Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 08:17 PM EDT

PDB ID	:	6DU6
Title	:	Crystal structure of the pyruvate kinase (PK1) from the mosquito Aedes aegypti
Authors	:	Pizarro, J.C.; Scaraffia, P.Y.; Petchampai, N.; Murillo-Solano, C.
Deposited on	:	2018-06-19
Resolution	:	3.51 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

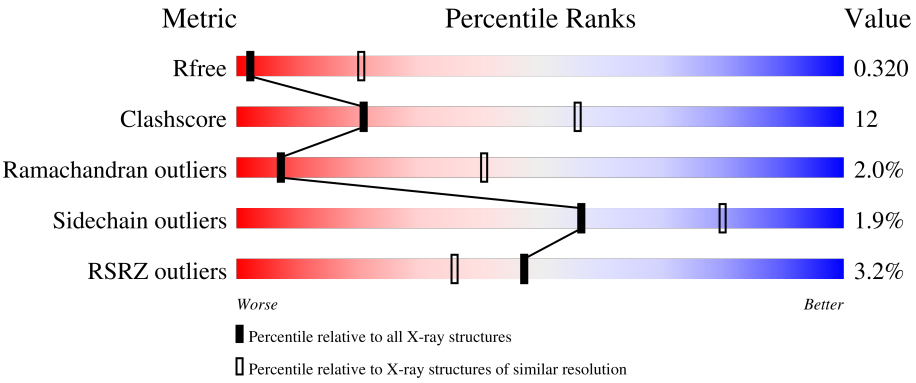
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.51 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	565	62% 24% • 11%
1	B	565	2% 63% 26% • 10%
1	C	565	4% 61% 28% • 9%
1	D	565	5% 62% 27% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15364 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	503	Total	C	N	O	S	0	0	0
			3786	2379	663	721	23			
1	B	509	Total	C	N	O	S	0	0	0
			3811	2393	663	732	23			
1	C	512	Total	C	N	O	S	0	0	0
			3873	2432	678	740	23			
1	D	505	Total	C	N	O	S	0	0	0
			3814	2396	666	729	23			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q16F38
A	-16	ALA	-	expression tag	UNP Q16F38
A	-15	SER	-	expression tag	UNP Q16F38
A	-14	TRP	-	expression tag	UNP Q16F38
A	-13	SER	-	expression tag	UNP Q16F38
A	-12	HIS	-	expression tag	UNP Q16F38
A	-11	PRO	-	expression tag	UNP Q16F38
A	-10	GLN	-	expression tag	UNP Q16F38
A	-9	PHE	-	expression tag	UNP Q16F38
A	-8	GLU	-	expression tag	UNP Q16F38
A	-7	LYS	-	expression tag	UNP Q16F38
A	-6	GLY	-	expression tag	UNP Q16F38
A	-5	ALA	-	expression tag	UNP Q16F38
A	-4	ASP	-	expression tag	UNP Q16F38
A	-3	ASP	-	expression tag	UNP Q16F38
A	-2	ASP	-	expression tag	UNP Q16F38
A	-1	ASP	-	expression tag	UNP Q16F38
A	0	LYS	-	expression tag	UNP Q16F38
A	530	PRO	-	expression tag	UNP Q16F38
A	531	GLY	-	expression tag	UNP Q16F38
A	532	PHE	-	expression tag	UNP Q16F38

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Chain	Residue	Modelled	Actual	Comment	Reference
A	533	SER	-	expression tag	UNP Q16F38
A	534	SER	-	expression tag	UNP Q16F38
A	535	ILE	-	expression tag	UNP Q16F38
A	536	SER	-	expression tag	UNP Q16F38
A	537	ALA	-	expression tag	UNP Q16F38
A	538	HIS	-	expression tag	UNP Q16F38
A	539	HIS	-	expression tag	UNP Q16F38
A	540	HIS	-	expression tag	UNP Q16F38
A	541	HIS	-	expression tag	UNP Q16F38
A	542	HIS	-	expression tag	UNP Q16F38
A	543	HIS	-	expression tag	UNP Q16F38
A	544	HIS	-	expression tag	UNP Q16F38
A	545	HIS	-	expression tag	UNP Q16F38
A	546	HIS	-	expression tag	UNP Q16F38
A	547	HIS	-	expression tag	UNP Q16F38
B	-17	MET	-	initiating methionine	UNP Q16F38
B	-16	ALA	-	expression tag	UNP Q16F38
B	-15	SER	-	expression tag	UNP Q16F38
B	-14	TRP	-	expression tag	UNP Q16F38
B	-13	SER	-	expression tag	UNP Q16F38
B	-12	HIS	-	expression tag	UNP Q16F38
B	-11	PRO	-	expression tag	UNP Q16F38
B	-10	GLN	-	expression tag	UNP Q16F38
B	-9	PHE	-	expression tag	UNP Q16F38
B	-8	GLU	-	expression tag	UNP Q16F38
B	-7	LYS	-	expression tag	UNP Q16F38
B	-6	GLY	-	expression tag	UNP Q16F38
B	-5	ALA	-	expression tag	UNP Q16F38
B	-4	ASP	-	expression tag	UNP Q16F38
B	-3	ASP	-	expression tag	UNP Q16F38
B	-2	ASP	-	expression tag	UNP Q16F38
B	-1	ASP	-	expression tag	UNP Q16F38
B	0	LYS	-	expression tag	UNP Q16F38
B	530	PRO	-	expression tag	UNP Q16F38
B	531	GLY	-	expression tag	UNP Q16F38
B	532	PHE	-	expression tag	UNP Q16F38
B	533	SER	-	expression tag	UNP Q16F38
B	534	SER	-	expression tag	UNP Q16F38
B	535	ILE	-	expression tag	UNP Q16F38
B	536	SER	-	expression tag	UNP Q16F38
B	537	ALA	-	expression tag	UNP Q16F38
B	538	HIS	-	expression tag	UNP Q16F38

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Chain	Residue	Modelled	Actual	Comment	Reference
B	539	HIS	-	expression tag	UNP Q16F38
B	540	HIS	-	expression tag	UNP Q16F38
B	541	HIS	-	expression tag	UNP Q16F38
B	542	HIS	-	expression tag	UNP Q16F38
B	543	HIS	-	expression tag	UNP Q16F38
B	544	HIS	-	expression tag	UNP Q16F38
B	545	HIS	-	expression tag	UNP Q16F38
B	546	HIS	-	expression tag	UNP Q16F38
B	547	HIS	-	expression tag	UNP Q16F38
C	-17	MET	-	initiating methionine	UNP Q16F38
C	-16	ALA	-	expression tag	UNP Q16F38
C	-15	SER	-	expression tag	UNP Q16F38
C	-14	TRP	-	expression tag	UNP Q16F38
C	-13	SER	-	expression tag	UNP Q16F38
C	-12	HIS	-	expression tag	UNP Q16F38
C	-11	PRO	-	expression tag	UNP Q16F38
C	-10	GLN	-	expression tag	UNP Q16F38
C	-9	PHE	-	expression tag	UNP Q16F38
C	-8	GLU	-	expression tag	UNP Q16F38
C	-7	LYS	-	expression tag	UNP Q16F38
C	-6	GLY	-	expression tag	UNP Q16F38
C	-5	ALA	-	expression tag	UNP Q16F38
C	-4	ASP	-	expression tag	UNP Q16F38
C	-3	ASP	-	expression tag	UNP Q16F38
C	-2	ASP	-	expression tag	UNP Q16F38
C	-1	ASP	-	expression tag	UNP Q16F38
C	0	LYS	-	expression tag	UNP Q16F38
C	530	PRO	-	expression tag	UNP Q16F38
C	531	GLY	-	expression tag	UNP Q16F38
C	532	PHE	-	expression tag	UNP Q16F38
C	533	SER	-	expression tag	UNP Q16F38
C	534	SER	-	expression tag	UNP Q16F38
C	535	ILE	-	expression tag	UNP Q16F38
C	536	SER	-	expression tag	UNP Q16F38
C	537	ALA	-	expression tag	UNP Q16F38
C	538	HIS	-	expression tag	UNP Q16F38
C	539	HIS	-	expression tag	UNP Q16F38
C	540	HIS	-	expression tag	UNP Q16F38
C	541	HIS	-	expression tag	UNP Q16F38
C	542	HIS	-	expression tag	UNP Q16F38
C	543	HIS	-	expression tag	UNP Q16F38
C	544	HIS	-	expression tag	UNP Q16F38

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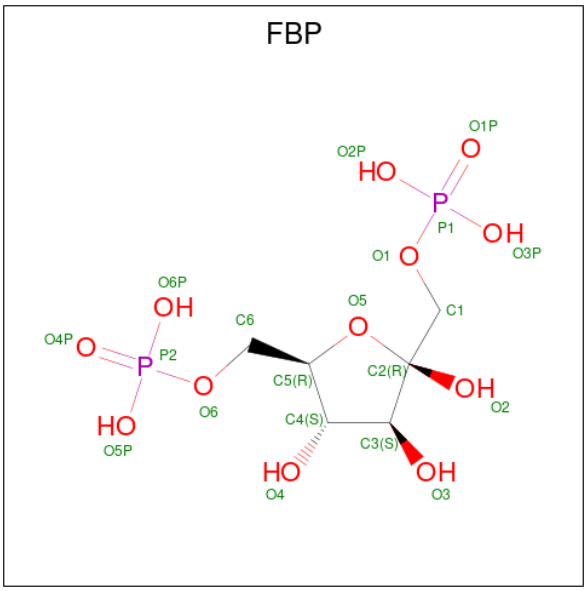
Chain	Residue	Modelled	Actual	Comment	Reference
C	545	HIS	-	expression tag	UNP Q16F38
C	546	HIS	-	expression tag	UNP Q16F38
C	547	HIS	-	expression tag	UNP Q16F38
D	-17	MET	-	initiating methionine	UNP Q16F38
D	-16	ALA	-	expression tag	UNP Q16F38
D	-15	SER	-	expression tag	UNP Q16F38
D	-14	TRP	-	expression tag	UNP Q16F38
D	-13	SER	-	expression tag	UNP Q16F38
D	-12	HIS	-	expression tag	UNP Q16F38
D	-11	PRO	-	expression tag	UNP Q16F38
D	-10	GLN	-	expression tag	UNP Q16F38
D	-9	PHE	-	expression tag	UNP Q16F38
D	-8	GLU	-	expression tag	UNP Q16F38
D	-7	LYS	-	expression tag	UNP Q16F38
D	-6	GLY	-	expression tag	UNP Q16F38
D	-5	ALA	-	expression tag	UNP Q16F38
D	-4	ASP	-	expression tag	UNP Q16F38
D	-3	ASP	-	expression tag	UNP Q16F38
D	-2	ASP	-	expression tag	UNP Q16F38
D	-1	ASP	-	expression tag	UNP Q16F38
D	0	LYS	-	expression tag	UNP Q16F38
D	530	PRO	-	expression tag	UNP Q16F38
D	531	GLY	-	expression tag	UNP Q16F38
D	532	PHE	-	expression tag	UNP Q16F38
D	533	SER	-	expression tag	UNP Q16F38
D	534	SER	-	expression tag	UNP Q16F38
D	535	ILE	-	expression tag	UNP Q16F38
D	536	SER	-	expression tag	UNP Q16F38
D	537	ALA	-	expression tag	UNP Q16F38
D	538	HIS	-	expression tag	UNP Q16F38
D	539	HIS	-	expression tag	UNP Q16F38
D	540	HIS	-	expression tag	UNP Q16F38
D	541	HIS	-	expression tag	UNP Q16F38
D	542	HIS	-	expression tag	UNP Q16F38
D	543	HIS	-	expression tag	UNP Q16F38
D	544	HIS	-	expression tag	UNP Q16F38
D	545	HIS	-	expression tag	UNP Q16F38
D	546	HIS	-	expression tag	UNP Q16F38
D	547	HIS	-	expression tag	UNP Q16F38

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



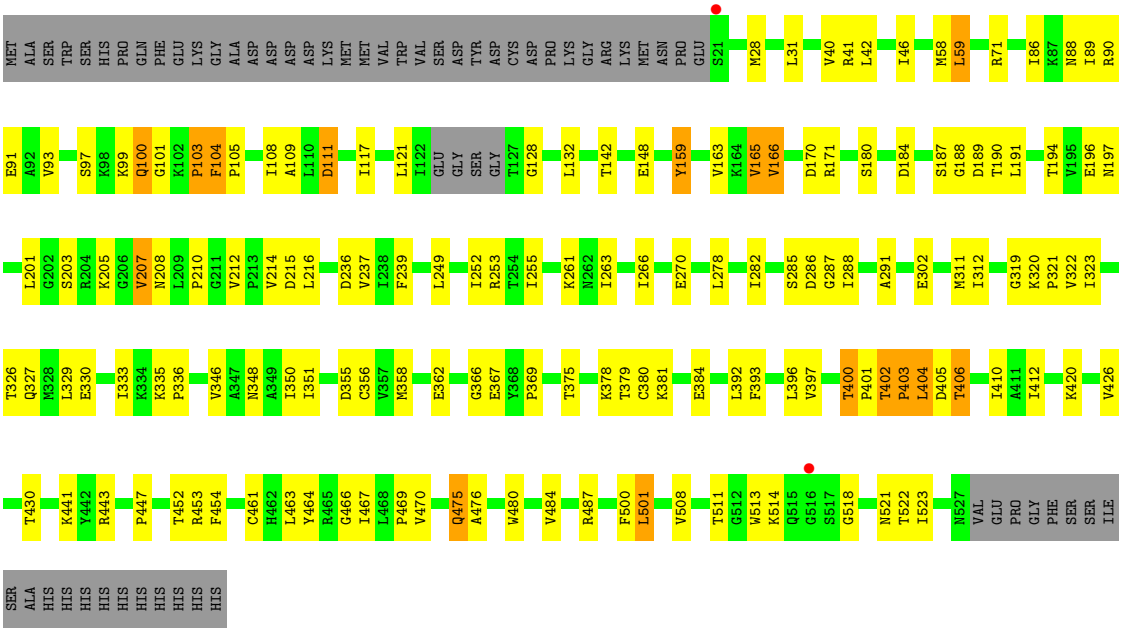
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

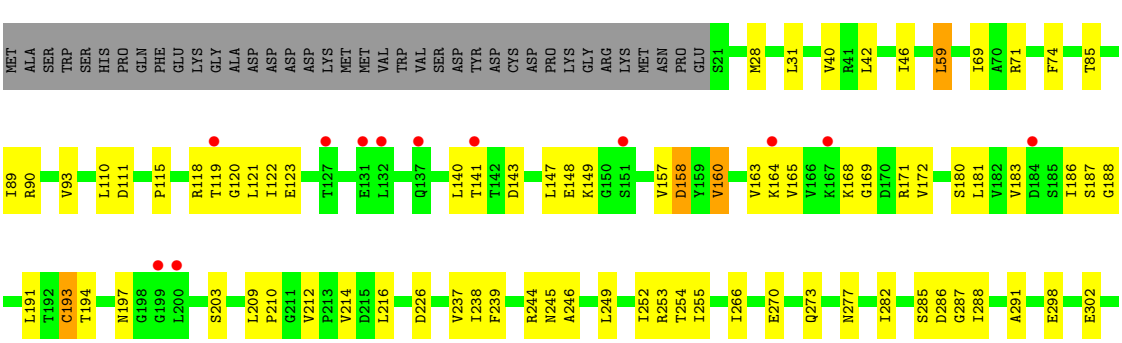
• Molecule 1: Pyruvate kinase

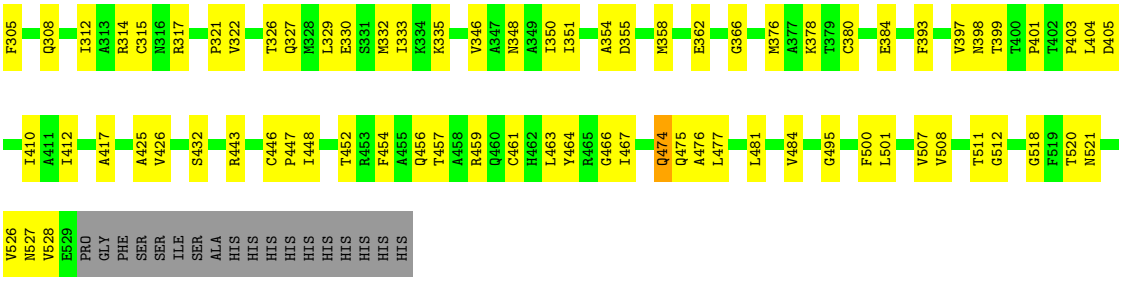
Chain A:



• Molecule 1: Pyruvate kinase

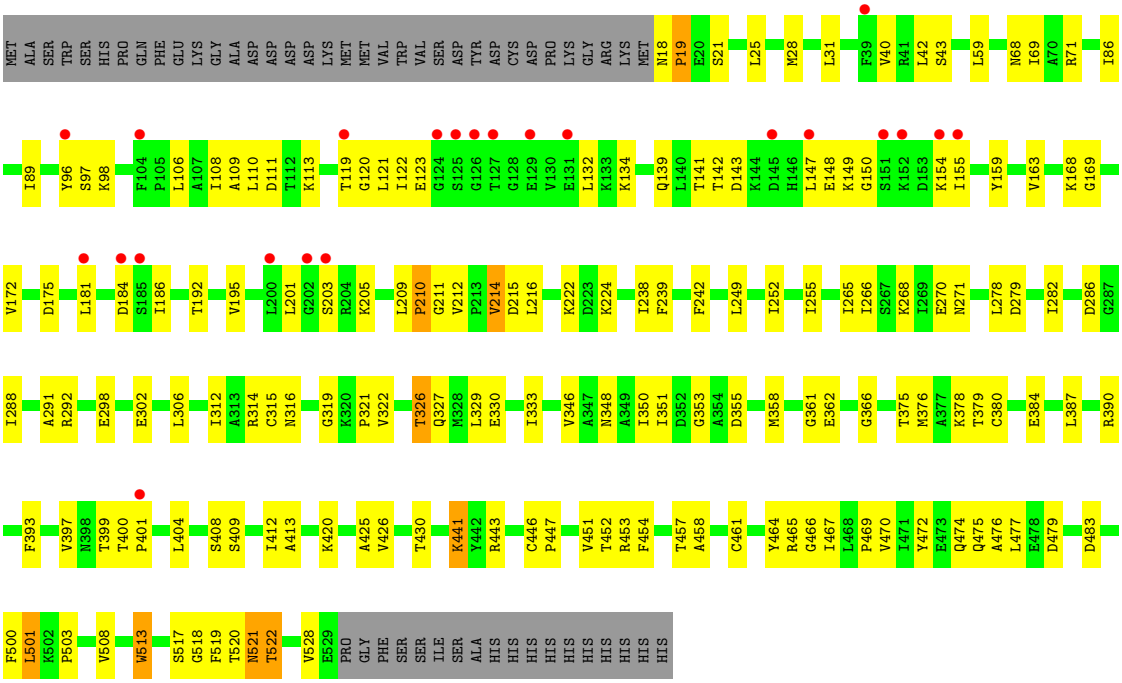
Chain B:





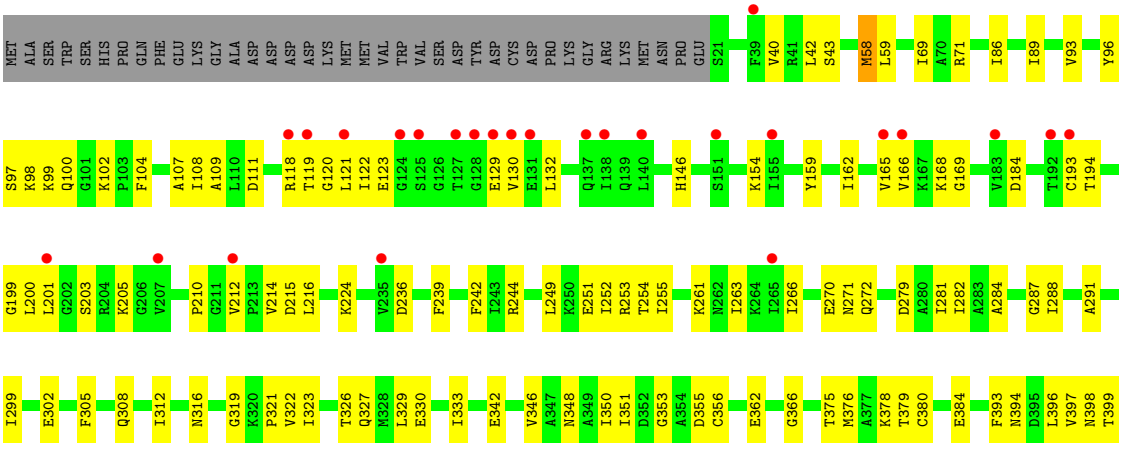
• Molecule 1: Pyruvate kinase

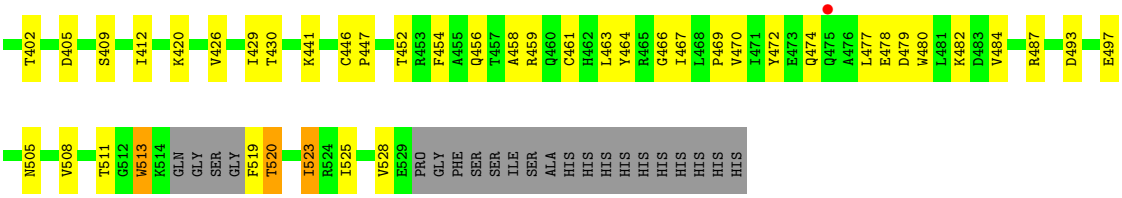
Chain C:



• Molecule 1: Pyruvate kinase

Chain D:




T402
D405
S409
I412
K420
V426
I429
T430
K441
C446
P447
T452
R453
F454
A455
Q456
T457
A458
R459
Q460
C461
H462
L463
Y464
R465
G466
I467
L468
P469
V470
I471
Y472
E473
Q474
Q475
A476
L477
E478
D479
W480
L481
K482
D483
V484
R487
D493
E497
N505
V508
T511
G512
W513
K514
GLN
GLY
SER
GLY
F519
T520
I523
R524
I525
V528
E529
PRO
GLY
PHE
SER
SER
ILE
SER
ALA
HIS
HIS
HIS
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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.23Å 113.65Å 202.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.53 – 3.51 49.53 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.53-3.51) 87.0 (49.53-3.51)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.42 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.271 , 0.319 0.272 , 0.320	Depositor DCC
R_{free} test set	2557 reflections (7.98%)	wwPDB-VP
Wilson B-factor (Å^2)	79.1	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	15364	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.26	0/3841	0.49	0/5196
1	B	0.27	0/3867	0.49	0/5236
1	C	0.26	0/3930	0.47	0/5313
1	D	0.25	0/3868	0.47	0/5230
All	All	0.26	0/15506	0.48	0/20975

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3786	0	3844	88	0
1	B	3811	0	3851	101	0
1	C	3873	0	3958	104	0
1	D	3814	0	3896	99	0
2	A	20	0	10	1	0
2	B	20	0	10	3	0
2	C	20	0	10	2	0
2	D	20	0	10	5	0
All	All	15364	0	15589	379	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 12.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ILE:HG13	1:B:521:ASN:HA	1.52	0.92
1:A:402:THR:HB	1:A:403:PRO:HD2	1.63	0.80
1:A:513:TRP:HE1	1:A:521:ASN:HD21	1.29	0.80
1:A:302:GLU:HG2	1:C:378:LYS:HB3	1.63	0.78
1:B:378:LYS:HB3	1:D:302:GLU:HG2	1.67	0.76
1:B:475:GLN:HG2	1:B:476:ALA:H	1.50	0.76
1:B:426:VAL:HG12	1:B:508:VAL:HB	1.66	0.76
1:B:495:GLY:HA2	1:B:500:PHE:HD2	1.50	0.76
1:A:180:SER:OG	1:A:196:GLU:O	2.02	0.76
1:B:452:THR:HG22	1:B:454:PHE:H	1.50	0.75
1:C:249:LEU:HD22	1:C:265:ILE:HD12	1.67	0.75
1:D:282:ILE:HG13	1:D:288:ILE:HD13	1.67	0.75
1:B:140:LEU:HD21	1:B:157:VAL:HG23	1.69	0.74
1:D:96:TYR:O	1:D:98:LYS:N	2.19	0.74
1:A:378:LYS:HB3	1:C:302:GLU:HG2	1.68	0.74
1:C:452:THR:HG22	1:C:454:PHE:H	1.53	0.74
1:B:327:GLN:HA	1:B:330:GLU:HG2	1.71	0.73
1:C:503:PRO:HA	1:C:528:VAL:HB	1.71	0.73
1:C:426:VAL:HG12	1:C:508:VAL:HB	1.70	0.72
1:A:327:GLN:HA	1:A:330:GLU:HG2	1.70	0.72
1:A:452:THR:HG22	1:A:454:PHE:H	1.53	0.72
1:A:333:ILE:HG23	1:A:366:GLY:HA2	1.71	0.71
1:A:410:ILE:HG13	1:A:521:ASN:HA	1.72	0.70
1:B:302:GLU:HG2	1:D:378:LYS:HB3	1.73	0.70
1:A:100:GLN:HB3	1:A:103:PRO:HG3	1.74	0.69
1:C:397:VAL:HG22	1:C:412:ILE:HD11	1.73	0.69
1:B:456:GLN:HA	1:B:459:ARG:HD3	1.74	0.69
1:D:456:GLN:HA	1:D:459:ARG:HD3	1.74	0.68
1:C:282:ILE:HD11	1:C:315:CYS:HA	1.75	0.68
1:B:181:LEU:HB3	1:B:193:CYS:SG	2.34	0.68
1:D:40:VAL:HG11	1:D:447:PRO:HB3	1.75	0.67
1:D:122:ILE:HG22	1:D:123:GLU:H	1.58	0.67
1:B:501:LEU:HD13	1:B:528:VAL:HG21	1.77	0.67
1:B:397:VAL:HG22	1:B:412:ILE:HD11	1.75	0.67
1:C:327:GLN:HA	1:C:330:GLU:HG2	1.77	0.66
1:D:333:ILE:HG23	1:D:366:GLY:HA2	1.76	0.66
1:B:40:VAL:HG21	1:B:447:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ILE:HG23	1:C:366:GLY:HA2	1.78	0.66
1:D:430:THR:HA	2:D:601:FBP:H61	1.78	0.65
1:B:333:ILE:HG23	1:B:366:GLY:HA2	1.79	0.65
1:A:165:VAL:HG23	1:A:166:VAL:HG23	1.78	0.64
1:C:134:LYS:HA	1:C:195:VAL:HB	1.78	0.64
1:B:380:CYS:O	1:B:384:GLU:HB2	1.96	0.64
1:D:327:GLN:HA	1:D:330:GLU:HG2	1.80	0.64
1:A:163:VAL:HG22	1:A:191:LEU:HD11	1.79	0.63
1:D:224:LYS:HG3	1:D:255:ILE:HD11	1.80	0.63
1:A:426:VAL:HG12	1:A:508:VAL:HB	1.81	0.63
1:C:500:PHE:HB2	1:C:501:LEU:HD23	1.79	0.63
1:B:245:ASN:HA	1:B:277:ASN:HD21	1.63	0.62
1:C:329:LEU:HB2	1:C:362:GLU:HG2	1.80	0.62
1:A:401:PRO:HB3	1:A:404:LEU:HD13	1.80	0.62
1:B:237:VAL:HG21	1:B:463:LEU:HD11	1.81	0.61
1:B:526:VAL:HG13	1:C:513:TRP:HZ3	1.65	0.61
1:B:282:ILE:HD11	1:B:315:CYS:HA	1.82	0.61
1:B:115:PRO:HB2	1:B:216:LEU:HD13	1.83	0.61
1:C:430:THR:OG1	2:C:601:FBP:O4P	2.12	0.60
1:B:40:VAL:HG11	1:B:447:PRO:HB3	1.82	0.60
1:D:323:ILE:HG12	1:D:356:CYS:HB2	1.83	0.60
1:D:397:VAL:HG22	1:D:412:ILE:HD11	1.83	0.60
1:A:253:ARG:NH2	1:A:261:LYS:O	2.34	0.60
1:C:119:THR:HG23	1:C:155:ILE:HG13	1.84	0.60
1:D:93:VAL:HG23	1:D:104:PHE:HD2	1.66	0.60
1:A:117:ILE:HB	1:A:207:VAL:CB	2.31	0.60
1:A:400:THR:H	1:A:401:PRO:CD	2.15	0.59
1:C:355:ASP:OD1	1:C:443:ARG:NH2	2.35	0.59
1:D:458:ALA:HB1	1:D:469:PRO:HB2	1.82	0.59
1:D:319:GLY:HA2	1:D:441:LYS:HG3	1.82	0.59
1:B:121:LEU:HA	1:B:203:SER:HB2	1.84	0.59
1:B:239:PHE:HD1	1:B:266:ILE:HB	1.68	0.59
1:B:412:ILE:HD13	1:C:420:LYS:HG3	1.83	0.59
1:D:472:TYR:CE2	1:D:474:GLN:HB3	2.37	0.59
1:C:348:ASN:HA	1:C:351:ILE:HG22	1.85	0.59
1:D:58:MET:SD	1:D:58:MET:N	2.75	0.59
1:D:69:ILE:HD11	1:D:109:ALA:HB2	1.83	0.59
1:D:216:LEU:O	1:D:244:ARG:NH2	2.35	0.59
1:C:361:GLY:O	1:C:366:GLY:N	2.36	0.59
1:C:270:GLU:HG2	1:C:291:ALA:HB3	1.83	0.58
1:A:380:CYS:O	1:A:384:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:OH	1:A:215:ASP:OD1	2.12	0.58
1:A:480:TRP:O	1:A:484:VAL:HG12	2.04	0.58
1:B:147:LEU:HD12	1:B:148:GLU:HG2	1.85	0.58
1:D:519:PHE:N	2:D:601:FBP:HO4	2.01	0.58
1:B:464:TYR:HB2	1:B:467:ILE:HD12	1.83	0.58
1:A:239:PHE:HD1	1:A:266:ILE:HB	1.69	0.57
1:B:512:GLY:HA2	1:B:520:THR:O	2.05	0.57
1:B:282:ILE:HA	1:B:288:ILE:HD11	1.86	0.57
1:D:71:ARG:NH2	1:D:111:ASP:OD2	2.38	0.57
1:B:183:VAL:HG22	1:B:191:LEU:HD11	1.86	0.57
1:A:99:LYS:O	1:A:101:GLY:N	2.37	0.57
1:B:214:VAL:HG12	1:B:216:LEU:H	1.68	0.57
1:C:71:ARG:NH2	1:C:111:ASP:OD2	2.39	0.56
1:C:517:SER:O	1:C:519:PHE:N	2.38	0.56
1:D:253:ARG:NH2	1:D:261:LYS:O	2.39	0.56
1:A:184:ASP:OD2	1:A:194:THR:OG1	2.23	0.56
1:A:282:ILE:HA	1:A:288:ILE:HD11	1.87	0.56
1:B:355:ASP:OD1	1:B:443:ARG:NH2	2.38	0.56
1:C:464:TYR:HB2	1:C:467:ILE:HD12	1.87	0.56
1:C:453:ARG:NH2	1:C:483:ASP:OD2	2.38	0.56
1:D:99:LYS:HB2	1:D:102:LYS:HB2	1.88	0.56
1:B:346:VAL:O	1:B:350:ILE:HG22	2.06	0.56
1:C:121:LEU:HA	1:C:203:SER:HB2	1.88	0.55
1:B:348:ASN:HA	1:B:351:ILE:HG22	1.88	0.55
1:C:430:THR:HA	2:C:601:FBP:H61	1.88	0.55
1:A:253:ARG:NH1	1:A:263:ILE:O	2.36	0.55
1:B:270:GLU:HG2	1:B:291:ALA:HB3	1.88	0.55
1:D:430:THR:OG1	2:D:601:FBP:O4P	2.16	0.55
1:A:278:LEU:O	1:A:282:ILE:HG13	2.07	0.55
1:D:119:THR:HG22	1:D:120:GLY:H	1.71	0.55
1:D:346:VAL:O	1:D:350:ILE:HG22	2.06	0.55
1:B:180:SER:HB3	1:B:197:ASN:HB3	1.87	0.55
1:D:165:VAL:HG12	1:D:212:VAL:HB	1.88	0.55
1:D:316:ASN:HD21	1:D:353:GLY:HA3	1.71	0.55
1:D:426:VAL:HG12	1:D:508:VAL:HB	1.87	0.55
1:D:43:SER:HB2	1:D:380:CYS:SG	2.47	0.55
1:C:475:GLN:HG2	1:C:476:ALA:H	1.71	0.55
1:B:123:GLU:HG3	1:B:149:LYS:HA	1.88	0.55
1:C:239:PHE:HD1	1:C:266:ILE:HB	1.72	0.55
1:D:348:ASN:HA	1:D:351:ILE:HG22	1.88	0.54
1:A:348:ASN:HA	1:A:351:ILE:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:VAL:HG22	1:C:209:LEU:HG	1.89	0.54
1:A:59:LEU:HD11	1:A:89:ILE:HG13	1.89	0.54
1:A:71:ARG:HA	1:A:109:ALA:HB3	1.89	0.54
1:C:316:ASN:HD21	1:C:353:GLY:HA3	1.72	0.54
1:C:461:CYS:HB3	1:C:467:ILE:HG21	1.90	0.54
1:C:141:THR:HG23	1:C:143:ASP:H	1.73	0.53
1:C:271:ASN:HA	1:C:298:GLU:HG3	1.89	0.53
1:C:451:VAL:HA	1:C:470:VAL:HG12	1.90	0.53
1:A:464:TYR:HB2	1:A:467:ILE:HD12	1.89	0.53
1:D:429:ILE:HD11	1:D:487:ARG:NE	2.23	0.53
1:C:69:ILE:HD11	1:C:109:ALA:HB2	1.91	0.53
1:D:513:TRP:HD1	1:D:513:TRP:H	1.57	0.53
1:B:40:VAL:HG22	1:B:500:PHE:HD1	1.74	0.52
1:C:346:VAL:O	1:C:350:ILE:HG22	2.09	0.52
1:D:511:THR:O	1:D:520:THR:HG22	2.10	0.52
1:D:452:THR:HG22	1:D:454:PHE:H	1.72	0.52
1:A:321:PRO:HA	1:A:355:ASP:OD2	2.09	0.52
1:B:187:SER:OG	1:B:188:GLY:N	2.42	0.52
1:B:193:CYS:SG	1:B:194:THR:N	2.83	0.52
1:D:132:LEU:HB2	1:D:199:GLY:O	2.10	0.52
1:A:346:VAL:O	1:A:350:ILE:HG22	2.09	0.52
1:C:40:VAL:HG11	1:C:447:PRO:HB3	1.92	0.52
1:C:380:CYS:O	1:C:384:GLU:HB2	2.09	0.52
1:C:521:ASN:OD1	1:C:522:THR:N	2.37	0.52
1:D:461:CYS:HB3	1:D:467:ILE:HG21	1.91	0.52
1:C:159:TYR:OH	1:C:215:ASP:OD1	2.23	0.52
1:A:500:PHE:HB2	1:A:501:LEU:HD23	1.92	0.52
1:A:355:ASP:OD1	1:A:443:ARG:NH2	2.43	0.51
1:C:458:ALA:HB1	1:C:469:PRO:HB2	1.92	0.51
1:C:110:LEU:HB3	1:C:238:ILE:HG13	1.91	0.51
1:B:501:LEU:HD22	1:B:507:VAL:HG11	1.92	0.51
1:A:214:VAL:HG12	1:A:216:LEU:H	1.76	0.51
1:D:252:ILE:O	1:D:255:ILE:HG22	2.11	0.51
1:B:288:ILE:O	1:B:322:VAL:HA	2.11	0.51
1:A:397:VAL:HG22	1:A:412:ILE:HD11	1.92	0.51
1:C:18:ASN:N	1:C:19:PRO:HD3	2.26	0.51
1:D:394:ASN:OD1	1:D:398:ASN:ND2	2.43	0.51
1:B:322:VAL:HG13	1:B:354:ALA:HA	1.93	0.50
1:D:214:VAL:HG12	1:D:216:LEU:H	1.76	0.50
1:D:329:LEU:HD23	1:D:342:GLU:HB3	1.92	0.50
1:A:511:THR:OG1	1:A:522:THR:OG1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ARG:HA	1:D:205:LYS:O	2.12	0.50
1:B:286:ASP:O	1:B:321:PRO:HD2	2.11	0.50
1:C:43:SER:HB2	1:C:380:CYS:SG	2.51	0.50
1:A:393:PHE:O	1:A:397:VAL:HG23	2.11	0.50
1:A:430:THR:OG1	2:A:601:FBP:O4P	2.18	0.50
1:A:405:ASP:O	1:A:406:THR:HB	2.12	0.50
1:B:511:THR:O	1:B:520:THR:HA	2.12	0.50
1:D:159:TYR:CD2	1:D:162:ILE:HG22	2.47	0.50
1:D:159:TYR:OH	1:D:215:ASP:OD1	2.20	0.50
1:C:147:LEU:HD12	1:C:148:GLU:HG2	1.93	0.49
1:D:244:ARG:O	1:D:281:ILE:HD11	2.11	0.49
1:A:420:LYS:HG3	1:D:412:ILE:HD13	1.95	0.49
1:A:396:LEU:HD12	1:C:25:LEU:HD22	1.94	0.49
1:A:278:LEU:HD21	1:A:311:MET:HG3	1.93	0.49
1:A:335:LYS:HG3	1:A:336:PRO:HD2	1.94	0.49
1:C:119:THR:HG22	1:C:120:GLY:H	1.77	0.49
1:A:323:ILE:HG12	1:A:356:CYS:HB2	1.95	0.49
1:A:475:GLN:HG2	1:A:476:ALA:N	2.27	0.49
1:B:119:THR:HG22	1:B:120:GLY:H	1.78	0.49
1:A:111:ASP:HA	1:A:239:PHE:O	2.13	0.48
1:B:165:VAL:HG12	1:B:212:VAL:HB	1.95	0.48
1:B:314:ARG:HG2	1:B:317:ARG:HH12	1.78	0.48
1:D:122:ILE:HG22	1:D:123:GLU:N	2.26	0.48
1:A:108:ILE:H	1:A:236:ASP:HB2	1.79	0.48
1:B:452:THR:HG21	1:B:457:THR:OG1	2.12	0.48
1:C:96:TYR:O	1:C:98:LYS:N	2.39	0.48
1:A:171:ARG:O	1:A:210:PRO:HD2	2.13	0.48
1:A:207:VAL:O	1:A:208:ASN:HB2	2.14	0.48
1:B:59:LEU:HD22	1:B:89:ILE:HA	1.95	0.48
1:C:319:GLY:HA2	1:C:441:LYS:HG3	1.95	0.48
1:C:475:GLN:HG2	1:C:476:ALA:N	2.29	0.48
1:A:187:SER:HB3	1:A:190:THR:OG1	2.13	0.48
1:B:71:ARG:NH2	1:B:111:ASP:OD2	2.45	0.48
1:A:46:ILE:HG21	1:A:358:MET:HE2	1.96	0.48
1:A:523:ILE:HB	1:D:523:ILE:HG23	1.96	0.48
1:B:287:GLY:C	1:B:288:ILE:HD12	2.35	0.48
1:D:146:HIS:NE2	1:D:154:LYS:HB2	2.28	0.48
1:A:288:ILE:O	1:A:322:VAL:HA	2.13	0.47
1:D:429:ILE:HD13	1:D:484:VAL:HG23	1.96	0.47
1:A:187:SER:OG	1:A:188:GLY:N	2.47	0.47
1:B:393:PHE:O	1:B:397:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:HA	1:B:93:VAL:HG12	1.96	0.47
1:C:71:ARG:NH1	1:C:358:MET:HE3	2.30	0.47
1:A:40:VAL:HG11	1:A:447:PRO:HB3	1.96	0.47
1:A:42:LEU:HB3	1:A:466:GLY:HA2	1.97	0.47
1:A:286:ASP:O	1:A:321:PRO:HD2	2.14	0.47
1:B:417:ALA:HB2	1:C:413:ALA:HB2	1.96	0.47
1:C:163:VAL:HG13	1:C:186:ILE:HD11	1.96	0.47
1:C:175:ASP:OD1	1:C:205:LYS:HD2	2.14	0.47
1:D:249:LEU:O	1:D:253:ARG:HG2	2.15	0.47
1:C:42:LEU:HD22	1:C:466:GLY:HA2	1.97	0.47
1:C:89:ILE:HD13	1:C:108:ILE:HG22	1.97	0.47
1:D:119:THR:HG22	1:D:120:GLY:N	2.29	0.47
1:D:420:LYS:HA	1:D:420:LYS:HD3	1.61	0.47
1:B:425:ALA:HA	1:B:446:CYS:HB2	1.96	0.47
1:B:474:GLN:OE1	1:B:474:GLN:N	2.44	0.47
1:C:121:LEU:HD23	1:C:203:SER:HB2	1.96	0.47
1:C:132:LEU:HD11	1:C:201:LEU:HD22	1.96	0.47
1:B:141:THR:C	1:B:143:ASP:H	2.18	0.46
1:D:168:LYS:HG3	1:D:169:GLY:H	1.80	0.46
1:D:505:ASN:O	1:D:528:VAL:HG23	2.15	0.46
1:A:121:LEU:HD23	1:A:203:SER:HB2	1.97	0.46
1:A:249:LEU:HD21	1:A:285:SER:OG	2.16	0.46
1:B:140:LEU:HB3	1:B:191:LEU:HB3	1.96	0.46
1:A:86:ILE:HA	1:A:89:ILE:HG22	1.98	0.46
1:C:123:GLU:HG2	1:C:149:LYS:HA	1.98	0.46
1:C:210:PRO:O	1:C:212:VAL:N	2.49	0.46
1:D:42:LEU:H	1:D:384:GLU:CD	2.19	0.46
1:B:432:SER:N	2:B:601:FBP:O5P	2.46	0.46
1:D:239:PHE:HD1	1:D:266:ILE:HB	1.80	0.46
1:D:477:LEU:HD13	1:D:479:ASP:H	1.81	0.46
1:A:237:VAL:HG21	1:A:463:LEU:HD11	1.97	0.46
1:A:312:ILE:HG23	1:A:322:VAL:HG11	1.98	0.46
1:C:168:LYS:HG3	1:C:169:GLY:H	1.81	0.46
1:D:166:VAL:HA	1:D:212:VAL:HG11	1.97	0.46
1:D:321:PRO:HB3	1:D:463:LEU:O	2.16	0.46
1:A:103:PRO:HB2	1:A:104:PHE:H	1.42	0.46
1:B:312:ILE:HA	1:B:322:VAL:HG21	1.96	0.46
1:D:287:GLY:C	1:D:288:ILE:HD12	2.36	0.46
1:B:59:LEU:HD11	1:B:89:ILE:HG12	1.98	0.45
1:B:122:ILE:HG12	1:B:203:SER:HB3	1.96	0.45
1:D:270:GLU:HG2	1:D:291:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ILE:HG23	1:D:322:VAL:HG11	1.98	0.45
1:D:393:PHE:O	1:D:397:VAL:HG23	2.15	0.45
1:A:329:LEU:HB2	1:A:362:GLU:HG2	1.97	0.45
1:C:214:VAL:HG23	1:C:216:LEU:H	1.82	0.45
1:C:288:ILE:O	1:C:322:VAL:HA	2.16	0.45
1:A:90:ARG:HA	1:A:93:VAL:HG12	1.97	0.45
1:C:113:LYS:HD3	1:C:222:LYS:HD3	1.97	0.45
1:C:224:LYS:HG3	1:C:255:ILE:HD11	1.97	0.45
1:C:404:LEU:HG	1:C:408:SER:HB2	1.99	0.45
1:C:121:LEU:HD12	1:C:147:LEU:O	2.17	0.45
1:C:278:LEU:HD23	1:C:314:ARG:HD2	1.98	0.45
1:C:139:GLN:OE1	1:C:154:LYS:NZ	2.41	0.45
1:D:242:PHE:HD1	1:D:271:ASN:HD22	1.64	0.45
1:A:319:GLY:HA2	1:A:441:LYS:HG3	1.98	0.45
1:B:42:LEU:HD22	1:B:466:GLY:HA2	1.99	0.45
1:B:249:LEU:HD21	1:B:285:SER:OG	2.16	0.45
1:C:312:ILE:HA	1:C:322:VAL:HG21	1.99	0.45
1:D:122:ILE:HD11	1:D:201:LEU:HG	1.99	0.45
1:B:85:THR:O	1:B:89:ILE:HG13	2.17	0.45
1:B:398:ASN:HD21	1:C:390:ARG:NH1	2.14	0.45
1:B:512:GLY:HA3	2:B:601:FBP:O3	2.16	0.45
1:D:329:LEU:HB2	1:D:362:GLU:HG2	1.99	0.45
1:A:105:PRO:HG2	1:A:469:PRO:HG2	1.98	0.44
1:B:163:VAL:HG23	1:B:164:LYS:HD2	1.99	0.44
1:D:130:VAL:O	1:D:200:LEU:HD13	2.16	0.44
1:D:482:LYS:HD3	1:D:482:LYS:HA	1.79	0.44
1:D:107:ALA:HB2	1:D:459:ARG:O	2.18	0.44
1:B:302:GLU:HG2	1:D:378:LYS:CB	2.45	0.44
1:C:181:LEU:HD13	1:C:195:VAL:HA	2.00	0.44
1:A:28:MET:HA	1:A:31:LEU:HD13	1.99	0.44
1:A:132:LEU:HD11	1:A:201:LEU:HD22	1.99	0.44
1:A:287:GLY:HA2	1:A:320:LYS:HB3	1.99	0.44
1:A:461:CYS:HB3	1:A:467:ILE:HG21	1.98	0.44
1:C:393:PHE:O	1:C:397:VAL:HG23	2.18	0.44
1:D:251:GLU:O	1:D:254:THR:HG22	2.17	0.44
1:D:464:TYR:HB2	1:D:467:ILE:HD12	1.99	0.44
1:A:117:ILE:HG23	1:A:159:TYR:H	1.81	0.44
1:C:472:TYR:CE2	1:C:474:GLN:HB3	2.53	0.44
1:C:312:ILE:HG23	1:C:322:VAL:HG11	2.00	0.44
1:D:121:LEU:HD23	1:D:203:SER:HB2	1.99	0.44
1:A:86:ILE:O	1:A:89:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:GLY:HA2	2:B:601:FBP:O6P	2.18	0.44
1:D:42:LEU:HD22	1:D:466:GLY:HA2	2.00	0.44
1:D:409:SER:HA	1:D:412:ILE:HG22	2.00	0.44
1:C:210:PRO:HB3	1:C:298:GLU:O	2.18	0.43
1:B:329:LEU:HB2	1:B:362:GLU:HG2	2.01	0.43
1:C:122:ILE:H	1:C:203:SER:HB3	1.83	0.43
1:A:287:GLY:C	1:A:288:ILE:HD12	2.38	0.43
1:C:350:ILE:HG13	1:C:465:ARG:HH22	1.83	0.43
1:A:484:VAL:HA	1:A:487:ARG:HE	1.83	0.43
1:B:168:LYS:HG3	1:B:169:GLY:N	2.33	0.43
1:B:28:MET:HA	1:B:31:LEU:HD13	2.00	0.43
1:B:141:THR:O	1:B:143:ASP:N	2.42	0.43
1:B:282:ILE:HG13	1:B:288:ILE:HD13	2.00	0.43
1:B:426:VAL:HG23	1:B:448:ILE:HA	2.00	0.43
1:D:108:ILE:HG12	1:D:459:ARG:HH21	1.83	0.43
1:D:184:ASP:H	1:D:193:CYS:HA	1.84	0.43
1:D:380:CYS:O	1:D:384:GLU:HB2	2.19	0.43
1:A:252:ILE:O	1:A:255:ILE:HG22	2.18	0.43
1:B:74:PHE:HD2	1:B:226:ASP:HB3	1.84	0.43
1:A:392:LEU:O	1:A:396:LEU:HD13	2.19	0.43
1:B:71:ARG:NH1	1:B:358:MET:HE3	2.34	0.43
1:C:123:GLU:HG3	1:C:150:GLY:O	2.18	0.43
1:C:375:THR:O	1:C:379:THR:HG22	2.19	0.43
1:B:46:ILE:HG12	1:B:69:ILE:CG2	2.48	0.43
1:D:86:ILE:O	1:D:89:ILE:HG22	2.19	0.43
1:D:288:ILE:O	1:D:322:VAL:HA	2.18	0.43
1:B:252:ILE:O	1:B:255:ILE:HG22	2.19	0.43
1:D:508:VAL:HG22	1:D:525:ILE:HD13	2.00	0.43
1:D:508:VAL:HG22	1:D:525:ILE:CD1	2.49	0.43
1:C:121:LEU:CD2	1:C:203:SER:HB2	2.49	0.42
1:B:118:ARG:O	1:B:158:ASP:N	2.52	0.42
1:B:171:ARG:HG3	1:B:210:PRO:HG2	2.01	0.42
1:C:141:THR:OG1	1:C:142:THR:N	2.52	0.42
1:D:480:TRP:CH2	2:D:601:FBP:H11	2.54	0.42
1:B:110:LEU:HB3	1:B:238:ILE:HG13	2.00	0.42
1:C:452:THR:HG21	1:C:457:THR:OG1	2.19	0.42
1:B:244:ARG:HD2	1:B:273:GLN:OE1	2.19	0.42
1:C:149:LYS:HA	1:C:149:LYS:HD2	1.83	0.42
1:C:452:THR:HG22	1:C:454:PHE:N	2.29	0.42
1:D:249:LEU:HD11	1:D:284:ALA:HB1	2.00	0.42
1:B:249:LEU:O	1:B:253:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LEU:HD23	1:C:252:ILE:HD12	2.01	0.42
1:C:279:ASP:O	1:C:282:ILE:HG22	2.19	0.42
1:D:426:VAL:HG13	1:D:446:CYS:SG	2.59	0.42
1:B:210:PRO:HB3	1:B:298:GLU:O	2.19	0.42
1:D:493:ASP:O	1:D:497:GLU:HG2	2.19	0.42
1:B:447:PRO:HG3	1:B:500:PHE:CD1	2.54	0.42
1:D:279:ASP:O	1:D:282:ILE:HG22	2.19	0.42
1:A:375:THR:O	1:A:379:THR:HG22	2.20	0.42
1:C:86:ILE:O	1:C:89:ILE:HG22	2.19	0.42
1:C:184:ASP:N	1:C:192:THR:O	2.45	0.42
1:D:321:PRO:HA	1:D:355:ASP:OD2	2.20	0.42
1:C:28:MET:HA	1:C:31:LEU:HD13	2.02	0.42
1:D:129:GLU:HB3	1:D:200:LEU:HD22	2.01	0.42
1:B:40:VAL:HG22	1:B:500:PHE:CD1	2.54	0.42
1:C:425:ALA:HA	1:C:446:CYS:HB2	2.01	0.42
1:A:31:LEU:HD23	1:C:306:LEU:HA	2.02	0.41
1:B:461:CYS:HB3	1:B:467:ILE:HG21	2.02	0.41
1:B:481:LEU:O	1:B:484:VAL:HG12	2.20	0.41
1:D:405:ASP:OD1	1:D:405:ASP:N	2.51	0.41
1:A:270:GLU:HG2	1:A:291:ALA:HB3	2.01	0.41
1:D:305:PHE:O	1:D:308:GLN:HG2	2.20	0.41
1:B:160:VAL:HG21	1:B:216:LEU:HD23	2.01	0.41
1:C:239:PHE:HB3	1:C:268:LYS:HD2	2.02	0.41
1:D:396:LEU:O	1:D:399:THR:HG22	2.20	0.41
1:A:402:THR:HB	1:A:403:PRO:CD	2.41	0.41
1:B:90:ARG:O	1:B:93:VAL:HG12	2.20	0.41
1:C:409:SER:HA	1:C:412:ILE:HG22	2.03	0.41
1:B:305:PHE:O	1:B:308:GLN:HG2	2.20	0.41
1:C:205:LYS:HD3	1:C:205:LYS:HA	1.67	0.41
1:C:477:LEU:HD13	1:C:479:ASP:H	1.86	0.41
1:B:332:MET:HA	1:B:335:LYS:O	2.21	0.41
1:C:68:ASN:O	1:C:106:LEU:HD12	2.20	0.41
1:C:453:ARG:NH2	1:C:476:ALA:HA	2.35	0.41
1:B:122:ILE:H	1:B:203:SER:HB3	1.85	0.41
1:A:41:ARG:HB2	1:A:381:LYS:HG2	2.03	0.41
1:A:142:THR:HG22	1:A:189:ASP:HB2	2.03	0.41
1:B:405:ASP:N	1:B:405:ASP:OD1	2.54	0.41
1:C:286:ASP:O	1:C:321:PRO:HD2	2.21	0.41
1:C:351:ILE:HG13	1:C:387:LEU:HD23	2.02	0.41
1:C:399:THR:O	1:C:401:PRO:HD3	2.21	0.41
1:B:119:THR:HG22	1:B:120:GLY:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:VAL:HB	1:B:186:ILE:HD11	2.03	0.41
1:B:172:VAL:HG22	1:B:209:LEU:HD22	2.03	0.41
1:D:272:GLN:HG3	1:D:299:ILE:HG22	2.03	0.41
1:A:88:ASN:O	1:A:91:GLU:HG2	2.21	0.40
1:A:367:GLU:C	1:A:369:PRO:HD3	2.41	0.40
1:D:375:THR:O	1:D:379:THR:HG22	2.21	0.40
1:D:480:TRP:CZ2	2:D:601:FBP:H11	2.56	0.40
1:C:242:PHE:HD1	1:C:271:ASN:HD22	1.68	0.40
1:C:292:ARG:HB2	1:C:326:THR:OG1	2.21	0.40
1:B:118:ARG:H	1:B:158:ASP:CB	2.34	0.40
1:D:236:ASP:O	1:D:263:ILE:HG23	2.21	0.40
1:A:205:LYS:HA	1:A:205:LYS:HD3	1.77	0.40
1:A:249:LEU:O	1:A:253:ARG:HG2	2.22	0.40
1:D:477:LEU:HD13	1:D:478:GLU:N	2.37	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	499/565 (88%)	459 (92%)	21 (4%)	19 (4%)	3 27
1	B	507/565 (90%)	474 (94%)	26 (5%)	7 (1%)	11 47
1	C	510/565 (90%)	475 (93%)	25 (5%)	10 (2%)	7 41
1	D	501/565 (89%)	474 (95%)	22 (4%)	5 (1%)	15 54
All	All	2017/2260 (89%)	1882 (93%)	94 (5%)	41 (2%)	7 41

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	THR

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Mol	Chain	Res	Type
1	A	402	THR
1	B	401	PRO
1	B	474	GLN
1	C	210	PRO
1	A	103	PRO
1	A	111	ASP
1	A	166	VAL
1	A	406	THR
1	B	158	ASP
1	B	160	VAL
1	C	97	SER
1	C	211	GLY
1	C	518	GLY
1	C	520	THR
1	D	97	SER
1	D	100	GLN
1	A	170	ASP
1	A	197	ASN
1	A	475	GLN
1	C	19	PRO
1	C	522	THR
1	A	97	SER
1	A	100	GLN
1	A	326	THR
1	B	246	ALA
1	B	326	THR
1	C	326	THR
1	D	326	THR
1	D	402	THR
1	A	404	LEU
1	A	514	LYS
1	C	21	SER
1	C	521	ASN
1	A	207	VAL
1	B	403	PRO
1	D	210	PRO
1	A	128	GLY
1	A	518	GLY
1	A	104	PHE
1	A	165	VAL

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	407/470 (87%)	398 (98%)	9 (2%)	52 77
1	B	409/470 (87%)	401 (98%)	8 (2%)	55 79
1	C	421/470 (90%)	414 (98%)	7 (2%)	60 82
1	D	414/470 (88%)	406 (98%)	8 (2%)	57 80
All	All	1651/1880 (88%)	1619 (98%)	32 (2%)	57 80

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	MET
1	A	59	LEU
1	A	148	GLU
1	A	159	TYR
1	A	212	VAL
1	A	403	PRO
1	A	453	ARG
1	A	470	VAL
1	A	501	LEU
1	B	59	LEU
1	B	193	CYS
1	B	254	THR
1	B	376	MET
1	B	399	THR
1	B	404	LEU
1	B	477	LEU
1	B	527	ASN
1	C	59	LEU
1	C	214	VAL
1	C	376	MET
1	C	400	THR
1	C	441	LYS
1	C	501	LEU
1	C	513	TRP

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Mol	Chain	Res	Type
1	D	58	MET
1	D	59	LEU
1	D	194	THR
1	D	376	MET
1	D	470	VAL
1	D	513	TRP
1	D	520	THR
1	D	523	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FBP	C	601	-	18,20,20	0.90	1 (5%)	23,32,32	0.74	0
2	FBP	D	601	-	18,20,20	0.92	1 (5%)	23,32,32	0.89	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FBP	A	601	-	18,20,20	0.92	1 (5%)	23,32,32	0.77	0
2	FBP	B	601	-	18,20,20	0.90	1 (5%)	23,32,32	0.78	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	FBP	C	601	-	-	7/13/32/32	0/1/1/1
2	FBP	D	601	-	-	7/13/32/32	0/1/1/1
2	FBP	A	601	-	-	8/13/32/32	0/1/1/1
2	FBP	B	601	-	-	8/13/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FBP	O2-C2	2.72	1.45	1.40
2	A	601	FBP	O2-C2	2.72	1.45	1.40
2	B	601	FBP	O2-C2	2.68	1.45	1.40
2	C	601	FBP	O2-C2	2.68	1.45	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	FBP	O5-C5-C6	2.20	114.29	109.45

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C1-O1-P1-O1P
2	A	601	FBP	C1-O1-P1-O2P
2	A	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	O1-C1-C2-O2
2	A	601	FBP	O1-C1-C2-C3
2	A	601	FBP	O1-C1-C2-O5
2	A	601	FBP	C4-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	601	FBP	O1-C1-C2-C3
2	B	601	FBP	O1-C1-C2-O5
2	B	601	FBP	C6-O6-P2-O4P
2	B	601	FBP	C6-O6-P2-O5P
2	B	601	FBP	C6-O6-P2-O6P
2	C	601	FBP	O1-C1-C2-O2
2	C	601	FBP	O1-C1-C2-C3
2	C	601	FBP	O1-C1-C2-O5
2	C	601	FBP	C6-O6-P2-O4P
2	C	601	FBP	C6-O6-P2-O5P
2	C	601	FBP	C6-O6-P2-O6P
2	D	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C1-O1-P1-O2P
2	D	601	FBP	C1-O1-P1-O3P
2	D	601	FBP	C6-O6-P2-O5P
2	B	601	FBP	C4-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	D	601	FBP	C6-O6-P2-O6P
2	D	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O1-C1-C2-C3
2	C	601	FBP	O5-C5-C6-O6

There are no ring outliers.

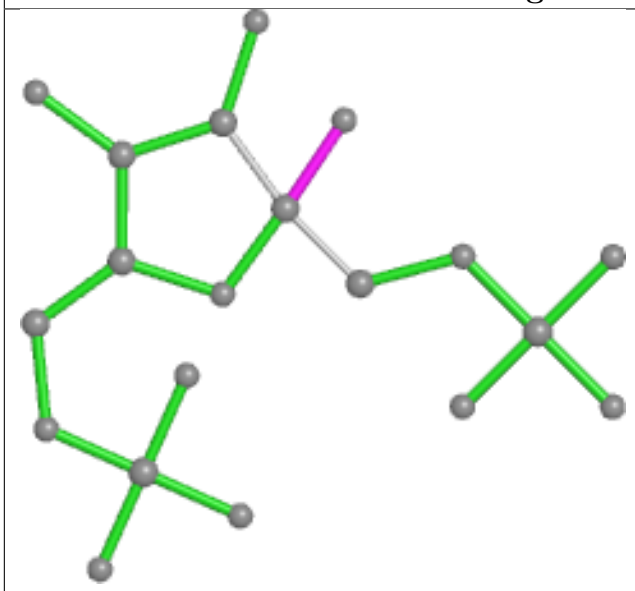
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	FBP	2	0
2	D	601	FBP	5	0
2	A	601	FBP	1	0
2	B	601	FBP	3	0

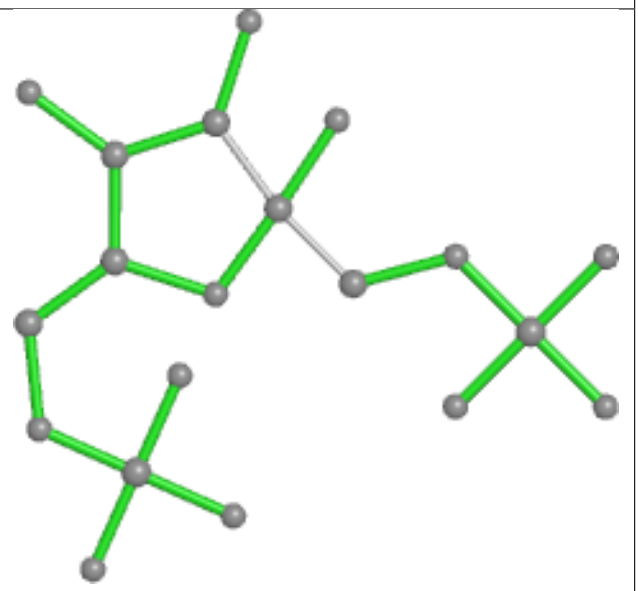
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

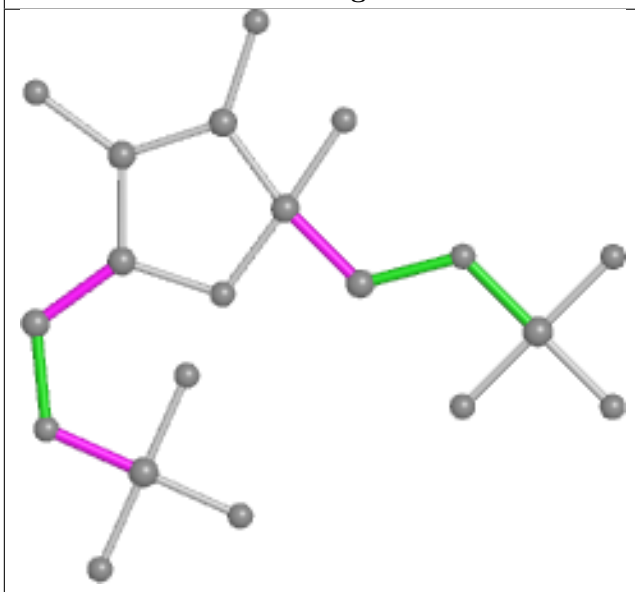
Ligand FBP C 601



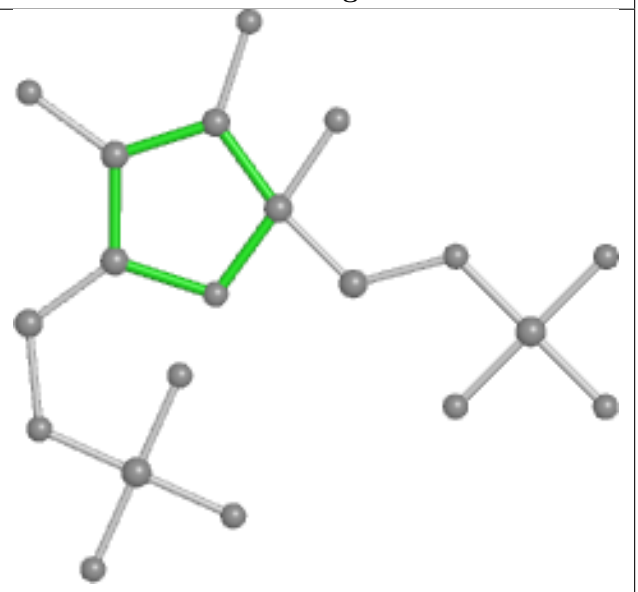
Bond lengths



Bond angles

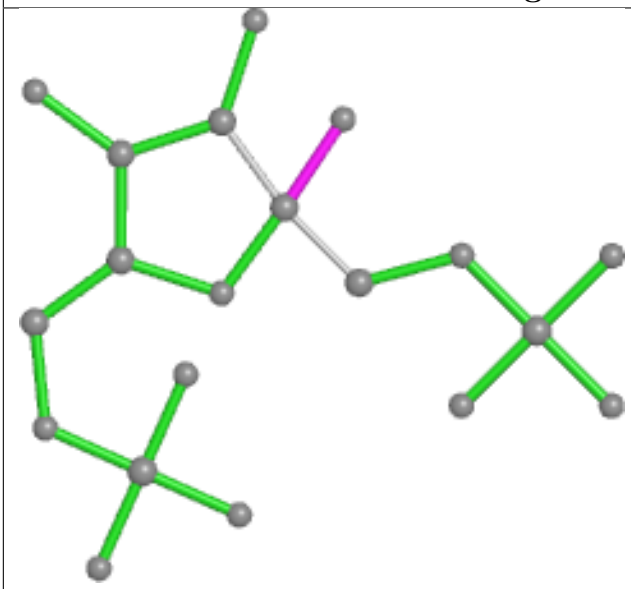


Torsions

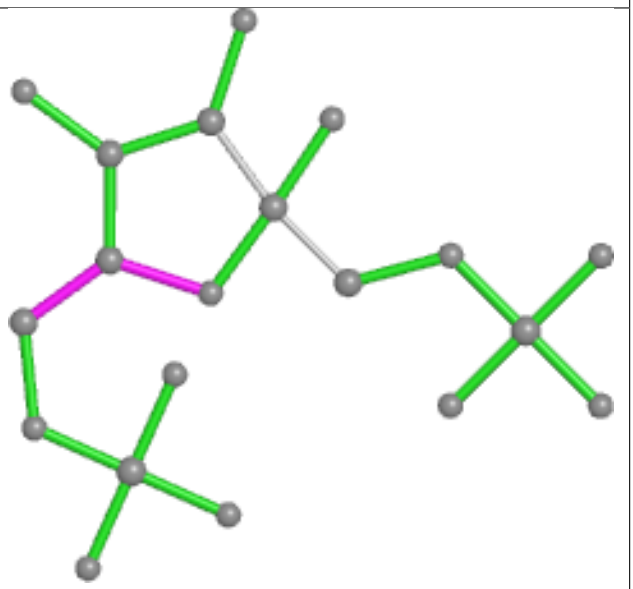


Rings

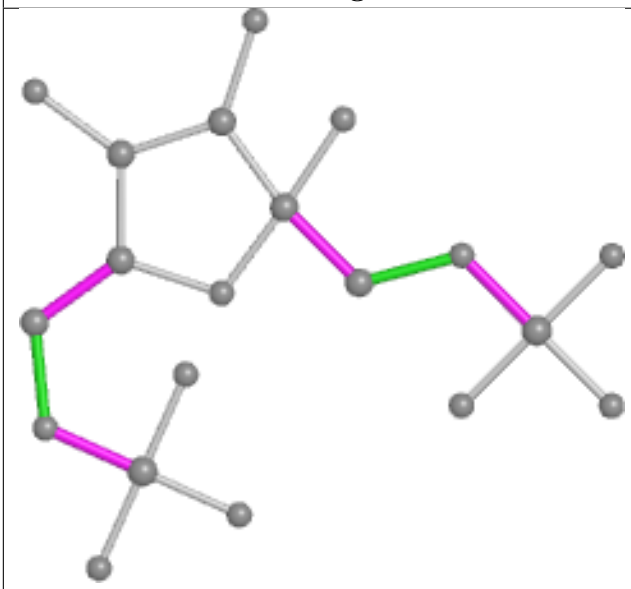
Ligand FBP D 601



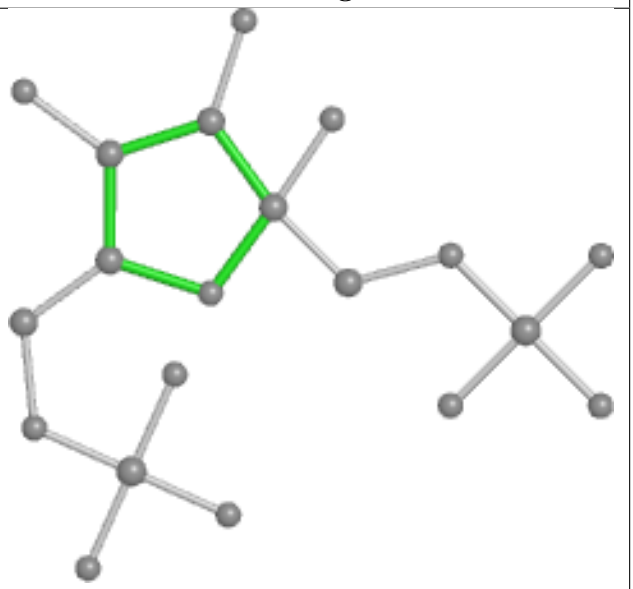
Bond lengths



Bond angles

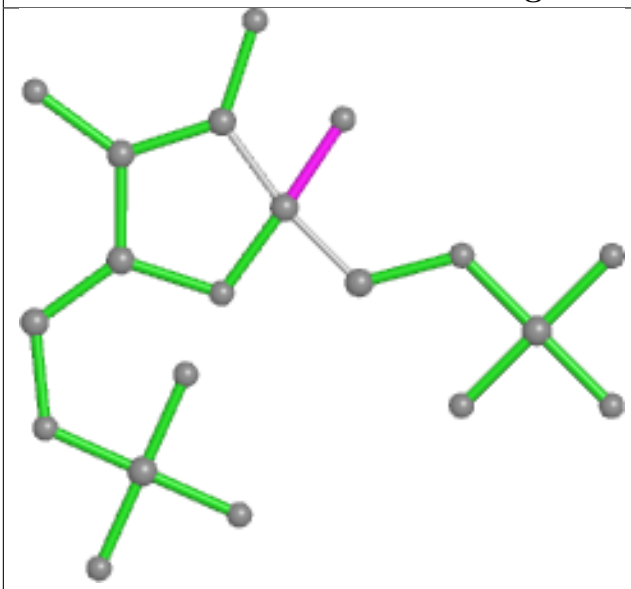


Torsions

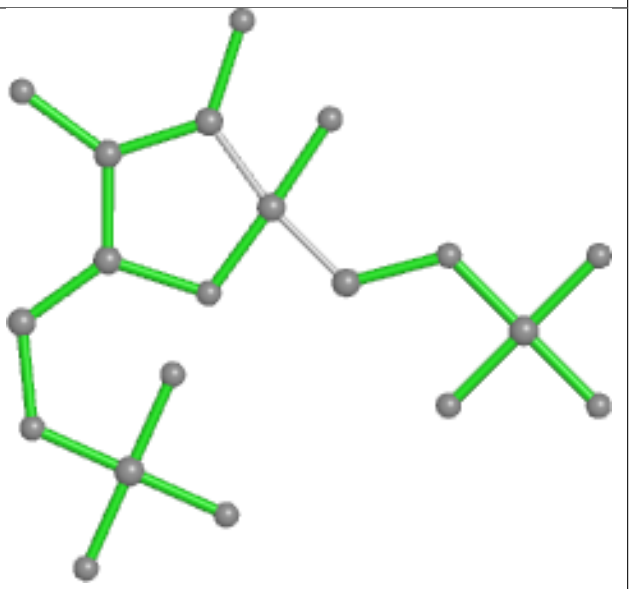


Rings

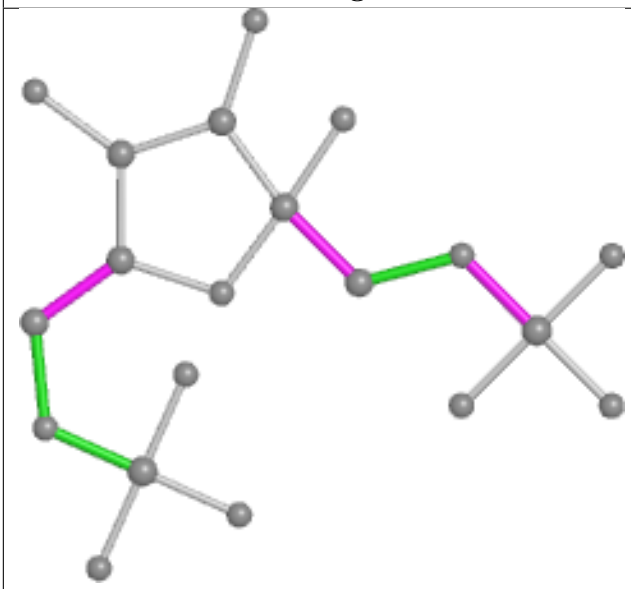
Ligand FBP A 601



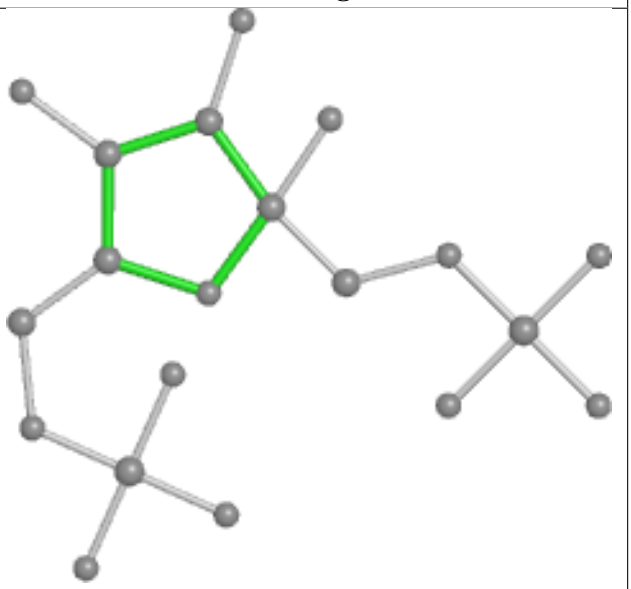
Bond lengths



Bond angles

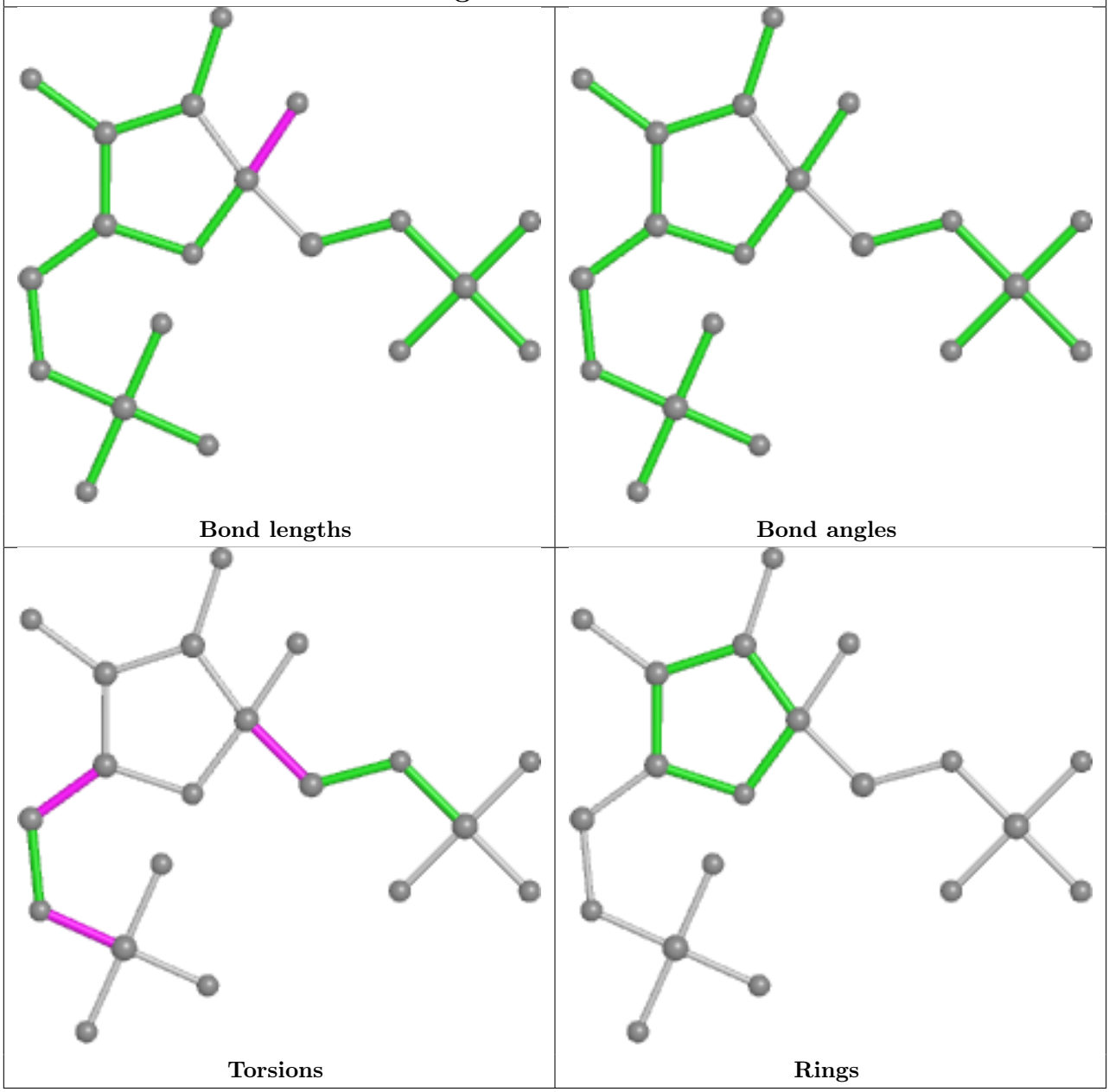


Torsions



Rings

Ligand FBP B 601



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, 95^{th} 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	503/565 (89%)	-0.04	2 (0%)	92	87	47, 100, 157, 250	0
1	B	509/565 (90%)	-0.02	12 (2%)	59	45	44, 93, 205, 297	0
1	C	512/565 (90%)	0.19	23 (4%)	33	24	40, 114, 244, 406	0
1	D	505/565 (89%)	0.38	27 (5%)	26	20	70, 141, 255, 343	0
All	All	2029/2260 (89%)	0.13	64 (3%)	47	36	40, 111, 220, 406	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	151	SER	8.4
1	C	125	SER	7.4
1	D	131	GLU	7.1
1	C	126	GLY	6.8
1	D	127	THR	6.5
1	D	128	GLY	6.1
1	D	129	GLU	6.0
1	D	125	SER	5.5
1	C	119	THR	4.8
1	C	152	LYS	4.5
1	C	127	THR	4.4
1	B	151	SER	4.3
1	B	184	ASP	3.9
1	C	147	LEU	3.9
1	B	119	THR	3.6
1	C	200	LEU	3.6
1	A	516	GLY	3.6
1	C	145	ASP	3.4
1	A	21	SER	3.4
1	C	401	PRO	3.2
1	D	155	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	130	VAL	3.2
1	C	129	GLU	3.1
1	C	203	SER	3.1
1	D	118	ARG	3.0
1	C	104	PHE	3.0
1	D	212	VAL	2.9
1	D	201	LEU	2.7
1	C	181	LEU	2.7
1	C	131	GLU	2.7
1	B	164	LYS	2.7
1	C	185	SER	2.7
1	C	39	PHE	2.7
1	C	154	LYS	2.6
1	B	141	THR	2.6
1	D	235	VAL	2.6
1	D	166	VAL	2.5
1	D	137	GLN	2.5
1	B	137	GLN	2.5
1	D	124	GLY	2.5
1	C	155	ILE	2.4
1	D	165	VAL	2.4
1	D	193	CYS	2.4
1	B	127	THR	2.4
1	D	121	LEU	2.4
1	C	124	GLY	2.4
1	D	192	THR	2.4
1	D	183	VAL	2.4
1	C	202	GLY	2.4
1	D	119	THR	2.4
1	D	39	PHE	2.3
1	B	167	LYS	2.3
1	B	200	LEU	2.3
1	D	207	VAL	2.3
1	D	138	ILE	2.2
1	D	151	SER	2.2
1	B	199	GLY	2.1
1	B	132	LEU	2.1
1	D	265	ILE	2.1
1	C	96	TYR	2.1
1	C	184	ASP	2.1
1	D	140	LEU	2.1
1	B	131	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	475	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

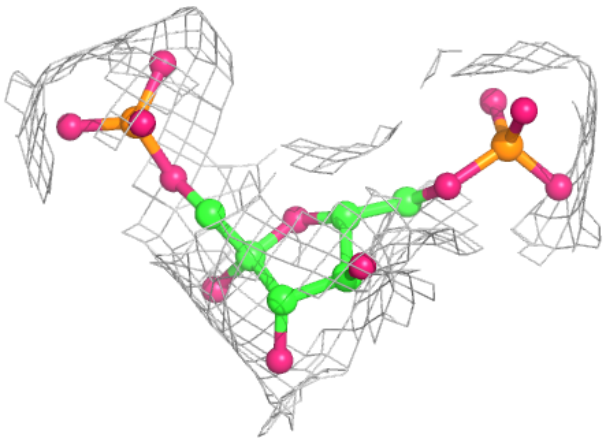
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

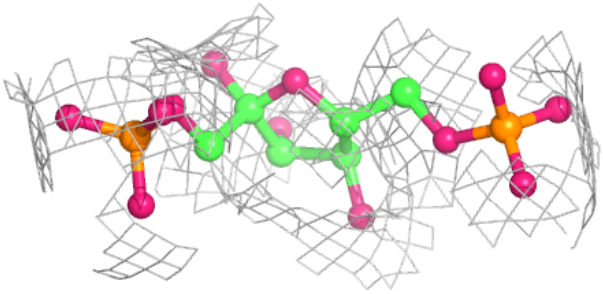
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FBP	D	601	20/20	0.85	0.21	102,106,111,113	0
2	FBP	B	601	20/20	0.89	0.18	70,76,80,84	0
2	FBP	A	601	20/20	0.92	0.12	89,110,115,115	0
2	FBP	C	601	20/20	0.93	0.15	64,88,95,95	0

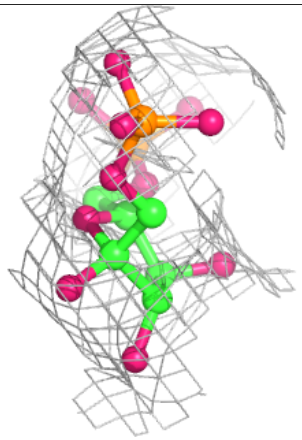
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP D 601:

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

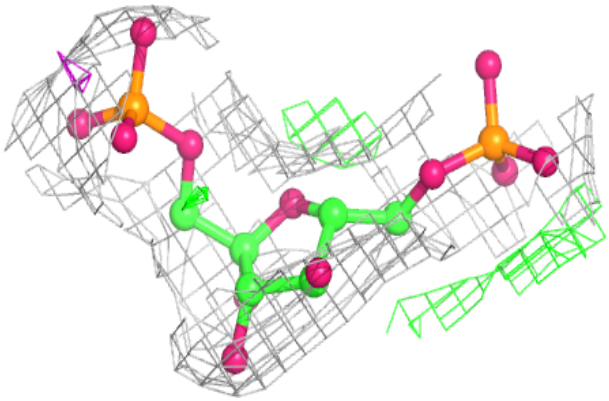


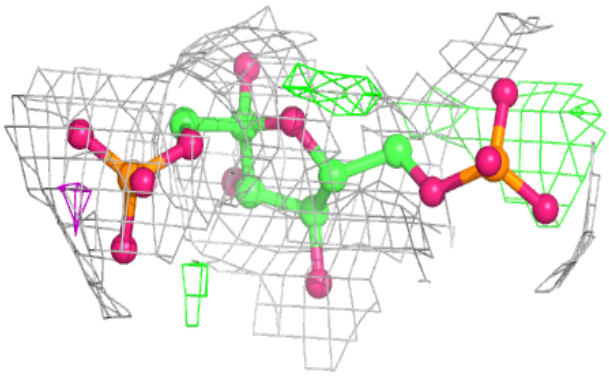


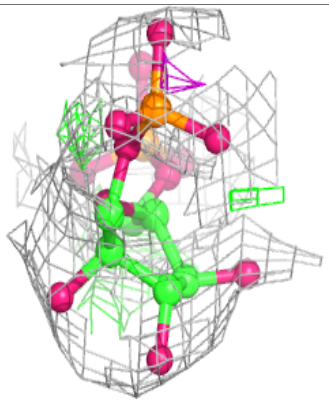


Electron density around FBP B 601:

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

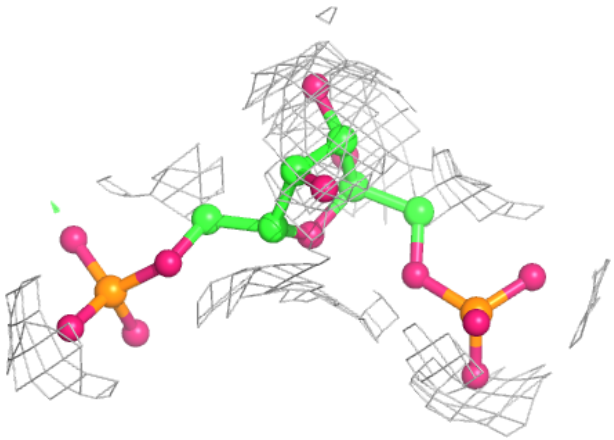


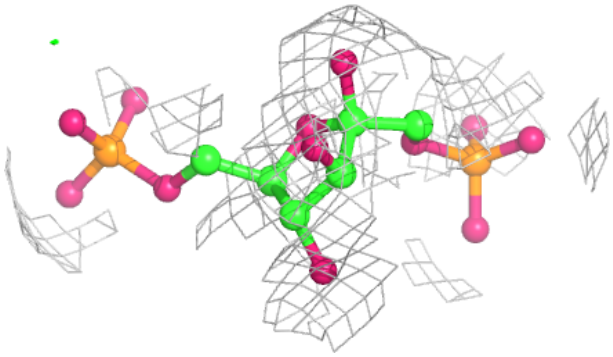


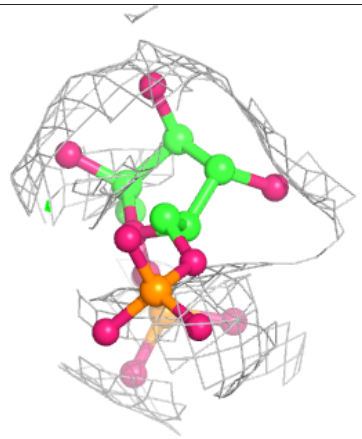


Electron density around FBP A 601:

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

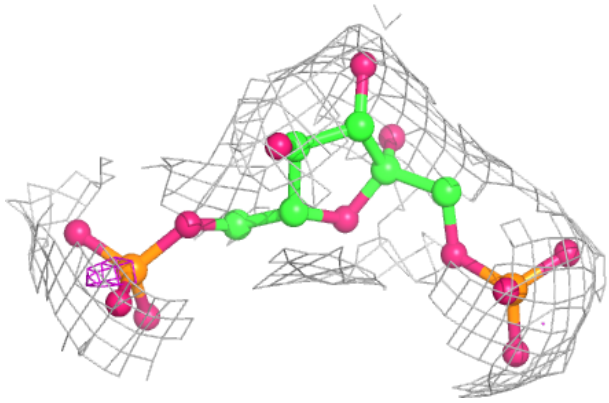


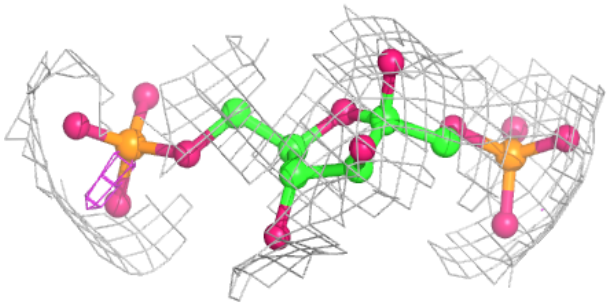


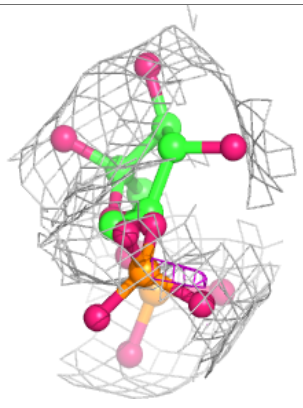


Electron density around FBP C 601:

$2mF_o$-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.