	542	10/10	0.93	0.09	-0.40	22,26,28,30	0
2	FBP	D	541	20/20	0.98	0.05	-0.82	13,15,17,18	0
2	FBP	B	541	20/20	0.97	0.06	-1.06	15,19,24,24	0
5	UNX	C	533	1/1	0.12	1.88	-	2,2,2,2	1
5	UNX	A	537	1/1	0.22	1.42	-	2,2,2,2	1
5	UNX	A	533	1/1	0.02	2.72	-	2,2,2,2	1
5	UNX	B	537	1/1	0.31	1.41	-	2,2,2,2	1
5	UNX	A	536	1/1	0.59	2.08	-	2,2,2,2	1

6.5 Other polymers ⓘ

There are no such residues in this entry.