Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2017 – 08:26 AM EDT

PDB ID	:	5X1V
Title	:	PKM2 in complex with compound 2
Authors	:	Matsui, Y.; Hanzawa, H.
Deposited on	:	2017-01-27
Resolution	:	2.10 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:

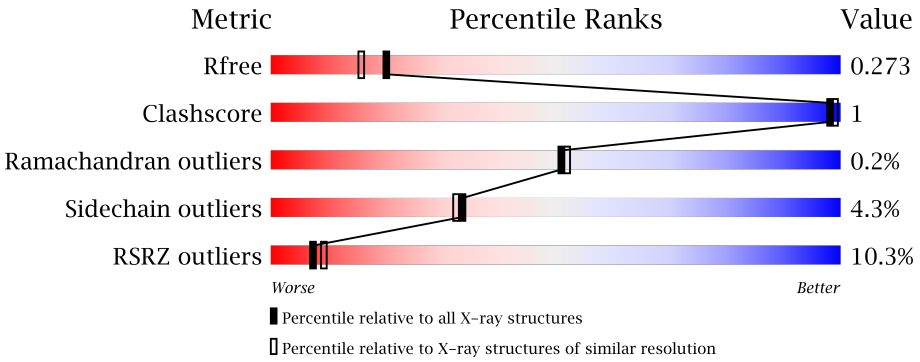
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 <=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	14% 88% 5% 7%
1	B	550	10% 86% 7% 7%
1	C	550	4% 89% 5% 6%
1	D	550	11% 88% 5% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16367 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	512	Total	C	N	O	S	0	0	0
			3919	2463	696	735	25			
1	B	513	Total	C	N	O	S	0	0	0
			3935	2475	698	737	25			
1	C	518	Total	C	N	O	S	0	0	0
			3965	2492	704	744	25			
1	D	511	Total	C	N	O	S	0	0	0
			3919	2463	696	735	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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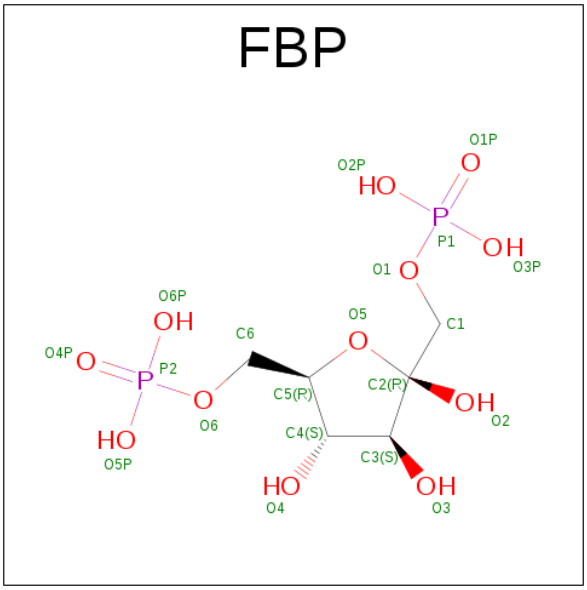
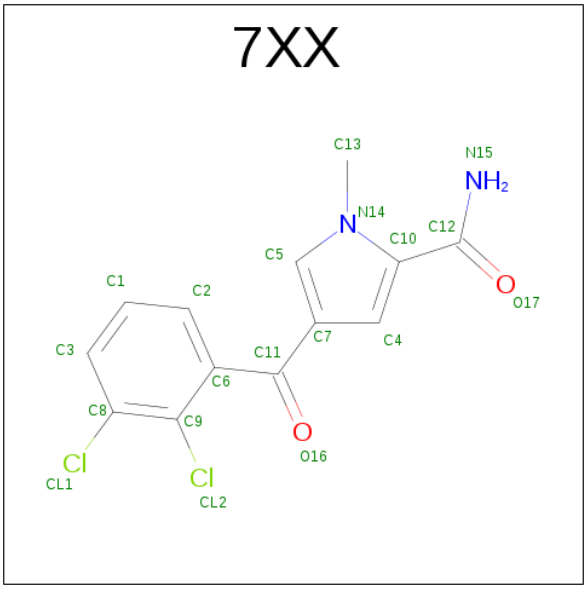
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP 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 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
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is 4-[2,3-bis(chloranyl)phenyl]carbonyl-1-methyl-pyrrole-2-carboxamide (three-letter code: 7XX) (formula: $C_{13}H_{10}Cl_2N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			19	13	2	2	2		
3	B	1	Total	C	Cl	N	O	0	0
			19	13	2	2	2		
3	C	1	Total	C	Cl	N	O	0	0
			19	13	2	2	2		
3	D	1	Total	C	Cl	N	O	0	0
			19	13	2	2	2		

- Molecule 4 is water.

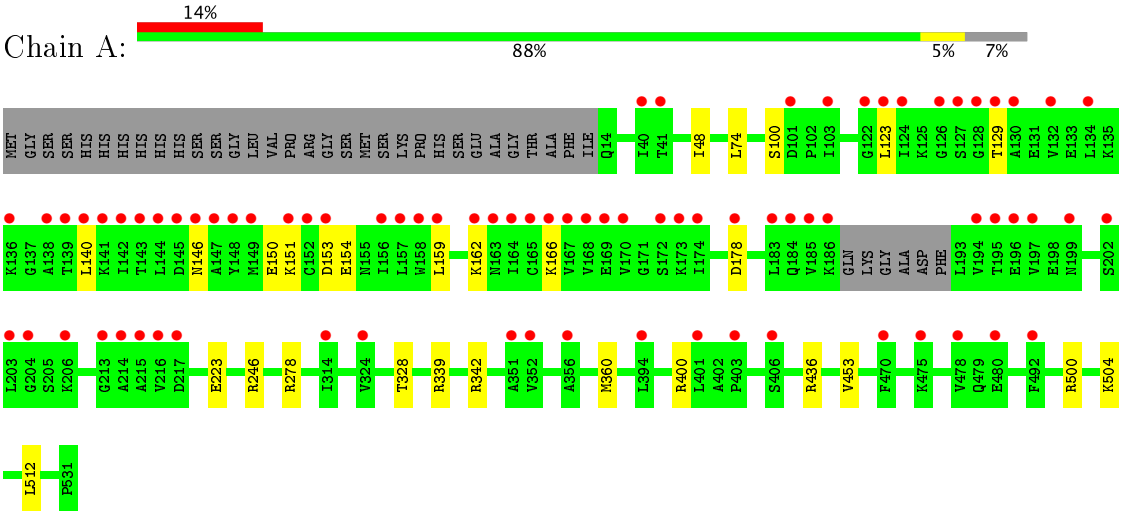
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	120	Total	O	0	0
			120	120		
4	C	127	Total	O	0	0
			127	127		
4	D	132	Total	O	0	0
			132	132		

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 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.

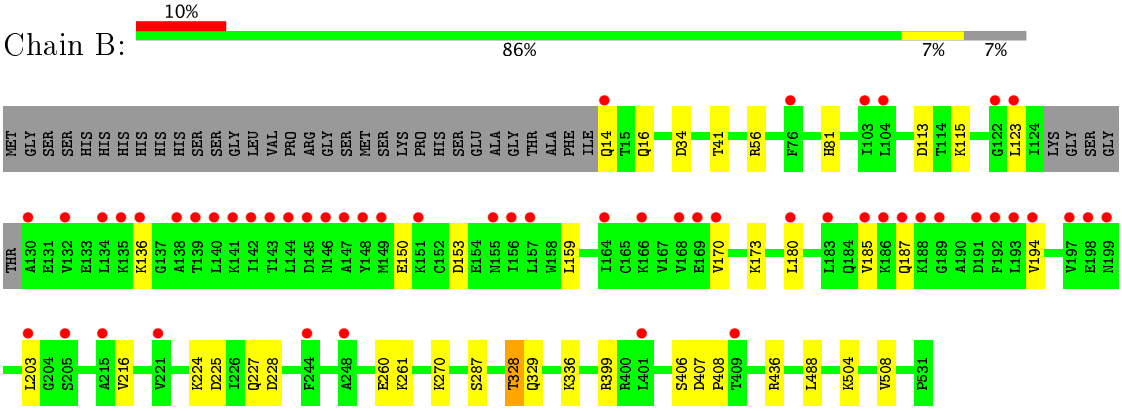
- Molecule 1: Pyruvate kinase PKM

Chain A:



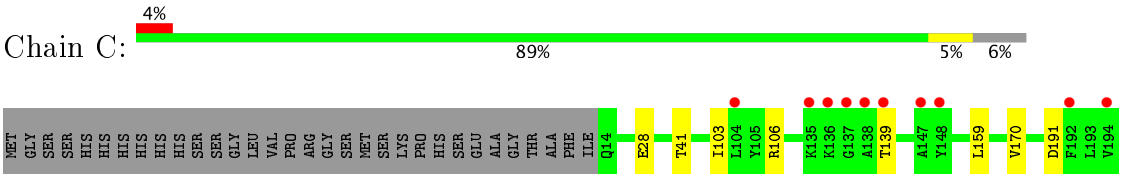
- Molecule 1: Pyruvate kinase PKM

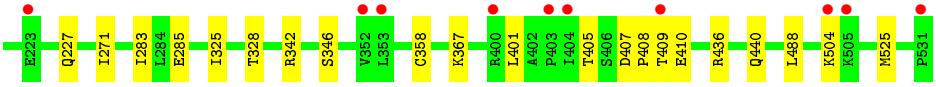
Chain B:



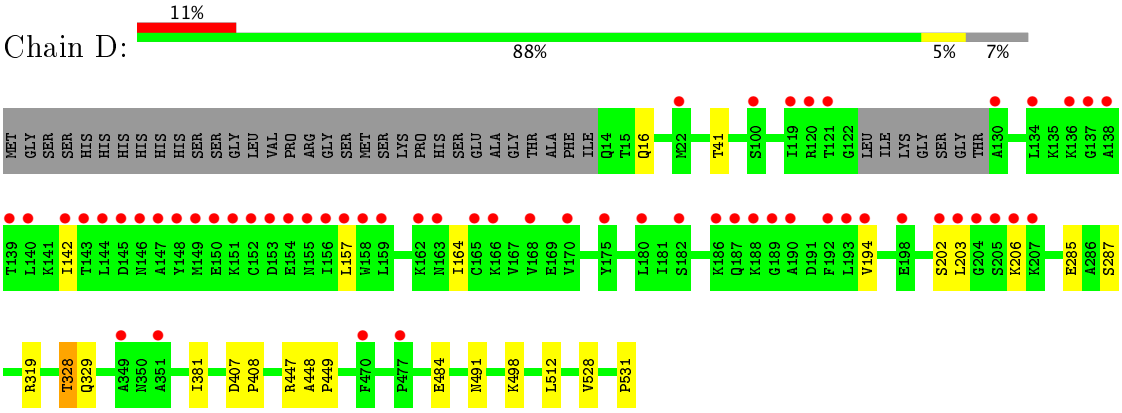
- Molecule 1: Pyruvate kinase PKM

Chain C:





- Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.47Å 151.66Å 92.08Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 40.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.10) 98.0 (40.29-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.234 , 0.274 0.233 , 0.273	Depositor DCC
R_{free} test set	12239 reflections (11.07%)	DCC
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16367	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: FBP, 7XX

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	0.48	0/3981	0.78	0/5376
1	B	0.54	0/3998	0.83	2/5399 (0.0%)
1	C	0.49	0/4029	0.80	0/5441
1	D	0.50	0/3982	0.79	1/5377 (0.0%)
All	All	0.50	0/15990	0.80	3/21593 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	381	ILE	CG1-CB-CG2	-5.54	99.22	111.40
1	B	225	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	34	ASP	CB-CG-OD2	5.41	123.17	118.30

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	3919	0	4006	4	0
1	B	3935	0	4017	8	0
1	C	3965	0	4049	7	0
1	D	3919	0	3995	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
3	C	19	0	0	0	0
3	D	19	0	0	0	0
4	A	94	0	0	0	0
4	B	120	0	0	0	0
4	C	127	0	0	0	0
4	D	132	0	0	0	0
All	All	16367	0	16107	24	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 1.

All (24) 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:81:HIS:NE2	1:B:228:ASP:OD1	2.29	0.56
1:B:115:LYS:HD3	1:B:224:LYS:HE2	1.89	0.55
1:D:498:LYS:NZ	1:D:531:PRO:O	2.40	0.55
1:C:342:ARG:HG2	1:D:329:GLN:HE21	1.74	0.52
1:C:325:ILE:HG12	1:C:358:CYS:HB2	1.93	0.51
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.92	0.50
1:A:123:LEU:HD12	1:A:150:GLU:HG2	1.95	0.49
1:B:328:THR:HG22	1:B:329:GLN:HG3	1.96	0.47
1:B:123:LEU:HD13	1:B:150:GLU:HG2	1.97	0.46
1:A:48:ILE:HB	1:A:360:MET:HG3	2.00	0.44
1:C:28:GLU:OE1	1:D:319:ARG:NH2	2.52	0.43
1:B:113:ASP:OD1	1:B:270:LYS:NZ	2.49	0.42
1:D:157:LEU:HD13	1:D:203:LEU:HD21	2.01	0.42
1:A:342:ARG:HG2	1:B:329:GLN:HE21	1.84	0.42
1:B:407:ASP:HA	1:B:408:PRO:HD3	1.83	0.42
1:C:407:ASP:OD1	1:C:409:THR:OG1	2.28	0.42
1:D:407:ASP:HA	1:D:408:PRO:HD3	1.92	0.41
1:C:407:ASP:HA	1:C:408:PRO:HD3	1.88	0.41
1:A:153:ASP:HB2	1:A:154:GLU:H	1.68	0.41
1:B:187:GLN:HB3	1:B:194:VAL:HB	2.02	0.41
1:C:410:GLU:HG2	1:C:440:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:ALA:HA	1:D:449:PRO:HD2	1.88	0.40
1:D:16:GLN:O	1:D:447:ARG:NH2	2.52	0.40
1:C:271:ILE:HD11	1:C:283:ILE:HG21	2.03	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	508/550 (92%)	495 (97%)	12 (2%)	1 (0%)	51	52
1	B	509/550 (92%)	496 (97%)	12 (2%)	1 (0%)	51	52
1	C	516/550 (94%)	504 (98%)	11 (2%)	1 (0%)	51	52
1	D	507/550 (92%)	495 (98%)	11 (2%)	1 (0%)	51	52
All	All	2040/2200 (93%)	1990 (98%)	46 (2%)	4 (0%)	51	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	C	328	THR
1	B	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	422/452 (93%)	402 (95%)	20 (5%)	30	28
1	B	423/452 (94%)	399 (94%)	24 (6%)	24	21
1	C	426/452 (94%)	409 (96%)	17 (4%)	36	36
1	D	421/452 (93%)	409 (97%)	12 (3%)	48	51
All	All	1692/1808 (94%)	1619 (96%)	73 (4%)	33	32

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	100	SER
1	A	129	THR
1	A	140	LEU
1	A	146	ASN
1	A	151	LYS
1	A	159	LEU
1	A	162	LYS
1	A	166	LYS
1	A	178	ASP
1	A	223	GLU
1	A	246	ARG
1	A	278	ARG
1	A	339	ARG
1	A	400	ARG
1	A	436	ARG
1	A	453	VAL
1	A	500	ARG
1	A	504	LYS
1	A	512	LEU
1	B	14	GLN
1	B	16	GLN
1	B	41	THR
1	B	56	ARG
1	B	136	LYS
1	B	153	ASP
1	B	159	LEU
1	B	170	VAL
1	B	173	LYS
1	B	180	LEU
1	B	185	VAL

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Mol	Chain	Res	Type
1	B	203	LEU
1	B	216	VAL
1	B	227	GLN
1	B	260	GLU
1	B	261	LYS
1	B	287	SER
1	B	336	LYS
1	B	399	ARG
1	B	406	SER
1	B	436	ARG
1	B	488	LEU
1	B	504	LYS
1	B	508	VAL
1	C	41	THR
1	C	103	ILE
1	C	106	ARG
1	C	139	THR
1	C	159	LEU
1	C	170	VAL
1	C	191	ASP
1	C	227	GLN
1	C	285	GLU
1	C	346	SER
1	C	367	LYS
1	C	401	LEU
1	C	405	THR
1	C	436	ARG
1	C	488	LEU
1	C	504	LYS
1	C	525	MET
1	D	41	THR
1	D	142	ILE
1	D	164	ILE
1	D	194	VAL
1	D	202	SER
1	D	206	LYS
1	D	285	GLU
1	D	287	SER
1	D	484	GLU
1	D	491	ASN
1	D	512	LEU
1	D	528	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	329	GLN
1	D	329	GLN
1	D	440	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 carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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	FBP	A	601	-	18,20,20	0.64	0	23,32,32	0.99	2 (8%)
3	7XX	A	602	-	17,20,20	1.03	2 (11%)	22,29,29	3.12	10 (45%)
2	FBP	B	601	-	18,20,20	0.65	0	23,32,32	1.05	1 (4%)
3	7XX	B	602	-	17,20,20	1.07	1 (5%)	22,29,29	3.06	10 (45%)
2	FBP	C	601	-	18,20,20	0.70	0	23,32,32	0.97	0
3	7XX	C	602	-	17,20,20	1.04	2 (11%)	22,29,29	3.19	9 (40%)
2	FBP	D	601	-	18,20,20	0.79	0	23,32,32	1.03	1 (4%)
3	7XX	D	602	-	17,20,20	1.05	2 (11%)	22,29,29	2.70	7 (31%)

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
2	FBP	A	601	-	-	0/13/32/32	0/1/1/1
3	7XX	A	602	-	-	0/4/12/12	0/2/2/2
2	FBP	B	601	-	-	0/13/32/32	0/1/1/1
3	7XX	B	602	-	-	0/4/12/12	0/2/2/2
2	FBP	C	601	-	-	0/13/32/32	0/1/1/1
3	7XX	C	602	-	-	0/4/12/12	0/2/2/2
2	FBP	D	601	-	-	0/13/32/32	0/1/1/1
3	7XX	D	602	-	-	0/4/12/12	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602	7XX	C7-C11	-2.31	1.45	1.49
3	C	602	7XX	C7-C11	-2.31	1.45	1.49
3	A	602	7XX	C7-C11	-2.27	1.45	1.49
3	A	602	7XX	C12-N15	2.03	1.36	1.33
3	C	602	7XX	C12-N15	2.13	1.37	1.33
3	B	602	7XX	C12-N15	2.43	1.37	1.33
3	D	602	7XX	C12-N15	2.64	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	7XX	C10-C12-N15	-5.47	110.40	116.30
3	C	602	7XX	C10-C12-N15	-5.27	110.62	116.30
3	B	602	7XX	C10-C12-N15	-5.04	110.87	116.30
3	D	602	7XX	C10-C12-N15	-4.35	111.61	116.30
3	B	602	7XX	C6-C9-C8	-4.02	117.32	120.19
3	B	602	7XX	C13-N14-C5	-3.07	119.17	124.90
3	C	602	7XX	C13-N14-C5	-3.01	119.28	124.90
3	A	602	7XX	C13-N14-C5	-2.98	119.34	124.90
3	B	602	7XX	O16-C11-C6	-2.84	114.77	119.82
3	D	602	7XX	C13-N14-C5	-2.83	119.62	124.90
3	C	602	7XX	O16-C11-C6	-2.56	115.27	119.82
3	C	602	7XX	C6-C9-C8	-2.35	118.51	120.19
3	A	602	7XX	O16-C11-C6	-2.19	115.91	119.82
2	A	601	FBP	O3P-P1-O1	-2.12	101.08	106.73
3	A	602	7XX	C6-C9-C8	-2.12	118.68	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	602	7XX	O17-C12-N15	-2.03	119.70	122.58
2	B	601	FBP	O1-P1-O1P	-2.02	100.82	106.47
3	A	602	7XX	C1-C2-C6	2.09	123.79	119.83
3	B	602	7XX	C1-C2-C6	2.11	123.84	119.83
3	D	602	7XX	C1-C2-C6	2.24	124.09	119.83
2	D	601	FBP	O6P-P2-O5P	2.30	116.90	107.61
2	A	601	FBP	O3P-P1-O2P	2.32	116.97	107.61
3	A	602	7XX	C3-C8-C9	2.40	123.32	120.58
3	C	602	7XX	C6-C9-CL2	2.52	122.41	119.71
3	D	602	7XX	C4-C7-C11	2.66	133.49	125.34
3	B	602	7XX	C3-C8-C9	2.75	123.72	120.58
3	C	602	7XX	C4-C7-C11	2.85	134.05	125.34
3	B	602	7XX	C4-C7-C11	2.89	134.18	125.34
3	A	602	7XX	C4-C7-C11	3.02	134.59	125.34
3	D	602	7XX	C6-C11-C7	3.09	124.69	119.47
3	D	602	7XX	C6-C9-CL2	3.17	123.12	119.71
3	B	602	7XX	C6-C11-C7	3.24	124.95	119.47
3	A	602	7XX	C6-C11-C7	3.47	125.33	119.47
3	B	602	7XX	C6-C9-CL2	3.57	123.54	119.71
3	A	602	7XX	C6-C9-CL2	3.69	123.68	119.71
3	C	602	7XX	C6-C11-C7	4.13	126.45	119.47
3	D	602	7XX	O17-C12-C10	8.74	127.54	119.60
3	B	602	7XX	O17-C12-C10	9.62	128.34	119.60
3	A	602	7XX	O17-C12-C10	10.33	128.99	119.60
3	C	602	7XX	O17-C12-C10	11.09	129.68	119.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	512/550 (93%)	0.97	79 (15%) 2 3	19, 42, 95, 108	0
1	B	513/550 (93%)	0.69	54 (10%) 7 9	22, 37, 82, 103	1 (0%)
1	C	518/550 (94%)	0.36	20 (3%) 40 47	23, 36, 55, 69	0
1	D	511/550 (92%)	0.69	58 (11%) 6 7	24, 36, 80, 97	0
All	All	2054/2200 (93%)	0.68	211 (10%) 7 9	19, 38, 81, 108	1 (0%)

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	LEU	9.5
1	D	155	ASN	7.8
1	A	144	LEU	7.8
1	A	126	GLY	7.6
1	A	213	GLY	7.5
1	A	170	VAL	7.2
1	A	148	TYR	7.1
1	B	147	ALA	7.1
1	D	192	PHE	6.8
1	B	156	ILE	6.6
1	A	159	LEU	6.5
1	B	148	TYR	6.4
1	D	148	TYR	6.3
1	A	151	LYS	6.1
1	D	190	ALA	5.9
1	B	142	ILE	5.8
1	A	152	CYS	5.8
1	B	140	LEU	5.7
1	B	143	THR	5.7
1	D	207	LYS	5.5
1	D	156	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	147	ALA	5.3
1	D	204	GLY	5.2
1	A	168	VAL	5.2
1	A	194	VAL	5.0
1	B	192	PHE	4.9
1	D	157	LEU	4.9
1	B	185	VAL	4.7
1	B	193	LEU	4.7
1	D	138	ALA	4.7
1	A	203	LEU	4.6
1	D	203	LEU	4.5
1	A	184	GLN	4.5
1	A	166	LYS	4.5
1	D	137	GLY	4.4
1	A	167	VAL	4.4
1	A	165	CYS	4.3
1	A	196	GLU	4.3
1	A	158	TRP	4.3
1	A	141	LYS	4.2
1	D	158	TRP	4.2
1	D	180	LEU	4.2
1	A	172	SER	4.2
1	D	168	VAL	4.1
1	A	164	ILE	4.1
1	D	166	LYS	4.1
1	A	139	THR	4.0
1	D	193	LEU	4.0
1	B	144	LEU	4.0
1	B	205	SER	4.0
1	B	170	VAL	4.0
1	D	149	MET	4.0
1	A	204	GLY	3.9
1	A	149	MET	3.9
1	B	168	VAL	3.9
1	D	142	ILE	3.9
1	A	403	PRO	3.8
1	A	138	ALA	3.8
1	A	185	VAL	3.8
1	B	139	THR	3.8
1	A	183	LEU	3.8
1	D	151	LYS	3.7
1	B	194	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	150	GLU	3.7
1	D	189	GLY	3.7
1	A	186	LYS	3.7
1	D	163	ASN	3.7
1	A	157	LEU	3.7
1	B	145	ASP	3.7
1	A	136	LYS	3.6
1	A	132	VAL	3.6
1	D	154	GLU	3.6
1	B	132	VAL	3.6
1	D	205	SER	3.6
1	A	351	ALA	3.6
1	A	215	ALA	3.5
1	A	156	ILE	3.5
1	D	153	ASP	3.5
1	A	128	GLY	3.5
1	A	214	ALA	3.5
1	A	122	GLY	3.5
1	B	151	LYS	3.5
1	D	121	THR	3.5
1	D	143	THR	3.4
1	A	147	ALA	3.4
1	A	123	LEU	3.4
1	A	195	THR	3.4
1	A	406	SER	3.3
1	A	169	GLU	3.3
1	A	324	VAL	3.3
1	B	183	LEU	3.3
1	D	139	THR	3.3
1	A	401	LEU	3.3
1	A	470	PHE	3.2
1	A	40	ILE	3.2
1	B	122	GLY	3.2
1	B	149	MET	3.2
1	B	197	VAL	3.2
1	A	146	ASN	3.1
1	D	170	VAL	3.1
1	B	130	ALA	3.1
1	A	145	ASP	3.1
1	D	165	CYS	3.1
1	D	140	LEU	3.0
1	A	143	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	217	ASP	3.0
1	B	188	LYS	3.0
1	B	123	LEU	3.0
1	D	194	VAL	3.0
1	C	135	LYS	3.0
1	A	153	ASP	2.9
1	D	130	ALA	2.9
1	B	134	LEU	2.9
1	B	157	LEU	2.9
1	A	103	ILE	2.9
1	C	148	TYR	2.9
1	B	191	ASP	2.9
1	D	146	ASN	2.9
1	D	186	LYS	2.9
1	A	480	GLU	2.9
1	A	41	THR	2.9
1	B	135	LYS	2.8
1	C	403	PRO	2.8
1	D	144	LEU	2.8
1	B	141	LYS	2.8
1	C	192	PHE	2.8
1	A	129	THR	2.8
1	D	145	ASP	2.8
1	D	134	LEU	2.7
1	D	198	GLU	2.7
1	D	119	ILE	2.7
1	B	198	GLU	2.7
1	D	206	LYS	2.7
1	C	194	VAL	2.7
1	D	162	LYS	2.7
1	B	187	GLN	2.7
1	B	244	PHE	2.7
1	D	136	LYS	2.7
1	C	531	PRO	2.6
1	D	477	PRO	2.6
1	D	470	PHE	2.6
1	D	120	ARG	2.6
1	A	206	LYS	2.6
1	B	155	ASN	2.6
1	A	134	LEU	2.6
1	C	353	LEU	2.5
1	D	152	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	404	ILE	2.5
1	B	221	VAL	2.5
1	C	139	THR	2.5
1	A	162	LYS	2.5
1	C	147	ALA	2.5
1	B	203	LEU	2.5
1	C	138	ALA	2.5
1	C	137	GLY	2.5
1	A	130	ALA	2.5
1	C	223	GLU	2.4
1	A	127	SER	2.4
1	A	197	VAL	2.4
1	B	199	ASN	2.4
1	B	136	LYS	2.4
1	B	76	PHE	2.4
1	B	186	LYS	2.4
1	A	216	VAL	2.4
1	D	159	LEU	2.3
1	A	178	ASP	2.3
1	A	173	LYS	2.3
1	D	22	MET	2.3
1	D	188	LYS	2.3
1	A	478	VAL	2.3
1	B	169	GLU	2.3
1	A	475	LYS	2.3
1	B	166	LYS	2.3
1	D	182	SER	2.3
1	A	394	LEU	2.3
1	A	314	ILE	2.3
1	B	164	ILE	2.3
1	A	356	ALA	2.2
1	D	349	ALA	2.2
1	B	146	ASN	2.2
1	B	104	LEU	2.2
1	B	401	LEU	2.2
1	C	104	LEU	2.2
1	A	199	ASN	2.2
1	D	202	SER	2.2
1	B	14	GLN	2.2
1	A	142	ILE	2.2
1	C	352	VAL	2.2
1	C	400	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	504	LYS	2.2
1	B	215	ALA	2.2
1	B	189	GLY	2.2
1	B	248	ALA	2.2
1	A	202	SER	2.2
1	A	124	ILE	2.1
1	A	174	ILE	2.1
1	B	103	ILE	2.1
1	C	136	LYS	2.1
1	A	492	PHE	2.1
1	A	163	ASN	2.1
1	C	409	THR	2.1
1	A	352	VAL	2.0
1	B	138	ALA	2.0
1	D	175	TYR	2.0
1	A	101	ASP	2.0
1	B	180	LEU	2.0
1	D	100	SER	2.0
1	D	187	GLN	2.0
1	B	409	THR	2.0
1	D	351	ALA	2.0
1	C	505	LYS	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

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
2	FBP	D	601	20/20	0.97	0.14	0.54	31,32,39,40	0
2	FBP	B	601	20/20	0.95	0.14	0.48	33,39,44,45	0
2	FBP	C	601	20/20	0.95	0.17	0.48	39,44,49,49	0
3	7XX	A	602	19/19	0.96	0.16	0.34	37,41,48,52	0
3	7XX	D	602	19/19	0.92	0.14	-0.11	37,39,41,43	0
3	7XX	B	602	19/19	0.96	0.13	-0.70	35,38,39,40	0
3	7XX	C	602	19/19	0.94	0.13	-0.77	35,40,44,45	0
2	FBP	A	601	20/20	0.95	0.12	-0.88	41,46,52,53	0

6.5 Other polymers (i)

There are no such residues in this entry.