WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 11:15 am GMT

PDB ID	:	6GG6
Title	:	Crystal structure of M2 PYK in complex with Serine.
Authors	:	McNae, I.W.; Yuan, M.; Walkinshaw, M.D.
Deposited on	:	2018-05-02
Resolution	:	2.96 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:

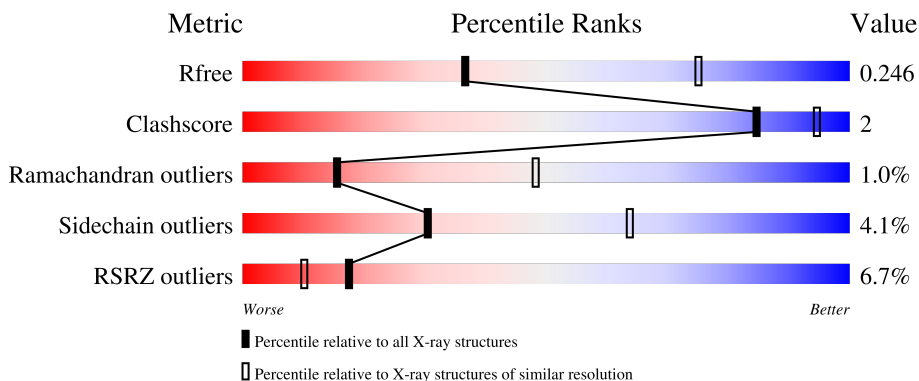|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.96 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.
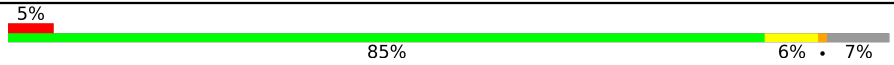
Metric	Percentile Ranks	Value
Rfree		0.246
Clashscore		2
Ramachandran outliers		1.0%
Sidechain outliers		4.1%
RSRZ outliers		6.7%

Worse *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	4% / 85% / 6% · 7%
1	B	551	8% / 85% / 7% · 7%
1	C	551	5% / 85% / 7% · 7%
1	D	551	10% / 85% / 6% · 7%
1	E	551	6% / 85% / 7% · 7%

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Mol	Chain	Length	Quality of chain
1	F	551	5% 85% 6% · 7%
1	G	551	6% 85% 6% · 7%
1	H	551	6% 85% 7% · 7%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 31408 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	510	Total	C	N	O	S	0	1	0
			3912	2460	694	733	25			
1	B	510	Total	C	N	O	S	0	1	0
			3912	2460	694	733	25			
1	C	510	Total	C	N	O	S	0	1	0
			3912	2460	694	733	25			
1	D	510	Total	C	N	O	S	0	1	0
			3912	2460	694	733	25			
1	E	510	Total	C	N	O	S	0	1	0
			3912	2460	694	733	25			
1	F	510	Total	C	N	O	S	0	1	0
			3912	2460	694	733	25			
1	G	510	Total	C	N	O	S	0	1	0
			3912	2460	694	733	25			
1	H	510	Total	C	N	O	S	0	1	0
			3912	2460	694	733	25			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	-19	MET	-	initiating methionine	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
C	-19	MET	-	initiating methionine	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	-19	MET	-	initiating methionine	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
E	-19	MET	-	initiating methionine	UNP P14618
E	-18	GLY	-	expression tag	UNP P14618
E	-17	SER	-	expression tag	UNP P14618
E	-16	SER	-	expression tag	UNP P14618
E	-15	HIS	-	expression tag	UNP P14618
E	-14	HIS	-	expression tag	UNP P14618
E	-13	HIS	-	expression tag	UNP P14618
E	-12	HIS	-	expression tag	UNP P14618
E	-11	HIS	-	expression tag	UNP P14618
E	-10	HIS	-	expression tag	UNP P14618
E	-9	SER	-	expression tag	UNP P14618
E	-8	SER	-	expression tag	UNP P14618
E	-7	GLY	-	expression tag	UNP P14618
E	-6	LEU	-	expression tag	UNP P14618
E	-5	VAL	-	expression tag	UNP P14618
E	-4	PRO	-	expression tag	UNP P14618
E	-3	ARG	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P14618
E	-1	SER	-	expression tag	UNP P14618
E	0	HIS	-	expression tag	UNP P14618
F	-19	MET	-	initiating methionine	UNP P14618
F	-18	GLY	-	expression tag	UNP P14618
F	-17	SER	-	expression tag	UNP P14618
F	-16	SER	-	expression tag	UNP P14618
F	-15	HIS	-	expression tag	UNP P14618
F	-14	HIS	-	expression tag	UNP P14618
F	-13	HIS	-	expression tag	UNP P14618
F	-12	HIS	-	expression tag	UNP P14618
F	-11	HIS	-	expression tag	UNP P14618
F	-10	HIS	-	expression tag	UNP P14618
F	-9	SER	-	expression tag	UNP P14618
F	-8	SER	-	expression tag	UNP P14618
F	-7	GLY	-	expression tag	UNP P14618
F	-6	LEU	-	expression tag	UNP P14618
F	-5	VAL	-	expression tag	UNP P14618
F	-4	PRO	-	expression tag	UNP P14618
F	-3	ARG	-	expression tag	UNP P14618
F	-2	GLY	-	expression tag	UNP P14618
F	-1	SER	-	expression tag	UNP P14618
F	0	HIS	-	expression tag	UNP P14618
G	-19	MET	-	initiating methionine	UNP P14618
G	-18	GLY	-	expression tag	UNP P14618
G	-17	SER	-	expression tag	UNP P14618
G	-16	SER	-	expression tag	UNP P14618
G	-15	HIS	-	expression tag	UNP P14618
G	-14	HIS	-	expression tag	UNP P14618
G	-13	HIS	-	expression tag	UNP P14618
G	-12	HIS	-	expression tag	UNP P14618
G	-11	HIS	-	expression tag	UNP P14618
G	-10	HIS	-	expression tag	UNP P14618
G	-9	SER	-	expression tag	UNP P14618
G	-8	SER	-	expression tag	UNP P14618
G	-7	GLY	-	expression tag	UNP P14618
G	-6	LEU	-	expression tag	UNP P14618
G	-5	VAL	-	expression tag	UNP P14618
G	-4	PRO	-	expression tag	UNP P14618
G	-3	ARG	-	expression tag	UNP P14618
G	-2	GLY	-	expression tag	UNP P14618
G	-1	SER	-	expression tag	UNP P14618

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

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	K 1	0	0
2	B	1	Total 1	K 1	0	0
2	C	1	Total 1	K 1	0	0
2	D	1	Total 1	K 1	0	0
2	E	1	Total 1	K 1	0	0
2	F	1	Total 1	K 1	0	0
2	G	1	Total 1	K 1	0	0
2	H	1	Total 1	K 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0
3	H	1	Total 1	Mg 1	0	0

- Molecule 4 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).
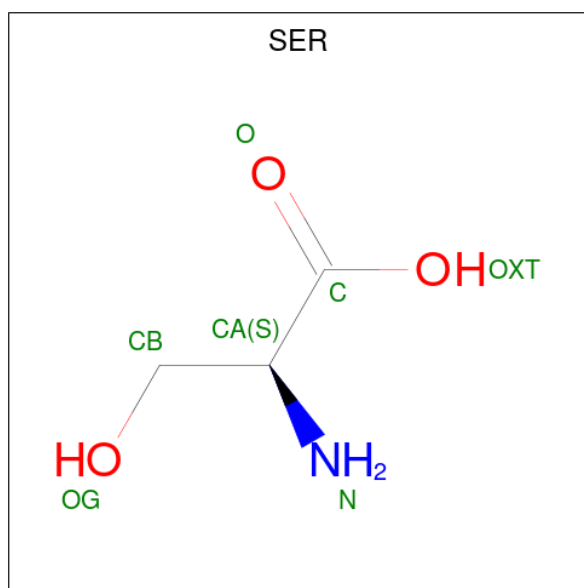
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 7	C 3	N 1	O 3	0	0
4	B	1	Total 7	C 3	N 1	O 3	0	0
4	C	1	Total 7	C 3	N 1	O 3	0	0
4	D	1	Total 7	C 3	N 1	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total 7	C 3	N 1	O 3	0	0
4	F	1	Total 7	C 3	N 1	O 3	0	0
4	G	1	Total 7	C 3	N 1	O 3	0	0
4	H	1	Total 7	C 3	N 1	O 3	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
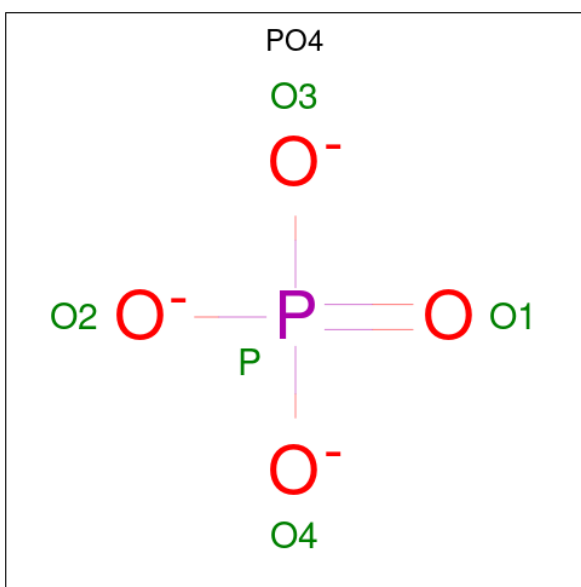
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0
5	B	1	Total 5	O 4	P 1	0	0
5	C	1	Total 5	O 4	P 1	0	0
5	D	1	Total 5	O 4	P 1	0	0
5	E	1	Total 5	O 4	P 1	0	0
5	F	1	Total 5	O 4	P 1	0	0
5	G	1	Total 5	O 4	P 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
5	H	1	5	4	1	0	0

3 Residue-property plots (i)

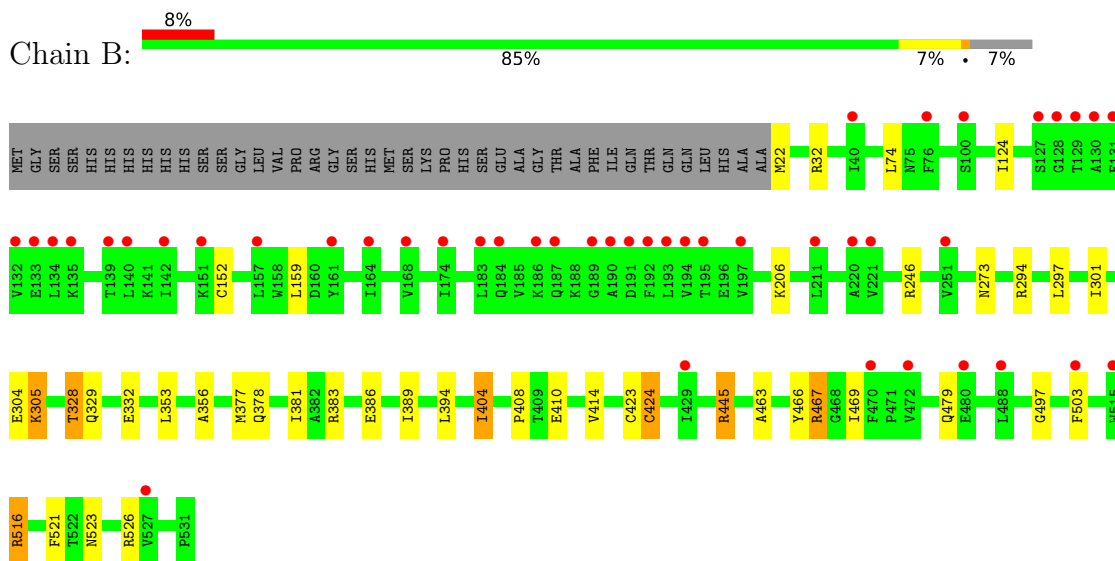These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
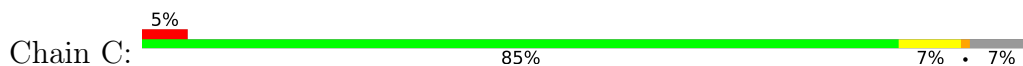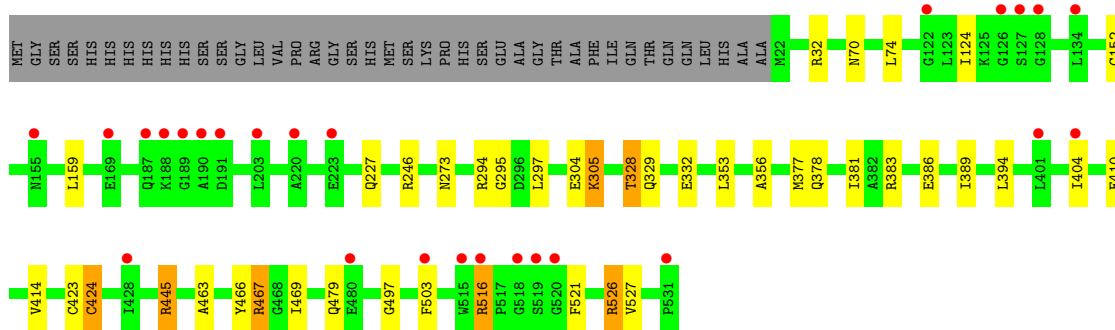
- Molecule 1: Pyruvate kinase PKM

Chain A:

- Molecule 1: Pyruvate kinase PKM

Chain B:

- Molecule 1: Pyruvate kinase PKM

Chain C:

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS PRO HIS SER GLU ALA GLY THR ALA PHE ILE GLN THR GLN LEU HIS ALA ALA M22 R32 N70 L74 G122 L123 I124 K125 G126 S127 G128 L134 C152

N155 L159 E169 Q187 K188 G189 A190 D191 L203 A220 E223 Q227 R246 N273 R294 G295 D296 L297 E304 K305 T328 Q329 E332 L353 A356 M377 Q378 I381 A382 R383 E386 I389 L394 L401 I404 E410

V414 C423 C424 I428 R445 A463 Y466 R467 G468 I469 Q479 E480 G497 F503 W515 R516 P517 G518 S519 G520 F521 R526 V527 P531

• Molecule 1: Pyruvate kinase PKM

Chain D:

10%
85%   6% • 7%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS PRO HIS SER GLU ALA GLY THR ALA PHE ILE GLN THR GLN LEU HIS ALA ALA M22 R32 L74 I119 R120 T121 G122 L123 I124 K125 G126 S127 G128 T129 A130 E131

V132 E133 L134 T139 L140 K141 I142 T143 L144 D145 N146 A147 Y148 M149 E150 K151 C152 N155 W158 L159 D160 Y161 I164 C165 K166 V167 V170 I174 K186 Q187 K188 G189 A190 D191 F192 L193 E198 S202 L203 G204 S205 K206 K207 G208 V209 V216 D217 E223

R246 K261 N273 R294 L297 I301 E304 K305 T328 Q329 E332 R342 L353 A356 M377 Q378 I381 A382 R383 E386 I389 L394 I404 E410 V414 C424 Q440 R445 A463 Y466 R467 G468 I469 Q479 E480
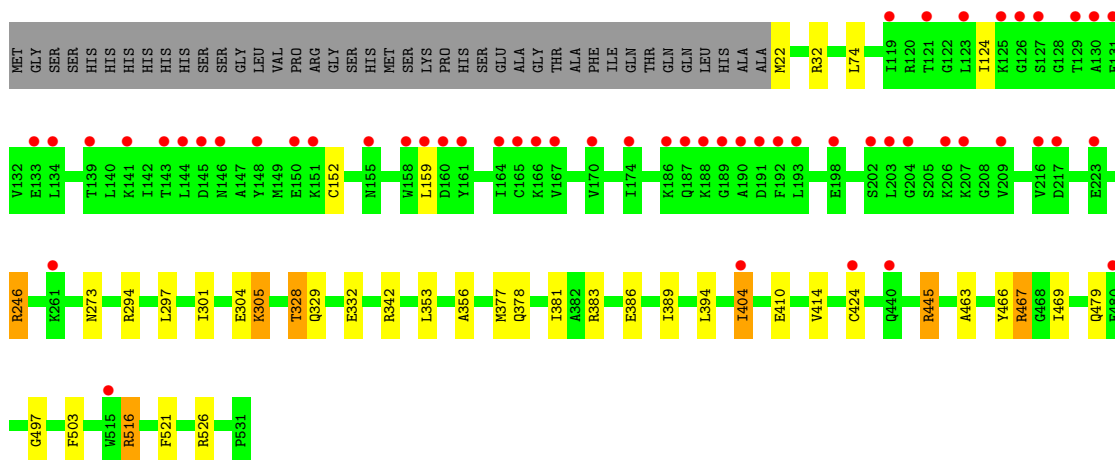
G497 F503 W515 R516 F521 R526 P531

• Molecule 1: Pyruvate kinase PKM

Chain E:

6%
85%   7% • 7%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS PRO HIS SER GLU ALA GLY THR ALA PHE ILE GLN THR GLN LEU HIS ALA ALA M22 R32 L74 R120 L123 I124 G128 T129 A130 E131 A138 A147

C152 N163 K166 V167 V168 I174 L183 Q184 V185 K186 Q187 K188 G189 A190 D191 F192 L193 V197 A220 R246 N273 R294 L297 I301 E304 K305 T328 Q329 E332 R342 L353 A356 M377 Q378 H379 L380 I381 A382 R383 E386

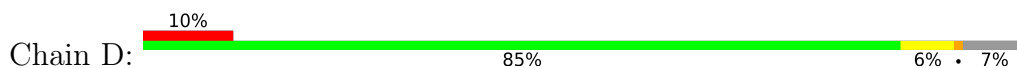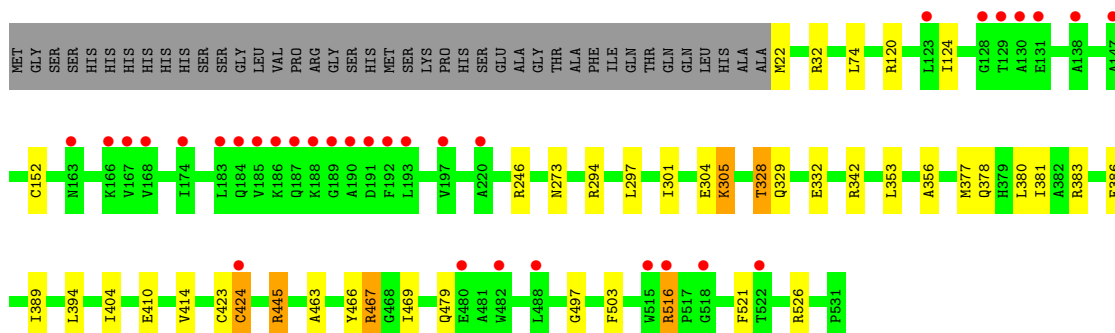I389 L394 I404 E410 V414 C423 C424 R445 A463 Y466 R467 G468 I469 Q479 E480 A481 W482 L488 G497 F503 W515 R516 P517 G518 F521 T522 R526 P531

• Molecule 1: Pyruvate kinase PKM

Chain F:

5%
85%   6% • 7%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS PRO HIS SER GLU ALA GLY THR ALA PHE ILE GLN THR GLN LEU HIS ALA ALA M22 R32 L74 V91 G122 L123 I124 K125 G126 S127 G128 I142 C152
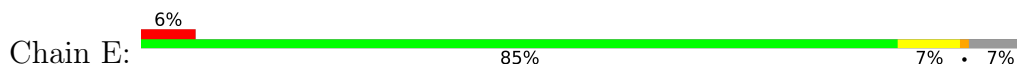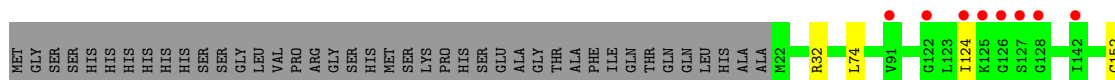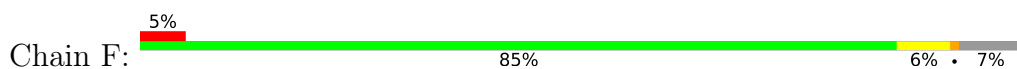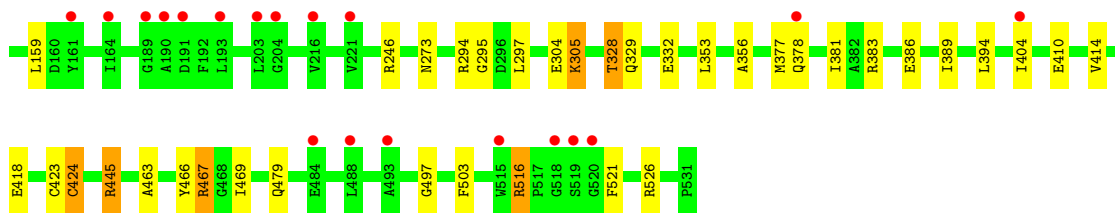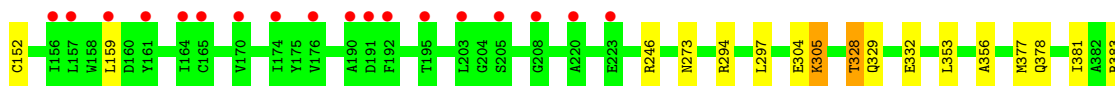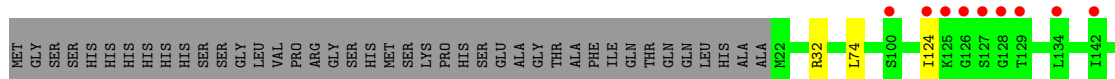
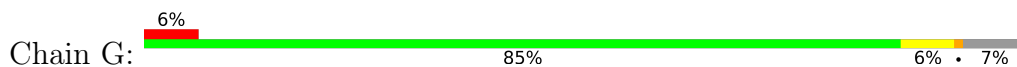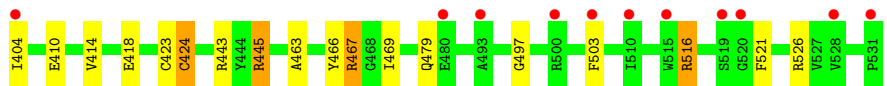• Molecule 1: Pyruvate kinase PKM

Chain G:

• Molecule 1: Pyruvate kinase PKM

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	93.35Å 108.94Å 124.34Å 89.72° 71.13° 66.94°	Depositor
Resolution (Å)	116.50 – 2.96 116.50 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.6 (116.50-2.96) 98.6 (116.50-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.236 , 0.252 0.233 , 0.246	Depositor DCC
R_{free} test set	4203 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	73.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 33.7	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31408	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9052e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: CSO, K, PO4, 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	0.39	0/3970	0.61	0/5359
1	B	0.38	0/3970	0.61	0/5359
1	C	0.39	0/3970	0.62	0/5359
1	D	0.44	0/3970	0.63	1/5359 (0.0%)
1	E	0.41	0/3970	0.63	1/5359 (0.0%)
1	F	0.39	0/3970	0.62	0/5359
1	G	0.38	0/3970	0.61	0/5359
1	H	0.41	0/3970	0.65	4/5359 (0.1%)
All	All	0.40	0/31760	0.62	6/42872 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	22	MET	CG-SD-CE	7.05	111.48	100.20
1	H	22	MET	CA-CB-CG	6.35	124.10	113.30
1	E	120	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	H	22	MET	CB-CG-SD	5.56	129.07	112.40
1	D	246	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	H	443	ARG	NE-CZ-NH1	5.01	122.81	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	3912	0	4001	18	1
1	B	3912	0	4001	20	0
1	C	3912	0	4001	22	1
1	D	3912	0	4001	18	0
1	E	3912	0	4002	19	0
1	F	3912	0	4001	19	0
1	G	3912	0	4001	17	0
1	H	3912	0	4001	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	7	0	4	1	0
4	B	7	0	4	0	0
4	C	7	0	4	1	0
4	D	7	0	4	0	0
4	E	7	0	4	0	0
4	F	7	0	4	0	0
4	G	7	0	4	0	0
4	H	7	0	4	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0
All	All	31408	0	32041	143	1

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 2.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445[A]:ARG:HH11	1:C:445[A]:ARG:HG3	1.20	1.07
1:E:445[A]:ARG:HH11	1:E:445[A]:ARG:HG3	1.14	1.06
1:B:445[A]:ARG:HG3	1:B:445[A]:ARG:HH11	1.15	1.06
1:F:445[A]:ARG:HG3	1:F:445[A]:ARG:HH11	1.20	1.06
1:G:445[A]:ARG:HH11	1:G:445[A]:ARG:HG3	1.16	1.04
1:H:445[A]:ARG:HH11	1:H:445[A]:ARG:HG3	1.19	1.04
1:D:445[A]:ARG:HH11	1:D:445[A]:ARG:HG3	1.18	1.02
1:A:445[A]:ARG:HG3	1:A:445[A]:ARG:HH11	1.18	1.02
1:E:445[A]:ARG:HH11	1:E:445[A]:ARG:CG	1.97	0.77
1:B:445[A]:ARG:HH11	1:B:445[A]:ARG:CG	1.97	0.76
1:A:445[A]:ARG:HG3	1:A:445[A]:ARG:NH1	1.98	0.75
1:B:445[A]:ARG:HG3	1:B:445[A]:ARG:NH1	1.95	0.75
1:E:445[A]:ARG:HG3	1:E:445[A]:ARG:NH1	1.94	0.75
1:H:445[A]:ARG:HH11	1:H:445[A]:ARG:CG	1.99	0.74
1:C:445[A]:ARG:HH11	1:C:445[A]:ARG:CG	2.01	0.73
1:F:445[A]:ARG:HH11	1:F:445[A]:ARG:CG	2.01	0.72
1:G:445[A]:ARG:HH11	1:G:445[A]:ARG:CG	1.97	0.70
1:H:445[A]:ARG:HG3	1:H:445[A]:ARG:NH1	2.00	0.70
1:D:445[A]:ARG:HG3	1:D:445[A]:ARG:NH1	1.98	0.69
1:G:445[A]:ARG:HG3	1:G:445[A]:ARG:NH1	1.97	0.68
1:D:445[A]:ARG:HH11	1:D:445[A]:ARG:CG	2.00	0.67
1:F:445[A]:ARG:HG3	1:F:445[A]:ARG:NH1	2.01	0.67
1:A:445[A]:ARG:HH11	1:A:445[A]:ARG:CG	2.00	0.65
1:C:445[A]:ARG:HG3	1:C:445[A]:ARG:NH1	2.00	0.64
1:D:304:GLU:O	1:D:305:LYS:HB2	2.04	0.57
1:B:304:GLU:O	1:B:305:LYS:HB2	2.05	0.57
1:A:304:GLU:O	1:A:305:LYS:HB2	2.05	0.56
1:C:304:GLU:O	1:C:305:LYS:HB2	2.05	0.56
1:G:304:GLU:O	1:G:305:LYS:HB2	2.05	0.56
1:H:304:GLU:O	1:H:305:LYS:HB2	2.05	0.56
1:B:445[A]:ARG:CG	1:B:445[A]:ARG:NH1	2.62	0.55
1:E:304:GLU:O	1:E:305:LYS:HB2	2.05	0.55
1:F:304:GLU:O	1:F:305:LYS:HB2	2.05	0.55
1:G:356:ALA:O	1:G:467:ARG:NH1	2.40	0.55
1:D:356:ALA:O	1:D:467:ARG:NH1	2.40	0.55
1:H:356:ALA:O	1:H:467:ARG:NH1	2.39	0.55
1:E:356:ALA:O	1:E:467:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ALA:O	1:A:467:ARG:NH1	2.40	0.54
1:C:356:ALA:O	1:C:467:ARG:NH1	2.40	0.54
1:F:356:ALA:O	1:F:467:ARG:NH1	2.40	0.54
1:G:445[A]:ARG:CG	1:G:445[A]:ARG:NH1	2.63	0.54
1:B:356:ALA:O	1:B:467:ARG:NH1	2.40	0.53
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.90	0.53
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.90	0.53
1:F:466:TYR:HB2	1:F:469:ILE:HD12	1.91	0.53
1:B:329:GLN:HA	1:B:332:GLU:HG2	1.91	0.53
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.90	0.53
1:E:329:GLN:HA	1:E:332:GLU:HG2	1.91	0.53
1:H:329:GLN:HA	1:H:332:GLU:HG2	1.91	0.53
1:C:329:GLN:HA	1:C:332:GLU:HG2	1.91	0.52
1:G:466:TYR:HB2	1:G:469:ILE:HD12	1.91	0.52
1:F:329:GLN:HA	1:F:332:GLU:HG2	1.90	0.52
1:D:329:GLN:HA	1:D:332:GLU:HG2	1.92	0.52
1:H:466:TYR:HB2	1:H:469:ILE:HD12	1.91	0.52
1:E:466:TYR:HB2	1:E:469:ILE:HD12	1.91	0.51
1:B:404:ILE:HD11	1:C:424:CYS:SG	2.50	0.51
1:A:329:GLN:HA	1:A:332:GLU:HG2	1.92	0.51
1:A:424:CYS:SG	1:D:404:ILE:HD11	2.50	0.51
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.92	0.51
1:G:329:GLN:HA	1:G:332:GLU:HG2	1.93	0.51
1:D:445[A]:ARG:NH1	1:D:445[A]:ARG:CG	2.66	0.50
1:E:445[A]:ARG:CG	1:E:445[A]:ARG:NH1	2.62	0.50
1:A:445[A]:ARG:NH1	1:A:445[A]:ARG:CG	2.66	0.49
1:C:70:ASN:ND2	4:C:603:SER:OXT	2.46	0.48
1:D:304:GLU:O	1:D:305:LYS:CB	2.63	0.47
1:B:304:GLU:O	1:B:305:LYS:CB	2.63	0.46
1:E:304:GLU:O	1:E:305:LYS:CB	2.63	0.46
1:E:377:MET:CE	1:E:381:ILE:HD11	2.45	0.46
1:D:377:MET:CE	1:D:381:ILE:HD11	2.46	0.46
1:A:377:MET:CE	1:A:381:ILE:HD11	2.45	0.46
1:B:408:PRO:HA	1:C:527:VAL:HG11	1.97	0.46
1:C:304:GLU:O	1:C:305:LYS:CB	2.63	0.46
1:B:523:ASN:O	1:C:526:ARG:HA	2.16	0.46
1:G:304:GLU:O	1:G:305:LYS:CB	2.63	0.46
1:A:304:GLU:O	1:A:305:LYS:CB	2.63	0.46
1:F:304:GLU:O	1:F:305:LYS:CB	2.63	0.46
1:B:377:MET:CE	1:B:381:ILE:HD11	2.46	0.45
1:H:304:GLU:O	1:H:305:LYS:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:MET:CE	1:C:381:ILE:HD11	2.47	0.44
1:E:342:ARG:NH2	1:F:295:GLY:O	2.50	0.44
1:H:410:GLU:O	1:H:414:VAL:HG23	2.18	0.44
1:G:377:MET:CE	1:G:381:ILE:HD11	2.47	0.44
1:D:410:GLU:O	1:D:414:VAL:HG23	2.18	0.44
1:F:377:MET:CE	1:F:381:ILE:HD11	2.47	0.44
1:G:410:GLU:O	1:G:414:VAL:HG23	2.18	0.44
1:A:410:GLU:O	1:A:414:VAL:HG23	2.18	0.44
1:B:410:GLU:O	1:B:414:VAL:HG23	2.18	0.44
1:E:353:LEU:HD23	1:E:389:ILE:HD13	1.99	0.44
1:C:445[A]:ARG:CG	1:C:445[A]:ARG:NH1	2.66	0.44
1:D:124:ILE:HD13	1:D:152:CYS:HB2	2.00	0.44
1:G:124:ILE:HD13	1:G:152:CYS:HB2	2.00	0.44
1:E:410:GLU:O	1:E:414:VAL:HG23	2.18	0.43
1:F:353:LEU:HD23	1:F:389:ILE:HD13	2.00	0.43
1:G:353:LEU:HD23	1:G:389:ILE:HD13	2.00	0.43
1:C:124:ILE:HD13	1:C:152:CYS:HB2	2.01	0.43
1:F:124:ILE:HD13	1:F:152:CYS:HB2	2.01	0.43
1:F:410:GLU:O	1:F:414:VAL:HG23	2.17	0.43
1:H:377:MET:CE	1:H:381:ILE:HD11	2.48	0.43
1:A:353:LEU:HD23	1:A:389:ILE:HD13	2.00	0.43
1:H:353:LEU:HD23	1:H:389:ILE:HD13	2.00	0.43
1:A:124:ILE:HD13	1:A:152:CYS:HB2	2.01	0.43
1:H:124:ILE:HD13	1:H:152:CYS:HB2	2.01	0.43
1:H:497:GLY:HA3	1:H:503:PHE:CZ	2.54	0.43
1:C:353:LEU:HD23	1:C:389:ILE:HD13	1.99	0.43
1:D:353:LEU:HD23	1:D:389:ILE:HD13	1.99	0.42
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.54	0.42
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.55	0.42
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.54	0.42
1:C:295:GLY:O	1:D:342:ARG:NH1	2.52	0.42
1:C:410:GLU:O	1:C:414:VAL:HG23	2.18	0.42
1:E:124:ILE:HD13	1:E:152:CYS:HB2	2.01	0.42
1:F:497:GLY:HA3	1:F:503:PHE:CZ	2.54	0.42
1:G:497:GLY:HA3	1:G:503:PHE:CZ	2.54	0.42
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.54	0.42
1:B:353:LEU:HD23	1:B:389:ILE:HD13	2.00	0.42
1:B:124:ILE:HD13	1:B:152:CYS:HB2	2.01	0.42
1:F:418:GLU:HG2	1:H:418:GLU:HB2	2.01	0.42
1:D:463:ALA:HB1	1:D:469:ILE:HG21	2.02	0.42
1:E:463:ALA:HB1	1:E:469:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ARG:CG	1:C:273:ASN:HD21	2.33	0.42
1:D:246:ARG:CG	1:D:273:ASN:HD21	2.33	0.42
1:E:497:GLY:HA3	1:E:503:PHE:CZ	2.54	0.42
1:F:246:ARG:CG	1:F:273:ASN:HD21	2.33	0.42
1:H:463:ALA:HB1	1:H:469:ILE:HG21	2.01	0.42
1:B:463:ALA:HB1	1:B:469:ILE:HG21	2.02	0.41
1:H:246:ARG:CG	1:H:273:ASN:HD21	2.33	0.41
1:G:246:ARG:CG	1:G:273:ASN:HD21	2.33	0.41
1:A:463:ALA:HB1	1:A:469:ILE:HG21	2.01	0.41
1:B:246:ARG:CG	1:B:273:ASN:HD21	2.34	0.41
1:E:246:ARG:CG	1:E:273:ASN:HD21	2.34	0.41
1:G:463:ALA:HB1	1:G:469:ILE:HG21	2.03	0.41
1:C:423:CYS:O	1:C:424:CYS:C	2.60	0.41
1:H:445[A]:ARG:CG	1:H:445[A]:ARG:NH1	2.66	0.41
1:A:423:CYS:O	1:A:424:CYS:C	2.60	0.41
1:C:463:ALA:HB1	1:C:469:ILE:HG21	2.01	0.41
1:G:423:CYS:O	1:G:424:CYS:C	2.60	0.41
1:B:423:CYS:O	1:B:424:CYS:C	2.60	0.40
1:H:423:CYS:O	1:H:424:CYS:C	2.60	0.40
1:F:423:CYS:O	1:F:424:CYS:C	2.60	0.40
1:F:463:ALA:HB1	1:F:469:ILE:HG21	2.01	0.40
1:E:423:CYS:O	1:E:424:CYS:C	2.60	0.40
1:E:380:LEU:HB3	1:F:304:GLU:HG3	2.03	0.40
1:A:43:ARG:O	4:A:603:SER:OG	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:LYS:O	1:C:227:GLN:NE2[1_455]	2.16	0.04

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	508/551 (92%)	483 (95%)	20 (4%)	5 (1%)	15	48
1	B	508/551 (92%)	483 (95%)	20 (4%)	5 (1%)	15	48
1	C	508/551 (92%)	484 (95%)	19 (4%)	5 (1%)	15	48
1	D	508/551 (92%)	482 (95%)	21 (4%)	5 (1%)	15	48
1	E	508/551 (92%)	484 (95%)	19 (4%)	5 (1%)	15	48
1	F	508/551 (92%)	482 (95%)	21 (4%)	5 (1%)	15	48
1	G	508/551 (92%)	483 (95%)	20 (4%)	5 (1%)	15	48
1	H	508/551 (92%)	484 (95%)	19 (4%)	5 (1%)	15	48
All	All	4064/4408 (92%)	3865 (95%)	159 (4%)	40 (1%)	15	48

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	CYS
1	B	424	CYS
1	C	424	CYS
1	D	424	CYS
1	E	424	CYS
1	F	424	CYS
1	G	424	CYS
1	H	424	CYS
1	A	305	LYS
1	B	305	LYS
1	C	305	LYS
1	D	305	LYS
1	E	305	LYS
1	F	305	LYS
1	G	305	LYS
1	H	305	LYS
1	A	328	THR
1	B	328	THR
1	C	328	THR
1	D	328	THR
1	E	328	THR
1	F	328	THR
1	G	328	THR
1	H	328	THR
1	A	516	ARG

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Mol	Chain	Res	Type
1	B	516	ARG
1	C	516	ARG
1	D	516	ARG
1	E	516	ARG
1	F	516	ARG
1	G	516	ARG
1	H	516	ARG
1	A	404	ILE
1	B	404	ILE
1	C	404	ILE
1	D	404	ILE
1	E	404	ILE
1	F	404	ILE
1	G	404	ILE
1	H	404	ILE

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	420/452 (93%)	402 (96%)	18 (4%)	29	62
1	B	420/452 (93%)	400 (95%)	20 (5%)	25	59
1	C	420/452 (93%)	403 (96%)	17 (4%)	31	64
1	D	420/452 (93%)	401 (96%)	19 (4%)	27	61
1	E	420/452 (93%)	402 (96%)	18 (4%)	29	62
1	F	420/452 (93%)	403 (96%)	17 (4%)	31	64
1	G	420/452 (93%)	402 (96%)	18 (4%)	29	62
1	H	420/452 (93%)	401 (96%)	19 (4%)	27	61
All	All	3360/3616 (93%)	3214 (96%)	146 (4%)	30	62

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	74	LEU
1	A	159	LEU
1	A	294	ARG
1	A	297	LEU
1	A	328	THR
1	A	378	GLN
1	A	383	ARG
1	A	386	GLU
1	A	394	LEU
1	A	436	ARG
1	A	445[A]	ARG
1	A	445[B]	ARG
1	A	467	ARG
1	A	479	GLN
1	A	516	ARG
1	A	521	PHE
1	A	526	ARG
1	B	22	MET
1	B	32	ARG
1	B	74	LEU
1	B	159	LEU
1	B	206	LYS
1	B	294	ARG
1	B	297	LEU
1	B	301	ILE
1	B	328	THR
1	B	378	GLN
1	B	383	ARG
1	B	386	GLU
1	B	394	LEU
1	B	445[A]	ARG
1	B	445[B]	ARG
1	B	467	ARG
1	B	479	GLN
1	B	516	ARG
1	B	521	PHE
1	B	526	ARG
1	C	32	ARG
1	C	74	LEU
1	C	159	LEU
1	C	294	ARG
1	C	297	LEU

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Mol	Chain	Res	Type
1	C	328	THR
1	C	378	GLN
1	C	383	ARG
1	C	386	GLU
1	C	394	LEU
1	C	445[A]	ARG
1	C	445[B]	ARG
1	C	467	ARG
1	C	479	GLN
1	C	516	ARG
1	C	521	PHE
1	C	526	ARG
1	D	22	MET
1	D	32	ARG
1	D	74	LEU
1	D	159	LEU
1	D	294	ARG
1	D	297	LEU
1	D	301	ILE
1	D	328	THR
1	D	378	GLN
1	D	383	ARG
1	D	386	GLU
1	D	394	LEU
1	D	445[A]	ARG
1	D	445[B]	ARG
1	D	467	ARG
1	D	479	GLN
1	D	516	ARG
1	D	521	PHE
1	D	526	ARG
1	E	22	MET
1	E	32	ARG
1	E	74	LEU
1	E	294	ARG
1	E	297	LEU
1	E	301	ILE
1	E	328	THR
1	E	378	GLN
1	E	383	ARG
1	E	386	GLU
1	E	394	LEU

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Mol	Chain	Res	Type
1	E	445[A]	ARG
1	E	445[B]	ARG
1	E	467	ARG
1	E	479	GLN
1	E	516	ARG
1	E	521	PHE
1	E	526	ARG
1	F	32	ARG
1	F	74	LEU
1	F	159	LEU
1	F	294	ARG
1	F	297	LEU
1	F	328	THR
1	F	378	GLN
1	F	383	ARG
1	F	386	GLU
1	F	394	LEU
1	F	445[A]	ARG
1	F	445[B]	ARG
1	F	467	ARG
1	F	479	GLN
1	F	516	ARG
1	F	521	PHE
1	F	526	ARG
1	G	32	ARG
1	G	74	LEU
1	G	159	LEU
1	G	294	ARG
1	G	297	LEU
1	G	328	THR
1	G	378	GLN
1	G	383	ARG
1	G	386	GLU
1	G	394	LEU
1	G	436	ARG
1	G	445[A]	ARG
1	G	445[B]	ARG
1	G	467	ARG
1	G	479	GLN
1	G	516	ARG
1	G	521	PHE
1	G	526	ARG

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Mol	Chain	Res	Type
1	H	22	MET
1	H	32	ARG
1	H	74	LEU
1	H	159	LEU
1	H	294	ARG
1	H	297	LEU
1	H	301	ILE
1	H	328	THR
1	H	378	GLN
1	H	383	ARG
1	H	386	GLU
1	H	394	LEU
1	H	445[A]	ARG
1	H	445[B]	ARG
1	H	467	ARG
1	H	479	GLN
1	H	516	ARG
1	H	521	PHE
1	H	526	ARG

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

Mol	Chain	Res	Type
1	F	318	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	CSO	C	474	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	H	474	1	3,6,7	0.57	0	0,6,8	-	-
1	CSO	F	474	1	3,6,7	0.65	0	0,6,8	-	-
1	CSO	E	474	1	3,6,7	0.72	0	0,6,8	-	-
1	CSO	D	474	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	B	474	1	3,6,7	0.66	0	0,6,8	-	-
1	CSO	G	474	1	3,6,7	0.65	0	0,6,8	-	-
1	CSO	A	474	1	3,6,7	0.61	0	0,6,8	-	-

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
1	CSO	C	474	1	-	0/1/5/7	-
1	CSO	H	474	1	-	0/1/5/7	-
1	CSO	F	474	1	-	0/1/5/7	-
1	CSO	E	474	1	-	0/1/5/7	-
1	CSO	D	474	1	-	0/1/5/7	-
1	CSO	B	474	1	-	0/1/5/7	-
1	CSO	G	474	1	-	0/1/5/7	-
1	CSO	A	474	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5　Carbohydrates　ⓘ

There are no monosaccharides in this entry.

5.6　Ligand geometry　ⓘ

Of 32 ligands modelled in this entry, 16 are monoatomic - 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	#$|Z| > 2$
5	PO4	G	604	-	4,4,4	0.91	0	6,6,6	0.63	0
4	SER	F	603	-	5,6,6	0.97	1 (20%)	5,7,7	1.56	2 (40%)
5	PO4	A	604	-	4,4,4	0.96	0	6,6,6	0.49	0
5	PO4	F	604	-	4,4,4	0.96	0	6,6,6	0.59	0
5	PO4	E	604	-	4,4,4	0.89	0	6,6,6	0.49	0
5	PO4	D	604	-	4,4,4	0.95	0	6,6,6	0.43	0
4	SER	A	603	-	5,6,6	1.06	1 (20%)	5,7,7	1.60	2 (40%)
4	SER	H	603	-	5,6,6	1.00	1 (20%)	5,7,7	1.63	2 (40%)
5	PO4	H	604	-	4,4,4	0.88	0	6,6,6	0.53	0
4	SER	E	603	-	5,6,6	1.08	1 (20%)	5,7,7	1.69	2 (40%)
4	SER	D	603	-	5,6,6	1.07	1 (20%)	5,7,7	1.73	2 (40%)
4	SER	C	603	-	5,6,6	1.03	1 (20%)	5,7,7	1.98	2 (40%)
4	SER	B	603	-	5,6,6	1.10	1 (20%)	5,7,7	1.48	1 (20%)
5	PO4	C	604	-	4,4,4	0.88	0	6,6,6	0.52	0
5	PO4	B	604	-	4,4,4	0.83	0	6,6,6	0.57	0
4	SER	G	603	-	5,6,6	1.02	1 (20%)	5,7,7	1.50	2 (40%)

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
4	SER	F	603	-	-	0/6/6/6	-
4	SER	A	603	-	-	2/6/6/6	-
4	SER	H	603	-	-	0/6/6/6	-
4	SER	E	603	-	-	2/6/6/6	-
4	SER	D	603	-	-	2/6/6/6	-
4	SER	C	603	-	-	2/6/6/6	-
4	SER	B	603	-	-	1/6/6/6	-
4	SER	G	603	-	-	2/6/6/6	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	SER	OXT-C	-2.40	1.22	1.30
4	E	603	SER	OXT-C	-2.36	1.22	1.30
4	D	603	SER	OXT-C	-2.34	1.22	1.30
4	A	603	SER	OXT-C	-2.30	1.23	1.30
4	C	603	SER	OXT-C	-2.25	1.23	1.30
4	G	603	SER	OXT-C	-2.17	1.23	1.30
4	H	603	SER	OXT-C	-2.12	1.23	1.30
4	F	603	SER	OXT-C	-2.11	1.23	1.30

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	603	SER	OXT-C-O	-3.62	115.87	124.09
4	D	603	SER	OXT-C-O	-2.88	117.55	124.09
4	E	603	SER	OXT-C-O	-2.82	117.69	124.09
4	A	603	SER	OXT-C-O	-2.81	117.71	124.09
4	H	603	SER	OXT-C-O	-2.54	118.33	124.09
4	F	603	SER	OXT-C-O	-2.54	118.33	124.09
4	B	603	SER	OXT-C-O	-2.52	118.36	124.09
4	G	603	SER	OXT-C-O	-2.49	118.42	124.09
4	C	603	SER	OXT-C-CA	2.44	121.68	113.38
4	D	603	SER	OXT-C-CA	2.42	121.62	113.38
4	E	603	SER	OXT-C-CA	2.32	121.30	113.38
4	H	603	SER	OXT-C-CA	2.27	121.11	113.38
4	F	603	SER	OXT-C-CA	2.19	120.84	113.38
4	A	603	SER	OXT-C-CA	2.14	120.68	113.38
4	G	603	SER	OXT-C-CA	2.11	120.58	113.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	SER	N-CA-CB-OG
4	C	603	SER	OXT-C-CA-N
4	D	603	SER	OXT-C-CA-N
4	E	603	SER	OXT-C-CA-N
4	C	603	SER	O-C-CA-N
4	D	603	SER	O-C-CA-N
4	E	603	SER	O-C-CA-N
4	G	603	SER	N-CA-CB-OG
4	A	603	SER	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
4	B	603	SER	OXT-C-CA-N
4	G	603	SER	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	SER	1	0
4	C	603	SER	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	509/551 (92%)	0.15	23 (4%)	33	21	45, 83, 132, 178	0
1	B	509/551 (92%)	0.38	45 (8%)	10	5	52, 99, 148, 187	0
1	C	509/551 (92%)	0.22	26 (5%)	28	17	48, 86, 147, 186	0
1	D	509/551 (92%)	0.57	55 (10%)	5	3	50, 88, 158, 188	0
1	E	509/551 (92%)	0.29	33 (6%)	18	11	52, 83, 130, 180	0
1	F	509/551 (92%)	0.23	27 (5%)	26	16	52, 94, 145, 183	0
1	G	509/551 (92%)	0.22	31 (6%)	21	12	46, 85, 146, 185	0
1	H	509/551 (92%)	0.18	31 (6%)	21	12	52, 88, 130, 176	0
All	All	4072/4408 (92%)	0.28	271 (6%)	17	10	45, 88, 145, 188	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	130	ALA	23.0
1	D	126	GLY	18.5
1	C	519	SER	16.4
1	H	128	GLY	13.4
1	D	121	THR	11.2
1	E	129	THR	10.7
1	G	127	SER	10.6
1	D	159	LEU	10.2
1	B	128	GLY	9.9
1	H	130	ALA	9.9
1	F	190	ALA	9.8
1	D	189	GLY	9.3
1	D	127	SER	9.2
1	D	188	LYS	8.9
1	F	518	GLY	8.9
1	F	519	SER	8.7

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Mol	Chain	Res	Type	RSRZ
1	C	520	GLY	8.6
1	A	128	GLY	8.4
1	D	190	ALA	8.4
1	D	131	GLU	7.8
1	H	129	THR	7.7
1	D	167	VAL	7.6
1	A	129	THR	7.6
1	D	424	CYS	7.2
1	D	125	LYS	7.2
1	G	157	LEU	7.1
1	G	128	GLY	7.0
1	A	127	SER	7.0
1	D	191	ASP	6.9
1	D	187	GLN	6.8
1	D	129	THR	6.6
1	D	192	PHE	6.5
1	H	127	SER	6.4
1	F	189	GLY	6.2
1	C	518	GLY	6.1
1	D	151	LYS	6.0
1	C	515	TRP	5.9
1	B	220	ALA	5.9
1	E	185	VAL	5.8
1	E	480	GLU	5.8
1	H	187	GLN	5.8
1	C	190	ALA	5.7
1	H	519	SER	5.7
1	F	520	GLY	5.7
1	C	126	GLY	5.6
1	D	203	LEU	5.6
1	B	195	THR	5.5
1	B	130	ALA	5.4
1	D	130	ALA	5.4
1	E	128	GLY	5.4
1	F	128	GLY	5.3
1	B	140	LEU	5.2
1	B	191	ASP	5.2
1	H	404	ILE	5.1
1	A	125	LYS	5.1
1	B	194	VAL	5.0
1	C	189	GLY	5.0
1	G	192	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	193	LEU	5.0
1	B	127	SER	4.9
1	E	131	GLU	4.9
1	D	161	TYR	4.8
1	D	193	LEU	4.7
1	G	165	CYS	4.7
1	C	127	SER	4.7
1	B	480	GLU	4.6
1	B	132	VAL	4.6
1	D	207	LYS	4.5
1	E	515	TRP	4.5
1	F	515	TRP	4.4
1	E	192	PHE	4.4
1	F	484	GLU	4.4
1	B	187	GLN	4.4
1	F	126	GLY	4.3
1	G	129	THR	4.3
1	E	184	GLN	4.3
1	A	191	ASP	4.3
1	C	404	ILE	4.3
1	G	164	ILE	4.2
1	B	174	ILE	4.1
1	B	168	VAL	4.1
1	D	158	TRP	4.0
1	D	404	ILE	4.0
1	B	197	VAL	3.9
1	G	191	ASP	3.9
1	E	190	ALA	3.9
1	D	145	ASP	3.9
1	E	187	GLN	3.9
1	D	144	LEU	3.9
1	B	190	ALA	3.8
1	D	515	TRP	3.8
1	A	424	CYS	3.8
1	B	184	GLN	3.8
1	F	191	ASP	3.7
1	E	174	ILE	3.7
1	D	217	ASP	3.7
1	E	424	CYS	3.7
1	D	480	GLU	3.7
1	C	191	ASP	3.6
1	A	192	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	203	LEU	3.6
1	F	127	SER	3.5
1	E	193	LEU	3.5
1	A	134	LEU	3.4
1	D	164	ILE	3.4
1	F	404	ILE	3.4
1	H	520	GLY	3.4
1	D	143	THR	3.3
1	C	203	LEU	3.3
1	G	125	LYS	3.3
1	D	204	GLY	3.3
1	D	119	ILE	3.3
1	B	183	LEU	3.2
1	E	183	LEU	3.2
1	D	186	LYS	3.2
1	G	520	GLY	3.1
1	E	138	ALA	3.1
1	C	128	GLY	3.1
1	B	192	PHE	3.1
1	E	197	VAL	3.1
1	B	131	GLU	3.1
1	G	531	PRO	3.1
1	A	142	ILE	3.1
1	D	134	LEU	3.0
1	B	134	LEU	3.0
1	E	123	LEU	3.0
1	G	174	ILE	3.0
1	A	126	GLY	3.0
1	F	125	LYS	3.0
1	A	193	LEU	3.0
1	D	139	THR	3.0
1	E	189	GLY	3.0
1	G	124	ILE	3.0
1	A	203	LEU	2.9
1	D	155	ASN	2.9
1	H	503	PHE	2.9
1	C	531	PRO	2.9
1	D	216	VAL	2.9
1	B	193	LEU	2.9
1	E	186	LYS	2.9
1	A	149	MET	2.9
1	G	156	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	187	GLN	2.9
1	H	531	PRO	2.9
1	D	166	LYS	2.9
1	C	169	GLU	2.9
1	G	404	ILE	2.8
1	H	131	GLU	2.8
1	F	221	VAL	2.8
1	E	147	ALA	2.8
1	B	142	ILE	2.8
1	A	185	VAL	2.8
1	H	515	TRP	2.7
1	A	221	VAL	2.7
1	H	192	PHE	2.7
1	H	157	LEU	2.7
1	A	195	THR	2.7
1	B	157	LEU	2.7
1	H	528	VAL	2.7
1	H	223	GLU	2.7
1	B	139	THR	2.7
1	G	134	LEU	2.7
1	D	150	GLU	2.7
1	G	203	LEU	2.6
1	E	220	ALA	2.6
1	D	170	VAL	2.6
1	A	220	ALA	2.6
1	E	188	LYS	2.6
1	C	480	GLU	2.6
1	H	480	GLU	2.6
1	C	428	ILE	2.6
1	H	132	VAL	2.6
1	H	493	ALA	2.6
1	F	122	GLY	2.6
1	B	251	VAL	2.6
1	G	190	ALA	2.5
1	C	155	ASN	2.5
1	B	189	GLY	2.5
1	A	205	SER	2.5
1	B	164	ILE	2.5
1	C	122	GLY	2.5
1	B	515	TRP	2.5
1	G	205	SER	2.5
1	F	164	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	186	LYS	2.5
1	G	176	VAL	2.5
1	D	165	CYS	2.5
1	F	378	GLN	2.5
1	G	126	GLY	2.5
1	B	527	VAL	2.4
1	D	209	VAL	2.4
1	H	125	LYS	2.4
1	D	198	GLU	2.4
1	D	141	LYS	2.4
1	F	216	VAL	2.4
1	D	206	LYS	2.4
1	D	174	ILE	2.4
1	E	166	LYS	2.4
1	G	159	LEU	2.4
1	B	76	PHE	2.4
1	D	223	GLU	2.4
1	E	522	THR	2.4
1	H	119	ILE	2.4
1	B	503	PHE	2.4
1	G	223	GLU	2.4
1	D	148	TYR	2.4
1	E	482	TRP	2.4
1	B	221	VAL	2.3
1	H	175	TYR	2.3
1	B	151	LYS	2.3
1	G	195	THR	2.3
1	B	470	PHE	2.3
1	F	124	ILE	2.3
1	B	161	TYR	2.3
1	G	142	ILE	2.3
1	H	184	GLN	2.3
1	E	191	ASP	2.3
1	D	202	SER	2.3
1	F	488	LEU	2.3
1	F	204	GLY	2.3
1	D	146	ASN	2.3
1	A	174	ILE	2.3
1	H	195	THR	2.2
1	C	188	LYS	2.2
1	D	133	GLU	2.2
1	H	148	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	197	VAL	2.2
1	H	186	LYS	2.2
1	B	129	THR	2.2
1	E	518	GLY	2.2
1	H	193	LEU	2.2
1	G	220	ALA	2.2
1	C	516	ARG	2.2
1	F	161	TYR	2.2
1	B	488	LEU	2.2
1	B	100	SER	2.2
1	F	142	ILE	2.2
1	F	91	VAL	2.2
1	G	170	VAL	2.2
1	B	40	ILE	2.2
1	A	519	SER	2.2
1	E	167	VAL	2.2
1	G	100	SER	2.1
1	B	472	VAL	2.1
1	A	183	LEU	2.1
1	C	223	GLU	2.1
1	E	163	ASN	2.1
1	C	503	PHE	2.1
1	D	123	LEU	2.1
1	E	516	ARG	2.1
1	F	493	ALA	2.1
1	B	429	ILE	2.1
1	D	261	LYS	2.1
1	E	168	VAL	2.1
1	E	488	LEU	2.1
1	G	484	GLU	2.1
1	B	211	LEU	2.1
1	C	134	LEU	2.1
1	D	440	GLN	2.1
1	G	161	TYR	2.1
1	G	208	GLY	2.1
1	B	135	LYS	2.1
1	C	401	LEU	2.1
1	B	133	GLU	2.0
1	H	141	LYS	2.0
1	A	204	GLY	2.0
1	H	510	ILE	2.0
1	D	160	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	164	ILE	2.0
1	C	220	ALA	2.0
1	H	500	ARG	2.0

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

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(Å^2)	Q<0.9
1	CSO	F	474	7/8	0.76	0.15	97,102,107,108	0
1	CSO	B	474	7/8	0.78	0.19	108,112,114,115	0
1	CSO	A	474	7/8	0.84	0.16	82,85,92,93	0
1	CSO	C	474	7/8	0.90	0.12	86,91,97,99	0
1	CSO	H	474	7/8	0.90	0.10	101,102,104,104	0
1	CSO	E	474	7/8	0.91	0.12	84,86,87,89	0
1	CSO	D	474	7/8	0.94	0.14	80,84,94,97	0
1	CSO	G	474	7/8	0.96	0.12	86,87,95,96	0

6.3　Carbohydrates ⓘ

There are no monosaccharides 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. 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(Å^2)	Q<0.9
3	MG	E	602	1/1	0.80	0.31	58,58,58,58	0
2	K	A	601	1/1	0.84	0.11	93,93,93,93	0
3	MG	B	602	1/1	0.86	0.21	49,49,49,49	0
2	K	C	601	1/1	0.88	0.13	70,70,70,70	0
3	MG	H	602	1/1	0.88	0.26	61,61,61,61	0
4	SER	H	603	7/7	0.88	0.17	74,77,77,79	0
2	K	G	601	1/1	0.90	0.08	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	SER	F	603	7/7	0.90	0.22	90,91,92,93	0
3	MG	F	602	1/1	0.90	0.37	66,66,66,66	0
4	SER	C	603	7/7	0.91	0.15	69,71,71,73	0
5	PO4	F	604	5/5	0.91	0.12	100,103,104,106	0
3	MG	C	602	1/1	0.92	0.34	58,58,58,58	0
5	PO4	B	604	5/5	0.93	0.09	119,121,122,123	0
3	MG	D	602	1/1	0.93	0.34	57,57,57,57	0
4	SER	E	603	7/7	0.94	0.18	79,82,86,88	0
3	MG	A	602	1/1	0.94	0.22	58,58,58,58	0
4	SER	B	603	7/7	0.94	0.19	85,86,86,87	0
3	MG	G	602	1/1	0.94	0.25	61,61,61,61	0
4	SER	D	603	7/7	0.94	0.18	69,72,75,76	0
4	SER	G	603	7/7	0.95	0.14	85,87,89,90	0
2	K	F	601	1/1	0.95	0.09	83,83,83,83	0
5	PO4	H	604	5/5	0.95	0.13	93,95,96,97	0
2	K	B	601	1/1	0.96	0.12	94,94,94,94	0
5	PO4	G	604	5/5	0.96	0.10	86,86,88,88	0
4	SER	A	603	7/7	0.96	0.15	81,83,86,88	0
5	PO4	A	604	5/5	0.97	0.10	87,88,89,90	0
2	K	E	601	1/1	0.97	0.11	72,72,72,72	0
5	PO4	E	604	5/5	0.97	0.10	83,83,84,86	0
2	K	H	601	1/1	0.98	0.09	80,80,80,80	0
5	PO4	D	604	5/5	0.98	0.10	86,87,88,90	0
2	K	D	601	1/1	0.98	0.04	77,77,77,77	0
5	PO4	C	604	5/5	0.99	0.07	72,72,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.