



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:07 pm BST

PDB ID : 3T07
Title : Crystal structure of *S. aureus* Pyruvate Kinase in complex with a naturally occurring bis-indole alkaloid
Authors : Worrall, L.J.; Vuckovic, M.; Strynadka, N.C.J.
Deposited on : 2011-07-19
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

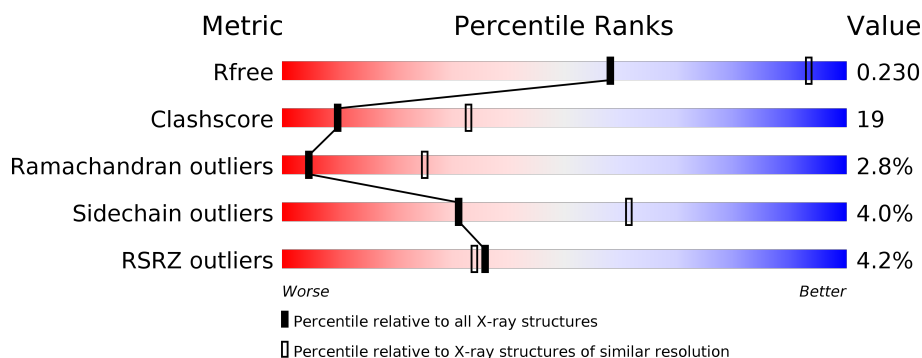
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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 $\leq 5\%$. 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>7%</div> <div> <div></div> <div>60%</div> <div>32%</div> <div>• •</div> </div> </div>
1	B	606	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>• •</div> </div> </div>
1	C	606	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>• •</div> </div> </div>
1	D	606	<div> <div>7%</div> <div> <div></div> <div>59%</div> <div>33%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	586	-	-	X	-
2	PO4	D	587	-	-	X	-
3	09C	B	586	X	-	-	-
3	09C	D	586	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17702 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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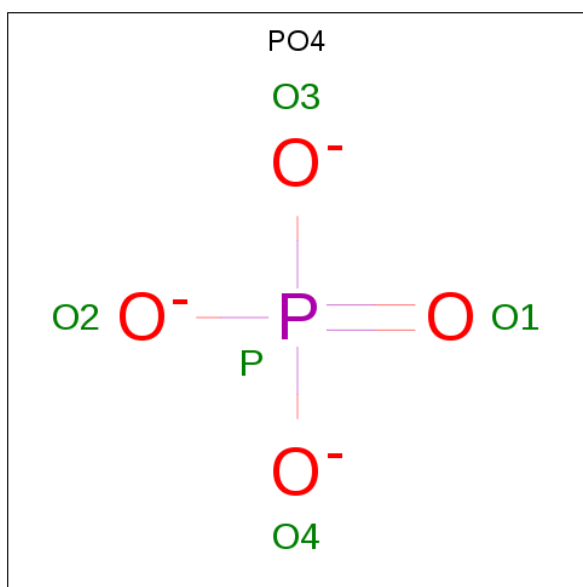
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP Q6GG09
B	-19	GLY	-	EXPRESSION TAG	UNP Q6GG09
B	-18	SER	-	EXPRESSION TAG	UNP Q6GG09
B	-17	SER	-	EXPRESSION TAG	UNP Q6GG09
B	-16	HIS	-	EXPRESSION TAG	UNP Q6GG09
B	-15	HIS	-	EXPRESSION TAG	UNP Q6GG09
B	-14	HIS	-	EXPRESSION TAG	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).



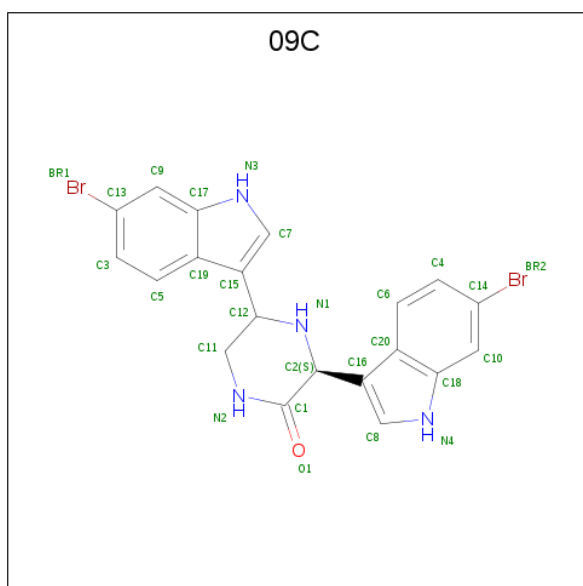
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

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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		

- Molecule 3 is (3S,5R)-3,5-bis(6-bromo-1H-indol-3-yl)piperazin-2-one (three-letter code: 09C) (formula: C₂₀H₁₆Br₂N₄O).

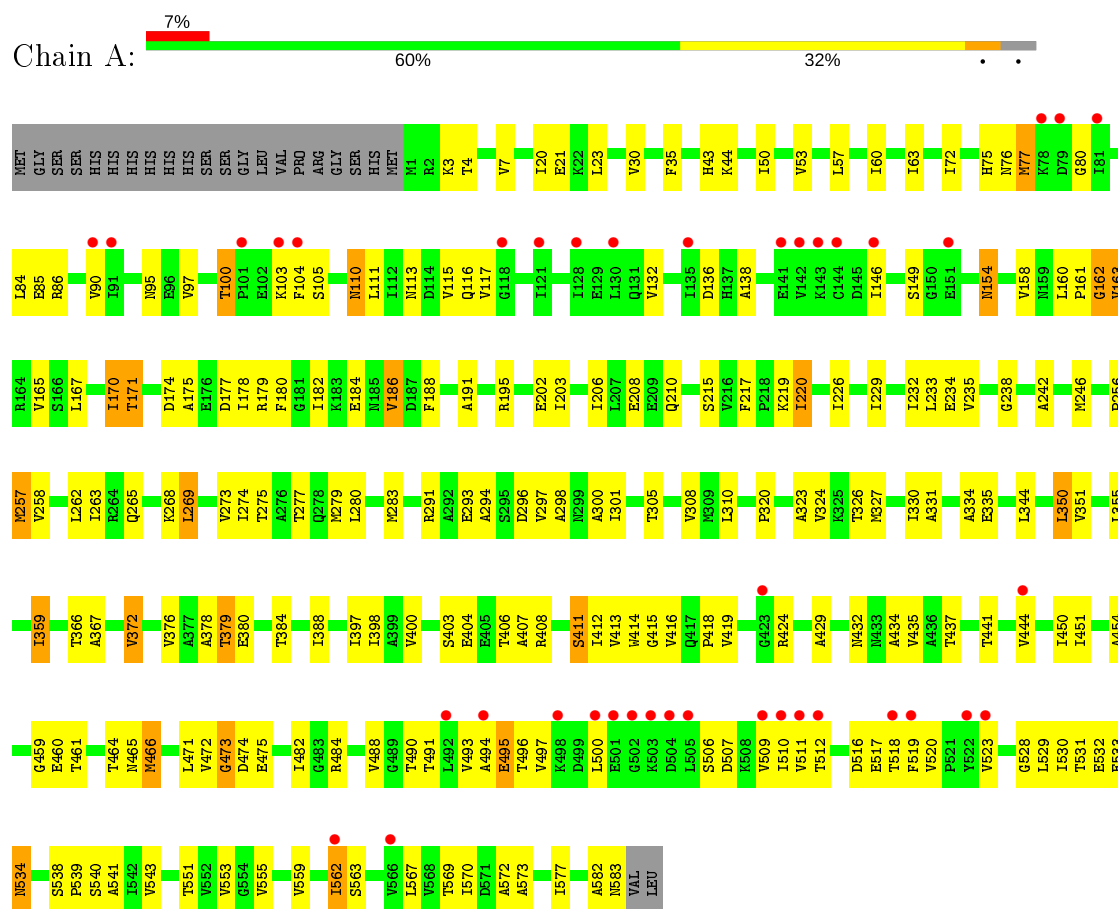


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	Br	C	N	O	0	0
			27	2	20	4	1		
3	D	1	Total	Br	C	N	O	0	0
			27	2	20	4	1		

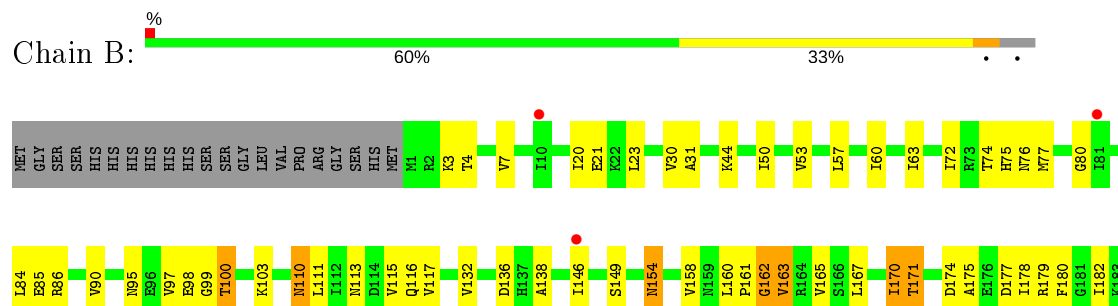
3 Residue-property plots

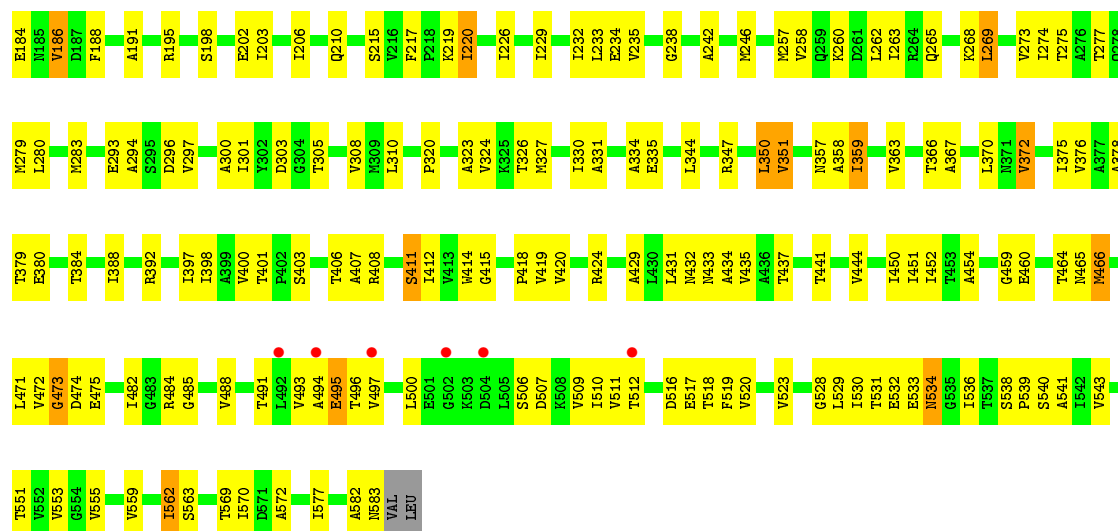
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

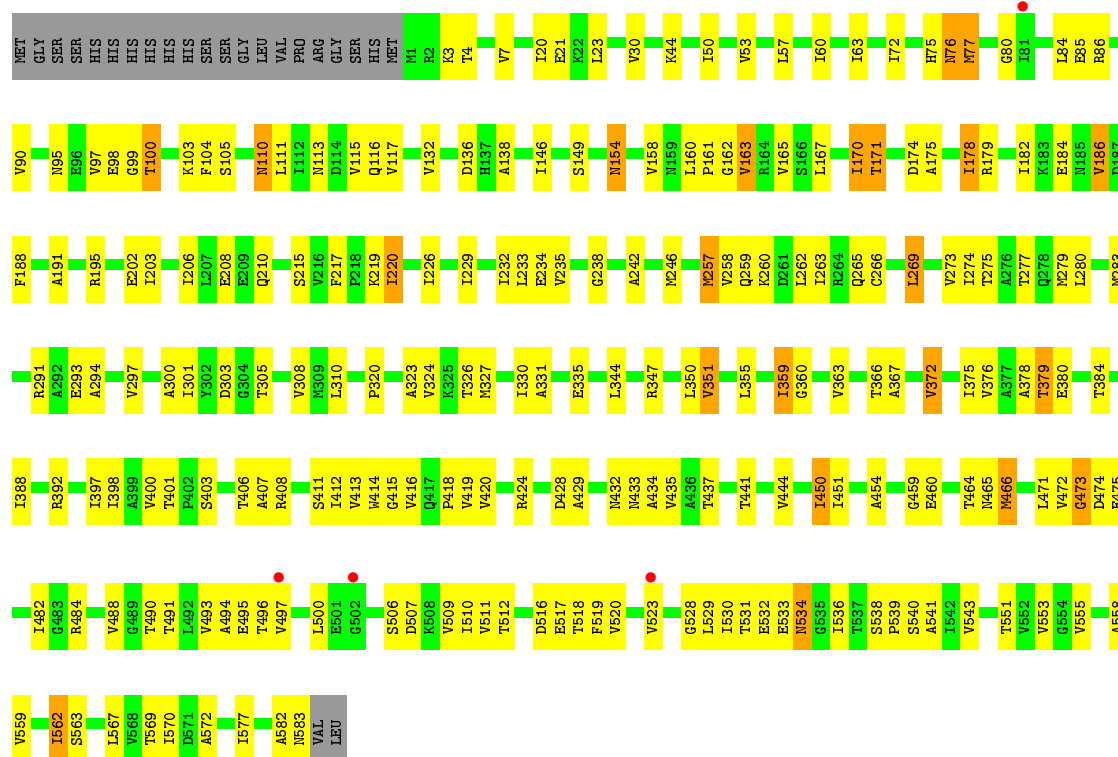


• Molecule 1: Pyruvate kinase



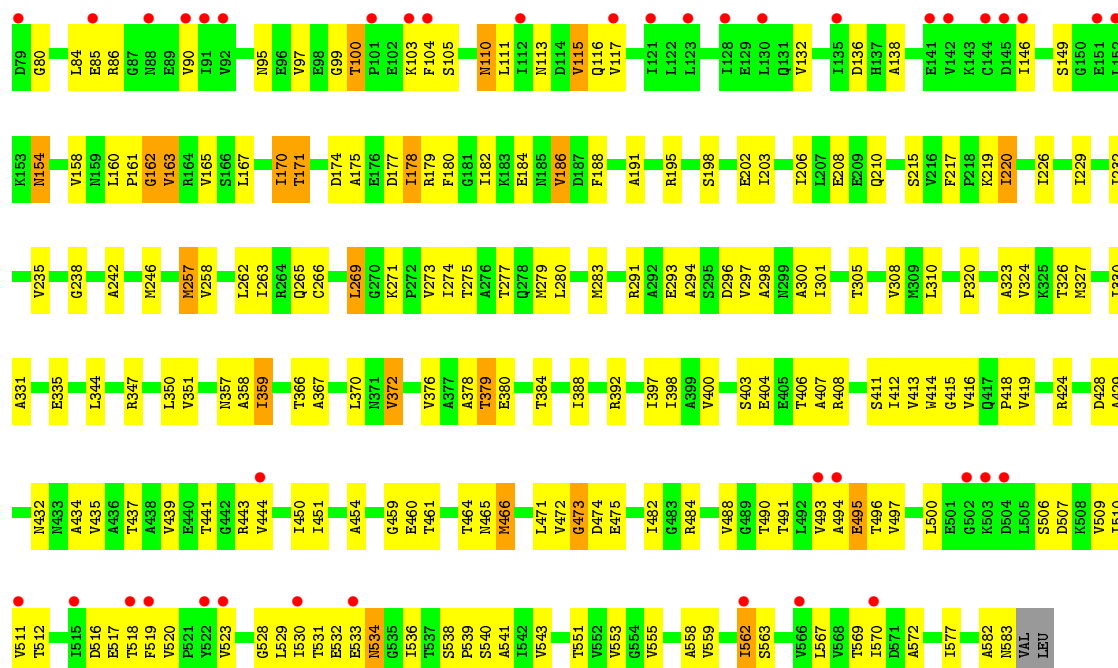


• Molecule 1: Pyruvate kinase



• 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	83.96Å 111.91Å 112.03Å 86.05° 72.14° 80.88°	Depositor
Resolution (Å)	60.00 – 3.30 48.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (60.00-3.30) 93.5 (48.62-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.226 0.202 , 0.230	Depositor DCC
R_{free} test set	2729 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	121.2	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 93.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17702	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 09C

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	0.53	0/4452	0.66	0/6022
1	B	0.57	0/4452	0.69	0/6022
1	C	0.58	1/4452 (0.0%)	0.69	0/6022
1	D	0.54	0/4452	0.67	0/6022
All	All	0.55	1/17808 (0.0%)	0.68	0/24088

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	CYS	CB-SG	-5.39	1.73	1.81

There are no bond angle outliers.

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	169	0
1	B	4407	0	4533	171	0
1	C	4407	0	4533	179	0
1	D	4407	0	4533	175	0
2	A	5	0	0	4	0
2	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	1	0
2	D	5	0	0	2	0
3	B	27	0	15	3	0
3	D	27	0	15	2	0
All	All	17702	0	18162	688	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 19.

All (688) 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)
3:D:586:09C:C7	3:D:586:09C:HAI	1.77	1.14
3:D:586:09C:C8	3:D:586:09C:HAH	1.77	1.14
3:B:586:09C:C7	3:B:586:09C:HAI	1.86	1.05
1:A:531:THR:HG21	1:A:540:SER:HB3	1.38	1.04
1:D:531:THR:HG21	1:D:540:SER:HB3	1.39	1.03
3:B:586:09C:C8	3:B:586:09C:HAH	1.88	1.03
1:B:84:LEU:HD23	1:B:90:VAL:HG21	1.40	1.03
1:B:531:THR:HG21	1:B:540:SER:HB3	1.42	1.00
1:C:84:LEU:HD23	1:C:90:VAL:HG21	1.47	0.97
1:A:84:LEU:HD23	1:A:90:VAL:HG21	1.47	0.96
1:C:531:THR:HG21	1:C:540:SER:HB3	1.44	0.96
1:D:84:LEU:HD23	1:D:90:VAL:HG21	1.45	0.95
1:C:366:THR:HG22	1:C:451:ILE:HD11	1.54	0.90
1:B:482:ILE:HD12	1:B:553:VAL:HG13	1.59	0.85
1:A:379:THR:HG22	2:A:586:PO4:O4	1.75	0.84
1:C:482:ILE:HD12	1:C:553:VAL:HG13	1.59	0.84
1:D:384:THR:OG1	1:D:464:THR:HB	1.77	0.83
1:B:283:MET:SD	1:B:326:THR:HG21	2.19	0.83
1:D:482:ILE:HD12	1:D:553:VAL:HG13	1.60	0.82
1:A:482:ILE:HD12	1:A:553:VAL:HG13	1.61	0.82
1:C:283:MET:SD	1:C:326:THR:HG21	2.21	0.80
1:C:21:GLU:HG3	1:C:57:LEU:HD11	1.61	0.80
1:C:384:THR:OG1	1:C:464:THR:HB	1.82	0.79
1:C:432:ASN:O	1:C:435:VAL:HG12	1.81	0.79
1:D:283:MET:SD	1:D:326:THR:HG21	2.22	0.79
1:A:384:THR:OG1	1:A:464:THR:HB	1.81	0.79
1:B:510:ILE:HD11	1:B:523:VAL:HG22	1.63	0.79
3:B:586:09C:HAH	3:B:586:09C:HAI	0.92	0.79
1:A:283:MET:SD	1:A:326:THR:HG21	2.23	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:THR:HG22	1:D:451:ILE:HD11	1.65	0.78
1:B:379:THR:HG22	2:B:587:PO4:O4	1.83	0.78
1:D:432:ASN:O	1:D:435:VAL:HG12	1.84	0.78
1:A:21:GLU:HG3	1:A:57:LEU:HD11	1.67	0.77
1:C:529:LEU:HD11	1:C:531:THR:HG22	1.67	0.77
1:C:510:ILE:HD11	1:C:523:VAL:HG22	1.67	0.77
1:A:366:THR:HG22	1:A:451:ILE:HD11	1.67	0.76
1:B:384:THR:OG1	1:B:464:THR:HB	1.86	0.76
1:D:582:ALA:O	1:D:583:ASN:ND2	2.18	0.76
1:A:432:ASN:O	1:A:435:VAL:HG12	1.85	0.76
1:D:21:GLU:HG3	1:D:57:LEU:HD11	1.67	0.76
1:A:510:ILE:HD11	1:A:523:VAL:HG22	1.67	0.76
1:D:529:LEU:HD11	1:D:531:THR:HG22	1.68	0.76
1:B:529:LEU:HD11	1:B:531:THR:HG22	1.68	0.76
1:B:21:GLU:HG3	1:B:57:LEU:HD11	1.66	0.75
1:C:582:ALA:O	1:C:583:ASN:ND2	2.19	0.75
1:D:510:ILE:HD11	1:D:523:VAL:HG22	1.67	0.75
1:A:569:THR:HG21	1:A:582:ALA:HB3	1.69	0.75
1:B:529:LEU:HB3	1:B:551:THR:HG22	1.68	0.74
1:A:582:ALA:O	1:A:583:ASN:ND2	2.20	0.74
1:A:275:THR:HG22	1:A:279:MET:HE2	1.67	0.73
1:B:432:ASN:O	1:B:435:VAL:HG12	1.88	0.73
1:B:582:ALA:O	1:B:583:ASN:ND2	2.22	0.73
1:C:378:ALA:HB3	1:C:454:ALA:HB2	1.71	0.73
1:C:529:LEU:HB3	1:C:551:THR:HG22	1.70	0.72
1:B:488:VAL:HG12	1:B:569:THR:OG1	1.89	0.72
1:D:275:THR:HG22	1:D:279:MET:HE2	1.70	0.72
1:D:569:THR:HG21	1:D:582:ALA:HB3	1.69	0.72
1:B:569:THR:HG21	1:B:582:ALA:HB3	1.71	0.72
1:A:529:LEU:HD11	1:A:531:THR:HG22	1.70	0.71
1:B:275:THR:HG22	1:B:279:MET:HE2	1.70	0.71
1:A:4:THR:HG21	1:A:301:ILE:HD13	1.73	0.71
1:B:366:THR:HG22	1:B:451:ILE:HD11	1.73	0.71
1:D:517:GLU:O	1:D:520:VAL:HG22	1.91	0.71
1:C:488:VAL:HG12	1:C:569:THR:OG1	1.90	0.70
1:D:100:THR:HG23	1:D:103:LYS:O	1.90	0.70
1:D:4:THR:HG21	1:D:301:ILE:HD13	1.74	0.70
1:C:4:THR:HG21	1:C:301:ILE:HD13	1.73	0.70
1:B:482:ILE:CD1	1:B:553:VAL:HG13	2.22	0.69
1:B:533:GLU:O	1:B:534:ASN:OD1	2.10	0.69
1:D:482:ILE:CD1	1:D:553:VAL:HG13	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:LEU:HB3	1:D:551:THR:HG22	1.73	0.69
1:C:533:GLU:O	1:C:534:ASN:OD1	2.11	0.69
1:A:539:PRO:O	1:A:543:VAL:HG13	1.93	0.69
1:B:378:ALA:HB3	1:B:454:ALA:HB2	1.75	0.69
1:A:533:GLU:O	1:A:534:ASN:OD1	2.09	0.69
1:C:72:ILE:HG22	1:C:158:VAL:HB	1.75	0.69
1:D:279:MET:HE3	1:D:308:VAL:HG13	1.74	0.69
1:A:482:ILE:CD1	1:A:553:VAL:HG13	2.22	0.68
1:C:482:ILE:CD1	1:C:553:VAL:HG13	2.23	0.68
1:D:539:PRO:O	1:D:543:VAL:HG13	1.92	0.68
1:B:4:THR:HG21	1:B:301:ILE:HD13	1.75	0.68
1:D:379:THR:HG22	2:D:587:PO4:O2	1.92	0.68
1:D:494:ALA:HB2	1:D:500:LEU:HD23	1.75	0.68
1:C:497:VAL:HG11	1:C:518:THR:OG1	1.93	0.68
1:C:494:ALA:HB2	1:C:500:LEU:HD23	1.76	0.68
1:A:529:LEU:HB3	1:A:551:THR:HG22	1.73	0.68
1:B:494:ALA:HB2	1:B:500:LEU:HD23	1.76	0.68
1:C:539:PRO:O	1:C:543:VAL:HG13	1.93	0.68
1:B:165:VAL:CG1	1:B:167:LEU:HD23	2.24	0.68
1:B:72:ILE:HG22	1:B:158:VAL:HB	1.76	0.67
1:D:533:GLU:O	1:D:534:ASN:OD1	2.13	0.67
1:B:497:VAL:HG11	1:B:518:THR:OG1	1.95	0.67
1:C:569:THR:HG21	1:C:582:ALA:HB3	1.77	0.67
1:D:23:LEU:HG	1:D:324:VAL:HG21	1.75	0.67
1:A:494:ALA:HB2	1:A:500:LEU:HD23	1.77	0.67
1:D:378:ALA:HB3	1:D:454:ALA:HB2	1.76	0.67
1:D:497:VAL:HG11	1:D:518:THR:OG1	1.94	0.67
1:A:165:VAL:CG1	1:A:167:LEU:HD23	2.25	0.67
1:A:517:GLU:O	1:A:520:VAL:HG22	1.95	0.67
1:C:494:ALA:HB3	1:C:512:THR:HG22	1.76	0.67
1:A:100:THR:HG23	1:A:103:LYS:O	1.95	0.67
1:A:23:LEU:HG	1:A:324:VAL:HG21	1.77	0.66
1:B:279:MET:HE3	1:B:308:VAL:HG13	1.76	0.66
1:B:60:ILE:HD12	1:B:418:PRO:HG2	1.77	0.66
1:C:275:THR:HG22	1:C:279:MET:HE2	1.78	0.66
1:D:72:ILE:HG22	1:D:158:VAL:HB	1.76	0.66
1:A:256:PRO:HB2	1:A:257:MET:HE3	1.78	0.66
1:C:165:VAL:CG1	1:C:167:LEU:HD23	2.26	0.65
1:B:539:PRO:O	1:B:543:VAL:HG13	1.95	0.65
1:A:497:VAL:HG11	1:A:518:THR:OG1	1.96	0.65
1:C:23:LEU:HG	1:C:324:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:ALA:HB3	1:D:512:THR:HG22	1.78	0.65
1:A:263:ILE:HG23	1:A:273:VAL:HG11	1.79	0.65
1:C:100:THR:HG23	1:C:103:LYS:O	1.97	0.65
1:D:488:VAL:HG12	1:D:569:THR:OG1	1.97	0.64
1:C:175:ALA:O	1:C:179:ARG:HG3	1.97	0.64
1:B:23:LEU:HG	1:B:324:VAL:HG21	1.79	0.64
1:B:494:ALA:HB3	1:B:512:THR:HG22	1.80	0.64
1:D:376:VAL:HG11	1:D:434:ALA:HB1	1.79	0.64
1:B:175:ALA:O	1:B:179:ARG:HG3	1.98	0.64
1:D:174:ASP:O	1:D:178:ILE:HG23	1.98	0.64
1:A:376:VAL:HG11	1:A:434:ALA:HB1	1.80	0.64
1:A:72:ILE:HG22	1:A:158:VAL:HB	1.79	0.64
1:A:403:SER:OG	1:A:406:THR:HG23	1.98	0.64
1:A:494:ALA:HB3	1:A:512:THR:HG22	1.80	0.64
1:A:60:ILE:HD12	1:A:418:PRO:HG2	1.78	0.64
1:D:165:VAL:CG1	1:D:167:LEU:HD23	2.27	0.63
1:C:7:VAL:HG22	1:C:30:VAL:HB	1.80	0.63
1:B:310:LEU:HD21	1:B:327:MET:CE	2.28	0.63
1:C:279:MET:HE3	1:C:308:VAL:HG13	1.79	0.63
1:C:471:LEU:HD23	1:C:472:VAL:N	2.12	0.63
1:C:174:ASP:O	1:C:178:ILE:HG23	1.97	0.63
1:A:175:ALA:O	1:A:179:ARG:HG3	1.99	0.62
1:B:482:ILE:HD13	1:B:541:ALA:CB	2.29	0.62
1:A:279:MET:HE3	1:A:308:VAL:HG13	1.80	0.62
1:A:471:LEU:HD23	1:A:472:VAL:N	2.13	0.62
1:A:50:ILE:HG21	1:A:63:ILE:HD11	1.82	0.62
1:A:220:ILE:CG2	1:A:226:ILE:HD13	2.30	0.62
1:D:530:ILE:HG23	1:D:555:VAL:HG21	1.81	0.62
1:A:160:LEU:HB3	1:A:163:VAL:HG11	1.81	0.62
1:A:274:ILE:HD11	1:A:412:ILE:HD11	1.82	0.62
1:C:60:ILE:HD12	1:C:418:PRO:HG2	1.81	0.62
1:C:80:GLY:HA2	1:C:154:ASN:HD21	1.65	0.62
1:D:175:ALA:O	1:D:179:ARG:HG3	2.00	0.62
1:B:471:LEU:HD23	1:B:472:VAL:N	2.15	0.62
1:C:310:LEU:HD21	1:C:327:MET:CE	2.29	0.62
1:A:310:LEU:HD21	1:A:327:MET:CE	2.30	0.61
1:A:488:VAL:HG12	1:A:569:THR:OG1	1.99	0.61
1:D:7:VAL:HG22	1:D:30:VAL:HB	1.81	0.61
1:D:50:ILE:HG21	1:D:63:ILE:HD11	1.80	0.61
1:A:291:ARG:HH12	1:D:296:ASP:CG	2.04	0.61
1:C:50:ILE:HG21	1:C:63:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:CG2	1:D:158:VAL:HB	2.30	0.61
1:B:246:MET:CE	1:B:258:VAL:HG11	2.30	0.61
1:D:344:LEU:O	1:D:344:LEU:HD12	2.00	0.61
1:D:471:LEU:HD23	1:D:472:VAL:N	2.14	0.61
1:B:160:LEU:HB3	1:B:163:VAL:HG11	1.82	0.61
1:A:80:GLY:HA2	1:A:154:ASN:HD21	1.65	0.61
1:B:72:ILE:CG2	1:B:158:VAL:HB	2.31	0.61
1:C:493:VAL:CG1	1:C:559:VAL:HG13	2.30	0.61
1:D:274:ILE:HD11	1:D:412:ILE:HD11	1.83	0.61
1:B:100:THR:HG23	1:B:103:LYS:O	2.00	0.60
1:D:160:LEU:HB3	1:D:163:VAL:HG11	1.83	0.60
1:A:482:ILE:HD13	1:A:541:ALA:CB	2.31	0.60
1:B:174:ASP:O	1:B:178:ILE:HG23	2.01	0.60
1:A:533:GLU:O	1:A:534:ASN:CG	2.39	0.60
1:B:398:ILE:HD13	1:B:441:THR:HG21	1.83	0.60
1:D:60:ILE:HD12	1:D:418:PRO:HG2	1.82	0.60
1:A:493:VAL:CG1	1:A:559:VAL:HG13	2.31	0.60
1:B:217:PHE:CE1	1:B:238:GLY:HA3	2.37	0.60
1:C:366:THR:HG22	1:C:451:ILE:CD1	2.29	0.60
1:C:72:ILE:CG2	1:C:158:VAL:HB	2.31	0.60
1:B:3:LYS:HB2	1:B:335:GLU:OE2	2.01	0.60
1:A:530:ILE:HG23	1:A:555:VAL:HG21	1.84	0.60
1:D:263:ILE:HG23	1:D:273:VAL:HG11	1.83	0.60
1:B:334:ALA:HB2	1:C:257:MET:HE2	1.84	0.59
1:B:517:GLU:O	1:B:520:VAL:HG22	2.02	0.59
1:D:220:ILE:CG2	1:D:226:ILE:HD13	2.31	0.59
1:C:274:ILE:HD11	1:C:412:ILE:HD11	1.84	0.59
1:C:482:ILE:HD13	1:C:541:ALA:CB	2.33	0.59
1:B:533:GLU:O	1:B:534:ASN:CG	2.41	0.59
1:A:174:ASP:O	1:A:178:ILE:HG23	2.01	0.59
1:C:246:MET:CE	1:C:258:VAL:HG11	2.33	0.59
1:B:80:GLY:HA2	1:B:154:ASN:HD21	1.67	0.59
1:B:84:LEU:CD2	1:B:90:VAL:HG21	2.27	0.59
1:C:160:LEU:HB3	1:C:163:VAL:HG11	1.85	0.59
1:C:482:ILE:CD1	1:C:553:VAL:CG1	2.81	0.59
1:D:493:VAL:CG1	1:D:559:VAL:HG13	2.32	0.59
1:A:72:ILE:CG2	1:A:158:VAL:HB	2.33	0.59
1:C:3:LYS:HB2	1:C:335:GLU:OE2	2.03	0.59
1:D:533:GLU:O	1:D:534:ASN:CG	2.41	0.59
1:B:493:VAL:CG1	1:B:559:VAL:HG13	2.33	0.58
1:B:220:ILE:CG2	1:B:226:ILE:HD13	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG22	1:A:30:VAL:HB	1.84	0.58
1:C:344:LEU:O	1:C:344:LEU:HD12	2.02	0.58
1:C:220:ILE:HD11	1:C:232:ILE:HD13	1.85	0.58
1:C:3:LYS:HA	1:C:415:GLY:HA2	1.86	0.58
1:C:217:PHE:CE1	1:C:238:GLY:HA3	2.38	0.58
1:C:376:VAL:HG11	1:C:434:ALA:HB1	1.84	0.58
1:B:246:MET:CE	1:B:258:VAL:CG1	2.82	0.58
1:C:509:VAL:HG12	1:C:528:GLY:HA3	1.86	0.58
1:D:310:LEU:HD21	1:D:327:MET:CE	2.33	0.58
1:A:3:LYS:HB2	1:A:335:GLU:OE2	2.03	0.58
1:D:80:GLY:HA2	1:D:154:ASN:HD21	1.68	0.57
1:D:380:GLU:O	1:D:406:THR:HG21	2.04	0.57
1:A:398:ILE:HD13	1:A:441:THR:HG21	1.86	0.57
1:D:246:MET:CE	1:D:258:VAL:HG11	2.34	0.57
1:D:482:ILE:CD1	1:D:553:VAL:CG1	2.83	0.57
1:D:3:LYS:HA	1:D:415:GLY:HA2	1.86	0.57
1:A:217:PHE:CE1	1:A:238:GLY:HA3	2.39	0.57
1:A:246:MET:CE	1:A:258:VAL:HG11	2.34	0.57
1:A:388:ILE:HG22	1:A:397:ILE:HD13	1.87	0.57
1:C:220:ILE:CG2	1:C:226:ILE:HD13	2.34	0.57
1:A:378:ALA:HB3	1:A:454:ALA:HB2	1.87	0.57
1:A:516:ASP:O	1:A:520:VAL:HG13	2.04	0.57
1:C:263:ILE:HG23	1:C:273:VAL:HG11	1.86	0.57
1:D:162:GLY:HA2	1:D:163:VAL:O	2.05	0.57
1:D:482:ILE:HD13	1:D:541:ALA:CB	2.35	0.57
1:A:509:VAL:HG12	1:A:528:GLY:HA3	1.87	0.56
1:A:482:ILE:CD1	1:A:553:VAL:CG1	2.84	0.56
1:A:359:ILE:HD12	1:A:466:MET:N	2.20	0.56
1:D:60:ILE:HG23	1:D:408:ARG:HG2	1.88	0.56
1:B:380:GLU:O	1:B:406:THR:HG21	2.04	0.56
1:C:171:THR:HB	1:C:174:ASP:H	1.70	0.56
1:C:517:GLU:O	1:C:520:VAL:HG22	2.06	0.56
1:B:50:ILE:HG21	1:B:63:ILE:HD11	1.88	0.56
1:C:533:GLU:O	1:C:534:ASN:CG	2.43	0.56
1:B:367:ALA:HA	1:B:372:VAL:HG13	1.88	0.56
1:C:246:MET:CE	1:C:258:VAL:CG1	2.83	0.56
1:C:530:ILE:HG23	1:C:555:VAL:HG21	1.88	0.56
1:A:511:VAL:HG21	1:A:562:ILE:HD11	1.88	0.56
1:B:482:ILE:CD1	1:B:553:VAL:CG1	2.83	0.55
1:D:3:LYS:HB2	1:D:335:GLU:OE2	2.06	0.55
1:D:403:SER:OG	1:D:406:THR:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:ILE:HD12	1:C:465:ASN:C	2.27	0.55
1:D:516:ASP:O	1:D:520:VAL:HG13	2.07	0.55
1:A:117:VAL:HA	1:A:132:VAL:HG12	1.88	0.55
1:B:191:ALA:HB2	1:B:203:ILE:CD1	2.36	0.55
1:C:162:GLY:HA2	1:C:163:VAL:O	2.07	0.55
1:A:380:GLU:O	1:A:406:THR:HG21	2.07	0.55
1:B:530:ILE:HG23	1:B:555:VAL:HG21	1.88	0.55
1:C:60:ILE:HG23	1:C:408:ARG:HG2	1.88	0.55
1:C:398:ILE:HD13	1:C:441:THR:HG21	1.88	0.55
1:D:400:VAL:CG2	1:D:437:THR:HG21	2.37	0.55
1:A:20:ILE:HG22	1:A:53:VAL:HG11	1.89	0.55
1:B:509:VAL:HG12	1:B:528:GLY:HA3	1.89	0.55
1:C:380:GLU:O	1:C:406:THR:HG21	2.06	0.55
1:D:191:ALA:HB2	1:D:203:ILE:CD1	2.37	0.55
1:D:509:VAL:HG12	1:D:528:GLY:HA3	1.88	0.55
1:C:229:ILE:HG12	1:C:262:LEU:HD23	1.89	0.54
1:A:60:ILE:HD13	1:A:407:ALA:HB1	1.88	0.54
1:C:117:VAL:HA	1:C:132:VAL:HG12	1.88	0.54
1:A:63:ILE:CG2	1:A:186:VAL:HG23	2.37	0.54
1:A:162:GLY:HA2	1:A:163:VAL:O	2.07	0.54
1:C:400:VAL:O	1:C:400:VAL:HG12	2.06	0.54
1:A:44:LYS:HE2	1:A:184:GLU:OE2	2.08	0.54
1:A:301:ILE:HA	1:A:305:THR:HG22	1.89	0.54
1:B:7:VAL:HG22	1:B:30:VAL:HB	1.89	0.54
1:C:4:THR:HG21	1:C:301:ILE:CD1	2.37	0.54
1:A:220:ILE:HG21	1:A:226:ILE:HD13	1.89	0.54
1:D:530:ILE:CG2	1:D:555:VAL:HG21	2.38	0.54
1:B:162:GLY:HA2	1:B:163:VAL:O	2.08	0.54
1:A:171:THR:HB	1:A:174:ASP:H	1.73	0.54
1:B:274:ILE:HD11	1:B:412:ILE:HD11	1.90	0.54
1:D:60:ILE:HD13	1:D:407:ALA:HB1	1.89	0.54
1:C:388:ILE:HG22	1:C:397:ILE:HD13	1.89	0.53
1:D:367:ALA:HA	1:D:372:VAL:HG13	1.90	0.53
1:D:44:LYS:HE2	1:D:184:GLU:OE2	2.09	0.53
1:B:403:SER:OG	1:B:406:THR:HG23	2.07	0.53
1:B:44:LYS:HE2	1:B:184:GLU:OE2	2.09	0.53
1:B:484:ARG:C	1:B:572:ALA:HB3	2.29	0.53
1:D:117:VAL:HA	1:D:132:VAL:HG12	1.90	0.53
1:B:3:LYS:HA	1:B:415:GLY:HA2	1.89	0.53
1:D:279:MET:CE	1:D:308:VAL:HG13	2.38	0.53
1:D:359:ILE:HD12	1:D:465:ASN:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:VAL:HG21	1:D:562:ILE:HD11	1.90	0.53
1:A:235:VAL:O	1:A:235:VAL:HG12	2.09	0.53
1:A:60:ILE:HG23	1:A:408:ARG:HG2	1.91	0.53
1:C:359:ILE:HD12	1:C:466:MET:N	2.24	0.53
1:B:4:THR:HG21	1:B:301:ILE:CD1	2.37	0.53
1:B:359:ILE:HD12	1:B:466:MET:N	2.23	0.53
1:A:512:THR:HG21	1:A:519:PHE:CE2	2.44	0.53
1:C:111:LEU:HD23	1:C:115:VAL:HG13	1.91	0.53
1:D:359:ILE:HD12	1:D:466:MET:N	2.24	0.53
1:C:301:ILE:HA	1:C:305:THR:HG22	1.90	0.53
1:D:111:LEU:HD23	1:D:115:VAL:HG13	1.89	0.53
1:A:246:MET:CE	1:A:258:VAL:CG1	2.87	0.53
1:A:242:ALA:HB1	1:A:277:THR:HG21	1.90	0.53
1:A:4:THR:HG21	1:A:301:ILE:CD1	2.37	0.53
1:B:344:LEU:HD12	1:B:344:LEU:O	2.09	0.53
1:C:367:ALA:HA	1:C:372:VAL:HG13	1.91	0.53
1:D:398:ILE:HD13	1:D:441:THR:HG21	1.90	0.53
1:B:376:VAL:HG11	1:B:434:ALA:HB1	1.91	0.52
1:C:582:ALA:C	1:C:583:ASN:HD22	2.12	0.52
1:A:182:ILE:HG21	1:A:210:GLN:HG2	1.90	0.52
1:B:60:ILE:HG23	1:B:408:ARG:HG2	1.90	0.52
1:C:115:VAL:HG23	1:C:116:GLN:N	2.25	0.52
1:C:191:ALA:HB2	1:C:203:ILE:CD1	2.40	0.52
1:D:301:ILE:HA	1:D:305:THR:HG22	1.90	0.52
1:D:582:ALA:C	1:D:583:ASN:HD22	2.13	0.52
1:A:461:THR:HG21	2:A:586:PO4:O3	2.09	0.52
1:D:532:GLU:O	1:D:555:VAL:N	2.43	0.52
1:C:4:THR:CG2	1:C:331:ALA:HB1	2.40	0.52
1:C:379:THR:CG2	1:C:384:THR:HB	2.40	0.52
1:B:63:ILE:CG2	1:B:186:VAL:HG23	2.39	0.52
1:D:242:ALA:HB1	1:D:277:THR:HG21	1.91	0.52
1:D:512:THR:HG21	1:D:519:PHE:CE2	2.45	0.52
1:A:220:ILE:HD11	1:A:232:ILE:HD13	1.91	0.52
1:C:44:LYS:HE2	1:C:184:GLU:OE2	2.09	0.52
1:D:220:ILE:HD11	1:D:232:ILE:HD13	1.90	0.52
1:A:279:MET:CE	1:A:308:VAL:HG13	2.40	0.52
1:C:509:VAL:HG12	1:C:528:GLY:CA	2.39	0.52
1:D:171:THR:HB	1:D:174:ASP:H	1.75	0.52
1:D:494:ALA:CB	1:D:500:LEU:HD23	2.40	0.52
1:B:220:ILE:HG21	1:B:226:ILE:HD13	1.91	0.51
1:B:310:LEU:HD21	1:B:327:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:O	1:A:344:LEU:HD12	2.10	0.51
1:A:532:GLU:O	1:A:555:VAL:N	2.44	0.51
1:B:115:VAL:HG23	1:B:116:GLN:N	2.26	0.51
1:B:4:THR:CG2	1:B:331:ALA:HB1	2.40	0.51
1:C:208:GLU:OE2	1:D:536:ILE:HG23	2.11	0.51
1:A:310:LEU:HD21	1:A:327:MET:HE2	1.92	0.51
1:C:512:THR:HG21	1:C:519:PHE:CE2	2.46	0.51
1:A:60:ILE:CD1	1:A:407:ALA:HB1	2.41	0.51
1:A:63:ILE:HG22	1:A:186:VAL:CG2	2.40	0.51
1:B:263:ILE:HG23	1:B:273:VAL:HG11	1.92	0.51
1:B:229:ILE:HG12	1:B:262:LEU:HD23	1.92	0.51
1:B:419:VAL:HG21	1:B:437:THR:CG2	2.41	0.51
1:D:444:VAL:HG21	1:D:450:ILE:HD11	1.91	0.51
1:D:4:THR:HG21	1:D:301:ILE:CD1	2.40	0.51
1:C:110:ASN:O	1:C:110:ASN:ND2	2.44	0.51
1:A:359:ILE:HD12	1:A:465:ASN:C	2.31	0.51
1:B:246:MET:HE2	1:B:258:VAL:CG1	2.41	0.51
1:C:265:GLN:O	1:C:269:LEU:HD12	2.10	0.51
1:C:494:ALA:CB	1:C:500:LEU:HD23	2.40	0.51
1:D:21:GLU:OE2	1:D:57:LEU:HD21	2.11	0.51
1:B:444:VAL:HG21	1:B:450:ILE:HD11	1.93	0.51
1:D:310:LEU:HD21	1:D:327:MET:HE2	1.92	0.51
1:B:265:GLN:O	1:B:269:LEU:HD12	2.11	0.51
1:A:191:ALA:HB2	1:A:203:ILE:CD1	2.41	0.50
1:B:60:ILE:HD13	1:B:407:ALA:HB1	1.93	0.50
1:D:217:PHE:CE1	1:D:238:GLY:HA3	2.46	0.50
1:D:388:ILE:HG22	1:D:397:ILE:HD13	1.93	0.50
1:A:165:VAL:HG12	1:A:167:LEU:HD23	1.93	0.50
1:A:3:LYS:HA	1:A:415:GLY:HA2	1.92	0.50
1:B:110:ASN:ND2	1:B:110:ASN:O	2.43	0.50
1:C:95:ASN:O	1:C:97:VAL:HG13	2.10	0.50
1:C:497:VAL:HG11	1:C:518:THR:CB	2.42	0.50
1:B:171:THR:HB	1:B:174:ASP:H	1.75	0.50
1:B:400:VAL:CG2	1:B:437:THR:HG21	2.41	0.50
1:B:359:ILE:HD12	1:B:465:ASN:C	2.31	0.50
1:B:63:ILE:HG22	1:B:186:VAL:CG2	2.41	0.50
1:D:491:THR:HG21	1:D:562:ILE:HD13	1.93	0.50
1:A:217:PHE:CZ	1:A:238:GLY:HA3	2.47	0.50
1:A:388:ILE:HG22	1:A:397:ILE:CD1	2.42	0.50
1:B:242:ALA:HB1	1:B:277:THR:HG21	1.91	0.50
1:B:424:ARG:HB3	1:B:429:ALA:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:SER:OG	1:C:406:THR:HG23	2.11	0.50
1:B:182:ILE:HG21	1:B:210:GLN:HG2	1.93	0.50
1:C:473:GLY:HA3	1:C:474:ASP:HB2	1.94	0.50
1:B:178:ILE:HD11	1:B:206:ILE:HG21	1.92	0.50
1:B:494:ALA:CB	1:B:500:LEU:HD23	2.42	0.50
1:B:497:VAL:HG11	1:B:518:THR:CB	2.42	0.50
1:B:20:ILE:HG22	1:B:53:VAL:HG11	1.93	0.50
1:D:111:LEU:HD21	1:D:115:VAL:HG11	1.93	0.50
1:D:246:MET:CE	1:D:258:VAL:CG1	2.89	0.50
1:A:494:ALA:CB	1:A:500:LEU:HD23	2.42	0.49
1:B:532:GLU:O	1:B:555:VAL:N	2.45	0.49
1:C:401:THR:O	1:C:420:VAL:HG13	2.12	0.49
1:C:533:GLU:O	1:C:534:ASN:CB	2.60	0.49
1:B:301:ILE:HA	1:B:305:THR:HG22	1.94	0.49
1:D:182:ILE:HG21	1:D:210:GLN:HG2	1.94	0.49
1:A:111:LEU:HD23	1:A:115:VAL:HG13	1.93	0.49
1:A:219:LYS:O	1:A:220:ILE:C	2.51	0.49
1:B:533:GLU:O	1:B:534:ASN:CB	2.60	0.49
1:C:220:ILE:HG21	1:C:226:ILE:HD13	1.94	0.49
1:C:242:ALA:HB1	1:C:277:THR:HG21	1.94	0.49
1:C:60:ILE:HD13	1:C:407:ALA:HB1	1.95	0.49
1:D:219:LYS:O	1:D:220:ILE:C	2.50	0.49
1:B:376:VAL:O	1:B:376:VAL:HG13	2.12	0.49
1:B:111:LEU:HD23	1:B:115:VAL:HG13	1.94	0.49
1:B:419:VAL:HG21	1:B:437:THR:HG21	1.94	0.49
1:C:99:GLY:C	1:C:100:THR:HG22	2.33	0.49
1:C:532:GLU:O	1:C:555:VAL:N	2.46	0.49
1:B:582:ALA:C	1:B:583:ASN:HD22	2.16	0.49
1:C:21:GLU:OE2	1:C:57:LEU:HD21	2.13	0.49
1:C:178:ILE:HD11	1:C:206:ILE:HG21	1.94	0.48
1:C:310:LEU:HD21	1:C:327:MET:HE2	1.94	0.48
1:C:491:THR:HG21	1:C:562:ILE:HD13	1.94	0.48
1:D:110:ASN:ND2	1:D:110:ASN:O	2.46	0.48
1:A:110:ASN:O	1:A:110:ASN:ND2	2.46	0.48
1:B:400:VAL:O	1:B:400:VAL:HG12	2.12	0.48
1:C:217:PHE:CZ	1:C:238:GLY:HA3	2.48	0.48
1:D:220:ILE:HG21	1:D:226:ILE:HD13	1.94	0.48
1:A:509:VAL:HG12	1:A:528:GLY:CA	2.42	0.48
1:C:111:LEU:HD23	1:C:111:LEU:C	2.34	0.48
1:C:20:ILE:HG22	1:C:53:VAL:HG11	1.95	0.48
1:B:165:VAL:HG12	1:B:167:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:THR:HG21	1:B:519:PHE:CE2	2.48	0.48
1:C:424:ARG:HB3	1:C:429:ALA:HB3	1.96	0.48
1:B:516:ASP:O	1:B:520:VAL:HG13	2.13	0.48
1:D:235:VAL:HG12	1:D:235:VAL:O	2.13	0.48
1:D:63:ILE:CG2	1:D:186:VAL:HG23	2.44	0.48
1:A:367:ALA:HA	1:A:372:VAL:HG13	1.94	0.48
1:B:401:THR:O	1:B:420:VAL:HG13	2.14	0.48
1:C:484:ARG:C	1:C:572:ALA:HB3	2.34	0.48
1:D:265:GLN:O	1:D:269:LEU:HD12	2.13	0.48
1:B:473:GLY:HA3	1:B:474:ASP:HB2	1.96	0.48
1:A:582:ALA:C	1:A:583:ASN:HD22	2.15	0.48
1:B:117:VAL:HA	1:B:132:VAL:HG12	1.95	0.48
1:B:217:PHE:CZ	1:B:238:GLY:HA3	2.48	0.48
1:B:530:ILE:CG2	1:B:555:VAL:HG21	2.44	0.48
1:C:235:VAL:O	1:C:235:VAL:HG12	2.14	0.48
1:C:419:VAL:HG21	1:C:437:THR:HG21	1.95	0.48
1:C:60:ILE:CD1	1:C:407:ALA:HB1	2.43	0.48
1:C:63:ILE:CG2	1:C:186:VAL:HG23	2.43	0.48
1:D:562:ILE:HD12	1:D:563:SER:O	2.14	0.48
1:B:379:THR:CG2	1:B:384:THR:HB	2.43	0.48
1:D:229:ILE:HG12	1:D:262:LEU:HD23	1.95	0.48
1:B:220:ILE:HD11	1:B:232:ILE:HD13	1.96	0.48
1:C:511:VAL:HG21	1:C:562:ILE:HD11	1.96	0.48
1:D:484:ARG:C	1:D:572:ALA:HB3	2.34	0.48
1:A:419:VAL:HG21	1:A:437:THR:CG2	2.45	0.47
1:D:188:PHE:CD1	1:D:215:SER:HB2	2.49	0.47
1:D:178:ILE:HD11	1:D:206:ILE:HG21	1.96	0.47
1:D:419:VAL:HG21	1:D:437:THR:CG2	2.44	0.47
1:D:509:VAL:HG12	1:D:528:GLY:CA	2.43	0.47
1:D:497:VAL:HG11	1:D:518:THR:CB	2.43	0.47
1:B:437:THR:O	1:B:441:THR:HG23	2.14	0.47
1:A:491:THR:HG21	1:A:562:ILE:HD13	1.96	0.47
1:B:165:VAL:HG11	1:B:167:LEU:HD23	1.95	0.47
1:B:188:PHE:CD1	1:B:215:SER:HB2	2.49	0.47
1:B:294:ALA:HA	1:B:330:ILE:HD13	1.96	0.47
1:B:347:ARG:O	1:B:351:VAL:HG13	2.14	0.47
1:C:379:THR:HG23	1:C:384:THR:HB	1.95	0.47
1:D:4:THR:CG2	1:D:331:ALA:HB1	2.44	0.47
1:C:165:VAL:HG12	1:C:167:LEU:HD23	1.94	0.47
1:C:182:ILE:HG21	1:C:210:GLN:HG2	1.95	0.47
1:A:473:GLY:HA3	1:A:474:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:VAL:HG11	1:A:518:THR:CB	2.44	0.47
1:B:279:MET:CE	1:B:308:VAL:HG13	2.43	0.47
1:A:178:ILE:HD11	1:A:206:ILE:HG21	1.95	0.47
1:B:219:LYS:O	1:B:220:ILE:C	2.53	0.47
1:D:533:GLU:O	1:D:534:ASN:CB	2.63	0.47
1:A:177:ASP:O	1:A:180:PHE:HB3	2.15	0.47
1:A:471:LEU:HD23	1:A:472:VAL:H	1.80	0.47
1:C:516:ASP:O	1:C:520:VAL:HG13	2.15	0.47
1:C:529:LEU:HD11	1:C:531:THR:CG2	2.43	0.47
1:A:229:ILE:HG12	1:A:262:LEU:HD23	1.97	0.47
1:C:111:LEU:HD21	1:C:115:VAL:HG11	1.97	0.47
1:D:294:ALA:HA	1:D:330:ILE:HD13	1.97	0.47
1:D:20:ILE:HG22	1:D:53:VAL:HG11	1.96	0.47
1:D:530:ILE:HD12	1:D:530:ILE:N	2.30	0.46
1:A:484:ARG:C	1:A:572:ALA:HB3	2.36	0.46
1:B:509:VAL:HG12	1:B:528:GLY:CA	2.45	0.46
1:B:538:SER:HB2	1:B:539:PRO:HD2	1.96	0.46
1:B:60:ILE:CD1	1:B:407:ALA:HB1	2.45	0.46
1:C:188:PHE:CD1	1:C:215:SER:HB2	2.50	0.46
1:A:111:LEU:HD21	1:A:115:VAL:HG11	1.96	0.46
1:A:294:ALA:HA	1:A:330:ILE:HD13	1.97	0.46
1:D:366:THR:HG22	1:D:451:ILE:CD1	2.42	0.46
1:D:95:ASN:O	1:D:97:VAL:HG13	2.15	0.46
1:A:533:GLU:O	1:A:534:ASN:CB	2.62	0.46
1:D:400:VAL:O	1:D:400:VAL:HG12	2.15	0.46
1:A:85:GLU:O	1:A:146:ILE:CG2	2.63	0.46
1:C:379:THR:HG22	2:C:586:PO4:O3	2.15	0.46
1:C:63:ILE:HG22	1:C:186:VAL:CG2	2.45	0.46
1:C:388:ILE:HG22	1:C:397:ILE:CD1	2.45	0.46
1:D:60:ILE:CD1	1:D:407:ALA:HB1	2.44	0.46
1:A:379:THR:CG2	1:A:384:THR:HB	2.45	0.46
1:A:419:VAL:HG21	1:A:437:THR:HG21	1.97	0.46
1:C:363:VAL:CG1	1:C:375:ILE:HD13	2.46	0.46
1:D:473:GLY:HA3	1:D:474:ASP:HB2	1.97	0.46
1:A:297:VAL:O	1:A:300:ALA:HB3	2.16	0.46
1:B:297:VAL:O	1:B:300:ALA:HB3	2.16	0.46
1:B:424:ARG:HB3	1:B:429:ALA:CB	2.46	0.46
1:C:538:SER:HB2	1:C:539:PRO:HD2	1.98	0.46
1:C:110:ASN:ND2	1:C:113:ASN:HB2	2.31	0.46
1:C:219:LYS:O	1:C:220:ILE:C	2.55	0.46
1:C:419:VAL:HG21	1:C:437:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:VAL:HG21	1:C:450:ILE:HD11	1.98	0.46
1:A:408:ARG:O	1:A:411:SER:OG	2.29	0.46
1:C:424:ARG:HB3	1:C:429:ALA:CB	2.46	0.46
1:C:530:ILE:CG2	1:C:555:VAL:HG21	2.46	0.46
1:A:4:THR:CG2	1:A:331:ALA:HB1	2.46	0.45
1:C:376:VAL:HG13	1:C:376:VAL:O	2.16	0.45
1:C:437:THR:O	1:C:441:THR:HG23	2.15	0.45
1:A:437:THR:O	1:A:441:THR:HG23	2.16	0.45
1:B:424:ARG:HD2	1:B:429:ALA:HB1	1.98	0.45
1:B:31:ALA:HB3	1:B:63:ILE:HD13	1.99	0.45
1:C:424:ARG:HD2	1:C:429:ALA:HB1	1.98	0.45
1:D:388:ILE:HG22	1:D:397:ILE:CD1	2.46	0.45
1:B:21:GLU:OE2	1:B:57:LEU:HD21	2.17	0.45
1:A:355:LEU:HD23	1:B:370:LEU:HD13	1.99	0.45
1:C:562:ILE:HD12	1:C:562:ILE:C	2.36	0.45
1:A:538:SER:HB2	1:A:539:PRO:HD2	1.98	0.45
1:A:84:LEU:CD2	1:A:90:VAL:HG21	2.34	0.45
1:B:471:LEU:HD23	1:B:472:VAL:H	1.81	0.45
1:B:95:ASN:O	1:B:97:VAL:HG13	2.17	0.45
1:C:562:ILE:HD12	1:C:563:SER:O	2.17	0.45
1:A:110:ASN:ND2	1:A:113:ASN:HB2	2.32	0.45
1:B:110:ASN:ND2	1:B:113:ASN:HB2	2.31	0.45
1:B:408:ARG:O	1:B:411:SER:OG	2.27	0.45
1:D:424:ARG:HB3	1:D:429:ALA:HB3	1.98	0.45
1:D:435:VAL:O	1:D:439:VAL:HG23	2.17	0.45
1:D:538:SER:HB2	1:D:539:PRO:HD2	1.98	0.45
1:B:178:ILE:HD11	1:B:206:ILE:HD12	1.99	0.45
1:B:235:VAL:HG12	1:B:235:VAL:O	2.17	0.45
1:B:85:GLU:O	1:B:146:ILE:CG2	2.65	0.45
1:C:305:THR:O	1:C:305:THR:HG23	2.17	0.45
1:A:334:ALA:HB2	1:D:257:MET:HE2	1.99	0.44
1:A:21:GLU:OE2	1:A:57:LEU:HD21	2.17	0.44
1:C:85:GLU:O	1:C:146:ILE:CG2	2.65	0.44
1:A:265:GLN:O	1:A:269:LEU:HD12	2.18	0.44
1:A:444:VAL:HG21	1:A:450:ILE:HD11	1.99	0.44
1:A:530:ILE:CG2	1:A:555:VAL:HG21	2.46	0.44
1:A:400:VAL:CG2	1:A:437:THR:HG21	2.47	0.44
1:A:296:ASP:CG	1:D:291:ARG:HH12	2.20	0.44
1:A:170:ILE:HD11	1:A:202:GLU:HB3	1.99	0.44
1:B:562:ILE:HD12	1:B:562:ILE:C	2.38	0.44
1:D:111:LEU:HD23	1:D:115:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:HD11	1:B:206:ILE:CD1	2.48	0.44
1:B:280:LEU:HD23	1:B:293:GLU:HB3	1.99	0.44
1:D:419:VAL:HG21	1:D:437:THR:HG21	1.98	0.44
1:B:111:LEU:HD21	1:B:115:VAL:HG11	2.00	0.44
1:B:63:ILE:CG2	1:B:186:VAL:CG2	2.96	0.44
1:D:85:GLU:O	1:D:146:ILE:CG2	2.65	0.44
1:A:208:GLU:OE2	1:B:536:ILE:HG23	2.18	0.44
1:B:491:THR:HG22	1:B:509:VAL:HG23	2.00	0.44
1:D:110:ASN:ND2	1:D:113:ASN:HB2	2.33	0.44
1:D:86:ARG:HG3	1:D:149:SER:H	1.83	0.44
1:D:165:VAL:HG12	1:D:167:LEU:HD23	1.97	0.44
1:D:10:ILE:HG13	1:D:50:ILE:HD11	2.00	0.44
1:A:424:ARG:HB3	1:A:429:ALA:HB3	2.00	0.44
1:C:111:LEU:HD23	1:C:115:VAL:CG1	2.48	0.44
1:C:178:ILE:HD11	1:C:206:ILE:CD1	2.48	0.44
1:D:280:LEU:HD23	1:D:293:GLU:HB3	2.00	0.44
1:D:379:THR:CG2	1:D:384:THR:HB	2.47	0.44
1:A:188:PHE:CD1	1:A:215:SER:HB2	2.52	0.43
1:B:529:LEU:HB3	1:B:551:THR:CG2	2.45	0.43
1:B:84:LEU:HD23	1:B:90:VAL:CG2	2.28	0.43
1:C:433:ASN:O	1:C:434:ALA:C	2.56	0.43
1:C:75:HIS:O	1:C:76:ASN:O	2.36	0.43
1:C:111:LEU:HD23	1:C:111:LEU:O	2.18	0.43
1:B:482:ILE:HD13	1:B:541:ALA:HA	1.99	0.43
1:B:562:ILE:HD12	1:B:563:SER:O	2.18	0.43
1:B:97:VAL:HG23	1:B:98:GLU:O	2.17	0.43
1:B:99:GLY:C	1:B:100:THR:HG22	2.38	0.43
1:C:279:MET:CE	1:C:308:VAL:HG13	2.46	0.43
1:D:461:THR:CG2	2:D:587:PO4:O3	2.66	0.43
1:A:482:ILE:HD13	1:A:541:ALA:HA	2.00	0.43
1:A:111:LEU:HD23	1:A:111:LEU:C	2.39	0.43
1:C:178:ILE:HD11	1:C:206:ILE:HD12	2.00	0.43
1:C:471:LEU:HD23	1:C:472:VAL:H	1.82	0.43
1:C:355:LEU:HD23	1:D:370:LEU:HD13	2.00	0.43
1:A:562:ILE:HD12	1:A:563:SER:O	2.18	0.43
1:B:511:VAL:HG21	1:B:562:ILE:HD11	2.01	0.43
1:B:491:THR:HG21	1:B:562:ILE:HD13	2.00	0.43
1:B:74:THR:HG22	1:B:75:HIS:O	2.19	0.43
1:C:428:ASP:OD2	1:D:428:ASP:OD2	2.36	0.43
1:B:233:LEU:O	1:B:234:GLU:C	2.57	0.43
1:C:482:ILE:HD13	1:C:541:ALA:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:VAL:O	1:D:300:ALA:HB3	2.19	0.43
1:D:555:VAL:HB	1:D:558:ALA:HB2	2.00	0.43
1:B:401:THR:CG2	1:B:407:ALA:HB2	2.49	0.43
1:C:170:ILE:HD11	1:C:202:GLU:HB3	2.00	0.43
1:A:86:ARG:HG3	1:A:149:SER:H	1.83	0.43
1:D:177:ASP:O	1:D:180:PHE:HB3	2.18	0.43
1:D:482:ILE:HD13	1:D:541:ALA:HA	2.01	0.43
1:D:582:ALA:O	1:D:583:ASN:CB	2.66	0.43
1:A:495:GLU:OE2	1:A:559:VAL:HG11	2.19	0.42
1:B:495:GLU:OE2	1:B:559:VAL:HG11	2.19	0.42
1:C:220:ILE:CD1	1:C:232:ILE:HD13	2.48	0.42
1:C:570:ILE:HG22	1:C:577:ILE:HG23	1.99	0.42
1:D:471:LEU:HD23	1:D:472:VAL:H	1.82	0.42
1:B:357:ASN:O	1:B:358:ALA:C	2.57	0.42
1:C:77:MET:HE1	1:C:104:PHE:CD2	2.55	0.42
1:D:323:ALA:HA	1:D:326:THR:HG22	2.01	0.42
1:A:570:ILE:HG22	1:A:577:ILE:HG23	2.01	0.42
1:B:363:VAL:CG1	1:B:375:ILE:HD13	2.49	0.42
1:C:294:ALA:HA	1:C:330:ILE:HD13	2.02	0.42
1:D:347:ARG:O	1:D:351:VAL:HG13	2.19	0.42
1:D:99:GLY:C	1:D:100:THR:HG22	2.40	0.42
1:A:305:THR:O	1:A:305:THR:HG23	2.19	0.42
1:C:86:ARG:HG3	1:C:149:SER:H	1.85	0.42
1:D:298:ALA:O	1:D:301:ILE:N	2.52	0.42
1:A:490:THR:HA	1:A:567:LEU:HA	2.01	0.42
1:A:530:ILE:HD12	1:A:530:ILE:N	2.34	0.42
1:A:355:LEU:O	1:A:355:LEU:HD13	2.19	0.42
1:C:536:ILE:HG23	1:D:208:GLU:OE2	2.19	0.42
1:B:4:THR:HG22	1:B:331:ALA:HB1	2.01	0.42
1:C:582:ALA:O	1:C:583:ASN:CB	2.67	0.42
1:D:404:GLU:O	1:D:407:ALA:HB3	2.19	0.42
1:A:63:ILE:CG2	1:A:186:VAL:CG2	2.98	0.42
1:B:268:LYS:HA	1:B:350:LEU:HD13	2.01	0.42
1:C:297:VAL:O	1:C:300:ALA:HB3	2.20	0.42
1:D:115:VAL:HG23	1:D:116:GLN:N	2.34	0.42
1:D:357:ASN:O	1:D:358:ALA:C	2.58	0.42
1:D:63:ILE:HG22	1:D:186:VAL:CG2	2.50	0.42
1:D:178:ILE:CD1	1:D:203:ILE:HG23	2.50	0.42
1:A:3:LYS:HD2	1:A:414:TRP:CH2	2.54	0.42
1:B:392:ARG:HD3	1:B:414:TRP:CE3	2.55	0.42
1:C:178:ILE:CD1	1:C:203:ILE:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PHE:CE1	1:A:43:HIS:CD2	3.08	0.41
1:A:3:LYS:HD2	1:A:414:TRP:CZ2	2.55	0.41
1:A:461:THR:HG21	2:A:586:PO4:P	2.60	0.41
1:B:431:LEU:HD23	1:B:452:ILE:HG21	2.00	0.41
1:D:170:ILE:HD11	1:D:202:GLU:HB3	2.01	0.41
1:D:413:VAL:HG23	1:D:416:VAL:CG2	2.50	0.41
1:D:424:ARG:HB3	1:D:429:ALA:CB	2.50	0.41
1:A:376:VAL:HG13	1:A:376:VAL:O	2.19	0.41
1:B:388:ILE:HG22	1:B:397:ILE:HD13	2.01	0.41
1:D:111:LEU:HD23	1:D:111:LEU:C	2.40	0.41
1:B:260:LYS:HG2	1:B:303:ASP:CG	2.41	0.41
1:D:305:THR:HG23	1:D:305:THR:O	2.20	0.41
1:D:347:ARG:NH1	1:D:392:ARG:HG3	2.36	0.41
1:A:233:LEU:O	1:A:234:GLU:C	2.59	0.41
1:A:404:GLU:O	1:A:407:ALA:HB3	2.20	0.41
1:D:226:ILE:HD11	1:D:246:MET:CE	2.49	0.41
1:D:392:ARG:HD3	1:D:414:TRP:CE3	2.56	0.41
1:A:403:SER:CB	1:A:406:THR:HG23	2.51	0.41
1:C:97:VAL:HG23	1:C:98:GLU:O	2.20	0.41
1:D:403:SER:CB	1:D:406:THR:HG23	2.51	0.41
1:A:178:ILE:CD1	1:A:203:ILE:HG23	2.50	0.41
1:A:298:ALA:O	1:A:301:ILE:N	2.53	0.41
1:A:268:LYS:HA	1:A:350:LEU:HD13	2.02	0.41
1:D:69:GLY:HA2	1:D:174:ASP:OD2	2.19	0.41
1:D:1:MET:N	1:D:443:ARG:HH12	2.19	0.41
1:D:246:MET:HE2	1:D:258:VAL:CG1	2.51	0.41
1:B:170:ILE:HD11	1:B:202:GLU:HB3	2.02	0.41
1:B:177:ASP:O	1:B:180:PHE:HB3	2.20	0.41
1:C:401:THR:CG2	1:C:407:ALA:HB2	2.51	0.41
1:C:530:ILE:N	1:C:530:ILE:HD12	2.36	0.41
1:C:75:HIS:HB2	1:C:105:SER:OG	2.21	0.41
1:D:75:HIS:HB2	1:D:105:SER:OG	2.21	0.41
1:D:72:ILE:HD12	1:D:160:LEU:HD13	2.03	0.41
1:D:490:THR:HA	1:D:567:LEU:HA	2.03	0.41
1:B:86:ARG:HG3	1:B:149:SER:H	1.86	0.41
1:D:84:LEU:HD23	1:D:90:VAL:CG2	2.33	0.41
1:A:280:LEU:HD23	1:A:293:GLU:HB3	2.02	0.41
1:C:280:LEU:HD23	1:C:293:GLU:HB3	2.03	0.41
1:D:111:LEU:CD2	1:D:115:VAL:HG11	2.50	0.41
1:A:413:VAL:CG2	1:A:416:VAL:CG2	2.98	0.41
1:B:323:ALA:HA	1:B:326:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LEU:HD11	1:B:531:THR:CG2	2.42	0.41
1:C:4:THR:HG22	1:C:331:ALA:HB1	2.03	0.41
1:D:3:LYS:HD2	1:D:414:TRP:CH2	2.56	0.41
1:D:77:MET:HE1	1:D:104:PHE:CD2	2.56	0.41
1:A:115:VAL:HG23	1:A:116:GLN:N	2.35	0.41
1:A:461:THR:CG2	2:A:586:PO4:O2	2.69	0.41
1:B:485:GLY:N	1:B:572:ALA:HB3	2.36	0.41
1:B:530:ILE:N	1:B:530:ILE:HD12	2.36	0.41
1:C:323:ALA:HA	1:C:326:THR:HG22	2.03	0.41
1:D:266:CYS:HB3	1:D:271:LYS:O	2.21	0.41
1:D:392:ARG:HA	1:D:414:TRP:CZ3	2.56	0.41
1:D:570:ILE:HG22	1:D:577:ILE:HG23	2.02	0.41
1:A:110:ASN:HD21	1:A:113:ASN:HB2	1.87	0.40
1:C:233:LEU:O	1:C:234:GLU:C	2.60	0.40
1:C:3:LYS:HD2	1:C:414:TRP:CH2	2.57	0.40
1:D:520:VAL:HG12	1:D:543:VAL:HG11	2.03	0.40
1:A:75:HIS:HB2	1:A:105:SER:OG	2.21	0.40
1:A:323:ALA:HA	1:A:326:THR:HG22	2.02	0.40
1:A:582:ALA:O	1:A:583:ASN:CB	2.68	0.40
1:C:355:LEU:HD13	1:C:355:LEU:O	2.21	0.40
1:C:413:VAL:CG2	1:C:416:VAL:CG2	2.99	0.40
1:D:217:PHE:CZ	1:D:238:GLY:HA3	2.56	0.40
1:D:495:GLU:OE2	1:D:559:VAL:HG11	2.21	0.40
1:A:379:THR:HG23	1:A:384:THR:HB	2.03	0.40
1:A:424:ARG:HB3	1:A:429:ALA:CB	2.51	0.40
1:B:433:ASN:O	1:B:434:ALA:C	2.57	0.40
1:B:570:ILE:HG22	1:B:577:ILE:HG23	2.04	0.40
1:C:260:LYS:HG2	1:C:303:ASP:CG	2.42	0.40
1:C:259:GLN:NE2	1:C:275:THR:HG21	2.36	0.40
1:C:392:ARG:HD3	1:C:414:TRP:CE3	2.57	0.40
1:C:529:LEU:HD12	1:C:530:ILE:N	2.36	0.40
1:C:555:VAL:HB	1:C:558:ALA:HB2	2.04	0.40
1:C:490:THR:HA	1:C:567:LEU:HA	2.03	0.40
1:A:72:ILE:HD12	1:A:160:LEU:HD13	2.04	0.40
1:C:246:MET:HE2	1:C:258:VAL:CG1	2.51	0.40
1:C:347:ARG:NH1	1:C:392:ARG:HG3	2.36	0.40
1:C:360:GLY:HA2	1:C:388:ILE:HD13	2.04	0.40
1:A:484:ARG:HG3	1:A:573:ALA:HB2	2.03	0.40
1:A:77:MET:HE1	1:A:104:PHE:CD2	2.57	0.40
1:A:95:ASN:O	1:A:97:VAL:HG13	2.21	0.40
1:B:482:ILE:HD13	1:B:541:ALA:CA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ASP:CG	1:C:291:ARG:HH12	2.25	0.40
1:C:347:ARG:O	1:C:351:VAL:HG13	2.22	0.40
1:C:471:LEU:HD22	1:C:473:GLY:O	2.21	0.40

There are no symmetry-related clashes.

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%)	512 (88%)	53 (9%)	16 (3%)	5	25
1	B	581/606 (96%)	514 (88%)	51 (9%)	16 (3%)	5	25
1	C	581/606 (96%)	511 (88%)	55 (10%)	15 (3%)	5	27
1	D	581/606 (96%)	512 (88%)	52 (9%)	17 (3%)	4	24
All	All	2324/2424 (96%)	2049 (88%)	211 (9%)	64 (3%)	5	25

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	220	ILE
1	B	154	ASN
1	B	220	ILE
1	C	154	ASN
1	C	220	ILE
1	D	154	ASN
1	D	220	ILE
1	A	534	ASN
1	B	534	ASN
1	C	76	ASN
1	C	506	SER

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Mol	Chain	Res	Type
1	C	534	ASN
1	D	534	ASN
1	A	475	GLU
1	A	506	SER
1	B	475	GLU
1	B	506	SER
1	C	475	GLU
1	D	475	GLU
1	D	506	SER
1	A	76	ASN
1	A	138	ALA
1	A	320	PRO
1	A	411	SER
1	A	460	GLU
1	B	76	ASN
1	B	320	PRO
1	B	411	SER
1	B	507	ASP
1	C	411	SER
1	C	507	ASP
1	D	76	ASN
1	D	138	ALA
1	D	161	PRO
1	A	161	PRO
1	A	163	VAL
1	A	507	ASP
1	B	138	ALA
1	B	161	PRO
1	B	163	VAL
1	B	460	GLU
1	C	138	ALA
1	C	161	PRO
1	C	163	VAL
1	C	320	PRO
1	C	460	GLU
1	D	163	VAL
1	D	320	PRO
1	D	411	SER
1	D	460	GLU
1	D	507	ASP
1	D	162	GLY
1	A	459	GLY

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Mol	Chain	Res	Type
1	B	473	GLY
1	D	473	GLY
1	B	459	GLY
1	D	459	GLY
1	B	162	GLY
1	C	459	GLY
1	C	473	GLY
1	D	115	VAL
1	A	162	GLY
1	A	473	GLY

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%)	471 (96%)	19 (4%)	32	62
1	B	490/510 (96%)	471 (96%)	19 (4%)	32	62
1	C	490/510 (96%)	469 (96%)	21 (4%)	29	59
1	D	490/510 (96%)	470 (96%)	20 (4%)	30	61
All	All	1960/2040 (96%)	1881 (96%)	79 (4%)	31	61

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	MET
1	A	100	THR
1	A	110	ASN
1	A	136	ASP
1	A	170	ILE
1	A	171	THR
1	A	186	VAL
1	A	195	ARG
1	A	257	MET
1	A	269	LEU
1	A	350	LEU

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Mol	Chain	Res	Type
1	A	351	VAL
1	A	359	ILE
1	A	372	VAL
1	A	379	THR
1	A	466	MET
1	A	495	GLU
1	A	496	THR
1	A	562	ILE
1	B	77	MET
1	B	100	THR
1	B	110	ASN
1	B	136	ASP
1	B	170	ILE
1	B	171	THR
1	B	186	VAL
1	B	195	ARG
1	B	198	SER
1	B	257	MET
1	B	269	LEU
1	B	350	LEU
1	B	351	VAL
1	B	359	ILE
1	B	372	VAL
1	B	466	MET
1	B	495	GLU
1	B	496	THR
1	B	562	ILE
1	C	77	MET
1	C	100	THR
1	C	110	ASN
1	C	136	ASP
1	C	170	ILE
1	C	171	THR
1	C	178	ILE
1	C	186	VAL
1	C	195	ARG
1	C	257	MET
1	C	269	LEU
1	C	350	LEU
1	C	351	VAL
1	C	359	ILE
1	C	372	VAL

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Mol	Chain	Res	Type
1	C	379	THR
1	C	450	ILE
1	C	466	MET
1	C	495	GLU
1	C	496	THR
1	C	562	ILE
1	D	77	MET
1	D	100	THR
1	D	110	ASN
1	D	136	ASP
1	D	170	ILE
1	D	171	THR
1	D	178	ILE
1	D	186	VAL
1	D	195	ARG
1	D	198	SER
1	D	257	MET
1	D	269	LEU
1	D	350	LEU
1	D	359	ILE
1	D	372	VAL
1	D	379	THR
1	D	466	MET
1	D	495	GLU
1	D	496	THR
1	D	562	ILE

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

Mol	Chain	Res	Type
1	A	43	HIS
1	A	409	GLN
1	A	583	ASN
1	B	43	HIS
1	B	409	GLN
1	B	583	ASN
1	C	43	HIS
1	C	110	ASN
1	C	409	GLN
1	C	583	ASN
1	D	43	HIS
1	D	409	GLN

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Mol	Chain	Res	Type
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](#)

6 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	$\# Z > 2$
3	09C	B	586	-	29,31,31	3.52	12 (41%)	32,46,46	3.18	13 (40%)
2	PO4	A	586	-	4,4,4	0.71	0	6,6,6	0.84	0
2	PO4	B	587	-	4,4,4	0.97	0	6,6,6	0.66	0
2	PO4	D	587	-	4,4,4	0.79	0	6,6,6	0.60	0
2	PO4	C	586	-	4,4,4	0.85	0	6,6,6	0.64	0
3	09C	D	586	-	29,31,31	3.57	13 (44%)	32,46,46	3.28	12 (37%)

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
3	09C	B	586	-	1/1/3/5	0/0/21/21	0/5/5/5
3	09C	D	586	-	1/1/3/5	0/0/21/21	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	586	09C	C12-N1	-13.28	1.32	1.46
3	B	586	09C	C12-N1	-12.99	1.32	1.46
3	B	586	09C	C15-C12	-6.98	1.40	1.52
3	D	586	09C	C15-C12	-6.93	1.40	1.52
3	B	586	09C	C1-N2	6.20	1.44	1.33
3	D	586	09C	C1-N2	6.09	1.44	1.33
3	D	586	09C	C11-N2	5.22	1.51	1.46
3	B	586	09C	C11-N2	5.13	1.51	1.46
3	D	586	09C	C16-C2	3.98	1.57	1.52
3	B	586	09C	C9-C17	-3.60	1.36	1.41
3	B	586	09C	C16-C2	3.18	1.56	1.52
3	D	586	09C	C10-C18	-3.03	1.37	1.41
3	D	586	09C	C9-C17	-3.00	1.37	1.41
3	B	586	09C	C2-N1	-2.75	1.44	1.47
3	D	586	09C	C5-C3	2.57	1.42	1.36
3	B	586	09C	C10-C18	-2.48	1.38	1.41
3	D	586	09C	C2-N1	-2.47	1.45	1.47
3	B	586	09C	C6-C4	2.42	1.41	1.36
3	D	586	09C	C7-N3	-2.36	1.31	1.36
3	D	586	09C	C17-N3	-2.30	1.31	1.38
3	B	586	09C	C17-N3	-2.23	1.31	1.38
3	D	586	09C	C6-C4	2.14	1.41	1.36
3	D	586	09C	C18-N4	-2.11	1.32	1.38
3	B	586	09C	C8-N4	-2.10	1.32	1.36
3	B	586	09C	C5-C3	2.04	1.40	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	586	09C	C2-N1-C12	11.83	134.72	111.92
3	B	586	09C	C2-N1-C12	11.46	134.02	111.92
3	D	586	09C	BR1-C13-C3	5.91	127.89	119.30
3	B	586	09C	BR1-C13-C9	-5.70	111.34	119.72
3	B	586	09C	BR2-C14-C4	5.04	126.62	119.30
3	D	586	09C	C16-C2-C1	4.70	116.20	110.90
3	B	586	09C	BR1-C13-C3	4.59	125.97	119.30
3	D	586	09C	C15-C12-N1	-4.55	104.69	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	586	09C	BR1-C13-C9	-4.46	113.17	119.72
3	D	586	09C	BR2-C14-C4	4.31	125.56	119.30
3	D	586	09C	BR2-C14-C10	-3.96	113.90	119.72
3	B	586	09C	C16-C2-C1	3.74	115.12	110.90
3	B	586	09C	C15-C12-N1	-3.69	105.90	111.08
3	B	586	09C	BR2-C14-C10	-3.50	114.58	119.72
3	D	586	09C	C15-C19-C17	-3.23	103.47	106.83
3	B	586	09C	C15-C19-C17	-3.08	103.63	106.83
3	B	586	09C	C3-C5-C19	-2.99	116.97	121.13
3	B	586	09C	C16-C20-C18	-2.93	103.78	106.83
3	D	586	09C	C16-C20-C18	-2.65	104.08	106.83
3	B	586	09C	C1-C2-N1	-2.54	104.20	111.03
3	D	586	09C	C4-C6-C20	-2.51	117.64	121.13
3	D	586	09C	C5-C19-C15	2.32	139.31	134.68
3	B	586	09C	C4-C14-C10	-2.29	118.80	121.99
3	D	586	09C	C3-C13-C9	-2.19	118.94	121.99
3	B	586	09C	C15-C7-N3	2.17	112.94	108.79

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	586	09C	C12
3	D	586	09C	C12

There are no torsion outliers.

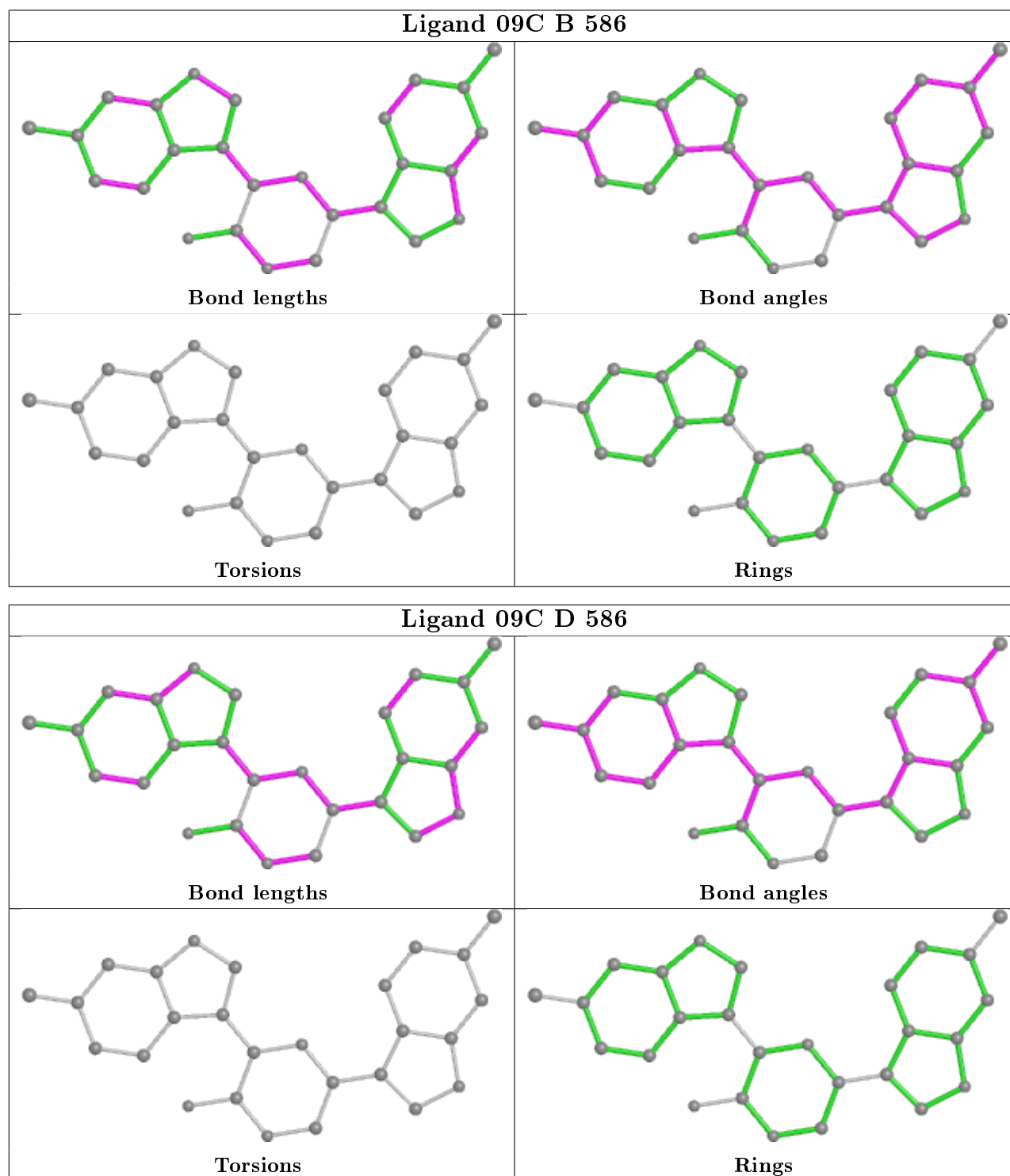
There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	586	09C	3	0
2	A	586	PO4	4	0
2	B	587	PO4	1	0
2	D	587	PO4	2	0
2	C	586	PO4	1	0
3	D	586	09C	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	583/606 (96%)	0.33	40 (6%) 16 16	90, 151, 212, 258	0
1	B	583/606 (96%)	0.03	9 (1%) 73 72	80, 135, 177, 220	0
1	C	583/606 (96%)	0.03	4 (0%) 87 88	85, 133, 175, 234	0
1	D	583/606 (96%)	0.38	44 (7%) 14 13	92, 154, 210, 236	0
All	All	2332/2424 (96%)	0.19	97 (4%) 36 34	80, 143, 202, 258	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	GLY	6.4
1	D	130	LEU	5.8
1	D	146	ILE	5.2
1	A	130	LEU	4.6
1	D	144	CYS	4.6
1	D	502	GLY	4.6
1	D	90	VAL	4.4
1	A	90	VAL	4.3
1	A	523	VAL	4.2
1	A	494	ALA	4.1
1	A	144	CYS	4.0
1	D	523	VAL	3.9
1	B	494	ALA	3.8
1	D	128	ILE	3.7
1	D	494	ALA	3.7
1	A	121	ILE	3.6
1	A	128	ILE	3.5
1	D	104	PHE	3.5
1	A	141	GLU	3.4
1	A	146	ILE	3.4
1	A	518	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	142	VAL	3.1
1	A	104	PHE	3.1
1	D	61	VAL	3.1
1	D	92	VAL	3.0
1	D	522	TYR	3.0
1	A	91	ILE	2.9
1	A	498	LYS	2.9
1	D	27	GLY	2.9
1	D	101	PRO	2.9
1	D	504	ASP	2.9
1	D	121	ILE	2.9
1	D	91	ILE	2.8
1	A	79	ASP	2.8
1	A	423	GLY	2.8
1	A	103	LYS	2.8
1	A	511	VAL	2.7
1	A	492	LEU	2.7
1	A	504	ASP	2.7
1	A	135	ILE	2.6
1	A	522	TYR	2.6
1	D	117	VAL	2.6
1	D	145	ASP	2.6
1	A	519	PHE	2.6
1	B	497	VAL	2.6
1	A	81	ILE	2.6
1	D	112	ILE	2.6
1	A	500	LEU	2.6
1	D	519	PHE	2.6
1	A	503	LYS	2.5
1	D	79	ASP	2.5
1	D	511	VAL	2.5
1	C	523	VAL	2.5
1	A	501	GLU	2.5
1	B	81	ILE	2.5
1	A	101	PRO	2.4
1	D	142	VAL	2.4
1	D	515	ILE	2.4
1	A	510	ILE	2.4
1	D	444	VAL	2.3
1	B	146	ILE	2.3
1	A	78	LYS	2.3
1	D	533	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	60	ILE	2.3
1	D	493	VAL	2.3
1	D	151	GLU	2.3
1	D	141	GLU	2.3
1	A	562	ILE	2.3
1	B	502	GLY	2.3
1	D	78	LYS	2.3
1	D	562	ILE	2.3
1	C	502	GLY	2.2
1	D	123	LEU	2.2
1	A	566	VAL	2.2
1	D	85	GLU	2.2
1	A	444	VAL	2.2
1	D	103	LYS	2.2
1	A	509	VAL	2.2
1	D	88	ASN	2.2
1	B	492	LEU	2.2
1	D	152	LEU	2.2
1	C	497	VAL	2.2
1	A	118	GLY	2.2
1	A	512	THR	2.2
1	D	570	ILE	2.1
1	C	81	ILE	2.1
1	B	10	ILE	2.1
1	D	530	ILE	2.1
1	D	503	LYS	2.1
1	B	504	ASP	2.1
1	D	518	THR	2.1
1	D	135	ILE	2.1
1	D	566	VAL	2.0
1	A	143	LYS	2.0
1	B	512	THR	2.0
1	A	151	GLU	2.0
1	A	505	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](#)

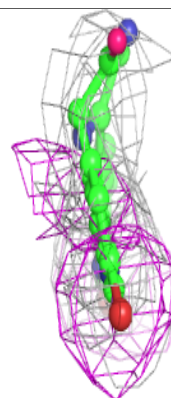
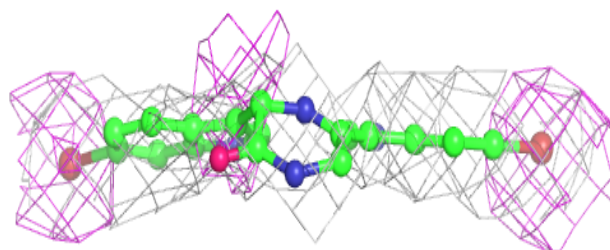
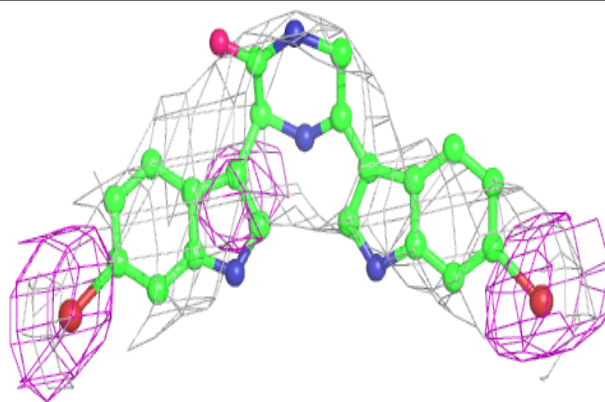
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	09C	D	586	27/27	0.90	0.39	123,160,180,182	0
2	PO4	B	587	5/5	0.91	0.19	143,161,175,179	0
3	09C	B	586	27/27	0.93	0.24	125,145,174,182	0
2	PO4	A	586	5/5	0.93	0.33	118,135,167,168	0
2	PO4	D	587	5/5	0.95	0.18	149,154,164,170	0
2	PO4	C	586	5/5	0.98	0.21	143,150,162,169	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

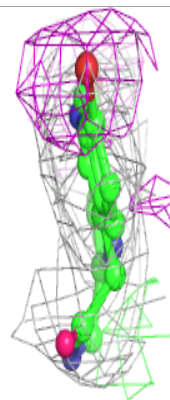
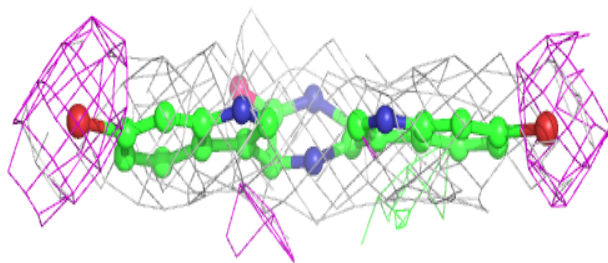
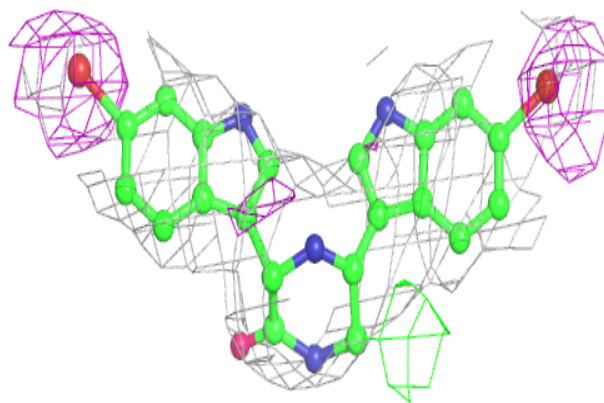
Electron density around 09C D 586:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 09C B 586:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.