



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:07 PM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

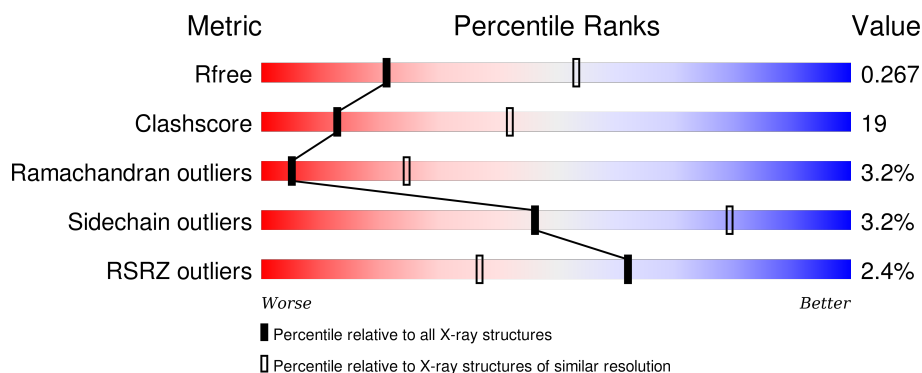
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	606	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>.</div> <div>.</div> </div> </div>
1	B	606	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>.</div> <div>.</div> </div> </div>
1	C	606	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>32%</div> <div>.</div> <div>.</div> </div> </div>
1	D	606	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>.</div> <div>.</div> </div> </div>

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

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

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

2 Entry composition

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
1	A	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	B	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	C	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			
1	D	583	Total	C	N	O	S	0	0	0
			4407	2745	764	880	18			

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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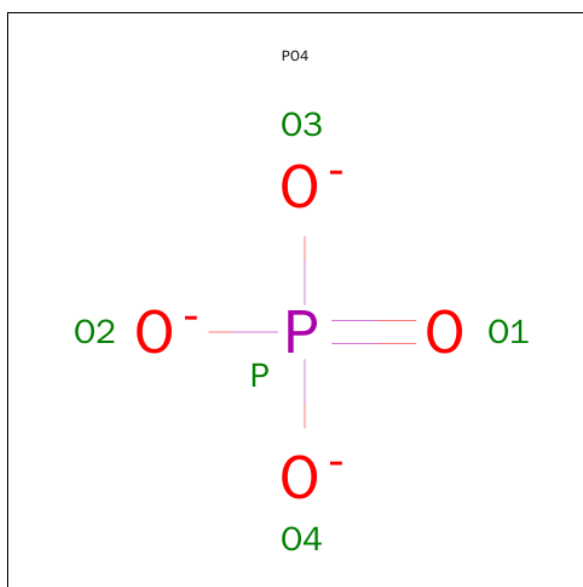
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP Q6GG09
B	-19	GLY	-	EXPRESSION TAG	UNP Q6GG09
B	-18	SER	-	EXPRESSION TAG	UNP Q6GG09
B	-17	SER	-	EXPRESSION TAG	UNP Q6GG09
B	-16	HIS	-	EXPRESSION TAG	UNP Q6GG09
B	-15	HIS	-	EXPRESSION TAG	UNP Q6GG09
B	-14	HIS	-	EXPRESSION TAG	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: O₄P).



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

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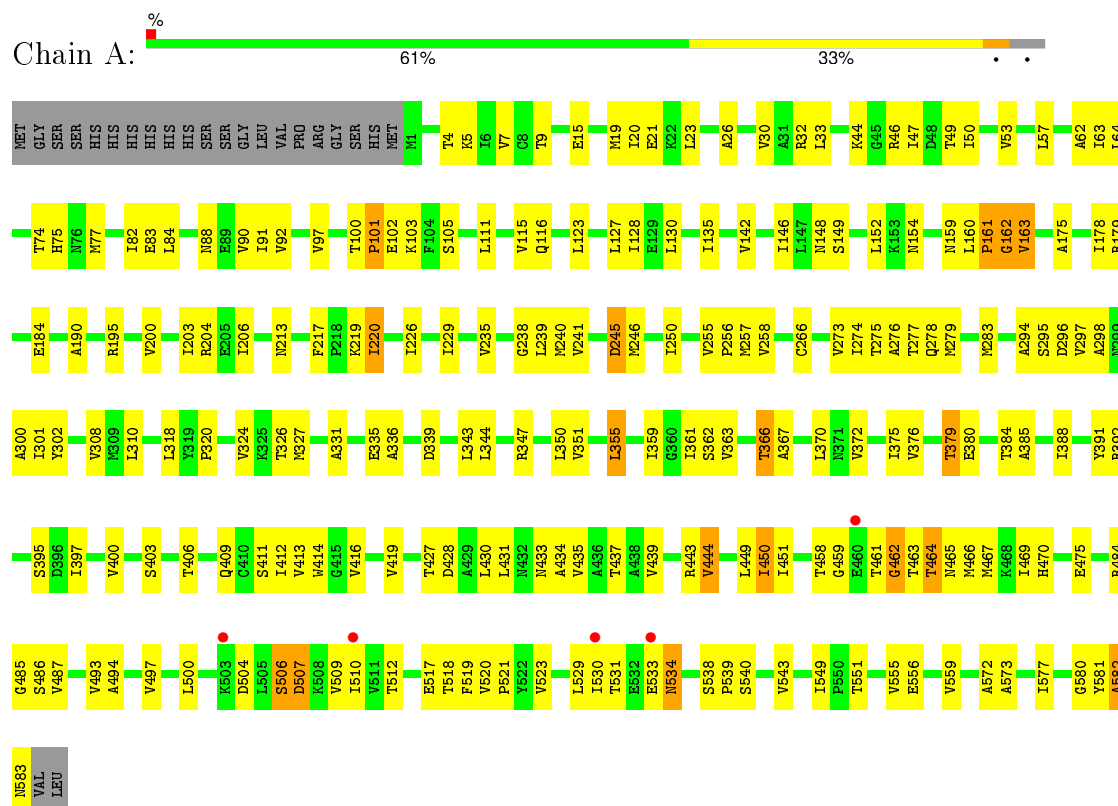
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

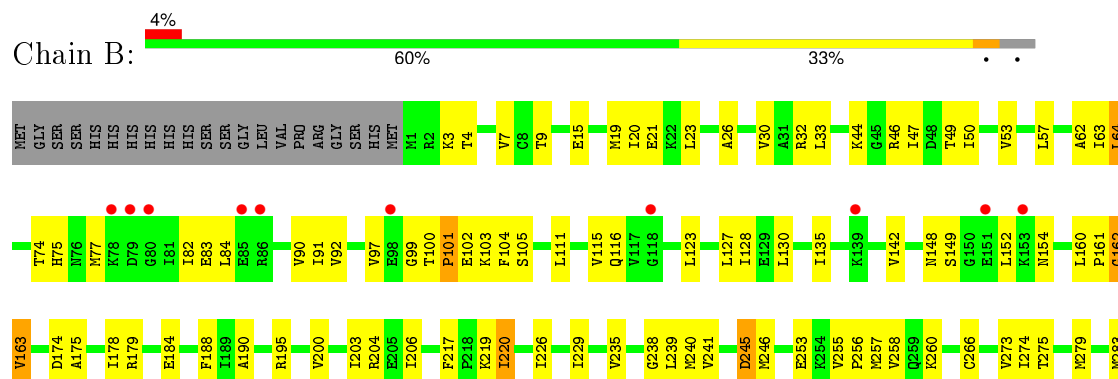
3 Residue-property plots

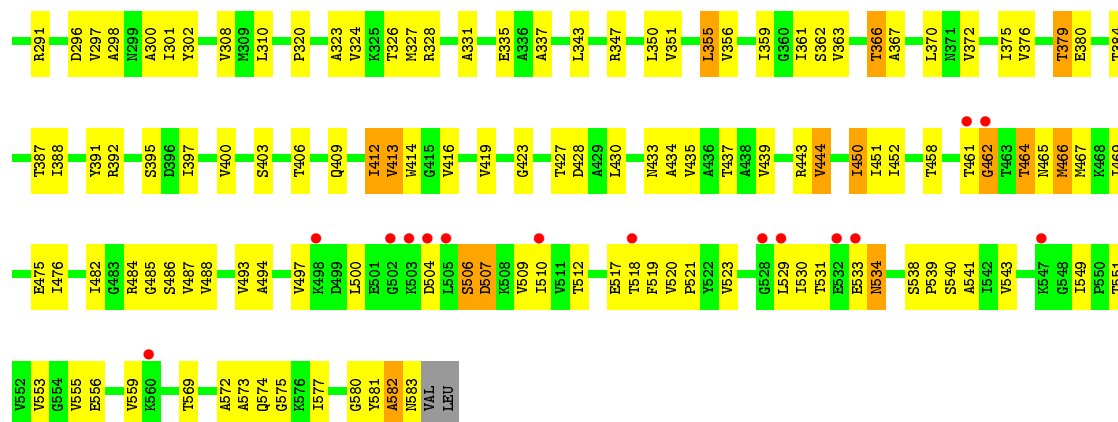
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

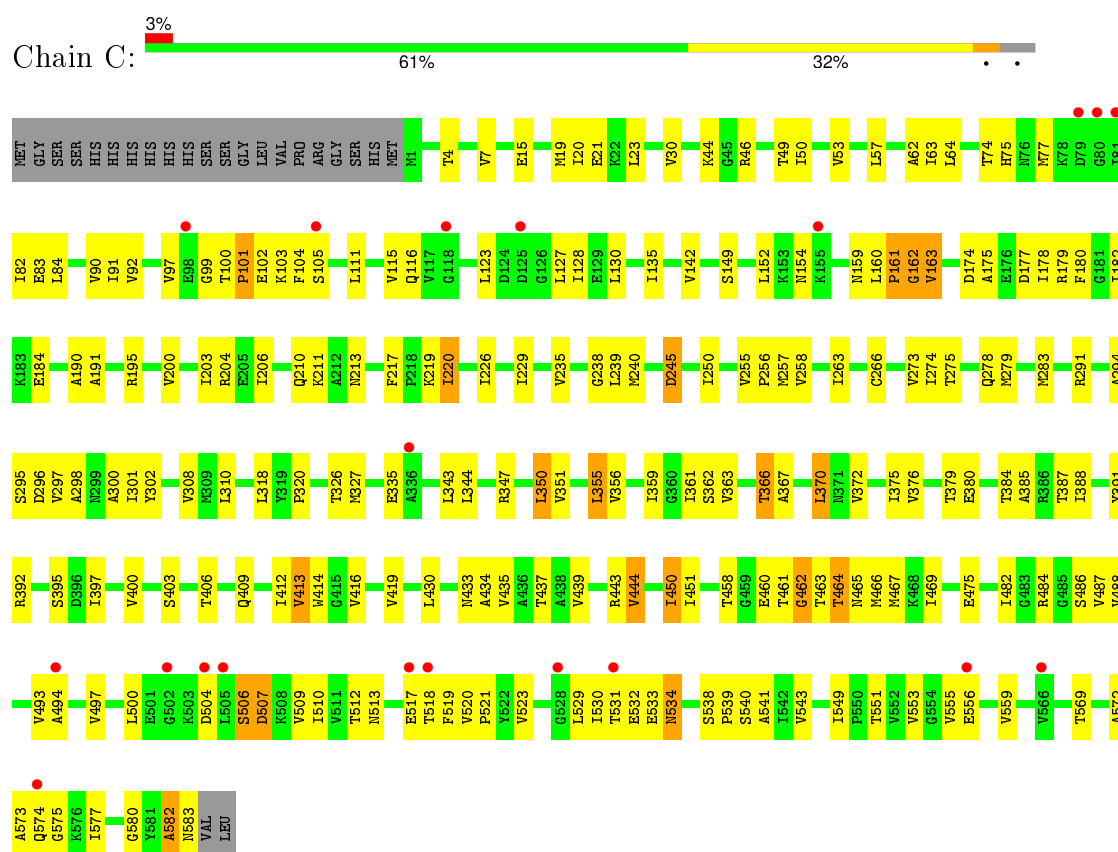


• Molecule 1: Pyruvate kinase

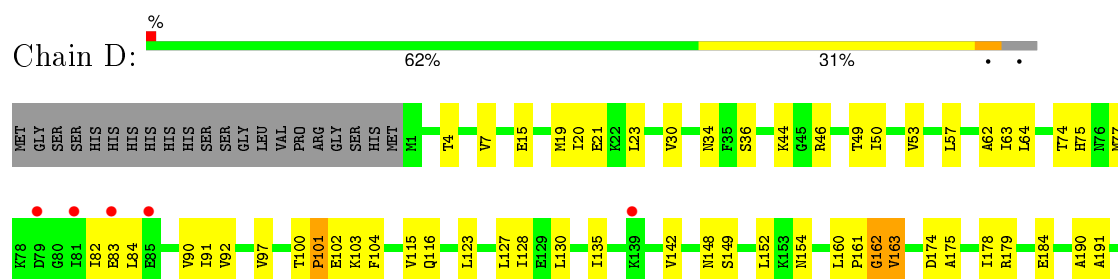


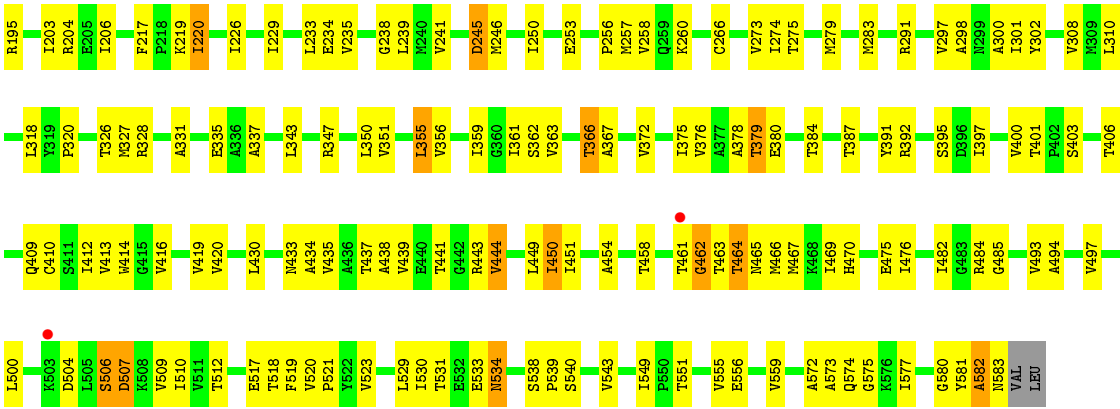


• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase





4 Data and refinement statistics

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) 97.1 (19.83-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.6.0107	Depositor
R, R_{free}	0.236 , 0.264 0.238 , 0.267	Depositor DCC
R_{free} test set	3539 reflections (5.37%)	DCC
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 , 62.4	EDS
Estimated twinning fraction	0.000 for -h,-h+k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 69483 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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.

All (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:CG1	1:A:388:ILE:CD1	1.82	1.53
1:C:388:ILE:CD1	1:C:388:ILE:CG1	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
1:D:4:THR:HG22	1:D:335:GLU:OE2	1.67	0.94
1:C:379:THR:HG22	2:C:586:PO4:O3	1.68	0.93
1:A:4:THR:HG22	1:A:335:GLU:OE2	1.67	0.93
1:A:363:VAL:HG22	1:A:451:ILE:HD11	1.53	0.91
1:A:379:THR:HG22	2:A:586:PO4:O1	1.72	0.89
1:B:308:VAL:HG11	1:B:327:MET:SD	2.15	0.86
1:B:4:THR:HG22	1:B:335:GLU:OE2	1.75	0.86
1:D:74:THR:HG22	1:D:75:HIS:O	1.75	0.86
1:C:363:VAL:HG22	1:C:451:ILE:HD11	1.57	0.86
1:A:74:THR:HG22	1:A:75:HIS:O	1.76	0.85
1:B:74:THR:HG22	1:B:75:HIS:O	1.75	0.85
1:C:74:THR:HG22	1:C:75:HIS:O	1.77	0.84
1:B:363:VAL:HG22	1:B:451:ILE:HD11	1.59	0.84
1:B:257:MET:CE	1:C:302:TYR:OH	2.26	0.84
1:A:123:LEU:HD11	1:A:130:LEU:HD11	1.59	0.83
1:D:419:VAL:HG21	1:D:437:THR:HG21	1.60	0.82
1:B:531:THR:HG21	1:B:540:SER:HB3	1.61	0.82
1:A:92:VAL:HG23	1:A:142:VAL:HB	1.62	0.81
1:C:419:VAL:HG21	1:C:437:THR:HG21	1.60	0.81
1:A:419:VAL:HG21	1:A:437:THR:HG21	1.62	0.80
1:C:4:THR:HG22	1:C:335:GLU:OE2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:THR:HG21	1:C:540:SER:HB3	1.62	0.79
1:B:419:VAL:HG21	1:B:437:THR:HG21	1.65	0.78
1:B:92:VAL:HG23	1:B:142:VAL:HB	1.65	0.77
1:A:531:THR:HG21	1:A:540:SER:HB3	1.67	0.77
1:C:92:VAL:HG23	1:C:142:VAL:HB	1.65	0.77
1:D:510:ILE:HD11	1:D:523:VAL:HG22	1.66	0.77
1:D:92:VAL:HG23	1:D:142:VAL:HB	1.65	0.77
1:D:275:THR:HG22	1:D:279:MET:CE	2.14	0.77
1:D:363:VAL:HG22	1:D:451:ILE:HD11	1.67	0.77
1:C:308:VAL:HG11	1:C:327:MET:SD	2.25	0.76
1:D:123:LEU:HD11	1:D:130:LEU:HD11	1.68	0.76
1:B:123:LEU:HD11	1:B:130:LEU:HD11	1.68	0.76
1:D:308:VAL:HG11	1:D:327:MET:SD	2.25	0.76
1:D:379:THR:HG23	1:D:384:THR:HB	1.68	0.76
1:C:123:LEU:HD11	1:C:130:LEU:HD11	1.66	0.75
1:D:531:THR:HG21	1:D:540:SER:HB3	1.69	0.74
1:B:510:ILE:HD11	1:B:523:VAL:HG22	1.68	0.74
1:A:257:MET:HG2	1:D:337:ALA:HB1	1.67	0.74
1:C:510:ILE:HD11	1:C:523:VAL:HG22	1.68	0.74
1:B:275:THR:HG22	1:B:279:MET:CE	2.18	0.74
1:A:275:THR:HG22	1:A:279:MET:CE	2.18	0.74
1:A:19:MET:O	1:A:23:LEU:HD13	1.87	0.74
1:B:379:THR:HG23	1:B:384:THR:HB	1.68	0.73
1:A:379:THR:HG23	1:A:384:THR:HB	1.68	0.73
1:D:351:VAL:HG21	1:D:391:TYR:OH	1.89	0.72
1:D:257:MET:HE1	1:D:260:LYS:HD2	1.72	0.71
1:A:510:ILE:HD11	1:A:523:VAL:HG22	1.72	0.71
1:A:302:TYR:OH	1:D:257:MET:HE2	1.90	0.71
1:B:351:VAL:HG21	1:B:391:TYR:OH	1.91	0.71
1:A:367:ALA:HA	1:A:372:VAL:HG22	1.70	0.71
1:A:302:TYR:OH	1:D:257:MET:CE	2.38	0.71
1:A:77:MET:HE2	1:A:82:ILE:HG21	1.73	0.70
1:C:351:VAL:HG21	1:C:391:TYR:OH	1.91	0.70
1:D:84:LEU:HD23	1:D:90:VAL:HG21	1.74	0.69
1:A:308:VAL:HG11	1:A:327:MET:SD	2.33	0.69
1:A:302:TYR:CZ	1:D:257:MET:HE3	2.27	0.69
1:D:274:ILE:HD11	1:D:412:ILE:HD11	1.74	0.69
1:C:84:LEU:HD23	1:C:90:VAL:HG21	1.74	0.69
1:D:419:VAL:HG21	1:D:437:THR:CG2	2.22	0.69
1:C:419:VAL:HG21	1:C:437:THR:CG2	2.23	0.69
1:D:19:MET:O	1:D:23:LEU:HD13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HD23	1:B:90:VAL:HG21	1.76	0.68
1:B:257:MET:HE1	1:C:302:TYR:CZ	2.29	0.67
1:D:77:MET:HE2	1:D:82:ILE:HG21	1.77	0.67
1:D:363:VAL:HG13	1:D:451:ILE:HD13	1.76	0.67
1:A:30:VAL:HG13	1:A:62:ALA:HB3	1.77	0.67
1:B:257:MET:CE	1:C:302:TYR:CZ	2.77	0.67
1:C:275:THR:HG22	1:C:279:MET:CE	2.25	0.67
1:B:362:SER:HB3	1:B:467:MET:HE1	1.77	0.66
1:B:77:MET:HE2	1:B:82:ILE:HG21	1.75	0.66
1:A:363:VAL:HG13	1:A:451:ILE:HD13	1.78	0.66
1:C:283:MET:SD	1:C:326:THR:HG21	2.36	0.66
1:B:337:ALA:HB1	1:C:257:MET:HG2	1.79	0.65
1:B:379:THR:CG2	2:B:586:PO4:O4	2.32	0.65
1:D:275:THR:HG22	1:D:279:MET:HE1	1.77	0.65
1:A:494:ALA:HB2	1:A:500:LEU:HD23	1.79	0.65
1:B:266:CYS:SG	1:B:273:VAL:CG2	2.85	0.64
1:C:7:VAL:HG22	1:C:30:VAL:HB	1.79	0.64
1:A:162:GLY:HA2	1:A:163:VAL:O	1.97	0.64
1:B:379:THR:CG2	1:B:384:THR:HB	2.27	0.64
1:A:275:THR:HG22	1:A:279:MET:HE1	1.79	0.64
1:C:77:MET:HE2	1:C:82:ILE:HG21	1.79	0.64
1:A:419:VAL:HG21	1:A:437:THR:CG2	2.26	0.64
1:A:274:ILE:HD11	1:A:412:ILE:HD11	1.80	0.64
1:C:379:THR:HG23	1:C:384:THR:HB	1.78	0.64
1:B:363:VAL:HG13	1:B:451:ILE:HD13	1.80	0.64
1:C:530:ILE:HG23	1:C:555:VAL:HG21	1.79	0.64
1:A:379:THR:CG2	1:A:384:THR:HB	2.27	0.63
1:B:530:ILE:HG23	1:B:555:VAL:HG21	1.79	0.63
1:D:162:GLY:HA2	1:D:163:VAL:O	1.99	0.63
1:A:363:VAL:CG1	1:A:375:ILE:HD13	2.28	0.63
1:B:419:VAL:HG21	1:B:437:THR:CG2	2.28	0.63
1:C:274:ILE:HD11	1:C:412:ILE:HD11	1.80	0.63
1:A:430:LEU:HD23	1:A:430:LEU:C	2.19	0.63
1:B:403:SER:OG	1:B:406:THR:HG23	1.97	0.63
1:C:297:VAL:O	1:C:300:ALA:HB3	1.99	0.63
1:D:355:LEU:O	1:D:355:LEU:HD22	1.98	0.63
1:A:115:VAL:HG12	1:A:160:LEU:HD23	1.81	0.63
1:B:517:GLU:O	1:B:520:VAL:HG22	1.98	0.62
1:A:7:VAL:HG22	1:A:30:VAL:HB	1.80	0.62
1:B:253:GLU:HA	1:C:294:ALA:CB	2.29	0.62
1:A:582:ALA:O	1:A:583:ASN:ND2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:VAL:CG1	1:C:375:ILE:HD13	2.30	0.62
1:C:162:GLY:HA2	1:C:163:VAL:O	1.98	0.62
1:D:509:VAL:O	1:D:509:VAL:HG23	2.00	0.62
1:B:127:LEU:HD22	1:B:128:ILE:HG23	1.82	0.62
1:C:367:ALA:HA	1:C:372:VAL:HG22	1.81	0.62
1:A:297:VAL:O	1:A:300:ALA:HB3	2.00	0.62
1:D:379:THR:CG2	1:D:384:THR:HB	2.28	0.61
1:A:400:VAL:HG22	1:A:419:VAL:CG2	2.30	0.61
1:D:266:CYS:SG	1:D:273:VAL:CG2	2.88	0.61
1:C:219:LYS:O	1:C:220:ILE:C	2.39	0.61
1:D:30:VAL:HG13	1:D:62:ALA:HB3	1.82	0.61
1:D:274:ILE:CD1	1:D:412:ILE:HD11	2.31	0.61
1:A:219:LYS:O	1:A:220:ILE:C	2.38	0.61
1:B:19:MET:O	1:B:23:LEU:HD13	2.01	0.61
1:C:115:VAL:HG12	1:C:160:LEU:HD23	1.83	0.61
1:D:297:VAL:O	1:D:300:ALA:HB3	2.01	0.61
1:A:413:VAL:HG12	1:A:416:VAL:HG23	1.83	0.61
1:C:19:MET:O	1:C:23:LEU:HD13	2.01	0.60
1:B:430:LEU:HD23	1:B:430:LEU:C	2.22	0.60
1:A:84:LEU:HD23	1:A:90:VAL:HG21	1.82	0.60
1:A:283:MET:SD	1:A:326:THR:HG21	2.42	0.60
1:D:7:VAL:HG22	1:D:30:VAL:HB	1.84	0.60
1:A:530:ILE:HG23	1:A:555:VAL:HG21	1.84	0.60
1:C:266:CYS:SG	1:C:273:VAL:CG2	2.90	0.60
1:D:283:MET:SD	1:D:326:THR:HG21	2.42	0.60
1:D:539:PRO:O	1:D:543:VAL:HG13	2.01	0.60
1:B:494:ALA:HB2	1:B:500:LEU:HD23	1.83	0.60
1:A:302:TYR:CZ	1:D:257:MET:CE	2.84	0.60
1:C:517:GLU:O	1:C:520:VAL:HG22	2.01	0.59
1:D:494:ALA:HB2	1:D:500:LEU:HD23	1.84	0.59
1:A:294:ALA:CB	1:D:253:GLU:HA	2.32	0.59
1:D:530:ILE:HG23	1:D:555:VAL:HG21	1.84	0.59
1:A:278:GLN:HB3	1:D:291:ARG:NH2	2.17	0.59
1:D:83:GLU:C	1:D:84:LEU:HD12	2.23	0.59
1:A:403:SER:OG	1:A:406:THR:HG23	2.03	0.59
1:D:430:LEU:C	1:D:430:LEU:HD23	2.23	0.59
1:B:20:ILE:HG22	1:B:53:VAL:HG11	1.85	0.59
1:C:400:VAL:HG22	1:C:419:VAL:CG2	2.33	0.59
1:B:539:PRO:O	1:B:543:VAL:HG13	2.03	0.58
1:C:379:THR:CG2	1:C:384:THR:HB	2.33	0.58
1:B:275:THR:HG22	1:B:279:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:VAL:HG21	1:A:450:ILE:HD11	1.85	0.58
1:B:283:MET:SD	1:B:326:THR:HG21	2.43	0.58
1:D:178:ILE:HD11	1:D:206:ILE:CD1	2.32	0.58
1:C:376:VAL:HG11	1:C:434:ALA:HB1	1.84	0.58
1:B:367:ALA:HA	1:B:372:VAL:HG22	1.86	0.58
1:A:384:THR:OG1	1:A:464:THR:HB	2.03	0.58
1:B:162:GLY:HA2	1:B:163:VAL:O	2.02	0.58
1:B:363:VAL:CG1	1:B:375:ILE:HD13	2.34	0.58
1:B:115:VAL:HG12	1:B:160:LEU:HD23	1.85	0.58
1:C:380:GLU:O	1:C:406:THR:HG21	2.04	0.58
1:C:384:THR:OG1	1:C:464:THR:HB	2.04	0.58
1:B:82:ILE:HG22	1:B:152:LEU:HB3	1.86	0.58
1:D:497:VAL:HG11	1:D:518:THR:OG1	2.04	0.58
1:A:539:PRO:O	1:A:543:VAL:HG13	2.03	0.58
1:A:549:ILE:O	1:A:551:THR:HG23	2.03	0.58
1:D:367:ALA:HA	1:D:372:VAL:HG22	1.86	0.58
1:C:355:LEU:O	1:C:355:LEU:HD22	2.04	0.58
1:D:403:SER:OG	1:D:406:THR:HG23	2.03	0.57
1:D:115:VAL:HG12	1:D:160:LEU:HD23	1.85	0.57
1:C:494:ALA:HB2	1:C:500:LEU:HD23	1.86	0.57
1:B:178:ILE:HD11	1:B:206:ILE:CD1	2.35	0.57
1:C:549:ILE:O	1:C:551:THR:HG23	2.03	0.57
1:C:539:PRO:O	1:C:543:VAL:HG13	2.04	0.57
1:C:275:THR:HG22	1:C:279:MET:HE1	1.86	0.57
1:D:517:GLU:O	1:D:520:VAL:HG22	2.04	0.57
1:A:509:VAL:O	1:A:509:VAL:HG23	2.04	0.57
1:C:435:VAL:O	1:C:439:VAL:HG23	2.05	0.57
1:D:362:SER:HB3	1:D:467:MET:HE1	1.87	0.57
1:C:127:LEU:HD22	1:C:128:ILE:HG23	1.86	0.57
1:A:376:VAL:HG11	1:A:434:ALA:HB1	1.86	0.57
1:D:275:THR:HG22	1:D:279:MET:HE3	1.86	0.56
1:B:235:VAL:HG12	1:B:235:VAL:O	2.05	0.56
1:A:351:VAL:HG21	1:A:391:TYR:OH	2.05	0.56
1:C:82:ILE:HG22	1:C:152:LEU:HB3	1.88	0.56
1:C:430:LEU:C	1:C:430:LEU:HD23	2.25	0.56
1:A:461:THR:HG23	1:A:462:GLY:H	1.70	0.56
1:B:274:ILE:CD1	1:B:412:ILE:HD11	2.36	0.56
1:B:274:ILE:HD11	1:B:412:ILE:HD11	1.86	0.56
1:B:308:VAL:CG1	1:B:327:MET:SD	2.93	0.56
1:D:582:ALA:O	1:D:583:ASN:ND2	2.38	0.56
1:D:20:ILE:HG22	1:D:53:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:GLN:HA	1:D:135:ILE:HD11	1.88	0.56
1:A:204:ARG:NH1	1:A:235:VAL:O	2.39	0.56
1:D:461:THR:HG23	1:D:462:GLY:H	1.70	0.56
1:A:127:LEU:HD22	1:A:128:ILE:HG23	1.87	0.56
1:C:204:ARG:NH1	1:C:235:VAL:O	2.39	0.56
1:D:444:VAL:HG21	1:D:450:ILE:HD11	1.86	0.56
1:C:461:THR:HG23	1:C:462:GLY:H	1.72	0.55
1:B:380:GLU:O	1:B:406:THR:HG21	2.05	0.55
1:C:363:VAL:HG13	1:C:451:ILE:HD13	1.86	0.55
1:A:178:ILE:HD11	1:A:206:ILE:CD1	2.36	0.55
1:A:82:ILE:HG22	1:A:152:LEU:HB3	1.88	0.55
1:A:529:LEU:HB3	1:A:551:THR:HG22	1.89	0.55
1:B:275:THR:HG22	1:B:279:MET:HE1	1.86	0.55
1:C:362:SER:HB3	1:C:467:MET:HE1	1.89	0.55
1:A:278:GLN:OE1	1:D:291:ARG:NE	2.40	0.54
1:D:549:ILE:O	1:D:551:THR:HG23	2.08	0.54
1:B:257:MET:HE2	1:B:260:LYS:HD2	1.89	0.54
1:D:82:ILE:HG22	1:D:152:LEU:HB3	1.89	0.54
1:D:494:ALA:HB3	1:D:512:THR:HG22	1.89	0.54
1:B:30:VAL:HG13	1:B:62:ALA:HB3	1.89	0.54
1:C:497:VAL:HG11	1:C:518:THR:OG1	2.07	0.54
1:B:529:LEU:HB3	1:B:551:THR:HG22	1.89	0.54
1:B:461:THR:HG23	1:B:462:GLY:H	1.72	0.54
1:D:351:VAL:HG21	1:D:391:TYR:CZ	2.42	0.54
1:A:362:SER:HB3	1:A:467:MET:HE1	1.90	0.54
1:B:444:VAL:HG21	1:B:450:ILE:HD11	1.90	0.54
1:B:20:ILE:CG2	1:B:53:VAL:HG11	2.38	0.54
1:B:235:VAL:CG1	1:B:235:VAL:O	2.55	0.54
1:B:97:VAL:HG11	1:B:103:LYS:HE3	1.88	0.54
1:D:127:LEU:HD22	1:D:128:ILE:HG23	1.90	0.54
1:A:486:SER:O	1:A:487:VAL:HG13	2.07	0.54
1:A:433:ASN:O	1:A:434:ALA:C	2.45	0.54
1:A:92:VAL:CG2	1:A:142:VAL:HB	2.37	0.54
1:D:274:ILE:HD11	1:D:412:ILE:CD1	2.37	0.54
1:B:77:MET:HE1	1:B:104:PHE:CD2	2.43	0.54
1:A:83:GLU:C	1:A:84:LEU:HD12	2.28	0.54
1:C:494:ALA:HB3	1:C:512:THR:HG22	1.90	0.54
1:B:174:ASP:O	1:B:178:ILE:HG23	2.07	0.54
1:C:444:VAL:HG21	1:C:450:ILE:HD11	1.90	0.54
1:A:275:THR:HG22	1:A:279:MET:HE3	1.89	0.54
1:B:361:ILE:HG13	1:B:391:TYR:CZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:CD1	1:A:412:ILE:HD11	2.37	0.53
1:B:274:ILE:HD11	1:B:412:ILE:CD1	2.39	0.53
1:C:44:LYS:HE2	1:C:184:GLU:OE2	2.08	0.53
1:A:159:ASN:O	1:A:161:PRO:HD3	2.09	0.53
1:D:435:VAL:O	1:D:439:VAL:HG23	2.07	0.53
1:A:517:GLU:O	1:A:520:VAL:HG22	2.08	0.53
1:D:400:VAL:HG22	1:D:419:VAL:CG2	2.38	0.53
1:B:175:ALA:O	1:B:179:ARG:HG3	2.09	0.53
1:D:384:THR:OG1	1:D:464:THR:HB	2.08	0.53
1:C:509:VAL:O	1:C:509:VAL:HG23	2.08	0.53
1:C:245:ASP:OD1	1:C:245:ASP:N	2.42	0.53
1:A:308:VAL:CG1	1:A:327:MET:CE	2.86	0.53
1:B:226:ILE:HD12	1:B:258:VAL:CG1	2.39	0.53
1:D:245:ASP:OD1	1:D:245:ASP:N	2.42	0.53
1:B:384:THR:OG1	1:B:464:THR:HB	2.09	0.53
1:A:367:ALA:CA	1:A:372:VAL:HG22	2.38	0.53
1:B:256:PRO:CG	1:C:295:SER:HB2	2.39	0.53
1:D:178:ILE:HD11	1:D:206:ILE:HD13	1.91	0.53
1:D:529:LEU:HB3	1:D:551:THR:HG22	1.92	0.52
1:A:428:ASP:OD2	1:B:427:THR:N	2.41	0.52
1:D:239:LEU:CD2	1:D:241:VAL:HG23	2.40	0.52
1:B:494:ALA:HB3	1:B:512:THR:HG22	1.90	0.52
1:A:380:GLU:O	1:A:406:THR:HG21	2.09	0.52
1:D:174:ASP:O	1:D:178:ILE:HG23	2.09	0.52
1:A:469:ILE:HG21	1:B:355:LEU:HD23	1.91	0.52
1:A:278:GLN:OE1	1:D:291:ARG:CZ	2.57	0.52
1:A:494:ALA:HB3	1:A:512:THR:HG22	1.91	0.52
1:D:219:LYS:O	1:D:220:ILE:C	2.47	0.52
1:A:44:LYS:HE2	1:A:184:GLU:OE2	2.09	0.52
1:C:226:ILE:HD12	1:C:258:VAL:CG1	2.39	0.52
1:A:392:ARG:HA	1:A:414:TRP:CZ3	2.44	0.52
1:C:30:VAL:HG13	1:C:62:ALA:HB3	1.92	0.52
1:B:127:LEU:CD2	1:B:128:ILE:HG23	2.39	0.52
1:A:463:THR:HG23	1:B:574:GLN:OE1	2.10	0.52
1:C:20:ILE:HG22	1:C:53:VAL:HG11	1.91	0.52
1:C:178:ILE:HD11	1:C:206:ILE:CD1	2.39	0.52
1:B:83:GLU:C	1:B:84:LEU:HD12	2.31	0.52
1:D:380:GLU:O	1:D:406:THR:HG21	2.10	0.52
1:C:20:ILE:HD12	1:C:49:THR:CG2	2.40	0.52
1:A:506:SER:OG	1:A:507:ASP:N	2.43	0.52
1:B:92:VAL:CG2	1:B:142:VAL:HB	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ILE:HB	1:A:416:VAL:HA	1.92	0.51
1:A:20:ILE:HG22	1:A:53:VAL:HG11	1.92	0.51
1:B:20:ILE:HD12	1:B:49:THR:CG2	2.40	0.51
1:A:359:ILE:HD12	1:A:465:ASN:HA	1.92	0.51
1:A:359:ILE:CD1	1:A:465:ASN:HA	2.40	0.51
1:B:297:VAL:O	1:B:300:ALA:HB3	2.10	0.51
1:A:116:GLN:HA	1:A:135:ILE:HD11	1.92	0.51
1:A:310:LEU:HD21	1:A:327:MET:HE2	1.93	0.51
1:B:509:VAL:O	1:B:509:VAL:HG23	2.10	0.51
1:C:15:GLU:HG2	1:C:46:ARG:HE	1.75	0.51
1:D:359:ILE:HD12	1:D:465:ASN:HA	1.93	0.51
1:D:92:VAL:CG2	1:D:142:VAL:HB	2.39	0.51
1:D:204:ARG:NH1	1:D:235:VAL:O	2.43	0.51
1:A:295:SER:HB2	1:D:256:PRO:HG3	1.91	0.51
1:B:484:ARG:C	1:B:572:ALA:HB3	2.31	0.51
1:D:506:SER:OG	1:D:507:ASP:N	2.43	0.51
1:C:77:MET:SD	1:C:99:GLY:HA3	2.51	0.51
1:B:253:GLU:HA	1:C:294:ALA:HB2	1.93	0.51
1:C:392:ARG:HA	1:C:414:TRP:CZ3	2.46	0.51
1:C:361:ILE:HG13	1:C:391:TYR:CZ	2.46	0.50
1:B:359:ILE:HD12	1:B:465:ASN:HA	1.93	0.50
1:A:497:VAL:HG11	1:A:518:THR:OG1	2.11	0.50
1:C:397:ILE:HB	1:C:416:VAL:HA	1.93	0.50
1:C:77:MET:HE1	1:C:104:PHE:CD2	2.47	0.50
1:D:20:ILE:CG2	1:D:53:VAL:HG11	2.41	0.50
1:B:44:LYS:HE2	1:B:184:GLU:OE2	2.11	0.50
1:D:376:VAL:HG11	1:D:434:ALA:HB1	1.94	0.50
1:D:493:VAL:CG1	1:D:559:VAL:HG13	2.42	0.50
1:A:400:VAL:HG22	1:A:419:VAL:HG23	1.93	0.50
1:A:175:ALA:O	1:A:179:ARG:HG3	2.11	0.50
1:B:351:VAL:HG21	1:B:391:TYR:CZ	2.46	0.50
1:B:257:MET:HE3	1:C:302:TYR:CZ	2.44	0.50
1:C:351:VAL:HG21	1:C:391:TYR:CZ	2.46	0.50
1:A:111:LEU:HD23	1:A:111:LEU:C	2.32	0.50
1:C:403:SER:OG	1:C:406:THR:HG23	2.12	0.50
1:D:239:LEU:HD21	1:D:241:VAL:HG23	1.94	0.50
1:D:484:ARG:C	1:D:572:ALA:HB3	2.32	0.50
1:C:50:ILE:HG21	1:C:63:ILE:HD11	1.94	0.50
1:D:400:VAL:O	1:D:400:VAL:HG12	2.11	0.49
1:C:229:ILE:HD11	1:C:239:LEU:CD1	2.42	0.49
1:A:344:LEU:HD12	1:A:344:LEU:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ALA:HA	1:A:372:VAL:CG2	2.40	0.49
1:B:484:ARG:HG3	1:B:573:ALA:HB2	1.94	0.49
1:D:363:VAL:CG1	1:D:375:ILE:HD13	2.42	0.49
1:C:175:ALA:O	1:C:179:ARG:HG3	2.13	0.49
1:D:298:ALA:HB1	1:D:302:TYR:CE2	2.47	0.49
1:C:127:LEU:CD2	1:C:128:ILE:HG23	2.42	0.49
1:D:582:ALA:O	1:D:583:ASN:CG	2.51	0.49
1:A:100:THR:HG23	1:A:101:PRO:HD2	1.94	0.49
1:B:291:ARG:CZ	1:C:278:GLN:OE1	2.60	0.49
1:C:363:VAL:HG22	1:C:451:ILE:CD1	2.38	0.49
1:A:92:VAL:HG22	1:A:142:VAL:O	2.12	0.49
1:D:538:SER:HB2	1:D:539:PRO:HD2	1.94	0.49
1:B:435:VAL:O	1:B:439:VAL:HG23	2.12	0.49
1:D:226:ILE:HD12	1:D:258:VAL:CG1	2.43	0.49
1:C:529:LEU:HB3	1:C:551:THR:HG22	1.94	0.49
1:B:256:PRO:HG3	1:C:295:SER:HB2	1.93	0.49
1:C:359:ILE:CD1	1:C:465:ASN:HA	2.42	0.49
1:D:359:ILE:CD1	1:D:465:ASN:HA	2.42	0.49
1:D:175:ALA:O	1:D:179:ARG:HG3	2.13	0.49
1:D:392:ARG:HA	1:D:414:TRP:CZ3	2.48	0.49
1:D:44:LYS:HE2	1:D:184:GLU:OE2	2.12	0.49
1:B:178:ILE:HD11	1:B:206:ILE:HD13	1.94	0.49
1:B:7:VAL:HG22	1:B:30:VAL:HB	1.95	0.49
1:B:549:ILE:O	1:B:551:THR:HG23	2.13	0.49
1:C:274:ILE:CD1	1:C:412:ILE:HD11	2.42	0.49
1:A:301:ILE:CD1	1:A:331:ALA:HA	2.43	0.48
1:C:400:VAL:HG22	1:C:419:VAL:HG23	1.94	0.48
1:D:97:VAL:HG11	1:D:103:LYS:HE3	1.95	0.48
1:B:219:LYS:O	1:B:220:ILE:C	2.51	0.48
1:D:100:THR:HG23	1:D:101:PRO:HD2	1.95	0.48
1:B:226:ILE:HD11	1:B:246:MET:HE3	1.95	0.48
1:D:15:GLU:HG2	1:D:46:ARG:HE	1.77	0.48
1:C:275:THR:HG22	1:C:279:MET:HE3	1.93	0.48
1:C:20:ILE:CG2	1:C:53:VAL:HG11	2.43	0.48
1:A:15:GLU:HG2	1:A:46:ARG:HE	1.78	0.48
1:C:116:GLN:HA	1:C:135:ILE:HD11	1.95	0.48
1:A:97:VAL:HG11	1:A:103:LYS:HE3	1.96	0.48
1:C:582:ALA:O	1:C:583:ASN:ND2	2.47	0.48
1:D:128:ILE:HG22	1:D:148:ASN:O	2.14	0.48
1:A:190:ALA:HA	1:A:217:PHE:O	2.13	0.48
1:D:400:VAL:CG2	1:D:437:THR:HG21	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:VAL:HG22	1:B:419:VAL:CG2	2.42	0.48
1:A:178:ILE:HD12	1:A:203:ILE:HG23	1.96	0.48
1:A:298:ALA:O	1:A:301:ILE:N	2.44	0.48
1:C:97:VAL:HG11	1:C:103:LYS:HE3	1.95	0.48
1:B:355:LEU:HD22	1:B:355:LEU:O	2.14	0.48
1:B:359:ILE:CD1	1:B:465:ASN:C	2.82	0.48
1:A:493:VAL:CG1	1:A:559:VAL:HG13	2.44	0.48
1:C:484:ARG:HG3	1:C:573:ALA:HB2	1.96	0.48
1:B:366:THR:HG22	1:B:367:ALA:N	2.29	0.48
1:A:127:LEU:CD2	1:A:128:ILE:HG23	2.44	0.48
1:C:178:ILE:HD12	1:C:203:ILE:HG23	1.96	0.48
1:B:493:VAL:CG1	1:B:559:VAL:HG13	2.43	0.48
1:A:20:ILE:HD12	1:A:49:THR:CG2	2.44	0.48
1:D:573:ALA:O	1:D:575:GLY:N	2.42	0.48
1:C:375:ILE:HG23	1:C:451:ILE:HG23	1.95	0.48
1:D:355:LEU:C	1:D:355:LEU:HD22	2.34	0.47
1:C:367:ALA:CA	1:C:372:VAL:HG22	2.44	0.47
1:C:83:GLU:C	1:C:84:LEU:HD12	2.34	0.47
1:B:497:VAL:HG11	1:B:518:THR:OG1	2.14	0.47
1:A:484:ARG:HG3	1:A:573:ALA:HB2	1.95	0.47
1:B:200:VAL:O	1:B:203:ILE:N	2.48	0.47
1:D:91:ILE:HD13	1:D:102:GLU:HG3	1.96	0.47
1:A:75:HIS:HB2	1:A:105:SER:OG	2.14	0.47
1:A:366:THR:HG22	1:A:367:ALA:N	2.29	0.47
1:D:375:ILE:HG23	1:D:451:ILE:HG23	1.96	0.47
1:A:274:ILE:HD11	1:A:412:ILE:CD1	2.43	0.47
1:D:266:CYS:SG	1:D:273:VAL:HG22	2.55	0.47
1:A:361:ILE:HG13	1:A:391:TYR:CZ	2.49	0.47
1:A:295:SER:HB2	1:D:256:PRO:CG	2.44	0.47
1:A:255:VAL:N	1:A:256:PRO:CD	2.77	0.47
1:B:15:GLU:HG2	1:B:46:ARG:HE	1.78	0.47
1:C:488:VAL:HG12	1:C:569:THR:OG1	2.14	0.47
1:C:530:ILE:HG12	1:C:577:ILE:HD13	1.97	0.47
1:A:351:VAL:HG21	1:A:391:TYR:CZ	2.50	0.47
1:A:435:VAL:O	1:A:439:VAL:HG23	2.14	0.47
1:C:400:VAL:CG2	1:C:437:THR:HG21	2.44	0.47
1:B:77:MET:HE2	1:B:82:ILE:CG2	2.45	0.47
1:A:494:ALA:CB	1:A:500:LEU:HD23	2.45	0.47
1:D:509:VAL:CG2	1:D:509:VAL:O	2.62	0.47
1:D:229:ILE:HD11	1:D:239:LEU:CD1	2.45	0.47
1:D:298:ALA:O	1:D:301:ILE:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ALA:O	1:C:301:ILE:N	2.46	0.47
1:B:91:ILE:HD13	1:B:102:GLU:HG3	1.97	0.47
1:B:21:GLU:HG3	1:B:57:LEU:HD11	1.96	0.47
1:A:50:ILE:HG21	1:A:63:ILE:HD11	1.96	0.47
1:C:356:VAL:HG12	1:C:387:THR:HG21	1.96	0.47
1:A:226:ILE:HD12	1:A:258:VAL:CG1	2.44	0.47
1:C:100:THR:HG23	1:C:101:PRO:HD2	1.96	0.47
1:C:379:THR:CG2	2:C:586:PO4:O3	2.52	0.47
1:A:302:TYR:OH	1:D:257:MET:HE3	2.08	0.47
1:D:485:GLY:N	1:D:572:ALA:HB3	2.30	0.47
1:C:217:PHE:CE1	1:C:238:GLY:HA3	2.50	0.47
1:C:91:ILE:HD13	1:C:102:GLU:HG3	1.97	0.47
1:A:239:LEU:CD2	1:A:241:VAL:HG23	2.45	0.47
1:A:520:VAL:HG12	1:A:543:VAL:HG11	1.97	0.47
1:B:239:LEU:CD2	1:B:241:VAL:HG23	2.45	0.47
1:A:266:CYS:SG	1:A:273:VAL:CG2	3.03	0.47
1:C:235:VAL:O	1:C:235:VAL:CG1	2.62	0.46
1:A:21:GLU:HG3	1:A:57:LEU:HD11	1.97	0.46
1:B:116:GLN:HA	1:B:135:ILE:HD11	1.97	0.46
1:B:266:CYS:SG	1:B:273:VAL:HG22	2.55	0.46
1:C:520:VAL:HG12	1:C:543:VAL:HG11	1.97	0.46
1:A:200:VAL:O	1:A:203:ILE:N	2.48	0.46
1:D:359:ILE:CD1	1:D:465:ASN:C	2.84	0.46
1:B:582:ALA:O	1:B:583:ASN:ND2	2.48	0.46
1:B:100:THR:HG23	1:B:101:PRO:HD2	1.96	0.46
1:D:497:VAL:HG11	1:D:518:THR:CB	2.45	0.46
1:B:226:ILE:HD12	1:B:258:VAL:HG11	1.97	0.46
1:A:240:MET:CE	1:A:274:ILE:HD12	2.45	0.46
1:D:226:ILE:HD12	1:D:258:VAL:HG11	1.96	0.46
1:A:91:ILE:HD13	1:A:102:GLU:HG3	1.98	0.46
1:A:245:ASP:OD1	1:A:245:ASP:N	2.48	0.46
1:C:92:VAL:CG2	1:C:142:VAL:HB	2.39	0.46
1:B:204:ARG:NH1	1:B:235:VAL:O	2.48	0.46
1:B:239:LEU:HD21	1:B:241:VAL:HG23	1.97	0.46
1:A:427:THR:N	1:B:428:ASP:OD2	2.48	0.46
1:C:486:SER:O	1:C:487:VAL:HG13	2.15	0.46
1:D:160:LEU:O	1:D:162:GLY:N	2.49	0.46
1:C:240:MET:CE	1:C:274:ILE:HD12	2.46	0.46
1:A:582:ALA:O	1:A:583:ASN:CG	2.54	0.46
1:B:433:ASN:O	1:B:434:ALA:C	2.54	0.46
1:A:520:VAL:N	1:A:521:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:ARG:C	1:C:572:ALA:HB3	2.36	0.46
1:A:257:MET:HG2	1:D:337:ALA:CB	2.41	0.46
1:D:20:ILE:HD12	1:D:49:THR:CG2	2.45	0.46
1:B:229:ILE:HD11	1:B:239:LEU:CD1	2.46	0.46
1:B:356:VAL:HG12	1:B:387:THR:HG21	1.98	0.46
1:A:372:VAL:HG23	1:A:395:SER:OG	2.15	0.46
1:D:266:CYS:CB	1:D:273:VAL:CG2	2.94	0.46
1:B:392:ARG:HA	1:B:414:TRP:CZ3	2.51	0.46
1:D:438:ALA:O	1:D:441:THR:OG1	2.34	0.46
1:C:308:VAL:CG1	1:C:327:MET:SD	3.00	0.46
1:D:366:THR:HG22	1:D:367:ALA:N	2.31	0.46
1:D:301:ILE:CD1	1:D:331:ALA:HA	2.46	0.46
1:B:323:ALA:O	1:B:326:THR:HG22	2.16	0.45
1:C:235:VAL:O	1:C:235:VAL:HG12	2.15	0.45
1:A:178:ILE:HD11	1:A:206:ILE:HD13	1.97	0.45
1:A:20:ILE:CG2	1:A:53:VAL:HG11	2.46	0.45
1:B:359:ILE:HD13	1:B:466:MET:N	2.30	0.45
1:B:376:VAL:HG11	1:B:434:ALA:HB1	1.96	0.45
1:C:574:GLN:OE1	1:D:463:THR:HG23	2.16	0.45
1:B:128:ILE:HG22	1:B:148:ASN:O	2.16	0.45
1:B:245:ASP:OD1	1:B:245:ASP:N	2.50	0.45
1:C:370:LEU:HD21	1:D:355:LEU:HA	1.98	0.45
1:C:497:VAL:HG11	1:C:518:THR:CB	2.47	0.45
1:C:92:VAL:HG22	1:C:142:VAL:O	2.17	0.45
1:B:77:MET:SD	1:B:99:GLY:HA3	2.57	0.45
1:C:359:ILE:HD12	1:C:465:ASN:HA	1.97	0.45
1:C:21:GLU:HG3	1:C:57:LEU:HD11	1.98	0.45
1:B:530:ILE:HG12	1:B:577:ILE:HD13	1.99	0.45
1:D:435:VAL:HG21	1:D:470:HIS:CE1	2.51	0.45
1:A:497:VAL:HG11	1:A:518:THR:CB	2.47	0.45
1:A:484:ARG:C	1:A:572:ALA:HB3	2.38	0.45
1:B:397:ILE:HB	1:B:416:VAL:HA	1.99	0.45
1:A:343:LEU:O	1:A:347:ARG:HG2	2.17	0.45
1:D:191:ALA:HB2	1:D:203:ILE:CD1	2.47	0.45
1:D:484:ARG:HG3	1:D:573:ALA:HB2	1.99	0.45
1:D:520:VAL:HG12	1:D:543:VAL:HG11	1.99	0.44
1:B:255:VAL:HB	1:C:291:ARG:HG2	1.99	0.44
1:C:226:ILE:HD12	1:C:258:VAL:HG11	1.98	0.44
1:B:64:LEU:HD12	1:B:188:PHE:CB	2.47	0.44
1:A:375:ILE:HG23	1:A:451:ILE:HG23	1.99	0.44
1:C:384:THR:O	1:C:385:ALA:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ILE:HD11	1:C:412:ILE:CD1	2.48	0.44
1:A:509:VAL:O	1:A:509:VAL:CG2	2.65	0.44
1:D:127:LEU:CD2	1:D:128:ILE:HG23	2.46	0.44
1:A:217:PHE:CE1	1:A:238:GLY:HA3	2.52	0.44
1:D:397:ILE:HB	1:D:416:VAL:HA	1.98	0.44
1:C:363:VAL:HG11	1:C:388:ILE:HD12	1.97	0.44
1:B:538:SER:HB2	1:B:539:PRO:HD2	1.99	0.44
1:D:372:VAL:HG23	1:D:395:SER:OG	2.17	0.44
1:A:359:ILE:CD1	1:A:465:ASN:C	2.85	0.44
1:B:573:ALA:O	1:B:575:GLY:N	2.46	0.44
1:C:413:VAL:HG12	1:C:416:VAL:HG23	1.99	0.44
1:D:367:ALA:CA	1:D:372:VAL:HG22	2.46	0.44
1:B:533:GLU:O	1:B:534:ASN:HB2	2.18	0.44
1:A:33:LEU:HD11	1:A:47:ILE:HG13	1.99	0.44
1:D:92:VAL:HG12	1:D:104:PHE:CD1	2.53	0.44
1:D:328:ARG:O	1:D:331:ALA:HB3	2.18	0.44
1:B:291:ARG:NH2	1:C:278:GLN:HB3	2.32	0.44
1:D:361:ILE:HG13	1:D:391:TYR:CZ	2.52	0.44
1:A:435:VAL:HG21	1:A:470:HIS:CE1	2.53	0.44
1:D:217:PHE:CE1	1:D:238:GLY:HA3	2.53	0.44
1:B:361:ILE:HG13	1:B:391:TYR:CE1	2.53	0.44
1:C:200:VAL:O	1:C:203:ILE:N	2.50	0.44
1:D:376:VAL:O	1:D:376:VAL:HG13	2.17	0.44
1:A:5:LYS:HG3	1:A:411:SER:O	2.17	0.44
1:A:335:GLU:O	1:A:336:ALA:C	2.56	0.44
1:C:111:LEU:HG	1:C:160:LEU:HD21	2.00	0.44
1:B:240:MET:CE	1:B:274:ILE:HD12	2.47	0.44
1:D:433:ASN:O	1:D:434:ALA:C	2.55	0.44
1:C:493:VAL:CG1	1:C:559:VAL:HG13	2.48	0.44
1:B:255:VAL:HB	1:C:291:ARG:CG	2.48	0.43
1:A:266:CYS:CB	1:A:273:VAL:CG2	2.96	0.43
1:A:276:ALA:C	1:A:277:THR:HG23	2.39	0.43
1:B:9:THR:OG1	1:B:32:ARG:NH1	2.45	0.43
1:B:33:LEU:HD11	1:B:47:ILE:HG13	2.00	0.43
1:C:482:ILE:HG13	1:C:541:ALA:HB1	1.99	0.43
1:B:310:LEU:HD21	1:B:327:MET:HE2	2.00	0.43
1:A:310:LEU:CD2	1:A:327:MET:HE2	2.49	0.43
1:B:266:CYS:CB	1:B:273:VAL:CG2	2.96	0.43
1:C:372:VAL:HG23	1:C:395:SER:OG	2.18	0.43
1:A:400:VAL:CG2	1:A:437:THR:HG21	2.47	0.43
1:C:308:VAL:CG1	1:C:327:MET:CE	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ILE:HG12	1:C:273:VAL:HG11	2.00	0.43
1:C:433:ASN:O	1:C:434:ALA:C	2.57	0.43
1:B:97:VAL:HG21	1:B:103:LYS:HG2	2.01	0.43
1:B:485:GLY:N	1:B:572:ALA:HB3	2.33	0.43
1:A:355:LEU:HD22	1:A:355:LEU:O	2.18	0.43
1:D:50:ILE:HG21	1:D:63:ILE:HD11	2.01	0.43
1:C:469:ILE:HG21	1:D:355:LEU:HD23	1.98	0.43
1:C:266:CYS:CB	1:C:273:VAL:CG2	2.96	0.43
1:B:512:THR:HG21	1:B:519:PHE:CE2	2.54	0.43
1:B:20:ILE:HD12	1:B:49:THR:HG22	2.00	0.43
1:A:485:GLY:N	1:A:572:ALA:HB3	2.33	0.43
1:D:533:GLU:O	1:D:534:ASN:CB	2.67	0.43
1:D:378:ALA:HB3	1:D:454:ALA:HB2	1.99	0.43
1:A:7:VAL:HG21	1:A:274:ILE:HD13	2.00	0.43
1:B:372:VAL:HG23	1:B:395:SER:OG	2.19	0.43
1:D:77:MET:HE1	1:D:104:PHE:CD2	2.53	0.43
1:D:413:VAL:HG12	1:D:416:VAL:HG23	2.00	0.43
1:D:190:ALA:HA	1:D:217:PHE:O	2.19	0.43
1:A:339:ASP:C	1:A:339:ASP:OD1	2.57	0.43
1:A:400:VAL:CG2	1:A:419:VAL:CG2	2.97	0.43
1:A:235:VAL:O	1:A:235:VAL:CG1	2.67	0.43
1:B:497:VAL:HG11	1:B:518:THR:CB	2.48	0.43
1:B:533:GLU:O	1:B:534:ASN:CB	2.67	0.43
1:C:255:VAL:N	1:C:256:PRO:CD	2.82	0.43
1:B:75:HIS:HB2	1:B:105:SER:OG	2.19	0.43
1:C:541:ALA:HB2	1:C:553:VAL:HG11	2.00	0.43
1:D:533:GLU:O	1:D:534:ASN:ND2	2.51	0.43
1:B:190:ALA:HA	1:B:217:PHE:O	2.19	0.43
1:D:449:LEU:HA	1:D:449:LEU:HD23	1.84	0.43
1:D:482:ILE:HD13	1:D:482:ILE:HA	1.92	0.43
1:C:355:LEU:HD13	1:C:356:VAL:N	2.34	0.43
1:C:160:LEU:O	1:C:162:GLY:N	2.51	0.43
1:C:174:ASP:O	1:C:178:ILE:HG23	2.19	0.43
1:C:359:ILE:CD1	1:C:465:ASN:C	2.87	0.43
1:B:497:VAL:HG11	1:B:518:THR:HB	2.01	0.43
1:B:217:PHE:CE1	1:B:238:GLY:HA3	2.53	0.43
1:B:328:ARG:O	1:B:331:ALA:HB3	2.19	0.43
1:A:160:LEU:O	1:A:162:GLY:N	2.52	0.43
1:C:512:THR:HG21	1:C:519:PHE:CE2	2.54	0.43
1:D:160:LEU:N	1:D:160:LEU:HD12	2.34	0.42
1:C:178:ILE:HD11	1:C:206:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:ALA:O	1:C:575:GLY:N	2.46	0.42
1:C:355:LEU:HD22	1:C:355:LEU:C	2.39	0.42
1:B:326:THR:HG23	1:B:327:MET:N	2.34	0.42
1:C:310:LEU:HD21	1:C:327:MET:HE2	2.00	0.42
1:B:7:VAL:HG21	1:B:274:ILE:HD13	2.00	0.42
1:B:376:VAL:O	1:B:376:VAL:HG13	2.19	0.42
1:A:533:GLU:O	1:A:534:ASN:CB	2.67	0.42
1:D:504:ASP:OD2	1:D:504:ASP:N	2.52	0.42
1:D:356:VAL:HG13	1:D:464:THR:HG23	2.02	0.42
1:B:92:VAL:HG22	1:B:142:VAL:O	2.19	0.42
1:B:520:VAL:HG12	1:B:543:VAL:HG11	2.01	0.42
1:D:497:VAL:HG11	1:D:518:THR:HB	2.02	0.42
1:B:291:ARG:NE	1:C:278:GLN:OE1	2.52	0.42
1:B:582:ALA:O	1:B:583:ASN:CG	2.58	0.42
1:D:530:ILE:HG12	1:D:577:ILE:HD13	2.01	0.42
1:C:363:VAL:CG1	1:C:388:ILE:HD12	2.50	0.42
1:C:355:LEU:HD23	1:D:469:ILE:HG21	2.00	0.42
1:B:367:ALA:CA	1:B:372:VAL:HG22	2.48	0.42
1:D:301:ILE:HD11	1:D:331:ALA:HA	2.01	0.42
1:A:229:ILE:HD11	1:A:239:LEU:CD1	2.50	0.42
1:A:9:THR:OG1	1:A:32:ARG:NH1	2.46	0.42
1:D:520:VAL:N	1:D:521:PRO:CD	2.83	0.42
1:A:533:GLU:O	1:A:534:ASN:HB2	2.20	0.42
1:A:88:ASN:C	1:A:146:ILE:HG22	2.40	0.42
1:B:494:ALA:CB	1:B:500:LEU:HD23	2.50	0.42
1:C:178:ILE:O	1:C:182:ILE:HG13	2.20	0.42
1:C:190:ALA:HA	1:C:217:PHE:O	2.19	0.42
1:C:210:GLN:O	1:C:211:LYS:C	2.57	0.42
1:D:533:GLU:O	1:D:534:ASN:HB2	2.19	0.42
1:C:533:GLU:O	1:C:534:ASN:HB2	2.20	0.42
1:A:449:LEU:HD23	1:A:449:LEU:HA	1.91	0.42
1:A:363:VAL:HG11	1:A:388:ILE:HD12	2.01	0.42
1:A:294:ALA:HB1	1:D:253:GLU:HA	2.02	0.42
1:B:255:VAL:N	1:B:256:PRO:CD	2.83	0.42
1:D:235:VAL:O	1:D:235:VAL:CG1	2.67	0.42
1:B:482:ILE:HG13	1:B:541:ALA:HB1	2.01	0.42
1:C:75:HIS:HB2	1:C:105:SER:OG	2.20	0.42
1:B:363:VAL:HG11	1:B:388:ILE:HD12	2.01	0.42
1:B:520:VAL:N	1:B:521:PRO:CD	2.83	0.42
1:A:295:SER:CA	1:D:256:PRO:HG2	2.50	0.42
1:A:504:ASP:N	1:A:504:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:GLU:HG3	1:D:57:LEU:HD11	2.01	0.42
1:C:266:CYS:SG	1:C:273:VAL:HG22	2.60	0.41
1:D:178:ILE:HD11	1:D:206:ILE:HD12	2.02	0.41
1:B:256:PRO:HG2	1:C:295:SER:CA	2.50	0.41
1:A:463:THR:CG2	1:B:574:GLN:OE1	2.68	0.41
1:B:359:ILE:CD1	1:B:465:ASN:HA	2.50	0.41
1:A:26:ALA:O	1:A:324:VAL:HG12	2.20	0.41
1:D:233:LEU:O	1:D:234:GLU:C	2.58	0.41
1:B:486:SER:O	1:B:487:VAL:HG13	2.21	0.41
1:A:400:VAL:HG12	1:A:400:VAL:O	2.20	0.41
1:A:538:SER:HB2	1:A:539:PRO:HD2	2.01	0.41
1:A:128:ILE:HG22	1:A:148:ASN:O	2.19	0.41
1:C:191:ALA:HB2	1:C:203:ILE:CD1	2.50	0.41
1:A:239:LEU:HD21	1:A:241:VAL:HG23	2.01	0.41
1:B:343:LEU:O	1:B:347:ARG:HG2	2.21	0.41
1:B:26:ALA:O	1:B:324:VAL:HG12	2.21	0.41
1:B:160:LEU:O	1:B:162:GLY:N	2.54	0.41
1:B:488:VAL:HG12	1:B:569:THR:OG1	2.20	0.41
1:D:34:ASN:ND2	1:D:36:SER:HB2	2.36	0.41
1:C:530:ILE:HG12	1:C:577:ILE:CD1	2.51	0.41
1:A:486:SER:O	1:A:487:VAL:CG1	2.69	0.41
1:C:513:ASN:HA	1:C:532:GLU:CG	2.51	0.41
1:A:530:ILE:HG12	1:A:577:ILE:HD13	2.02	0.41
1:A:226:ILE:HD11	1:A:246:MET:CE	2.50	0.41
1:A:355:LEU:HD23	1:B:469:ILE:HG21	2.02	0.41
1:C:463:THR:HG23	1:D:574:GLN:OE1	2.21	0.41
1:B:298:ALA:O	1:B:301:ILE:N	2.53	0.41
1:D:476:ILE:HA	1:D:476:ILE:HD13	1.90	0.41
1:A:384:THR:O	1:A:385:ALA:C	2.59	0.41
1:A:97:VAL:HG22	1:A:105:SER:HB3	2.03	0.41
1:C:97:VAL:HG22	1:C:105:SER:HB3	2.02	0.41
1:B:111:LEU:HG	1:B:160:LEU:HD21	2.02	0.41
1:B:482:ILE:HA	1:B:482:ILE:HD13	1.95	0.41
1:A:533:GLU:O	1:A:534:ASN:ND2	2.51	0.41
1:B:541:ALA:HB2	1:B:553:VAL:HG11	2.02	0.41
1:C:177:ASP:O	1:C:180:PHE:HB3	2.20	0.41
1:B:476:ILE:HD13	1:B:476:ILE:HA	1.91	0.41
1:D:355:LEU:HD13	1:D:356:VAL:N	2.35	0.41
1:C:356:VAL:HG13	1:C:464:THR:HG23	2.02	0.41
1:A:4:THR:CG2	1:A:331:ALA:HB1	2.50	0.41
1:B:266:CYS:SG	1:B:273:VAL:HG21	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HG	1:A:160:LEU:HD21	2.03	0.41
1:A:430:LEU:CD2	1:A:430:LEU:C	2.89	0.41
1:D:512:THR:HG21	1:D:519:PHE:CE2	2.56	0.41
1:D:494:ALA:CB	1:D:500:LEU:HD23	2.49	0.41
1:A:370:LEU:HD21	1:B:355:LEU:HA	2.02	0.41
1:C:20:ILE:HD12	1:C:49:THR:HG22	2.03	0.41
1:B:376:VAL:CG1	1:B:452:ILE:HG12	2.51	0.41
1:B:3:LYS:HD2	1:B:414:TRP:CZ2	2.56	0.41
1:C:343:LEU:O	1:C:347:ARG:HG2	2.21	0.41
1:D:401:THR:O	1:D:420:VAL:HA	2.21	0.41
1:B:504:ASP:OD2	1:B:504:ASP:N	2.53	0.41
1:D:400:VAL:HG22	1:D:419:VAL:HG23	2.02	0.41
1:A:512:THR:HG21	1:A:519:PHE:CE2	2.55	0.41
1:D:235:VAL:O	1:D:235:VAL:HG12	2.21	0.41
1:A:497:VAL:HG11	1:A:518:THR:HB	2.02	0.41
1:D:226:ILE:HD11	1:D:246:MET:CE	2.50	0.41
1:B:50:ILE:HG21	1:B:63:ILE:HD11	2.02	0.41
1:A:363:VAL:CG1	1:A:388:ILE:HD12	2.51	0.40
1:D:356:VAL:HG12	1:D:387:THR:HG21	2.03	0.40
1:C:400:VAL:CG2	1:C:419:VAL:CG2	2.99	0.40
1:D:530:ILE:HG12	1:D:577:ILE:CD1	2.52	0.40
1:C:509:VAL:CG2	1:C:509:VAL:O	2.68	0.40
1:B:226:ILE:HD11	1:B:246:MET:CE	2.50	0.40
1:B:413:VAL:HG12	1:B:416:VAL:HG23	2.03	0.40
1:D:343:LEU:O	1:D:347:ARG:HG2	2.20	0.40
1:C:344:LEU:HD12	1:C:344:LEU:O	2.22	0.40
1:C:366:THR:HG22	1:C:367:ALA:N	2.37	0.40
1:C:538:SER:HB2	1:C:539:PRO:HD2	2.03	0.40
1:C:159:ASN:O	1:C:161:PRO:HD3	2.21	0.40
1:C:520:VAL:N	1:C:521:PRO:CD	2.84	0.40
1:C:533:GLU:O	1:C:534:ASN:CB	2.69	0.40
1:B:298:ALA:HB1	1:B:302:TYR:CE2	2.57	0.40
1:C:506:SER:OG	1:C:507:ASP:N	2.49	0.40
1:C:504:ASP:OD2	1:C:504:ASP:N	2.54	0.40
1:D:92:VAL:HG12	1:D:104:PHE:CE1	2.56	0.40
1:C:361:ILE:HG13	1:C:391:TYR:CE1	2.56	0.40
1:D:178:ILE:HD12	1:D:203:ILE:HG23	2.02	0.40
1:A:235:VAL:HG12	1:A:235:VAL:O	2.20	0.40
1:A:392:ARG:HD2	1:A:414:TRP:CE2	2.56	0.40
1:C:583:ASN:HA	1:C:583:ASN:HD22	1.73	0.40
1:D:310:LEU:HD21	1:D:327:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:HD12	1:D:49:THR:HG22	2.04	0.40
1:C:497:VAL:HG11	1:C:518:THR:HB	2.03	0.40
1:B:91:ILE:HD12	1:B:91:ILE:N	2.36	0.40
1:B:506:SER:OG	1:B:507:ASP:N	2.52	0.40
1:A:431:LEU:HA	1:A:431:LEU:HD23	1.86	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:B:423:GLY:O	1:C:460:GLU:OE1[1_455]	2.15	0.05

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	581/606 (96%)	513 (88%)	48 (8%)	20 (3%)	5	23
1	B	581/606 (96%)	514 (88%)	49 (8%)	18 (3%)	5	25
1	C	581/606 (96%)	516 (89%)	47 (8%)	18 (3%)	5	25
1	D	581/606 (96%)	516 (89%)	47 (8%)	18 (3%)	5	25
All	All	2324/2424 (96%)	2059 (89%)	191 (8%)	74 (3%)	5	24

All (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

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Mol	Chain	Res	Type
1	B	154	ASN
1	B	220	ILE
1	B	320	PRO
1	B	475	GLU
1	B	556	GLU
1	C	154	ASN
1	C	220	ILE
1	C	320	PRO
1	C	475	GLU
1	C	556	GLU
1	D	154	ASN
1	D	220	ILE
1	D	320	PRO
1	D	475	GLU
1	D	556	GLU
1	A	149	SER
1	A	162	GLY
1	A	462	GLY
1	A	506	SER
1	A	507	ASP
1	B	149	SER
1	B	162	GLY
1	B	462	GLY
1	B	506	SER
1	B	507	ASP
1	C	149	SER
1	C	162	GLY
1	C	462	GLY
1	C	506	SER
1	C	507	ASP
1	D	149	SER
1	D	162	GLY
1	D	462	GLY
1	D	506	SER
1	D	507	ASP
1	A	534	ASN
1	B	195	ARG
1	B	534	ASN
1	C	534	ASN
1	D	534	ASN
1	A	195	ARG
1	C	195	ARG

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Mol	Chain	Res	Type
1	C	213	ASN
1	D	195	ARG
1	A	161	PRO
1	A	163	VAL
1	A	213	ASN
1	C	161	PRO
1	C	582	ALA
1	D	582	ALA
1	A	581	TYR
1	A	582	ALA
1	B	161	PRO
1	B	163	VAL
1	B	581	TYR
1	B	582	ALA
1	C	163	VAL
1	D	101	PRO
1	D	161	PRO
1	D	163	VAL
1	D	581	TYR
1	A	101	PRO
1	A	459	GLY
1	A	580	GLY
1	B	101	PRO
1	B	580	GLY
1	C	580	GLY
1	C	101	PRO
1	D	580	GLY

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	490/510 (96%)	474 (97%)	16 (3%)	45	79
1	B	490/510 (96%)	474 (97%)	16 (3%)	45	79
1	C	490/510 (96%)	474 (97%)	16 (3%)	45	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	490/510 (96%)	475 (97%)	15 (3%)	47 80
All	All	1960/2040 (96%)	1897 (97%)	63 (3%)	46 79

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	245	ASP
1	A	250	ILE
1	A	296	ASP
1	A	318	LEU
1	A	350	LEU
1	A	355	LEU
1	A	366	THR
1	A	379	THR
1	A	409	GLN
1	A	443	ARG
1	A	444	VAL
1	A	450	ILE
1	A	458	THR
1	A	464	THR
1	A	466	MET
1	B	64	LEU
1	B	245	ASP
1	B	296	ASP
1	B	350	LEU
1	B	355	LEU
1	B	366	THR
1	B	370	LEU
1	B	379	THR
1	B	409	GLN
1	B	412	ILE
1	B	443	ARG
1	B	444	VAL
1	B	450	ILE
1	B	458	THR
1	B	464	THR
1	B	466	MET
1	C	64	LEU
1	C	245	ASP
1	C	250	ILE
1	C	296	ASP

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Mol	Chain	Res	Type
1	C	318	LEU
1	C	350	LEU
1	C	355	LEU
1	C	366	THR
1	C	370	LEU
1	C	409	GLN
1	C	443	ARG
1	C	444	VAL
1	C	450	ILE
1	C	458	THR
1	C	464	THR
1	C	466	MET
1	D	64	LEU
1	D	245	ASP
1	D	250	ILE
1	D	318	LEU
1	D	350	LEU
1	D	355	LEU
1	D	366	THR
1	D	379	THR
1	D	409	GLN
1	D	443	ARG
1	D	444	VAL
1	D	450	ILE
1	D	458	THR
1	D	464	THR
1	D	466	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	148	ASN
1	A	470	HIS
1	A	583	ASN
1	B	299	ASN
1	B	583	ASN
1	C	110	ASN
1	C	299	ASN
1	C	470	HIS
1	C	583	ASN
1	D	34	ASN

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Mol	Chain	Res	Type
1	D	110	ASN
1	D	299	ASN
1	D	470	HIS
1	D	583	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 carbohydrates 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	A	586	-	4,4,4	0.35	0	6,6,6	0.27	0
2	PO4	B	586	-	4,4,4	0.38	0	6,6,6	0.29	0
2	PO4	C	586	-	4,4,4	0.38	0	6,6,6	0.28	0
2	PO4	D	586	-	4,4,4	0.38	0	6,6,6	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	586	-	-	0/0/0/0	0/0/0/0
2	PO4	B	586	-	-	0/0/0/0	0/0/0/0
2	PO4	C	586	-	-	0/0/0/0	0/0/0/0
2	PO4	D	586	-	-	0/0/0/0	0/0/0/0

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	A	586	PO4	1	0
2	B	586	PO4	2	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 ⓘ

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	583/606 (96%)	-0.29	5 (0%) 85 69	59, 108, 154, 195	0
1	B	583/606 (96%)	-0.07	25 (4%) 39 17	63, 123, 196, 226	0
1	C	583/606 (96%)	-0.10	20 (3%) 49 23	66, 126, 196, 226	0
1	D	583/606 (96%)	-0.24	7 (1%) 81 61	74, 116, 155, 218	0
All	All	2332/2424 (96%)	-0.18	57 (2%) 62 37	59, 117, 184, 226	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	ASP	9.5
1	B	118	GLY	6.9
1	B	80	GLY	4.9
1	B	504	ASP	4.1
1	C	504	ASP	4.0
1	B	78	LYS	3.9
1	B	533	GLU	3.9
1	D	461	THR	3.7
1	B	498	LYS	3.6
1	C	81	ILE	3.5
1	B	503	LYS	3.4
1	B	462	GLY	3.4
1	D	79	ASP	3.3
1	C	155	LYS	3.2
1	C	79	ASP	3.1
1	C	531	THR	3.0
1	B	98	GLU	3.0
1	B	505	LEU	3.0
1	B	86	ARG	3.0
1	C	336	ALA	2.9
1	A	503	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	151	GLU	2.9
1	A	460	GLU	2.9
1	C	505	LEU	2.9
1	B	153	LYS	2.8
1	B	139	LYS	2.7
1	C	80	GLY	2.7
1	C	98	GLU	2.7
1	B	85	GLU	2.7
1	C	502	GLY	2.6
1	D	83	GLU	2.6
1	B	528	GLY	2.6
1	C	528	GLY	2.6
1	C	556	GLU	2.6
1	D	81	ILE	2.6
1	D	503	LYS	2.6
1	D	85	GLU	2.5
1	B	461	THR	2.5
1	B	560	LYS	2.5
1	A	530	ILE	2.4
1	C	105	SER	2.4
1	B	510	ILE	2.3
1	B	502	GLY	2.3
1	C	518	THR	2.3
1	C	517	GLU	2.2
1	C	566	VAL	2.2
1	B	532	GLU	2.2
1	C	494	ALA	2.2
1	D	139	LYS	2.2
1	C	125	ASP	2.2
1	C	118	GLY	2.2
1	B	518	THR	2.1
1	C	574	GLN	2.1
1	A	533	GLU	2.1
1	A	510	ILE	2.1
1	B	547	LYS	2.0
1	B	529	LEU	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	D	586	5/5	0.88	0.15	-0.69	121,125,147,148	0
2	PO4	C	586	5/5	0.89	0.12	-0.79	111,127,142,143	0
2	PO4	B	586	5/5	0.95	0.11	-0.82	90,117,140,141	0
2	PO4	A	586	5/5	0.93	0.09	-1.40	93,107,128,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.