wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 01:45 PM EST

PDB ID	:	3T05
Title	:	Crystal structure of S. aureus Pyruvate Kinase
Authors	:	Worrall, L.J.; Vuckovic, M.; Strynadka, N.C.J.
Deposited on	:	2011-07-19
Resolution	:	3.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

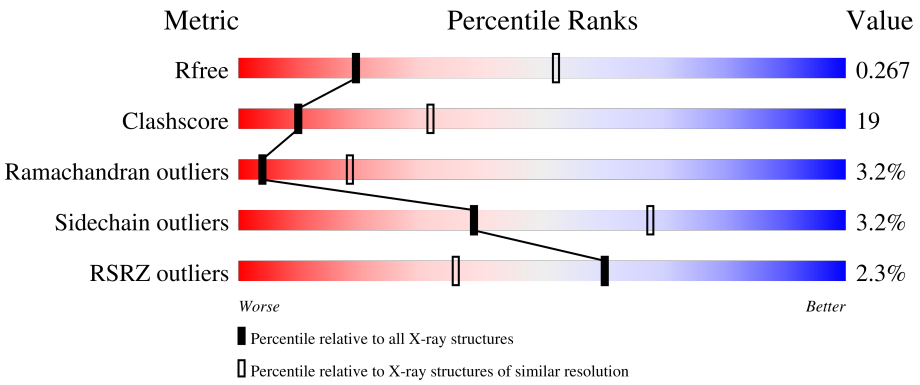
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	606	61% 33%
1	B	606	4% 60% 33%
1	C	606	3% 61% 32%
1	D	606	% 62% 31%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	586	-	-	X	-
2	PO4	C	586	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 17648 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	4407	2745	764	880	18	0	0	0
1	B	583	4407	2745	764	880	18	0	0	0
1	C	583	4407	2745	764	880	18	0	0	0
1	D	583	4407	2745	764	880	18	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q6GG09
A	-19	GLY	-	expression tag	UNP Q6GG09
A	-18	SER	-	expression tag	UNP Q6GG09
A	-17	SER	-	expression tag	UNP Q6GG09
A	-16	HIS	-	expression tag	UNP Q6GG09
A	-15	HIS	-	expression tag	UNP Q6GG09
A	-14	HIS	-	expression tag	UNP Q6GG09
A	-13	HIS	-	expression tag	UNP Q6GG09
A	-12	HIS	-	expression tag	UNP Q6GG09
A	-11	HIS	-	expression tag	UNP Q6GG09
A	-10	SER	-	expression tag	UNP Q6GG09
A	-9	SER	-	expression tag	UNP Q6GG09
A	-8	GLY	-	expression tag	UNP Q6GG09
A	-7	LEU	-	expression tag	UNP Q6GG09
A	-6	VAL	-	expression tag	UNP Q6GG09
A	-5	PRO	-	expression tag	UNP Q6GG09
A	-4	ARG	-	expression tag	UNP Q6GG09
A	-3	GLY	-	expression tag	UNP Q6GG09
A	-2	SER	-	expression tag	UNP Q6GG09
A	-1	HIS	-	expression tag	UNP Q6GG09
A	0	MET	-	expression tag	UNP Q6GG09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q6GG09
B	-19	GLY	-	expression tag	UNP Q6GG09
B	-18	SER	-	expression tag	UNP Q6GG09
B	-17	SER	-	expression tag	UNP Q6GG09
B	-16	HIS	-	expression tag	UNP Q6GG09
B	-15	HIS	-	expression tag	UNP Q6GG09
B	-14	HIS	-	expression tag	UNP Q6GG09
B	-13	HIS	-	expression tag	UNP Q6GG09
B	-12	HIS	-	expression tag	UNP Q6GG09
B	-11	HIS	-	expression tag	UNP Q6GG09
B	-10	SER	-	expression tag	UNP Q6GG09
B	-9	SER	-	expression tag	UNP Q6GG09
B	-8	GLY	-	expression tag	UNP Q6GG09
B	-7	LEU	-	expression tag	UNP Q6GG09
B	-6	VAL	-	expression tag	UNP Q6GG09
B	-5	PRO	-	expression tag	UNP Q6GG09
B	-4	ARG	-	expression tag	UNP Q6GG09
B	-3	GLY	-	expression tag	UNP Q6GG09
B	-2	SER	-	expression tag	UNP Q6GG09
B	-1	HIS	-	expression tag	UNP Q6GG09
B	0	MET	-	expression tag	UNP Q6GG09
C	-20	MET	-	expression tag	UNP Q6GG09
C	-19	GLY	-	expression tag	UNP Q6GG09
C	-18	SER	-	expression tag	UNP Q6GG09
C	-17	SER	-	expression tag	UNP Q6GG09
C	-16	HIS	-	expression tag	UNP Q6GG09
C	-15	HIS	-	expression tag	UNP Q6GG09
C	-14	HIS	-	expression tag	UNP Q6GG09
C	-13	HIS	-	expression tag	UNP Q6GG09
C	-12	HIS	-	expression tag	UNP Q6GG09
C	-11	HIS	-	expression tag	UNP Q6GG09
C	-10	SER	-	expression tag	UNP Q6GG09
C	-9	SER	-	expression tag	UNP Q6GG09
C	-8	GLY	-	expression tag	UNP Q6GG09
C	-7	LEU	-	expression tag	UNP Q6GG09
C	-6	VAL	-	expression tag	UNP Q6GG09
C	-5	PRO	-	expression tag	UNP Q6GG09
C	-4	ARG	-	expression tag	UNP Q6GG09
C	-3	GLY	-	expression tag	UNP Q6GG09
C	-2	SER	-	expression tag	UNP Q6GG09
C	-1	HIS	-	expression tag	UNP Q6GG09
C	0	MET	-	expression tag	UNP Q6GG09

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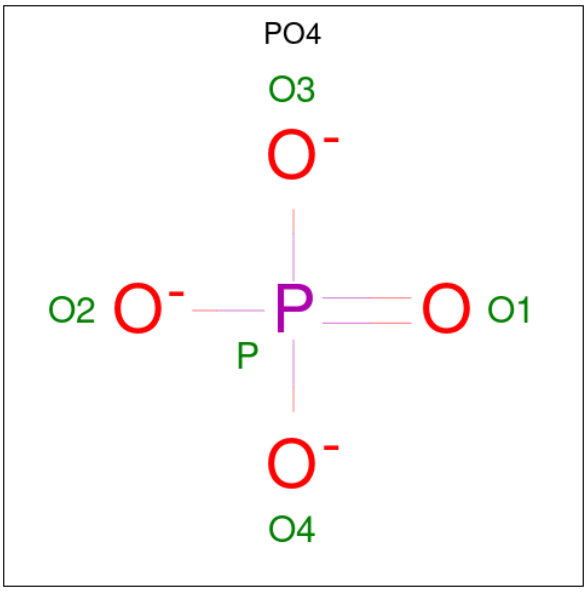
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q6GG09
D	-19	GLY	-	expression tag	UNP Q6GG09
D	-18	SER	-	expression tag	UNP Q6GG09
D	-17	SER	-	expression tag	UNP Q6GG09
D	-16	HIS	-	expression tag	UNP Q6GG09
D	-15	HIS	-	expression tag	UNP Q6GG09
D	-14	HIS	-	expression tag	UNP Q6GG09
D	-13	HIS	-	expression tag	UNP Q6GG09
D	-12	HIS	-	expression tag	UNP Q6GG09
D	-11	HIS	-	expression tag	UNP Q6GG09
D	-10	SER	-	expression tag	UNP Q6GG09
D	-9	SER	-	expression tag	UNP Q6GG09
D	-8	GLY	-	expression tag	UNP Q6GG09
D	-7	LEU	-	expression tag	UNP Q6GG09
D	-6	VAL	-	expression tag	UNP Q6GG09
D	-5	PRO	-	expression tag	UNP Q6GG09
D	-4	ARG	-	expression tag	UNP Q6GG09
D	-3	GLY	-	expression tag	UNP Q6GG09
D	-2	SER	-	expression tag	UNP Q6GG09
D	-1	HIS	-	expression tag	UNP Q6GG09
D	0	MET	-	expression tag	UNP Q6GG09

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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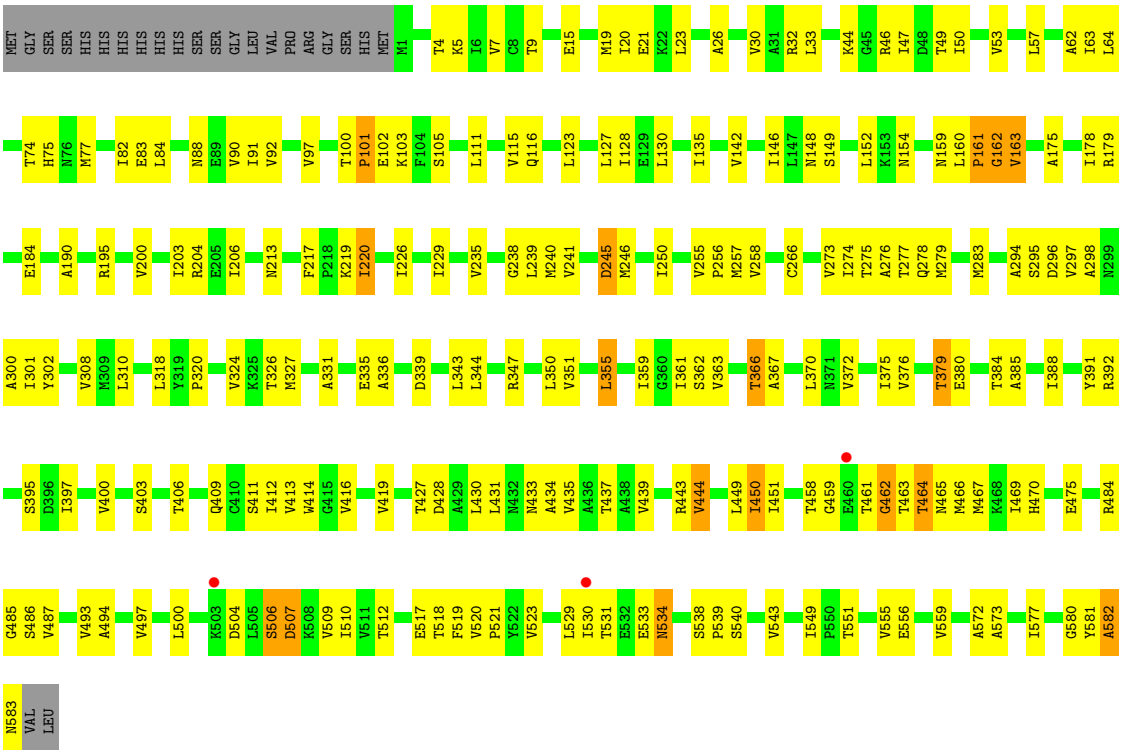
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	B	1	5	4	1	0	0
			Total	O	P		
2	C	1	5	4	1	0	0
			Total	O	P		
2	D	1	5	4	1	0	0

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.

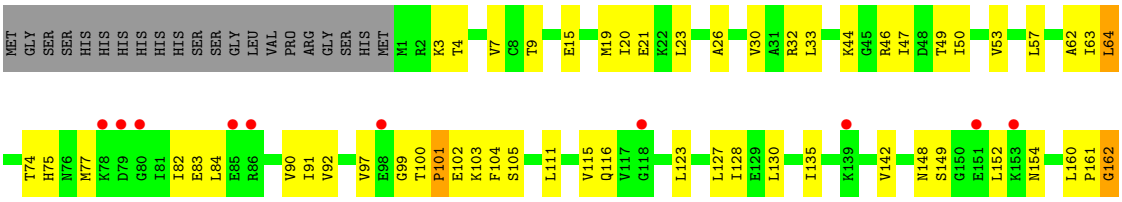
- Molecule 1: Pyruvate kinase

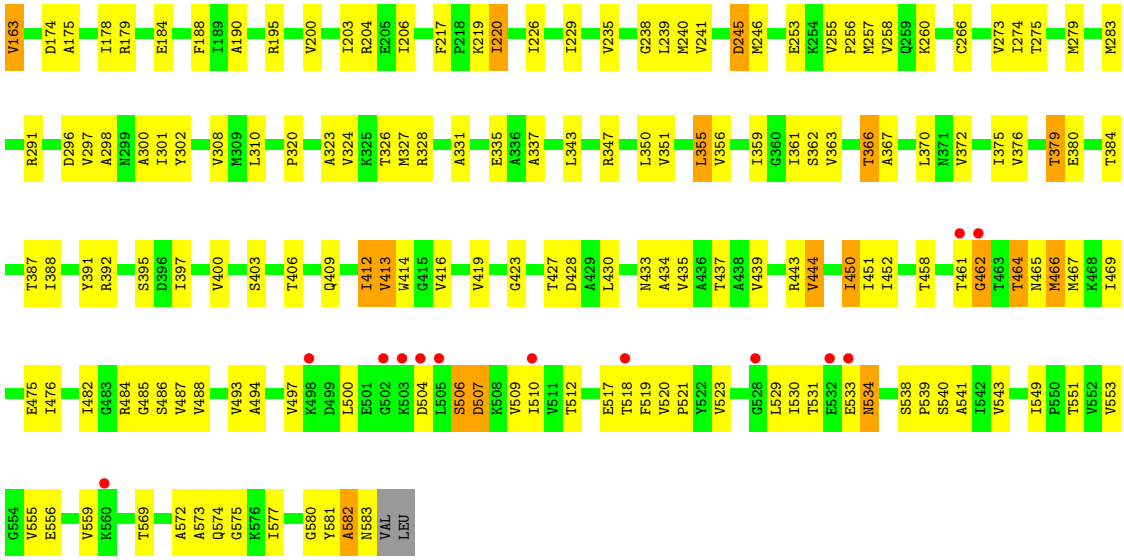
Chain A:



- Molecule 1: Pyruvate kinase

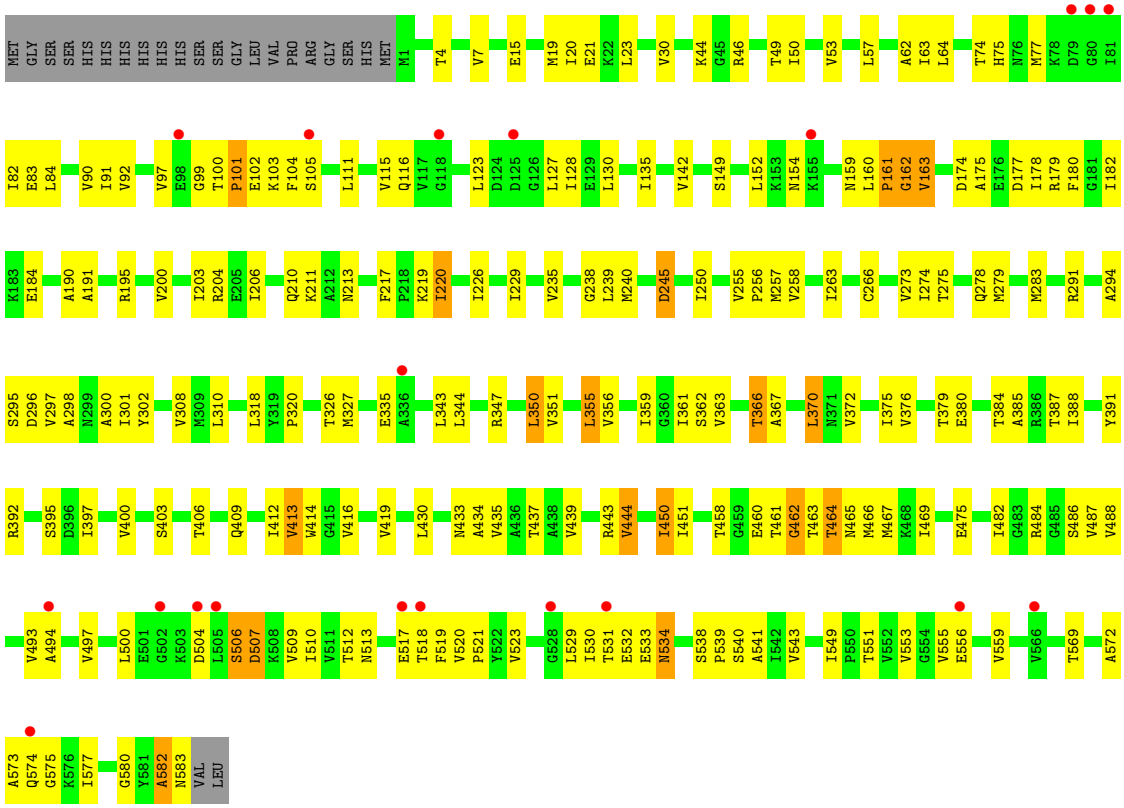
Chain B:





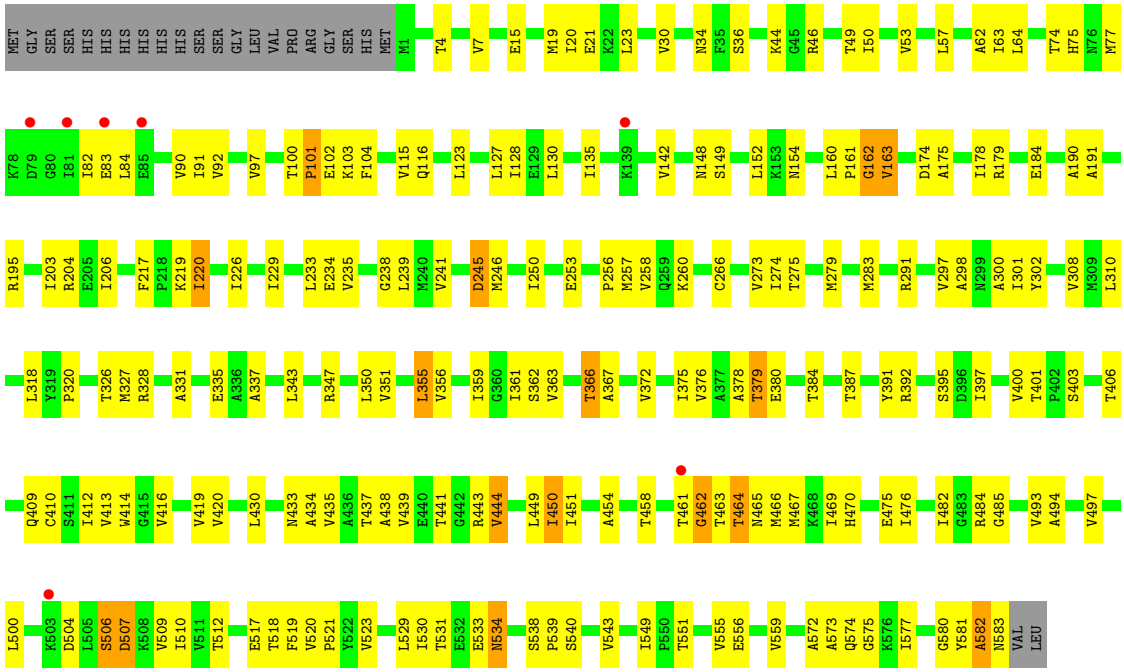
• Molecule 1: Pyruvate kinase

Chain C:



• Molecule 1: Pyruvate kinase

Chain D:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET M1 T4 V7 E15 M19 I20 E21 K22 L23 V30 M34 F35 S36 K44 G45 R46 T49 I50 V53 L57 A62 I63 L64 T74 H75 N76 M77
K78 D79 G80 I81 I82 E83 L84 E85 V90 I91 V92 V97 T100 P101 E102 K103 F104 V115 Q116 L123 L127 I128 E129 L130 I135 K139 V142 N148 S149 L152 K153 N154 L160 P161 G162 V163 D174 A175 I178 R179 E184 A190 A191
R195 I203 R204 E205 I206 F217 P218 K219 I220 I226 I229 L233 E234 V235 G238 L239 M240 V241 D245 M246 I250 E253 P256 M257 V258 Q259 K260 C266 V273 I274 T275 M279 M283 R291 V297 A298 N299 A300 I301 Y302 V308 M309 L310
L318 Y319 P320 T326 M327 R328 A331 E335 A336 A337 L343 R347 L350 V351 L355 V356 I359 G360 I361 S362 V363 T366 A367 V372 I375 V376 A377 A378 T379 E380 T384 T387 Y391 R392 S395 D396 I397 V400 T401 P402 S403 T406
Q409 C410 S411 I412 V413 W414 G415 V416 V419 V420 L430 N433 A434 V435 A436 T437 A438 V439 E440 T441 G442 R443 V444 L449 I450 I451 A454 T458 T461 G462 T463 T464 N465 M466 M467 K468 I469 H470 E475 I476 I482 G483 R484 G485 V493 A494 V497
L500 K503 D504 L505 S506 D507 K508 V509 I510 V511 T512 E517 T518 F519 V520 P521 V522 V523 L529 I530 T531 E532 E533 N534 S538 P539 S540 V543 I549 P550 T551 V555 E556 V559 A572 A573 Q574 G575 K576 I577 G580 Y581 A582 N583 VAL LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.02Å 111.26Å 111.16Å 85.36° 80.15° 70.46°	Depositor
Resolution (Å)	19.90 – 3.05 19.83 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.90-3.05) 97.9 (19.83-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 3.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.264 0.238 , 0.267	Depositor DCC
R_{free} test set	3539 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	95.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17648	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.70	0/4452	0.73	0/6022
1	B	0.62	1/4452 (0.0%)	0.70	0/6022
1	C	0.59	1/4452 (0.0%)	0.69	1/6022 (0.0%)
1	D	0.62	1/4452 (0.0%)	0.71	0/6022
All	All	0.63	3/17808 (0.0%)	0.71	1/24088 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	413	VAL	CB-CG1	6.88	1.67	1.52
1	B	413	VAL	CB-CG1	6.16	1.65	1.52
1	D	410	CYS	CB-SG	-5.74	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	350	LEU	CA-CB-CG	5.12	127.09	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4407	0	4533	185	0
1	B	4407	0	4533	186	1
1	C	4407	0	4533	181	1
1	D	4407	0	4533	178	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	2	0
2	D	5	0	0	1	0
All	All	17648	0	18132	687	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 19.

The worst 5 of 687 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:388:ILE:CD1	1:A:388:ILE:CG1	1.82	1.53
1:C:388:ILE:CG1	1:C:388:ILE:CD1	1.81	1.51
1:B:379:THR:HG22	2:B:586:PO4:O4	1.40	1.18
1:B:257:MET:HE3	1:C:302:TYR:OH	1.62	0.99
1:D:379:THR:HG22	2:D:586:PO4:O2	1.66	0.95

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:B:423:GLY:O	1:C:460:GLU:OE1[1_455]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/606 (96%)	513 (88%)	48 (8%)	20 (3%)	3	17
1	B	581/606 (96%)	514 (88%)	49 (8%)	18 (3%)	4	19
1	C	581/606 (96%)	516 (89%)	47 (8%)	18 (3%)	4	19
1	D	581/606 (96%)	516 (89%)	47 (8%)	18 (3%)	4	19
All	All	2324/2424 (96%)	2059 (89%)	191 (8%)	74 (3%)	4	18

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	220	ILE
1	A	320	PRO
1	A	475	GLU
1	A	556	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/510 (96%)	474 (97%)	16 (3%)	38	67
1	B	490/510 (96%)	474 (97%)	16 (3%)	38	67
1	C	490/510 (96%)	474 (97%)	16 (3%)	38	67
1	D	490/510 (96%)	475 (97%)	15 (3%)	40	68
All	All	1960/2040 (96%)	1897 (97%)	63 (3%)	39	68

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	450	ILE
1	D	379	THR
1	C	296	ASP
1	D	366	THR
1	D	450	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	299	ASN
1	D	470	HIS
1	C	470	HIS
1	D	583	ASN
1	D	110	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	PO4	B	586	-	4,4,4	0.84	0	6,6,6	0.86	0
2	PO4	A	586	-	4,4,4	0.79	0	6,6,6	0.72	0
2	PO4	C	586	-	4,4,4	0.80	0	6,6,6	0.65	0
2	PO4	D	586	-	4,4,4	0.82	0	6,6,6	0.55	0

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.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	586	PO4	2	0
2	A	586	PO4	1	0
2	C	586	PO4	2	0
2	D	586	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	583/606 (96%)	-0.31	3 (0%)	91	79	59, 108, 154, 195	0
1	B	583/606 (96%)	-0.10	23 (3%)	39	19	63, 123, 196, 226	0
1	C	583/606 (96%)	-0.12	20 (3%)	45	22	66, 126, 196, 226	0
1	D	583/606 (96%)	-0.26	7 (1%)	79	58	74, 116, 155, 218	0
All	All	2332/2424 (96%)	-0.20	53 (2%)	60	36	59, 117, 184, 226	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	ASP	9.4
1	B	118	GLY	6.6
1	B	80	GLY	5.0
1	B	504	ASP	4.0
1	C	504	ASP	4.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	D	586	5/5	0.88	0.15	121,125,147,148	0
2	PO4	C	586	5/5	0.89	0.12	111,127,142,143	0
2	PO4	A	586	5/5	0.93	0.09	93,107,128,132	0
2	PO4	B	586	5/5	0.95	0.11	90,117,140,141	0

6.5 Other polymers (i)

There are no such residues in this entry.