Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 09:36 PM EDT

PDB ID	:	5WRP
Title	:	T-state crystal structure of pyruvate kinase from Mycobacterium tuberculosis
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Deposited on	:	2016-12-02
Resolution	:	2.85 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 (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	:	2.37.1
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)	:	2.37.1

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 2.85 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		0.234
Clashscore		8
Ramachandran outliers		0.2%
Sidechain outliers		6.1%
RSRZ outliers		2.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution
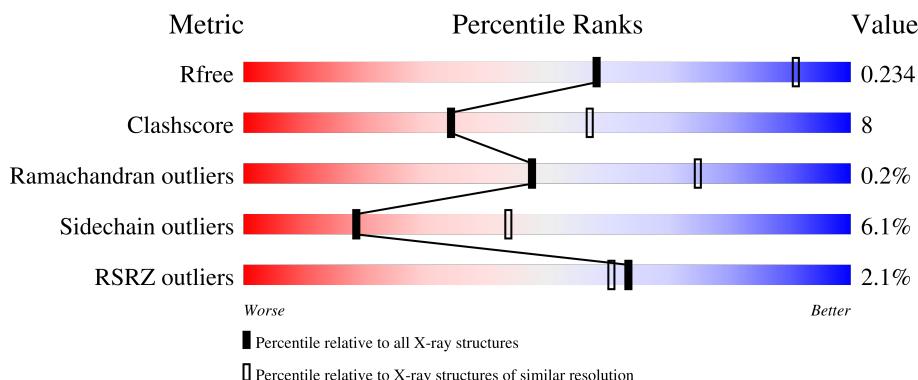
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	475	% / 82% 15% ·
1	B	475	5% / 81% 16% ··
1	C	475	% / 62% 16% · 20%
1	D	475	82% 16% ·
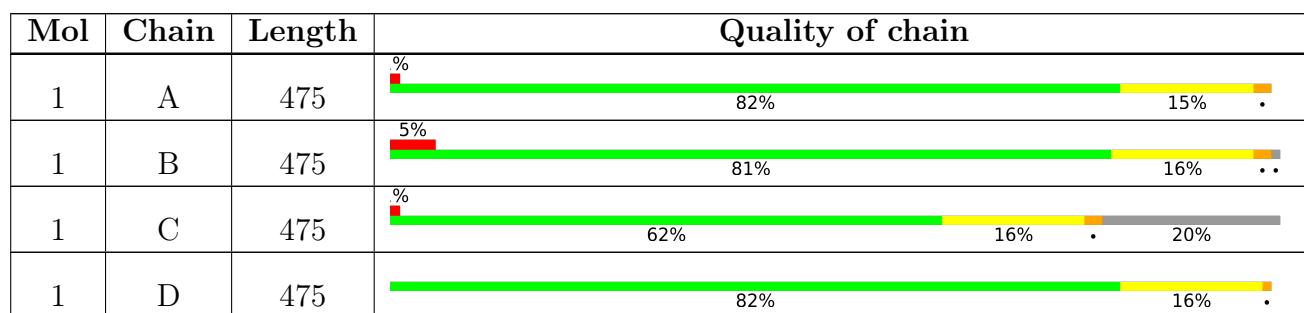
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13803 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
1	A	473	Total 3561	C 2217	N 644	O 681	S 19	0	0	0
1	B	472	Total 3551	C 2211	N 641	O 680	S 19	0	0	0
1	C	378	Total 2867	C 1792	N 517	O 543	S 15	0	0	0
1	D	473	Total 3570	C 2222	N 645	O 684	S 19	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P9WKE5
A	-1	GLY	-	expression tag	UNP P9WKE5
A	0	HIS	-	expression tag	UNP P9WKE5
B	-2	GLY	-	expression tag	UNP P9WKE5
B	-1	GLY	-	expression tag	UNP P9WKE5
B	0	HIS	-	expression tag	UNP P9WKE5
C	-2	GLY	-	expression tag	UNP P9WKE5
C	-1	GLY	-	expression tag	UNP P9WKE5
C	0	HIS	-	expression tag	UNP P9WKE5
D	-2	GLY	-	expression tag	UNP P9WKE5
D	-1	GLY	-	expression tag	UNP P9WKE5
D	0	HIS	-	expression tag	UNP P9WKE5

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
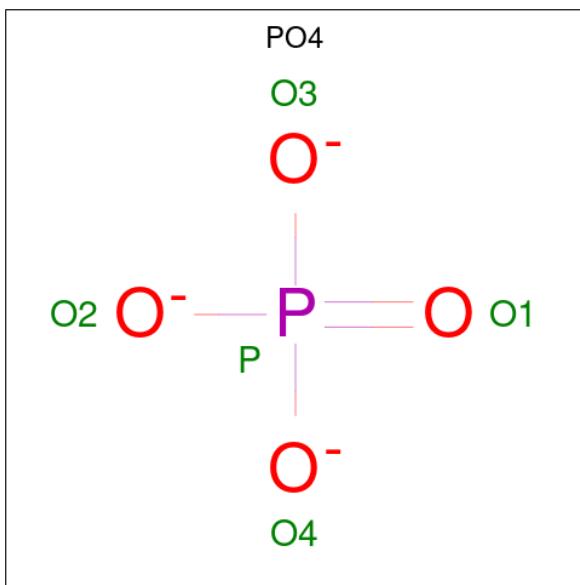
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total 66	O 66	0	0
3	B	70	Total 70	O 70	0	0
3	C	28	Total 28	O 28	0	0
3	D	70	Total 70	O 70	0	0

3 Residue-property plots ⓘ

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:

PRO GLY MET ASN VAL T165 I174 T178 D186 M187 V188 A189 F192 V202 M206 D207 R208 I209 V215 I216 A217 K218 K221 L228 F235 D236 A237 R242 L251 E252 E253 V254 P255 A261 M278 S281 E292 A293 V296 A297 V315 G316

K317 Y318 P319 L320 R324 T325 R328 I329 E335 N336 S337 T338 H345 I346 P347 R348 R351 I354 R359 D360 L370 F373 R382 L386 H387 W409 K418 M419 M425 D430 L433 L434 R441 L444 A449 G450 A451 P452 V456

G457 S458 T459 N460 L461 I462 H463 V464 H465 R466 I467 G468 E469 D470 D471 V472

• Molecule 1: Pyruvate kinase

Chain D:

82%   16%

GLY GLY H0 R4 G5 K6 C9 T10 T15 D18 D19 L20 M29 R33 F36 V46 R50 L65 L75 G76 R77 F78 A79 S80 T83 H84 W85 V91 R92 I93 T94 G100 R111 L112 A113 Q114 V117 V124 V129 A130 L131 V132

V133 E137 G138 D139 D140 V141 E147 D153 I157 S158 K172 M187 F192 A217 K221 L228 F235 R242 V254 P255 L256 V257 Q258 A261 A275 S281 R290 D305 E335 N336 H345 R348 R351 R364 L370

D378 R382 L383 A384 R385 L390 P399 T408 I415 M419 M425 Q428 L436 R441 A451 P452 N460 I461 I462 H463 I467 V472

4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.76Å　129.48Å　243.98Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	88.79　–　2.85 85.06　–　2.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (88.79-2.85) 99.1 (85.06-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.206　,　0.233 0.210　,　0.234	Depositor DCC
R_{free} test set	3479 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	65.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13803	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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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 (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	0.63	0/3612	0.63	0/4906
1	B	0.60	0/3601	0.63	2/4891 (0.0%)
1	C	0.67	0/2908	0.68	1/3949 (0.0%)
1	D	0.64	0/3621	0.65	1/4918 (0.0%)
All	All	0.63	0/13742	0.65	4/18664 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	461	LEU	CA-CB-CG	6.14	129.43	115.30
1	B	461	LEU	CA-CB-CG	5.76	128.56	115.30
1	C	242	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	385	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	3561	0	3627	61	0
1	B	3551	0	3620	59	0
1	C	2867	0	2936	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3570	0	3632	56	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	66	0	0	3	0
3	B	70	0	0	1	0
3	C	28	0	0	2	0
3	D	70	0	0	0	0
All	All	13803	0	13815	230	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 8.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:PHE:HA	1:B:100:GLY:HA3	1.31	1.11
1:B:33:ARG:HD2	1:B:308:MET:CE	1.98	0.94
1:C:451:ALA:HB2	1:C:460:ASN:HD21	1.35	0.91
1:D:451:ALA:HB2	1:D:460:ASN:HD21	1.35	0.89
1:D:370:LEU:HD21	1:D:383:LEU:HD22	1.54	0.89
1:B:451:ALA:HB2	1:B:460:ASN:HD21	1.37	0.88
1:B:33:ARG:HD2	1:B:308:MET:HE1	1.54	0.88
1:A:461:LEU:HD21	1:C:461:LEU:CD2	2.05	0.87
1:A:130:ALA:HB3	1:A:147:GLU:HG3	1.57	0.85
1:A:451:ALA:HB2	1:A:460:ASN:HD21	1.44	0.81
1:B:355:SER:HB2	1:B:383:LEU:CD1	2.12	0.78
1:A:185:VAL:O	1:A:211:ARG:NH2	2.16	0.78
1:D:78:PHE:HA	1:D:100:GLY:HA3	1.66	0.78
1:D:419:MET:HE1	1:D:428:GLN:HB2	1.66	0.78
1:A:78:PHE:HA	1:A:100:GLY:HA3	1.66	0.77
1:C:451:ALA:HB3	1:C:452:PRO:HD2	1.67	0.77
1:C:451:ALA:HB2	1:C:460:ASN:ND2	1.99	0.77
1:D:451:ALA:HB2	1:D:460:ASN:ND2	2.00	0.77
1:A:278:MET:HE3	1:A:296:VAL:HG22	1.68	0.74
1:B:451:ALA:HB2	1:B:460:ASN:ND2	2.01	0.72
1:C:336:ASN:HB3	1:D:256:LEU:CD1	2.19	0.72
1:D:451:ALA:HB3	1:D:452:PRO:HD2	1.71	0.72
1:C:433:LEU:HD23	1:C:467:ILE:HD13	1.71	0.71
1:C:451:ALA:CB	1:C:452:PRO:CD	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:MET:CE	1:D:428:GLN:HB2	2.20	0.71
1:A:451:ALA:HB3	1:A:452:PRO:HD2	1.71	0.71
1:D:6:LYS:NZ	1:D:408:THR:O	2.23	0.71
1:C:296:VAL:CG2	1:C:329:ILE:HG21	2.21	0.70
1:A:364:ARG:NH1	1:C:346:ILE:HD11	2.06	0.70
1:B:451:ALA:HB3	1:B:452:PRO:HD2	1.73	0.70
1:A:451:ALA:HB2	1:A:460:ASN:ND2	2.05	0.70
1:C:451:ALA:CB	1:C:452:PRO:HD2	2.22	0.69
1:B:33:ARG:HD2	1:B:308:MET:HE2	1.71	0.69
1:B:221:LYS:HE2	1:B:248:GLU:OE1	1.93	0.69
1:A:10:THR:OG1	1:A:33:ARG:NH2	2.25	0.69
1:D:451:ALA:CB	1:D:452:PRO:CD	2.71	0.69
1:A:461:LEU:HD21	1:C:461:LEU:HD21	1.76	0.68
1:A:160:PRO:HB3	1:A:248:GLU:CG	2.23	0.68
1:B:451:ALA:CB	1:B:452:PRO:CD	2.72	0.67
1:A:160:PRO:HB3	1:A:248:GLU:HG2	1.75	0.67
1:A:451:ALA:CB	1:A:452:PRO:CD	2.71	0.67
1:C:359:ARG:NH1	1:C:360:ASP:OD2	2.28	0.66
1:A:400:GLU:HG2	3:A:641:HOH:O	1.95	0.66
1:D:242:ARG:HD2	1:D:258:GLN:OE1	1.95	0.65
1:B:278:MET:HE3	1:B:296:VAL:HG22	1.78	0.65
1:B:451:ALA:CB	1:B:452:PRO:HD2	2.27	0.64
1:D:451:ALA:CB	1:D:452:PRO:HD2	2.28	0.64
1:A:461:LEU:CD2	1:C:461:LEU:CD2	2.76	0.63
1:A:451:ALA:CB	1:A:452:PRO:HD2	2.29	0.63
1:A:456:VAL:HG11	1:C:469:GLU:O	1.99	0.63
1:C:434:LEU:HD11	1:C:467:ILE:HG22	1.79	0.62
1:A:194:ARG:HG2	1:A:223:GLU:HG3	1.81	0.62
1:D:111:ARG:HD2	1:D:114:GLN:HE21	1.63	0.62
1:A:278:MET:CE	1:A:296:VAL:HG22	2.30	0.62
1:C:47:ALA:O	1:C:51:VAL:HG23	2.00	0.61
1:B:17:ARG:HB2	1:B:20:LEU:HD22	1.83	0.61
1:B:178:THR:HG23	1:B:209:ILE:HD11	1.83	0.60
1:A:85:TRP:CZ2	1:A:91:VAL:HG21	2.36	0.60
1:D:15:THR:HA	1:D:20:LEU:HD23	1.83	0.60
1:A:15:THR:HA	1:A:20:LEU:HD23	1.85	0.58
1:D:117:VAL:O	1:D:133:VAL:HG21	2.03	0.58
1:D:419:MET:CE	1:D:428:GLN:CB	2.80	0.58
1:A:186:ASP:C	1:A:187:MET:HG3	2.24	0.58
1:A:364:ARG:HH11	1:C:346:ILE:HD11	1.68	0.58
1:D:111:ARG:HD2	1:D:114:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:LEU:CD2	1:D:461:LEU:CD2	2.82	0.57
1:C:434:LEU:HD11	1:C:467:ILE:CG2	2.35	0.57
1:C:292:GLU:O	1:C:296:VAL:HG13	2.04	0.57
1:C:434:LEU:CD1	1:C:467:ILE:CG2	2.83	0.56
1:B:398:TRP:HE3	1:B:400:GLU:OE1	1.88	0.56
1:D:117:VAL:O	1:D:133:VAL:CG2	2.53	0.56
1:A:178:THR:HG23	1:A:209:ILE:HD11	1.86	0.56
1:A:441:ARG:NH2	1:A:471:ASP:OD1	2.39	0.56
1:A:3:ARG:NH1	1:A:30:ASP:OD1	2.39	0.56
1:D:461:LEU:HD13	1:D:461:LEU:C	2.26	0.56
1:C:293:ALA:O	1:C:296:VAL:HG22	2.06	0.55
1:C:278:MET:HE3	1:C:296:VAL:HG12	1.88	0.55
1:B:186:ASP:C	1:B:187:MET:HG3	2.25	0.55
1:C:251:LEU:CD1	1:D:290:ARG:HA	2.37	0.55
1:D:378:ASP:OD1	1:D:382:ARG:NE	2.39	0.54
1:C:451:ALA:HB1	1:C:452:PRO:CD	2.37	0.54
1:D:192:PHE:CZ	1:D:221:LYS:HE3	2.42	0.54
1:C:433:LEU:HD23	1:C:467:ILE:CD1	2.36	0.54
1:D:65:LEU:HD13	1:D:187:MET:HG3	1.90	0.54
1:A:85:TRP:CE2	1:A:91:VAL:HG21	2.43	0.54
1:B:157:ILE:HG22	1:B:159:LEU:HD13	1.90	0.54
1:C:67:ASP:OD1	1:C:218:LYS:NZ	2.40	0.53
1:C:178:THR:HG22	1:C:209:ILE:HD11	1.90	0.53
1:A:461:LEU:CD2	1:C:461:LEU:HD22	2.37	0.53
1:D:36:PHE:O	1:D:172:LYS:NZ	2.42	0.53
1:B:228:LEU:HD21	1:B:261:ALA:HA	1.90	0.53
1:C:281:SER:HB3	1:C:292:GLU:OE1	2.09	0.53
1:C:387:HIS:HA	1:C:409:TRP:CZ3	2.44	0.53
1:B:152:SER:HG	1:B:155:LYS:HZ3	1.55	0.53
1:B:414:PHE:CZ	1:B:436:LEU:HD21	2.44	0.53
1:B:412:GLU:OE1	1:B:438:ARG:NH1	2.43	0.52
1:A:124:VAL:HG22	1:A:157:ILE:HG22	1.91	0.52
1:B:242:ARG:HD3	1:B:258:GLN:OE1	2.08	0.52
1:C:46:VAL:O	1:C:50:ARG:HG3	2.08	0.52
1:D:451:ALA:HB3	1:D:452:PRO:CD	2.38	0.52
1:D:370:LEU:CD2	1:D:383:LEU:HD22	2.35	0.52
1:A:242:ARG:HD3	1:A:258:GLN:OE1	2.08	0.52
1:B:451:ALA:HB1	1:B:452:PRO:CD	2.40	0.52
1:C:325:THR:HG22	1:C:328:ARG:HH11	1.74	0.51
1:A:92:ARG:NH1	1:A:137:GLU:OE1	2.43	0.51
1:B:75:LEU:HD23	1:B:157:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:ILE:HD12	1:C:460:ASN:HA	1.91	0.51
1:D:92:ARG:NH1	1:D:137:GLU:OE2	2.39	0.51
1:D:364:ARG:CG	1:D:364:ARG:HH21	2.24	0.51
1:B:355:SER:HB2	1:B:383:LEU:HD12	1.89	0.51
1:D:419:MET:HE3	1:D:425:MET:HA	1.93	0.51
1:C:228:LEU:HD21	1:C:261:ALA:HA	1.93	0.50
1:B:112:LEU:HG	1:B:141:VAL:HG21	1.92	0.50
1:D:399:PRO:HA	1:D:415:ILE:HD13	1.93	0.50
1:A:359:ARG:NH1	1:A:360:ASP:OD1	2.44	0.50
1:C:451:ALA:CB	1:C:460:ASN:HD21	2.17	0.50
1:D:228:LEU:HD21	1:D:261:ALA:HA	1.93	0.50
1:A:259:LYS:HE2	1:B:301:LEU:HD13	1.92	0.50
1:D:77:ARG:HG3	1:D:153:ASP:CG	2.32	0.50
1:A:451:ALA:HB1	1:A:452:PRO:CD	2.41	0.50
1:C:65:LEU:HD11	1:C:189:ALA:HB2	1.94	0.50
1:A:112:LEU:HG	1:A:141:VAL:HG21	1.94	0.49
1:D:451:ALA:HB1	1:D:452:PRO:CD	2.41	0.49
1:B:3:ARG:NH2	1:B:30:ASP:OD2	2.45	0.49
1:A:160:PRO:HB3	1:A:248:GLU:HG3	1.91	0.49
1:B:36:PHE:O	1:B:172:LYS:NZ	2.45	0.49
1:A:73:ILE:HG22	1:A:157:ILE:CG1	2.43	0.49
1:A:461:LEU:HD22	1:A:462:ILE:N	2.28	0.49
1:D:83:THR:HG23	1:D:84:HIS:N	2.27	0.49
1:A:228:LEU:HD21	1:A:261:ALA:HA	1.95	0.49
1:B:160:PRO:HB3	1:B:248:GLU:HG2	1.93	0.49
1:C:335:GLU:O	1:C:335:GLU:HG2	2.12	0.49
1:C:17:ARG:HB2	1:C:20:LEU:HD13	1.95	0.49
1:C:3:ARG:NH2	1:C:30:ASP:OD2	2.46	0.48
1:C:434:LEU:CD1	1:C:467:ILE:HG21	2.44	0.48
1:C:208:ARG:HH21	1:C:208:ARG:HG3	1.78	0.48
1:A:254:VAL:N	1:A:255:PRO:CD	2.77	0.48
1:C:217:ALA:HB2	1:C:235:PHE:CG	2.49	0.48
1:B:461:LEU:HD13	1:B:461:LEU:C	2.34	0.48
1:A:456:VAL:CG1	1:C:469:GLU:O	2.62	0.48
1:A:456:VAL:HG13	1:C:469:GLU:HG3	1.96	0.48
1:A:73:ILE:HG22	1:A:157:ILE:HG13	1.96	0.47
1:B:254:VAL:N	1:B:255:PRO:CD	2.77	0.47
1:D:451:ALA:CB	1:D:460:ASN:HD21	2.16	0.47
1:C:296:VAL:HG21	1:C:329:ILE:HG21	1.96	0.47
1:A:194:ARG:CG	1:A:223:GLU:HG3	2.44	0.47
1:D:112:LEU:HG	1:D:141:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HD2	1:B:382:ARG:CZ	2.45	0.47
1:A:9:CYS:HB2	1:A:29:MET:SD	2.55	0.46
1:C:296:VAL:HG23	1:C:329:ILE:HG21	1.96	0.46
1:A:83:THR:HG23	1:A:84:HIS:N	2.30	0.46
1:A:461:LEU:CD2	1:C:461:LEU:HD21	2.44	0.46
1:B:9:CYS:HB2	1:B:29:MET:SD	2.56	0.46
1:C:351:ARG:HG2	3:C:619:HOH:O	2.15	0.46
1:C:465:HIS:HB2	1:C:469:GLU:OE2	2.15	0.46
1:A:290:ARG:NE	1:B:277:GLN:OE1	2.44	0.46
1:B:214:PRO:HA	1:B:236:ASP:OD1	2.16	0.46
1:D:364:ARG:HH21	1:D:364:ARG:HG2	1.81	0.46
1:A:469:GLU:O	1:C:456:VAL:HG21	2.15	0.46
1:D:217:ALA:HB2	1:D:235:PHE:CG	2.51	0.46
1:D:370:LEU:HD21	1:D:383:LEU:CD2	2.38	0.46
1:A:217:ALA:HB2	1:A:235:PHE:CG	2.50	0.45
1:B:217:ALA:HB2	1:B:235:PHE:CG	2.52	0.45
1:C:216:ILE:HG12	1:C:237:ALA:HB3	1.98	0.45
1:C:449:ALA:HB3	1:C:461:LEU:HD12	1.98	0.45
1:B:414:PHE:CE2	1:B:436:LEU:HD21	2.51	0.45
1:C:254:VAL:N	1:C:255:PRO:CD	2.80	0.45
1:D:124:VAL:HB	1:D:129:VAL:HG22	1.98	0.45
1:D:254:VAL:N	1:D:255:PRO:CD	2.80	0.45
1:C:174:ILE:O	1:C:178:THR:HG23	2.17	0.45
1:D:94:THR:OG1	1:D:139:ASP:HB3	2.18	0.44
1:B:78:PHE:CA	1:B:100:GLY:HA3	2.22	0.44
1:C:278:MET:CE	1:C:296:VAL:HG12	2.47	0.44
1:C:9:CYS:HB2	1:C:29:MET:SD	2.58	0.44
1:A:217:ALA:HB2	1:A:235:PHE:CD2	2.53	0.44
1:B:451:ALA:HB3	1:B:452:PRO:CD	2.42	0.43
1:C:192:PHE:CE2	1:C:221:LYS:HD3	2.53	0.43
1:D:9:CYS:HB2	1:D:29:MET:SD	2.58	0.43
1:D:75:LEU:HD23	1:D:157:ILE:HD11	2.00	0.43
1:B:217:ALA:HB2	1:B:235:PHE:CD2	2.53	0.43
1:C:217:ALA:HB2	1:C:235:PHE:CD2	2.53	0.43
1:B:157:ILE:HG22	1:B:159:LEU:CD1	2.48	0.43
1:C:336:ASN:HB3	1:D:256:LEU:HD13	1.96	0.43
1:C:444:LEU:HD12	1:C:444:LEU:HA	1.88	0.43
1:C:17:ARG:HG3	1:C:20:LEU:HD22	1.99	0.43
1:B:46:VAL:O	1:B:50:ARG:HG3	2.17	0.43
1:D:85:TRP:CZ2	1:D:91:VAL:HG11	2.54	0.43
1:A:46:VAL:O	1:A:50:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ILE:HG12	1:A:237:ALA:HB3	2.01	0.43
1:B:216:ILE:HG12	1:B:237:ALA:HB3	2.01	0.43
1:C:186:ASP:C	1:C:187:MET:HG3	2.38	0.43
1:C:434:LEU:CD1	1:C:467:ILE:HG22	2.45	0.43
1:D:46:VAL:O	1:D:50:ARG:HG3	2.18	0.43
1:D:419:MET:CE	1:D:425:MET:HA	2.48	0.43
1:C:251:LEU:CD1	1:D:290:ARG:CA	2.97	0.42
1:A:131:LEU:HD23	1:A:143:CYS:HB2	2.01	0.42
1:C:278:MET:HB3	1:C:278:MET:HE2	1.85	0.42
1:B:451:ALA:CB	1:B:460:ASN:HD21	2.20	0.42
1:B:83:THR:HG23	1:B:84:HIS:N	2.34	0.42
1:B:278:MET:HG3	1:B:308:MET:O	2.19	0.42
1:D:217:ALA:HB2	1:D:235:PHE:CD2	2.55	0.42
1:B:218:LYS:HE2	1:B:220:GLU:OE1	2.19	0.42
1:D:4:ARG:NH2	1:D:390:LEU:O	2.51	0.42
1:A:3:ARG:NH2	3:A:607:HOH:O	2.40	0.42
1:A:451:ALA:CB	1:A:460:ASN:HD21	2.24	0.42
1:C:206:MET:HE1	1:C:215:VAL:CG2	2.49	0.42
1:C:320:LEU:HB3	1:C:324:ARG:HH12	1.85	0.42
1:C:463:HIS:CE1	1:C:465:HIS:HB3	2.55	0.42
1:C:15:THR:HA	1:C:20:LEU:HD23	2.01	0.41
1:D:242:ARG:HG3	1:D:275:ALA:O	2.19	0.41
1:B:340:ALA:HB2	3:B:661:HOH:O	2.20	0.41
1:A:463:HIS:CE1	1:A:465:HIS:HB3	2.55	0.41
1:D:364:ARG:CG	1:D:364:ARG:NH2	2.83	0.41
1:A:211:ARG:NH1	1:A:400:GLU:OE1	2.54	0.41
1:D:10:THR:HA	1:D:33:ARG:HB3	2.03	0.41
1:B:278:MET:CE	1:B:296:VAL:HG22	2.48	0.41
1:B:92:ARG:NH1	1:B:137:GLU:OE1	2.45	0.41
1:B:399:PRO:HA	1:B:415:ILE:HD13	2.02	0.41
1:B:419:MET:SD	1:B:425:MET:HA	2.61	0.41
1:A:194:ARG:HG2	1:A:223:GLU:CG	2.49	0.40
1:C:360:ASP:HB3	3:C:616:HOH:O	2.22	0.40
1:A:186:ASP:HA	3:A:641:HOH:O	2.21	0.40
1:B:270:LYS:HA	1:B:271:PRO:HD3	1.95	0.40
1:C:419:MET:SD	1:C:425:MET:HA	2.61	0.40
1:B:355:SER:HB2	1:B:383:LEU:HD11	1.98	0.40
1:B:20:LEU:HA	1:B:20:LEU:HD12	1.84	0.40
1:B:114:GLN:HE21	1:B:114:GLN:HB2	1.72	0.40
1:C:296:VAL:CG2	1:C:297:ALA:N	2.84	0.40
1:B:451:ALA:CB	1:D:463:HIS:NE2	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:VAL:HG12	1:C:206:MET:CE	2.52	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	471/475 (99%)	458 (97%)	12 (2%)	1 (0%)	47	75
1	B	470/475 (99%)	456 (97%)	13 (3%)	1 (0%)	47	75
1	C	374/475 (79%)	362 (97%)	11 (3%)	1 (0%)	41	68
1	D	472/475 (99%)	460 (98%)	11 (2%)	1 (0%)	47	75
All	All	1787/1900 (94%)	1736 (97%)	47 (3%)	4 (0%)	47	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	ALA
1	B	451	ALA
1	C	451	ALA
1	D	451	ALA

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	381/381 (100%)	357 (94%)	24 (6%)	18	42
1	B	380/381 (100%)	359 (94%)	21 (6%)	21	49
1	C	307/381 (81%)	286 (93%)	21 (7%)	16	38
1	D	382/381 (100%)	360 (94%)	22 (6%)	20	46
All	All	1450/1524 (95%)	1362 (94%)	88 (6%)	18	43

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	77	ARG
1	A	80	SER
1	A	90	THR
1	A	91	VAL
1	A	147	GLU
1	A	158	SER
1	A	159	LEU
1	A	187	MET
1	A	195	SER
1	A	248	GLU
1	A	251	LEU
1	A	281	SER
1	A	305	ASP
1	A	336	ASN
1	A	351	ARG
1	A	364	ARG
1	A	385	ARG
1	A	400	GLU
1	A	408	THR
1	A	420	GLN
1	A	436	LEU
1	A	461	LEU
1	A	471	ASP
1	B	18	ASP
1	B	80	SER
1	B	111	ARG
1	B	158	SER
1	B	159	LEU
1	B	187	MET
1	B	201	LEU
1	B	281	SER
1	B	305	ASP

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Mol	Chain	Res	Type
1	B	335	GLU
1	B	345	HIS
1	B	351	ARG
1	B	368	LYS
1	B	375	GLN
1	B	383	LEU
1	B	385	ARG
1	B	400	GLU
1	B	408	THR
1	B	415	ILE
1	B	436	LEU
1	B	461	LEU
1	C	17	ARG
1	C	18	ASP
1	C	19	ASP
1	C	251	LEU
1	C	252	GLU
1	C	281	SER
1	C	335	GLU
1	C	345	HIS
1	C	348	ARG
1	C	370	LEU
1	C	373	PHE
1	C	382	ARG
1	C	385	ARG
1	C	418	LYS
1	C	430	ASP
1	C	441	ARG
1	C	444	LEU
1	C	458	SER
1	C	465	HIS
1	C	467	ILE
1	C	469	GLU
1	D	18	ASP
1	D	77	ARG
1	D	80	SER
1	D	111	ARG
1	D	131	LEU
1	D	147	GLU
1	D	158	SER
1	D	281	SER
1	D	290	ARG

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Mol	Chain	Res	Type
1	D	305	ASP
1	D	335	GLU
1	D	336	ASN
1	D	345	HIS
1	D	348	ARG
1	D	351	ARG
1	D	382	ARG
1	D	385	ARG
1	D	408	THR
1	D	436	LEU
1	D	441	ARG
1	D	461	LEU
1	D	467	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	B	69	GLN
1	B	84	HIS
1	B	114	GLN
1	C	69	GLN
1	C	203	HIS
1	C	336	ASN
1	C	404	GLN
1	C	420	GLN
1	D	69	GLN
1	D	84	HIS
1	D	114	GLN
1	D	182	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	501	-	4,4,4	0.73	0	6,6,6	0.43	0
2	PO4	C	501	-	4,4,4	0.82	0	6,6,6	0.63	0
2	PO4	D	501	-	4,4,4	0.59	0	6,6,6	0.62	0
2	PO4	A	501	-	4,4,4	0.95	0	6,6,6	0.35	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.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	473/475 (99%)	0.17	6 (1%)	77	76	43, 67, 107, 120	0
1	B	472/475 (99%)	0.27	24 (5%)	28	23	52, 79, 109, 118	0
1	C	378/475 (79%)	0.30	7 (1%)	66	64	47, 80, 116, 135	0
1	D	473/475 (99%)	-0.01	0	100	100	43, 66, 90, 109	0
All	All	1796/1900 (94%)	0.18	37 (2%)	63	60	43, 72, 108, 135	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	TRP	4.6
1	B	75	LEU	3.7
1	B	129	VAL	3.5
1	C	315	VAL	3.5
1	B	157	ILE	3.3
1	B	38	HIS	3.3
1	B	93	ILE	3.2
1	B	36	PHE	3.2
1	B	143	CYS	3.2
1	C	338	THR	3.0
1	C	36	PHE	2.9
1	B	123	LEU	2.9
1	A	151	VAL	2.9
1	B	156	GLY	2.8
1	A	0	HIS	2.8
1	C	317	LYS	2.7
1	B	126	ASP	2.7
1	B	124	VAL	2.7
1	B	91	VAL	2.6
1	C	470	ASP	2.6
1	C	320	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	141	VAL	2.5
1	B	131	LEU	2.4
1	A	169	LEU	2.3
1	B	155	LYS	2.3
1	B	125	ASP	2.3
1	B	151	VAL	2.2
1	B	81	GLY	2.2
1	A	472	VAL	2.2
1	B	121	ARG	2.1
1	A	85	TRP	2.1
1	C	318	TYR	2.1
1	B	74	ARG	2.1
1	B	78	PHE	2.0
1	B	169	LEU	2.0
1	B	107	THR	2.0
1	B	154	ASN	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 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
2	PO4	C	501	5/5	0.92	0.16	80,91,93,102	0
2	PO4	B	501	5/5	0.96	0.12	71,74,83,85	0
2	PO4	A	501	5/5	0.96	0.18	58,62,71,71	0
2	PO4	D	501	5/5	0.97	0.14	61,67,74,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.