



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2018 – 01:45 PM EST

PDB ID : 5X0I
Title : Crystal structure of PKM2 R399E mutant complexed with FBP and serine
Authors : Wang, W.C.; Chen, T.J.
Deposited on : 2017-01-20
Resolution : 2.64 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-20030736
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-20030736

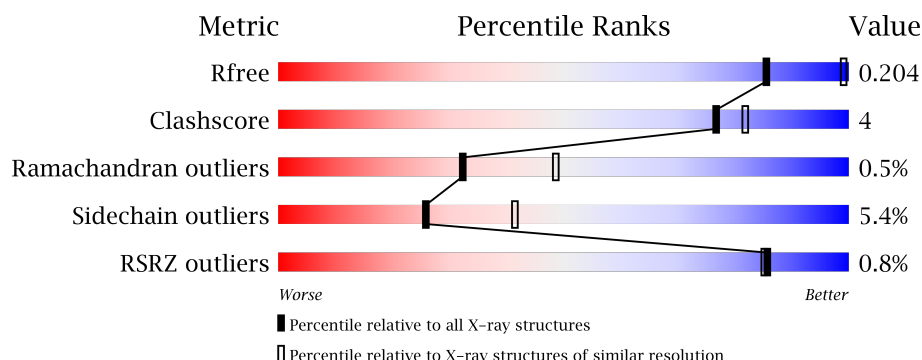
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1044 (2.66-2.62)
Clashscore	112137	1092 (2.66-2.62)
Ramachandran outliers	110173	1077 (2.66-2.62)
Sidechain outliers	110143	1077 (2.66-2.62)
RSRZ outliers	101464	1047 (2.66-2.62)

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	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 82%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 1% 82% 12% 6% </div> </div>
1	B	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 79%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 1% 79% 13% 7% </div> </div>
1	C	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 81%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 1% 81% 12% 6% </div> </div>
1	D	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 81%, yellow 11%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> 81% 11% 6% </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SER	B	602	-	-	-	X
3	SER	D	602	-	-	-	X
4	PYR	D	603	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16023 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	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			
1	B	515	Total	C	N	O	S	0	0	0
			3949	2484	698	742	25			
1	C	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			
1	D	518	Total	C	N	O	S	0	0	0
			3963	2491	701	746	25			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P14618
A	-18	GLY	-	expression tag	UNP P14618
A	-17	SER	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	HIS	-	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	SER	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	GLY	-	expression tag	UNP P14618
A	-6	LEU	-	expression tag	UNP P14618
A	-5	VAL	-	expression tag	UNP P14618
A	-4	PRO	-	expression tag	UNP P14618
A	-3	ARG	-	expression tag	UNP P14618
A	-2	GLY	-	expression tag	UNP P14618
A	-1	SER	-	expression tag	UNP P14618
A	0	HIS	-	expression tag	UNP P14618
A	399	GLU	ARG	engineered mutation	UNP P14618

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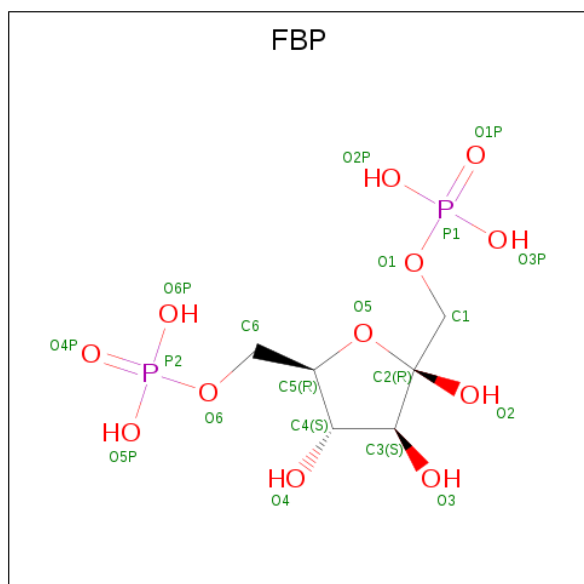
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP P14618
B	-18	GLY	-	expression tag	UNP P14618
B	-17	SER	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	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	SER	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	GLY	-	expression tag	UNP P14618
B	-6	LEU	-	expression tag	UNP P14618
B	-5	VAL	-	expression tag	UNP P14618
B	-4	PRO	-	expression tag	UNP P14618
B	-3	ARG	-	expression tag	UNP P14618
B	-2	GLY	-	expression tag	UNP P14618
B	-1	SER	-	expression tag	UNP P14618
B	0	HIS	-	expression tag	UNP P14618
B	399	GLU	ARG	engineered mutation	UNP P14618
C	-19	MET	-	expression tag	UNP P14618
C	-18	GLY	-	expression tag	UNP P14618
C	-17	SER	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	HIS	-	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	SER	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	GLY	-	expression tag	UNP P14618
C	-6	LEU	-	expression tag	UNP P14618
C	-5	VAL	-	expression tag	UNP P14618
C	-4	PRO	-	expression tag	UNP P14618
C	-3	ARG	-	expression tag	UNP P14618
C	-2	GLY	-	expression tag	UNP P14618
C	-1	SER	-	expression tag	UNP P14618
C	0	HIS	-	expression tag	UNP P14618
C	399	GLU	ARG	engineered mutation	UNP P14618

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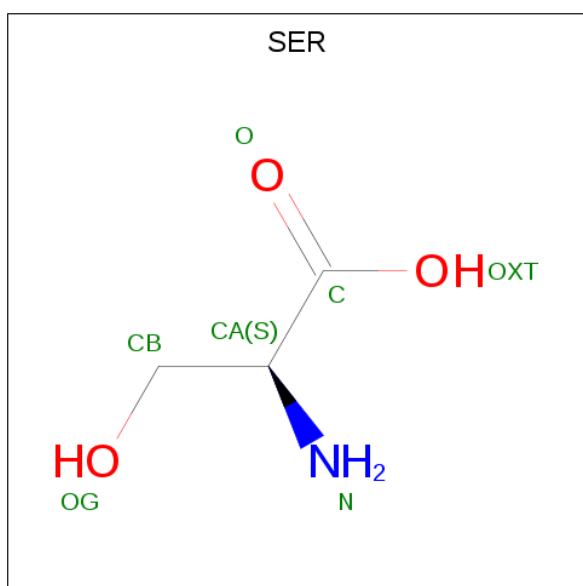
Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP P14618
D	-18	GLY	-	expression tag	UNP P14618
D	-17	SER	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	SER	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	GLY	-	expression tag	UNP P14618
D	-6	LEU	-	expression tag	UNP P14618
D	-5	VAL	-	expression tag	UNP P14618
D	-4	PRO	-	expression tag	UNP P14618
D	-3	ARG	-	expression tag	UNP P14618
D	-2	GLY	-	expression tag	UNP P14618
D	-1	SER	-	expression tag	UNP P14618
D	0	HIS	-	expression tag	UNP P14618
D	399	GLU	ARG	engineered mutation	UNP P14618

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



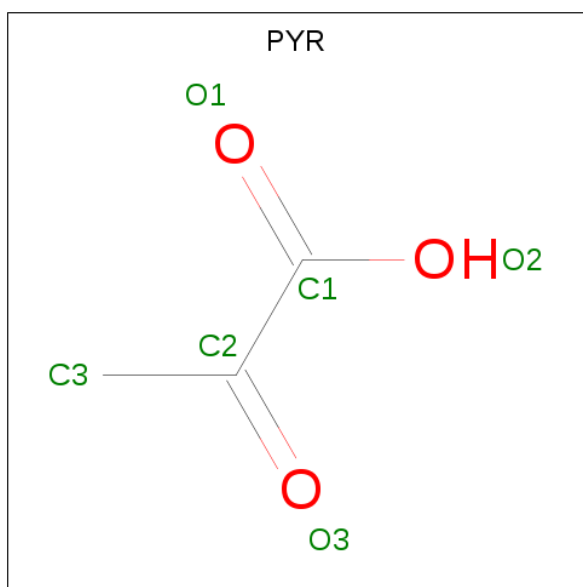
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	3	1	3		
3	B	1	Total	C	N	O	0	0
			7	3	1	3		
3	C	1	Total	C	N	O	0	0
			7	3	1	3		
3	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	K	0	0
			1	1		

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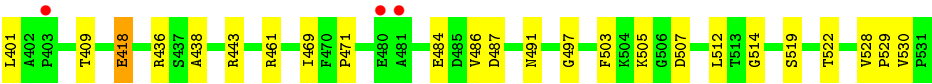
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0

- Molecule 7 is water.

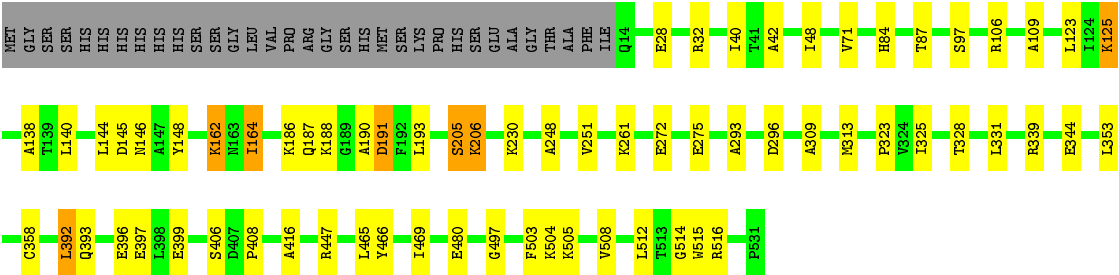
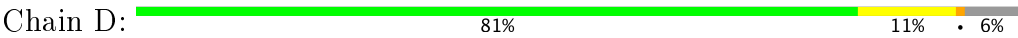
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	13	Total O 13 13	0	0
7	B	13	Total O 13 13	0	0
7	C	9	Total O 9 9	0	0
7	D	10	Total O 10 10	0	0

- Molecule 1: Pyruvate kinase PKM





● 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	116.60Å 137.88Å 149.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.64 29.68 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.64) 100.0 (29.68-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.180 , 0.218 0.185 , 0.204	Depositor DCC
R_{free} test set	3616 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16023	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: K, MG, FBP, PYR

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	0.87	0/4027	0.76	3/5439 (0.1%)
1	B	0.84	0/4012	0.74	2/5418 (0.0%)
1	C	0.81	0/4027	0.73	0/5439
1	D	0.82	1/4027 (0.0%)	0.73	3/5439 (0.1%)
All	All	0.83	1/16093 (0.0%)	0.74	8/21735 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	399	GLU	CG-CD	5.76	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	106	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	180	LEU	CA-CB-CG	6.26	129.69	115.30
1	D	447	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	106	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	319	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	D	106	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	526	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	GLY	Peptide

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	3963	0	4041	30	0
1	B	3949	0	4029	35	0
1	C	3963	0	4041	28	0
1	D	3963	0	4041	29	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	1	0
2	D	20	0	10	1	0
3	A	7	0	4	0	0
3	B	7	0	4	1	0
3	C	7	0	4	0	0
3	D	7	0	4	0	0
4	A	6	0	3	0	0
4	B	6	0	3	0	0
4	C	6	0	3	0	0
4	D	6	0	3	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	13	0	0	0	0
7	B	13	0	0	0	0
7	C	9	0	0	0	0
7	D	10	0	0	0	0
All	All	16023	0	16220	114	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 (114) 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:A:136:LYS:HG3	1:A:198:GLU:O	1.89	0.72
1:C:106:ARG:NH2	1:C:471:PRO:O	2.24	0.71
1:A:133:GLU:HG2	1:A:133:GLU:O	1.92	0.68
1:B:412:THR:HG22	1:B:512:LEU:HD21	1.74	0.68
1:C:218:LEU:O	1:C:219:PRO:C	2.37	0.62
1:D:123:LEU:HA	1:D:205:SER:HB3	1.82	0.61
1:D:515:TRP:CE3	1:D:516:ARG:HG2	2.35	0.61
1:D:323:PRO:HB3	1:D:465:LEU:O	2.00	0.60
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.84	0.59
1:B:143:THR:HA	1:B:191:ASP:O	2.02	0.59
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.87	0.57
1:D:515:TRP:CD2	1:D:516:ARG:HG2	2.40	0.56
1:C:393:GLN:O	1:C:397:GLU:HG3	2.06	0.56
1:A:243:SER:HA	1:A:270:LYS:HD3	1.89	0.55
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.42	0.55
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.42	0.54
1:A:370:TYR:N	1:A:371:PRO:CD	2.71	0.54
1:C:238:ASP:OD1	1:C:461:ARG:NE	2.40	0.54
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.90	0.52
1:B:92:ARG:O	1:B:96:GLU:HG2	2.10	0.52
1:A:334:MET:HA	1:A:337:LYS:O	2.11	0.51
1:A:50:THR:HG22	1:A:366:ALA:HB2	1.91	0.51
1:D:393:GLN:O	1:D:397:GLU:HG3	2.11	0.51
1:B:323:PRO:HB3	1:B:465:LEU:O	2.12	0.50
1:D:331:LEU:HD23	1:D:344:GLU:HB3	1.92	0.50
1:C:165:CYS:O	1:C:188:LYS:CE	2.60	0.50
1:D:28:GLU:O	1:D:32:ARG:HG3	2.11	0.50
1:C:311:LYS:HE3	1:D:353:LEU:CD1	2.41	0.50
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.94	0.50
1:D:514:GLY:HA3	2:D:601:FBP:O3	2.11	0.50
1:B:82:GLU:OE2	1:B:82:GLU:HA	2.11	0.50
1:D:145:ASP:HB3	1:D:148:TYR:HD2	1.77	0.49
1:C:321:GLY:HA2	1:C:443:ARG:HG2	1.94	0.49
1:A:331:LEU:HD23	1:A:344:GLU:HB3	1.95	0.49
1:B:516:ARG:HB2	1:B:517:PRO:CD	2.43	0.48
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.96	0.48
1:B:175:TYR:HE2	1:B:212:PRO:HG3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.96	0.47
1:A:36:ASP:O	1:A:38:PRO:HD3	2.15	0.47
1:D:309:ALA:HB1	1:D:313:MET:HE2	1.97	0.47
1:C:288:ASP:O	1:C:323:PRO:HD2	2.14	0.47
1:A:25:THR:HB	1:B:397:GLU:HG2	1.96	0.47
1:D:205:SER:O	1:D:206:LYS:HB2	2.15	0.47
1:D:272:GLU:HB3	1:D:293:ALA:HB3	1.96	0.47
1:A:443:ARG:HG2	1:A:443:ARG:O	2.15	0.47
1:C:528:VAL:HG12	1:C:529:PRO:O	2.16	0.46
1:A:397:GLU:CD	1:B:25:THR:HB	2.35	0.46
1:C:321:GLY:HA3	1:C:443:ARG:HD3	1.98	0.46
1:B:99:ALA:O	1:B:100:SER:C	2.54	0.46
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.98	0.46
1:D:325:ILE:HG12	1:D:358:CYS:HB2	1.98	0.46
1:B:400:ARG:CZ	1:D:392:LEU:HD21	2.46	0.45
1:A:418:GLU:HG2	1:C:418:GLU:OE1	2.17	0.45
1:D:144:LEU:HD13	1:D:162:LYS:O	2.17	0.45
1:A:25:THR:HB	1:B:397:GLU:CG	2.46	0.45
1:A:416:ALA:HB2	1:A:512:LEU:HD11	1.98	0.45
1:C:127:SER:HB3	1:C:130:ALA:HB2	1.98	0.45
1:B:516:ARG:HB2	1:B:517:PRO:HD2	1.98	0.45
1:D:416:ALA:HB2	1:D:512:LEU:HD11	1.99	0.45
1:B:36:ASP:O	1:B:38:PRO:HD3	2.17	0.44
1:C:409:THR:HG23	1:C:522:THR:HB	1.99	0.44
1:D:40:ILE:HD12	1:D:42:ALA:HB3	1.99	0.44
1:A:337:LYS:HD2	1:B:180:LEU:HD22	1.98	0.44
1:B:188:LYS:HG2	1:B:189:GLY:H	1.82	0.44
1:D:190:ALA:O	1:D:191:ASP:CB	2.65	0.44
1:C:438:ALA:HB1	1:C:469:ILE:HD13	1.99	0.44
1:C:321:GLY:CA	1:C:443:ARG:HG2	2.48	0.44
1:B:141:LYS:HB3	1:B:156:ILE:HD13	1.99	0.43
1:B:228:ASP:O	1:B:231:PHE:HB3	2.18	0.43
1:C:325:ILE:HG12	1:C:358:CYS:HB2	2.01	0.43
1:C:514:GLY:HA3	2:C:601:FBP:O3	2.17	0.43
1:D:296:ASP:OD2	4:D:603:PYR:O1	2.35	0.43
1:A:226:ILE:O	1:A:227:GLN:C	2.54	0.43
1:B:407:ASP:HA	1:B:408:PRO:HD2	1.90	0.43
1:B:325:ILE:HG12	1:B:358:CYS:HB2	2.00	0.43
1:A:136:LYS:CG	1:A:198:GLU:O	2.63	0.43
1:B:186:LYS:O	1:B:187:GLN:HG2	2.19	0.43
1:B:174:ILE:HG12	1:B:211:LEU:CD2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ALA:O	1:D:251:VAL:N	2.51	0.43
1:B:436:ARG:HG2	1:B:436:ARG:HH11	1.83	0.43
1:D:406:SER:O	1:D:408:PRO:HD3	2.19	0.43
1:C:486:VAL:O	1:C:487:ASP:C	2.57	0.43
1:D:71:VAL:HG22	1:D:109:ALA:HB3	2.00	0.43
1:B:503:PHE:CD1	1:B:530:VAL:HG21	2.53	0.42
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.53	0.42
1:A:301:ILE:HB	1:A:302:PRO:HD2	2.02	0.42
1:A:338:PRO:HB3	1:A:370:TYR:CE1	2.55	0.42
1:A:142:ILE:HA	1:A:157:LEU:O	2.20	0.42
1:D:84:HIS:O	1:D:87:THR:N	2.50	0.42
1:A:222:SER:O	1:A:226:ILE:HG13	2.19	0.42
1:D:164:ILE:HD12	1:D:193:LEU:HD11	2.02	0.42
1:B:190:ALA:O	1:B:191:ASP:CB	2.68	0.42
1:B:14:GLN:O	1:B:14:GLN:HG3	2.20	0.42
1:C:168:VAL:O	1:C:188:LYS:HE3	2.20	0.42
1:C:297:LEU:O	1:C:301:ILE:HG12	2.19	0.41
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.84	0.41
1:B:317:CYS:HB3	1:B:322:LYS:O	2.20	0.41
1:B:48:ILE:HG12	1:B:71:VAL:HB	2.00	0.41
1:C:507:ASP:O	1:C:530:VAL:HG23	2.20	0.41
1:B:178:ASP:OD1	1:B:178:ASP:N	2.53	0.41
1:B:175:TYR:CE2	1:B:212:PRO:HG3	2.55	0.41
1:A:400:ARG:NH2	1:C:22:MET:O	2.53	0.41
1:C:332:GLU:HA	1:C:332:GLU:OE1	2.20	0.41
1:B:142:ILE:O	1:B:192:PHE:HA	2.20	0.41
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.49	0.41
1:B:140:LEU:HD21	1:B:157:LEU:HD22	2.03	0.41
1:C:144:LEU:HD13	1:C:162:LYS:O	2.20	0.41
1:C:223:GLU:N	1:C:223:GLU:OE2	2.49	0.41
1:A:40:ILE:HD12	1:A:42:ALA:HB3	2.02	0.41
1:D:125:LYS:HG3	1:D:125:LYS:H	1.71	0.41
1:B:159:LEU:HD12	1:B:164:ILE:CD1	2.51	0.40
1:C:143:THR:HG21	1:C:156:ILE:HD11	2.04	0.40
1:B:43:ARG:O	3:B:602:SER:HB2	2.21	0.40
1:A:60:THR:O	1:A:64:MET:HG2	2.21	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	516/551 (94%)	493 (96%)	22 (4%)	1 (0%)	51	69
1	B	511/551 (93%)	490 (96%)	19 (4%)	2 (0%)	38	54
1	C	516/551 (94%)	494 (96%)	19 (4%)	3 (1%)	28	43
1	D	516/551 (94%)	487 (94%)	25 (5%)	4 (1%)	22	34
All	All	2059/2204 (93%)	1964 (95%)	85 (4%)	10 (0%)	32	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	D	191	ASP
1	C	125	LYS
1	D	138	ALA
1	B	191	ASP
1	C	126	GLY
1	C	328	THR
1	D	206	LYS
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	426/453 (94%)	404 (95%)	22 (5%)	27	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	425/453 (94%)	400 (94%)	25 (6%)	23	36
1	C	426/453 (94%)	400 (94%)	26 (6%)	22	34
1	D	426/453 (94%)	406 (95%)	20 (5%)	30	48
All	All	1703/1812 (94%)	1610 (94%)	93 (6%)	26	40

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	A	125	LYS
1	A	127	SER
1	A	133	GLU
1	A	134	LEU
1	A	135	LYS
1	A	139	THR
1	A	156	ILE
1	A	180	LEU
1	A	186	LYS
1	A	191	ASP
1	A	224	LYS
1	A	234	GLU
1	A	253	GLU
1	A	272	GLU
1	A	400	ARG
1	A	414	VAL
1	A	422	LYS
1	A	424	CYS
1	A	436	ARG
1	A	498	LYS
1	A	505	LYS
1	B	37	SER
1	B	56	ARG
1	B	74	LEU
1	B	134	LEU
1	B	139	THR
1	B	156	ILE
1	B	162	LYS
1	B	172	SER
1	B	182	SER
1	B	224	LYS
1	B	230	LYS

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Mol	Chain	Res	Type
1	B	260	GLU
1	B	261	LYS
1	B	272	GLU
1	B	275	GLU
1	B	337	LYS
1	B	396	GLU
1	B	400	ARG
1	B	401	LEU
1	B	424	CYS
1	B	436	ARG
1	B	443	ARG
1	B	504	LYS
1	B	505	LYS
1	B	508	VAL
1	C	14	GLN
1	C	24	ASP
1	C	56	ARG
1	C	59	GLU
1	C	135	LYS
1	C	154	GLU
1	C	155	ASN
1	C	173	LYS
1	C	186	LYS
1	C	187	GLN
1	C	188	LYS
1	C	191	ASP
1	C	202	SER
1	C	226	ILE
1	C	256	LYS
1	C	272	GLU
1	C	288	ASP
1	C	346	SER
1	C	401	LEU
1	C	418	GLU
1	C	436	ARG
1	C	484	GLU
1	C	491	ASN
1	C	505	LYS
1	C	512	LEU
1	C	519	SER
1	D	97	SER
1	D	125	LYS

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Mol	Chain	Res	Type
1	D	140	LEU
1	D	146	ASN
1	D	162	LYS
1	D	164	ILE
1	D	186	LYS
1	D	187	GLN
1	D	188	LYS
1	D	205	SER
1	D	230	LYS
1	D	261	LYS
1	D	275	GLU
1	D	339	ARG
1	D	392	LEU
1	D	396	GLU
1	D	480	GLU
1	D	504	LYS
1	D	505	LYS
1	D	508	VAL

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

Mol	Chain	Res	Type
1	A	479	GLN
1	B	264	ASN
1	C	155	ASN
1	C	184	GLN
1	D	146	ASN
1	D	187	GLN
1	D	318	ASN
1	D	479	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	FBP	A	601	-	18,20,20	0.65	0	23,32,32	1.36	3 (13%)
3	SER	A	602	-	2,6,6	0.18	0	1,7,7	0.69	0
4	PYR	A	603	5	2,5,5	0.55	0	2,6,6	1.17	0
2	FBP	B	601	-	18,20,20	0.73	0	23,32,32	1.11	2 (8%)
3	SER	B	602	-	2,6,6	0.43	0	1,7,7	0.47	0
4	PYR	B	603	5	2,5,5	0.59	0	2,6,6	1.31	0
2	FBP	C	601	-	18,20,20	0.73	0	23,32,32	1.22	4 (17%)
3	SER	C	602	-	2,6,6	0.67	0	1,7,7	1.05	0
4	PYR	C	603	5	2,5,5	0.97	0	2,6,6	1.16	0
2	FBP	D	601	-	18,20,20	1.02	1 (5%)	23,32,32	1.16	3 (13%)
3	SER	D	602	-	2,6,6	0.28	0	1,7,7	0.13	0
4	PYR	D	603	5	2,5,5	0.22	0	2,6,6	2.76	1 (50%)

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	SER	A	602	-	-	0/2/6/6	0/0/0/0
4	PYR	A	603	5	-	0/0/4/4	0/0/0/0
2	FBP	B	601	-	-	0/13/32/32	0/1/1/1
3	SER	B	602	-	-	0/2/6/6	0/0/0/0
4	PYR	B	603	5	-	0/0/4/4	0/0/0/0
2	FBP	C	601	-	-	0/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SER	C	602	-	-	0/2/6/6	0/0/0/0
4	PYR	C	603	5	-	0/0/4/4	0/0/0/0
2	FBP	D	601	-	-	0/13/32/32	0/1/1/1
3	SER	D	602	-	-	0/2/6/6	0/0/0/0
4	PYR	D	603	5	-	0/0/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FBP	O5-C2	2.52	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FBP	O3P-P1-O1	-2.76	99.39	106.73
2	A	601	FBP	O5P-P2-O6	-2.64	99.70	106.73
2	B	601	FBP	O3P-P1-O1	-2.58	99.87	106.73
2	C	601	FBP	O3P-P1-O1	-2.29	100.65	106.73
2	C	601	FBP	O5-C5-C6	2.02	114.06	109.54
2	C	601	FBP	O6P-P2-O5P	2.05	115.89	107.61
2	C	601	FBP	O3P-P1-O2P	2.08	116.01	107.61
2	D	601	FBP	O3P-P1-O2P	2.21	116.53	107.61
2	D	601	FBP	O6P-P2-O5P	2.29	116.86	107.61
2	B	601	FBP	O3P-P1-O2P	2.34	117.06	107.61
2	A	601	FBP	P1-O1-C1	2.42	124.96	118.30
2	A	601	FBP	O6P-P2-O5P	3.15	120.31	107.61
4	D	603	PYR	O3-C2-C3	3.41	127.93	120.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	SER	1	0
2	C	601	FBP	1	0
2	D	601	FBP	1	0
4	D	603	PYR	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	518/551 (94%)	-0.55	3 (0%) 89 88	19, 35, 61, 102	0
1	B	515/551 (93%)	-0.50	7 (1%) 75 72	23, 35, 81, 119	0
1	C	518/551 (94%)	-0.43	7 (1%) 75 72	23, 40, 77, 108	0
1	D	518/551 (94%)	-0.39	0 100 100	23, 41, 79, 100	0
All	All	2069/2204 (93%)	-0.47	17 (0%) 86 85	19, 38, 77, 119	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	ASP	3.4
1	C	403	PRO	3.2
1	B	191	ASP	3.0
1	B	215	ALA	2.9
1	A	133	GLU	2.9
1	C	480	GLU	2.8
1	B	130	ALA	2.6
1	B	129	THR	2.5
1	C	481	ALA	2.4
1	C	128	GLY	2.4
1	B	187	GLN	2.4
1	A	404	ILE	2.4
1	C	127	SER	2.4
1	A	129	THR	2.3
1	C	126	GLY	2.2
1	B	125	LYS	2.2
1	C	191	ASP	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, 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(Å ²)	Q<0.9
3	SER	D	602	7/7	0.95	0.31	3.41	42,46,50,55	0
3	SER	B	602	7/7	0.91	0.25	2.58	39,44,47,47	0
4	PYR	D	603	6/6	0.94	0.21	2.49	40,41,45,46	0
4	PYR	A	603	6/6	0.98	0.19	1.72	36,38,38,41	0
3	SER	C	602	7/7	0.93	0.21	0.88	44,44,50,51	0
3	SER	A	602	7/7	0.92	0.18	0.81	31,37,38,39	0
4	PYR	C	603	6/6	0.96	0.17	0.55	30,34,36,38	0
4	PYR	B	603	6/6	0.97	0.17	0.48	24,25,32,35	0
6	K	A	605	1/1	0.98	0.14	0.11	44,44,44,44	0
6	K	C	605	1/1	0.92	0.13	-0.24	44,44,44,44	0
2	FBP	D	601	20/20	0.98	0.09	-0.77	20,26,31,31	0
2	FBP	B	601	20/20	0.99	0.08	-0.97	21,25,32,34	0
2	FBP	A	601	20/20	0.98	0.09	-0.98	22,28,33,36	0
2	FBP	C	601	20/20	0.98	0.10	-1.21	27,31,40,41	0
6	K	D	605	1/1	0.97	0.08	-1.36	52,52,52,52	0
6	K	B	605	1/1	0.97	0.07	-2.42	42,42,42,42	0
5	MG	C	604	1/1	0.98	0.22	-	35,35,35,35	0
5	MG	D	604	1/1	0.97	0.27	-	46,46,46,46	0
5	MG	B	604	1/1	0.96	0.24	-	33,33,33,33	0
5	MG	A	604	1/1	0.96	0.23	-	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.