Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:51 AM GMT

PDB ID	:	3N25
Title	:	The structure of muscle pyruvate kinase in complex with proline, pyruvate, and Mn2+
Authors	:	Fenton, A.W.; Johnson, T.A.; Holyoak, T.
Deposited on	:	2010-05-17
Resolution	:	2.41 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

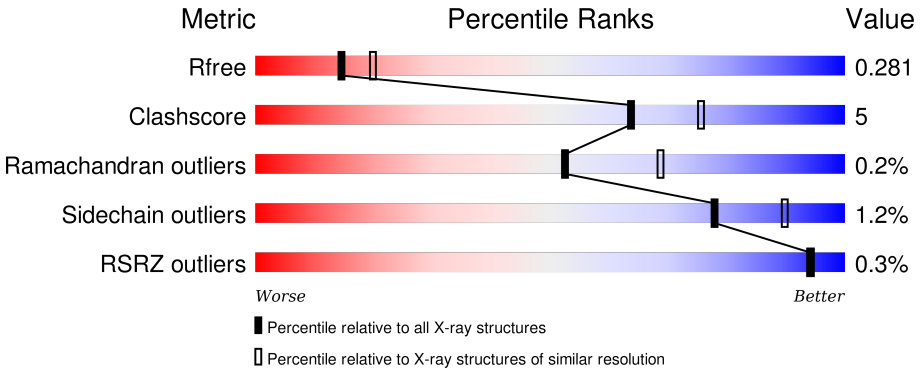
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	531	84% 14% •
1	B	531	81% 15% •
1	C	531	86% 10% •
1	D	531	88% 10% •
1	E	531	88% 10% •

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Mol	Chain	Length	Quality of chain
1	F	531	85% 12%
1	G	531	86% 10%
1	H	531	% 83% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	6002	-	-	-	X
7	GOL	A	6301	-	-	-	X
7	GOL	C	6055	-	-	-	X
7	GOL	C	6303	-	-	-	X
7	GOL	F	6306	-	-	-	X
7	GOL	H	6308	-	-	-	X
8	EDO	A	6043	-	-	-	X
8	EDO	D	6017	-	-	-	X
8	EDO	E	6046	-	-	-	X
8	EDO	E	6049	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33971 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 isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	14	0
			4061	2559	719	753	30			
1	B	508	Total	C	N	O	S	0	11	0
			3981	2508	709	736	28			
1	C	512	Total	C	N	O	S	0	14	0
			4033	2543	712	749	29			
1	D	521	Total	C	N	O	S	0	9	0
			4050	2547	718	756	29			
1	E	521	Total	C	N	O	S	0	8	0
			4049	2545	718	756	30			
1	F	515	Total	C	N	O	S	0	8	0
			4015	2525	711	750	29			
1	G	510	Total	C	N	O	S	0	6	0
			3961	2495	700	738	28			
1	H	519	Total	C	N	O	S	0	14	0
			4080	2570	722	759	29			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LYS	MET	SEE REMARK 999	UNP P11974
A	400	ALA	SER	SEE REMARK 999	UNP P11974
A	403	GLN	HIS	SEE REMARK 999	UNP P11974
B	29	LYS	MET	SEE REMARK 999	UNP P11974
B	400	ALA	SER	SEE REMARK 999	UNP P11974
B	403	GLN	HIS	SEE REMARK 999	UNP P11974
C	29	LYS	MET	SEE REMARK 999	UNP P11974
C	400	ALA	SER	SEE REMARK 999	UNP P11974
C	403	GLN	HIS	SEE REMARK 999	UNP P11974
D	29	LYS	MET	SEE REMARK 999	UNP P11974
D	400	ALA	SER	SEE REMARK 999	UNP P11974
D	403	GLN	HIS	SEE REMARK 999	UNP P11974
E	29	LYS	MET	SEE REMARK 999	UNP P11974

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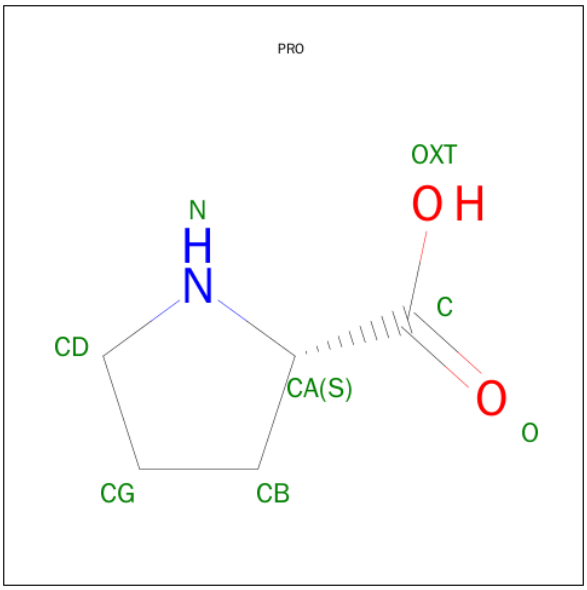
Chain	Residue	Modelled	Actual	Comment	Reference
E	400	ALA	SER	SEE REMARK 999	UNP P11974
E	403	GLN	HIS	SEE REMARK 999	UNP P11974
F	29	LYS	MET	SEE REMARK 999	UNP P11974
F	400	ALA	SER	SEE REMARK 999	UNP P11974
F	403	GLN	HIS	SEE REMARK 999	UNP P11974
G	29	LYS	MET	SEE REMARK 999	UNP P11974
G	400	ALA	SER	SEE REMARK 999	UNP P11974
G	403	GLN	HIS	SEE REMARK 999	UNP P11974
H	29	LYS	MET	SEE REMARK 999	UNP P11974
H	400	ALA	SER	SEE REMARK 999	UNP P11974
H	403	GLN	HIS	SEE REMARK 999	UNP P11974

- Molecule 2 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	5	1	2		
2	B	1	Total	C	N	O	0	0
			8	5	1	2		
2	C	1	Total	C	N	O	0	0
			8	5	1	2		
2	D	1	Total	C	N	O	0	0
			8	5	1	2		
2	E	1	Total	C	N	O	0	0
			8	5	1	2		
2	F	1	Total	C	N	O	0	0
			8	5	1	2		

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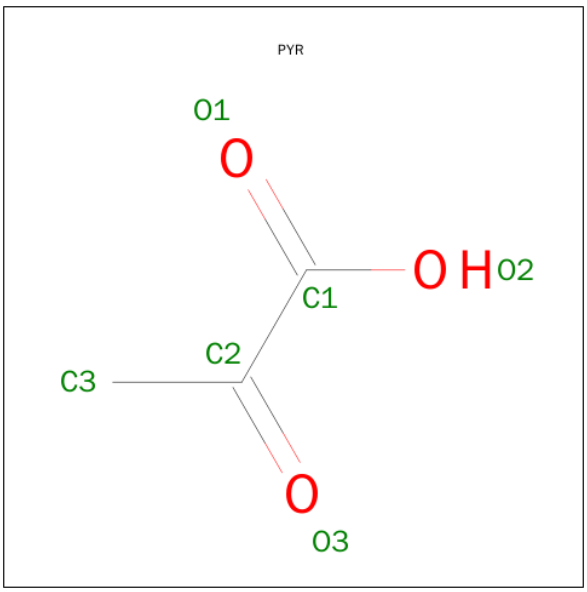
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C N O 8 5 1 2	0	0
2	H	1	Total C N O 8 5 1 2	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	H	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	E	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	A	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Na 1 1	0	0
6	D	2	Total Na 2 2	0	0

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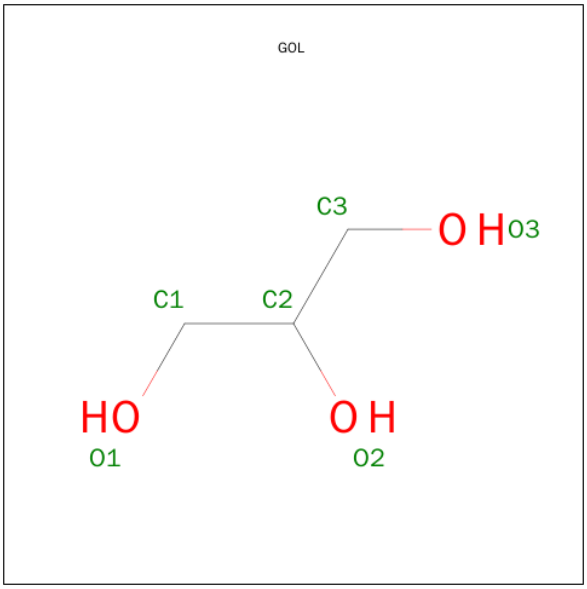
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	2	Total Na 2 2	0	0
6	H	2	Total Na 2 2	0	0
6	B	1	Total Na 1 1	0	0
6	C	1	Total Na 1 1	0	0
6	A	2	Total Na 2 2	0	0
6	F	1	Total Na 1 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

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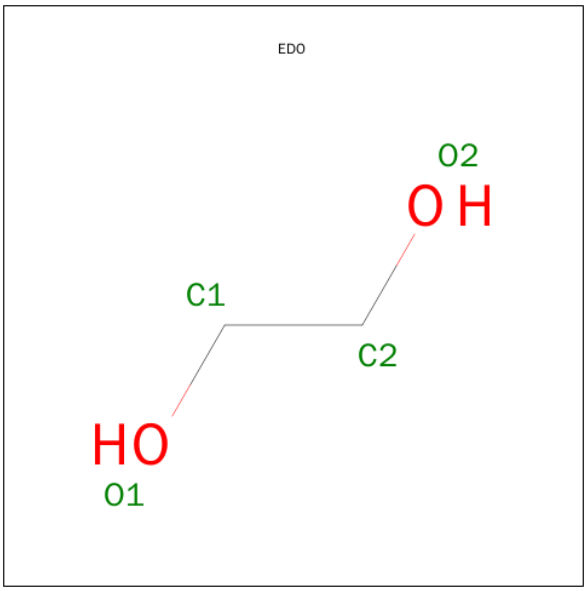
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	E	1	Total C O 4 2 2	0	0
8	F	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C O 4 2 2	0	0

- Molecule 9 is water.

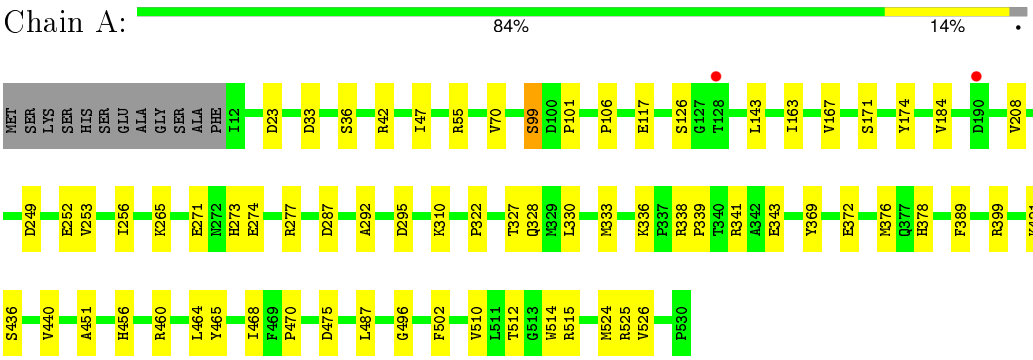
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	193	Total O 193 193	0	0
9	B	147	Total O 147 147	0	0
9	C	199	Total O 199 199	0	0
9	D	192	Total O 192 192	0	0
9	E	190	Total O 190 190	0	0
9	F	186	Total O 186 186	0	0
9	G	126	Total O 126 126	0	0
9	H	194	Total O 194 194	0	0

3 Residue-property plots (i)

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

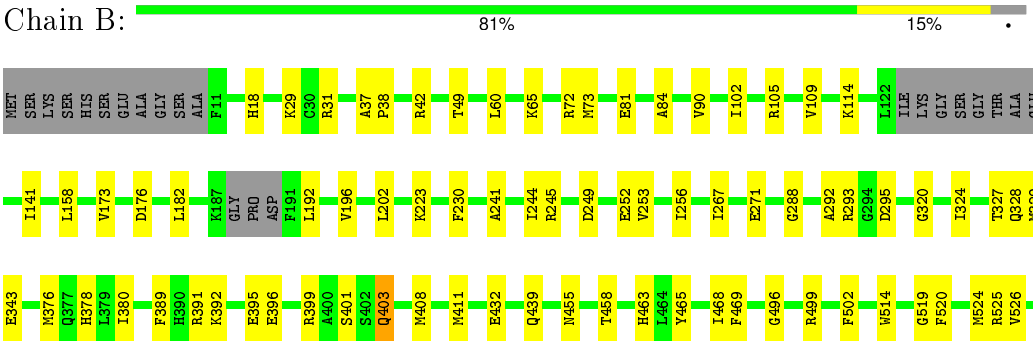
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain A:



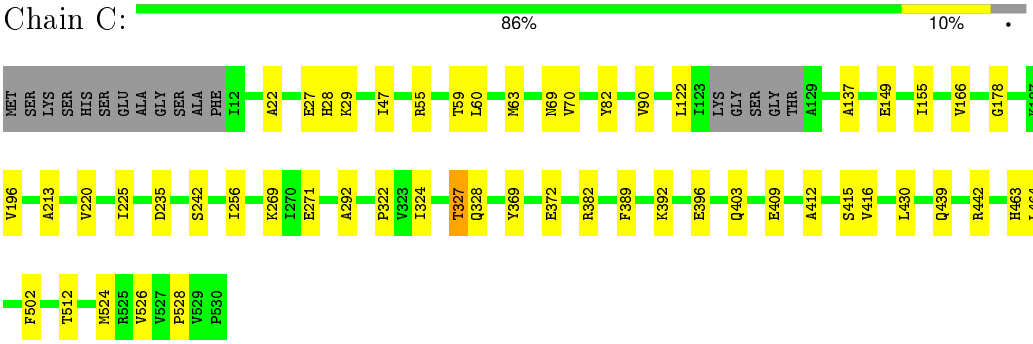
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain B:



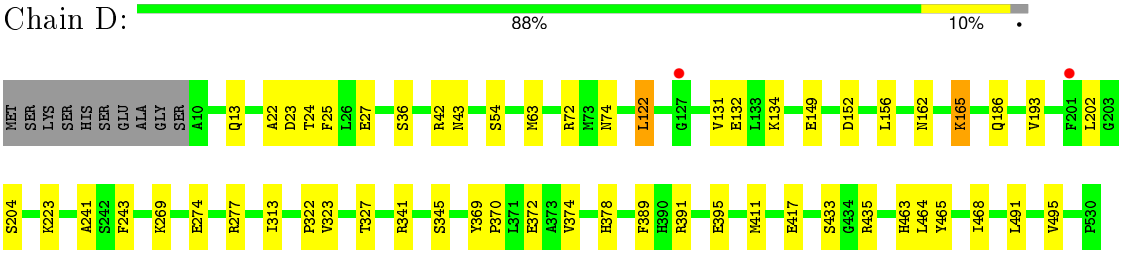
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain C:



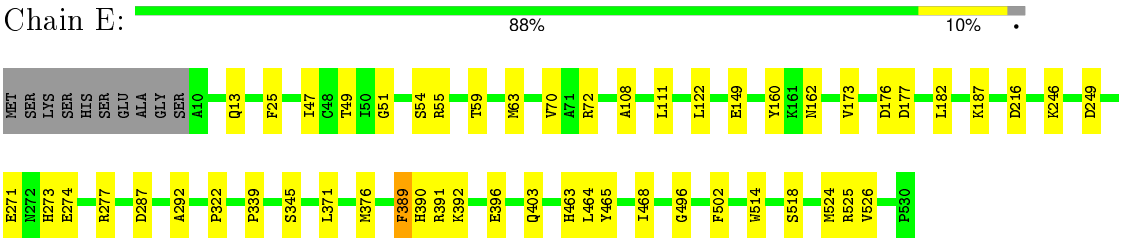
• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain D:



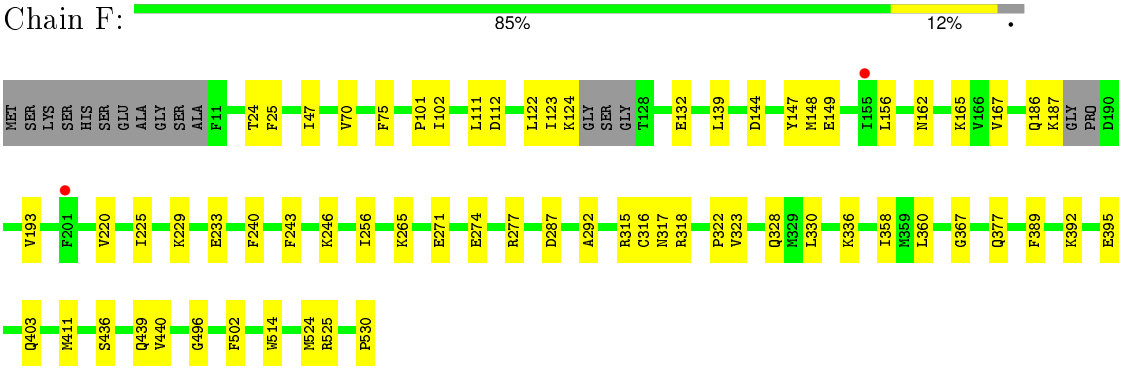
• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain E:



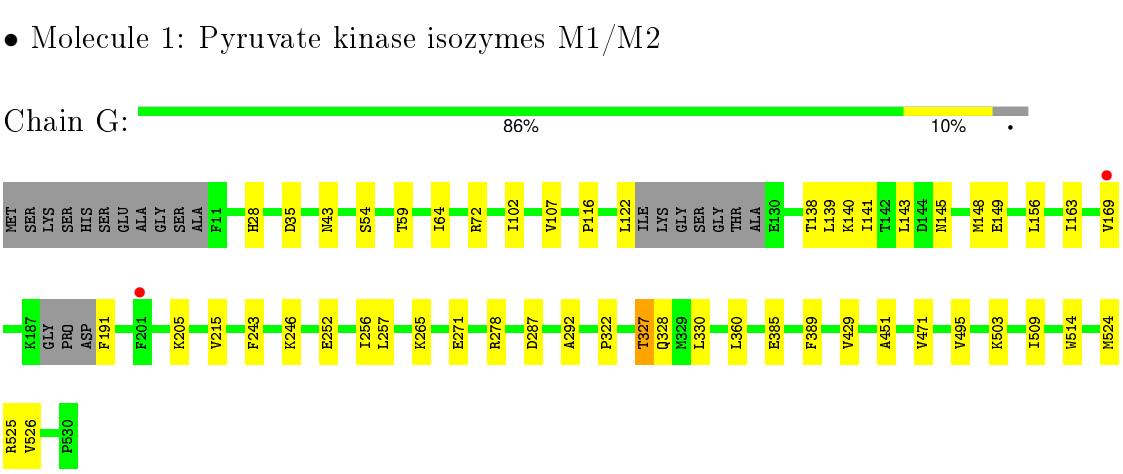
• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain F:



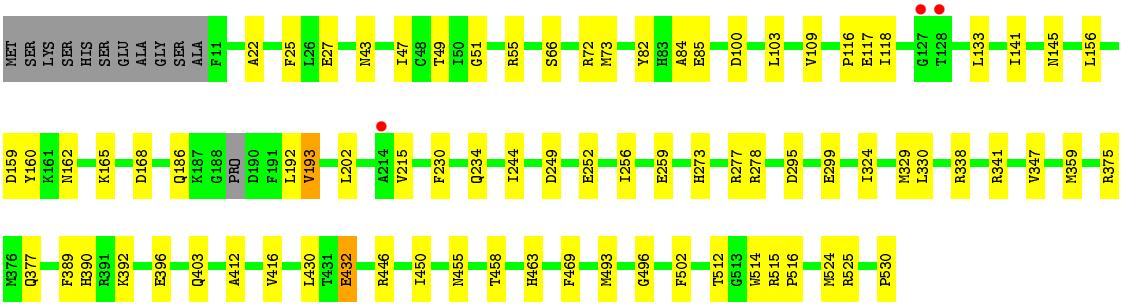
• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain G:



• Molecule 1: Pyruvate kinase isozymes M1/M2

Chain H:


MET SER LYS SER HIS SER GLU ALA GLY SER ALA F11 A22 F25 L26 E27 N43 I47 C48 T49 I50 G51 R55 S66 R72 M73 Y82 H83 A84 E85 D100 L103 V109 P116 E117 I118 G127 T128 L133 I141 N145 L156
D159 Y160 K161 N162 K165 D168 Q186 K187 G188 PRO D190 F191 L192 V193 L202 A214 V215 F230 Q234 I244 D249 E252 I256 E259 H273 R277 R278 D295 E299 I324 M329 L330 R338 R341 V347 M359 R375
M376 Q377 F389 H390 R391 K392 E396 Q403 A412 V416 L430 T431 E432 R446 I450 N455 T458 H463 F469 M493 G496 F502 T512 G513 W514 R515 P516 M524 R525 P530

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	82.37Å 108.75Å 144.26Å 95.18° 93.38° 112.23°	Depositor
Resolution (Å)	36.59 – 2.41 36.59 – 2.41	Depositor EDS
% Data completeness (in resolution range)	83.0 (36.59-2.41) 79.4 (36.59-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.268 0.218 , 0.281	Depositor DCC
R_{free} test set	7394 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , -3.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 146918 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	33971	wwPDB-VP
Average B, all atoms (Å^2)	5.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, NA, K, MN, EDO, PYR

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	0.44	0/4165	0.56	0/5614
1	B	0.42	0/4071	0.56	0/5484
1	C	0.45	0/4125	0.58	0/5561
1	D	0.44	0/4132	0.57	0/5572
1	E	0.45	0/4127	0.58	0/5563
1	F	0.45	0/4090	0.57	0/5511
1	G	0.41	0/4037	0.55	0/5440
1	H	0.44	0/4172	0.56	0/5618
All	All	0.44	0/32919	0.57	0/44363

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	4061	0	4191	63	0
1	B	3981	0	4092	67	0
1	C	4033	0	4127	40	0
1	D	4050	0	4138	33	0
1	E	4049	0	4138	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4015	0	4104	47	0
1	G	3961	0	4047	39	0
1	H	4080	0	4185	66	0
2	A	8	0	7	0	0
2	B	8	0	7	1	0
2	C	8	0	7	3	0
2	D	8	0	7	2	0
2	E	8	0	7	1	0
2	F	8	0	7	0	0
2	G	8	0	7	1	0
2	H	8	0	7	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	0	3	1	0
4	B	6	0	3	1	0
4	C	6	0	3	0	0
4	D	6	0	3	1	0
4	E	6	0	3	0	0
4	F	6	0	3	2	0
4	G	6	0	3	2	0
4	H	6	0	3	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	2	0	0	0	0
7	A	18	0	24	2	0
7	B	18	0	24	2	0
7	C	12	0	16	0	0
7	D	18	0	24	2	0
7	E	12	0	16	0	0
7	F	18	0	24	3	0
7	G	12	0	16	1	0
7	H	6	0	8	2	0
8	A	12	0	18	0	0
8	B	8	0	12	1	0
8	C	4	0	6	0	0
8	D	12	0	18	2	0
8	E	16	0	24	0	0
8	F	4	0	6	0	0
8	H	4	0	6	0	0
9	A	193	0	0	4	0
9	B	147	0	0	5	0
9	C	199	0	0	6	0
9	D	192	0	0	2	0
9	E	190	0	0	5	0
9	F	186	0	0	10	0
9	G	126	0	0	6	0
9	H	194	0	0	7	0
All	All	33971	0	33344	345	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 5.

All (345) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524[B]:MET:HE2	1:B:524[B]:MET:CE	1.89	1.02
1:A:524[B]:MET:HE2	1:B:524[B]:MET:HE2	1.36	1.01
1:F:274:GLU:HG3	1:F:277:ARG:NH2	1.88	0.88
1:A:524[B]:MET:CE	1:B:524[B]:MET:CE	2.54	0.86
1:A:524[B]:MET:HE2	1:B:524[B]:MET:HB3	1.56	0.86
1:F:101:PRO:HG2	9:F:1664:HOH:O	1.78	0.81
1:G:524[A]:MET:HE1	1:H:524[A]:MET:SD	2.23	0.79
1:G:524[A]:MET:CE	1:H:524[A]:MET:SD	2.71	0.79
1:B:526[B]:VAL:HG13	1:B:526[B]:VAL:O	1.82	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:GLN:HB3	9:C:1259:HOH:O	1.85	0.75
1:B:463:HIS:HD1	2:B:1600:PRO:N	1.85	0.74
1:B:526[B]:VAL:CG1	1:B:526[B]:VAL:O	2.36	0.73
1:H:73:MET:CE	1:H:109:VAL:HG13	2.18	0.73
1:G:246:LYS:HB3	9:G:1641:HOH:O	1.89	0.73
1:A:524[B]:MET:CE	1:B:524[B]:MET:SD	2.77	0.72
1:H:432[A]:GLU:OE2	9:H:1382:HOH:O	2.08	0.72
4:F:1500:PYR:H33	9:F:668:HOH:O	1.89	0.72
1:G:278:ARG:HD3	9:G:1641:HOH:O	1.88	0.72
1:A:399[A]:ARG:NE	1:B:391[A]:ARG:NH1	2.39	0.70
1:A:524[B]:MET:HE2	1:B:524[B]:MET:SD	2.30	0.70
1:G:524[A]:MET:HE2	1:H:524[A]:MET:HB3	1.75	0.69
1:A:42:ARG:HE	1:A:378:HIS:HD2	1.40	0.69
1:E:526:VAL:HG23	1:F:411:MET:SD	2.33	0.69
1:F:274:GLU:HG3	1:F:277:ARG:HH22	1.55	0.69
1:A:514:TRP:CE3	1:B:525:ARG:HD3	2.27	0.69
1:H:273:HIS:CE1	1:H:277[A]:ARG:HE	2.11	0.69
1:D:463:HIS:HD1	2:D:1600:PRO:N	1.91	0.69
7:F:6010:GOL:H32	1:H:341:ARG:HH12	1.56	0.69
1:A:369:TYR:HB3	1:A:372[B]:GLU:HG2	1.76	0.67
1:H:493:MET:HG2	1:H:530:PRO:HD2	1.76	0.67
1:G:524[A]:MET:HE2	1:H:524[A]:MET:SD	2.35	0.66
1:A:55:ARG:HD3	9:A:1222:HOH:O	1.95	0.66
1:C:220:VAL:HG11	1:C:256:ILE:CD1	2.27	0.65
1:F:233:GLU:OE2	9:F:798:HOH:O	2.13	0.65
1:C:496:GLY:HA3	1:C:502:PHE:CZ	2.33	0.64
1:F:220:VAL:HG11	1:F:256:ILE:HD11	1.79	0.64
1:A:524[B]:MET:CE	1:B:524[B]:MET:HB3	2.27	0.64
1:B:328:GLN:OE1	1:D:341:ARG:HG2	1.98	0.64
1:F:25:PHE:CE1	1:H:25[A]:PHE:CE2	2.85	0.63
1:D:274[A]:GLU:OE1	1:D:277:ARG:NH2	2.31	0.63
1:G:145:ASN:O	1:G:148:MET:HB2	1.98	0.63
1:D:391:ARG:O	1:D:395:GLU:HG3	1.98	0.63
1:A:524[B]:MET:HE2	1:B:524[B]:MET:CB	2.28	0.63
1:E:524[B]:MET:HB3	1:F:524[B]:MET:HE2	1.81	0.63
1:E:391:ARG:HD3	9:E:1287:HOH:O	1.99	0.62
1:H:463:HIS:HD1	2:H:1600:PRO:N	1.97	0.62
1:F:25:PHE:CE1	1:H:25[A]:PHE:CD2	2.87	0.62
1:E:390:HIS:HD2	9:E:1283:HOH:O	1.83	0.62
4:D:1500:PYR:H33	9:D:1625:HOH:O	1.98	0.62
1:A:524[B]:MET:CE	1:B:524[B]:MET:HE2	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:VAL:HG11	1:C:256:ILE:HD11	1.82	0.61
1:C:392:LYS:O	1:C:396:GLU:HG3	2.01	0.61
1:F:220:VAL:HG11	1:F:256:ILE:CD1	2.30	0.61
1:H:100:ASP:OD2	1:H:103:LEU:HD12	2.00	0.61
1:D:465:TYR:HB2	1:D:468:ILE:HD12	1.83	0.61
1:A:524[B]:MET:HE1	1:B:524[B]:MET:SD	2.40	0.60
1:A:341:ARG:HG2	1:C:328[A]:GLN:OE1	2.00	0.60
1:B:432[B]:GLU:OE2	1:B:455:ASN:HB2	2.02	0.60
1:C:439[B]:GLN:NE2	9:C:1386:HOH:O	2.09	0.60
1:H:244:ILE:HD12	1:H:249:ASP:HB3	1.84	0.60
1:D:22:ALA:HB1	1:D:27[B]:GLU:HB3	1.84	0.60
1:C:526[B]:VAL:HG23	1:D:411:MET:SD	2.42	0.59
1:F:496:GLY:HA3	1:F:502:PHE:CZ	2.37	0.59
1:A:338[B]:ARG:HD3	1:C:178:GLY:O	2.01	0.59
1:E:274:GLU:HG3	1:E:277[B]:ARG:HH22	1.67	0.59
1:G:122:LEU:HB2	1:G:149:GLU:HA	1.85	0.58
1:H:73:MET:HE3	1:H:109:VAL:HG13	1.84	0.58
1:E:51:GLY:O	1:E:55:ARG:HB2	2.04	0.58
1:E:274:GLU:HG3	1:E:277[B]:ARG:NH2	2.18	0.58
4:B:1500:PYR:H33	9:B:1604:HOH:O	2.03	0.58
1:F:225:ILE:HG22	1:F:229:LYS:HE3	1.86	0.57
1:G:102:ILE:HG12	9:G:1009:HOH:O	2.05	0.57
1:B:295:ASP:OD1	7:B:6302:GOL:H12	2.05	0.57
1:G:287:ASP:O	1:G:322:PRO:HD2	2.04	0.57
1:F:25:PHE:CD1	1:H:25[A]:PHE:CE2	2.92	0.57
1:E:463:HIS:HD1	2:E:1600:PRO:N	2.03	0.57
1:G:271:GLU:HB3	1:G:292:ALA:HB3	1.87	0.57
1:H:51:GLY:O	1:H:55:ARG:HG3	2.05	0.56
1:G:514:TRP:CE3	1:H:525:ARG:HD3	2.40	0.56
1:E:70:VAL:HG22	1:E:108:ALA:HB3	1.87	0.56
1:B:320:GLY:HA2	9:B:1611:HOH:O	2.04	0.56
1:D:156:LEU:HD13	1:D:202:LEU:HD21	1.86	0.56
9:B:929:HOH:O	1:D:23:ASP:HB2	2.05	0.56
1:A:465:TYR:HB2	1:A:468:ILE:HD12	1.88	0.56
1:D:132:GLU:HG2	1:D:134:LYS:HG2	1.87	0.56
1:G:215:VAL:HG21	7:G:6207:GOL:O2	2.06	0.56
1:C:463:HIS:HD1	2:C:1600:PRO:N	2.03	0.56
1:F:162:ASN:OD1	1:F:165:LYS:HG3	2.06	0.56
1:F:336:LYS:HE2	9:F:617:HOH:O	2.05	0.56
1:D:243:PHE:HZ	7:D:6304:GOL:H31	1.69	0.55
1:F:530:PRO:HG3	9:F:1671:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ALA:HB1	1:A:244:ILE:HD11	1.88	0.55
1:A:475:ASP:OD2	1:A:487:LEU:HD21	2.07	0.55
1:E:122:LEU:HD12	1:E:149:GLU:HG2	1.89	0.55
1:B:271:GLU:HB3	1:B:292:ALA:HB3	1.89	0.55
1:F:403:GLN:CD	1:F:403:GLN:H	2.10	0.55
1:B:42:ARG:HE	1:B:378:HIS:HD2	1.55	0.55
1:A:252[B]:GLU:OE1	1:A:252[B]:GLU:HA	2.06	0.54
1:E:339:PRO:HG3	1:E:376:MET:HG2	1.88	0.54
1:G:524[A]:MET:HE2	1:H:524[A]:MET:CB	2.37	0.54
1:H:162:ASN:OD1	1:H:165:LYS:HD3	2.08	0.54
1:D:243:PHE:CZ	7:D:6304:GOL:H31	2.42	0.54
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.43	0.54
1:D:54:SER:HB2	1:D:63[A]:MET:SD	2.47	0.54
1:F:102:ILE:HD13	9:F:1664:HOH:O	2.07	0.54
1:B:399[B]:ARG:CZ	9:B:929:HOH:O	2.54	0.54
1:H:186:GLN:HB3	1:H:193:VAL:HG13	1.89	0.54
1:D:223:LYS:HE2	9:D:1611:HOH:O	2.07	0.54
1:A:524[B]:MET:HB3	1:B:524[B]:MET:HE2	1.88	0.54
1:F:102:ILE:CD1	9:F:1664:HOH:O	2.55	0.54
1:F:403:GLN:HB3	9:F:1667:HOH:O	2.08	0.54
1:G:143:LEU:HD21	1:G:163:ILE:HG22	1.90	0.54
1:D:186:GLN:HB2	1:D:193:VAL:HB	1.89	0.53
1:C:166:VAL:HG12	1:C:213:ALA:HB1	1.89	0.53
1:G:43:ASN:O	2:G:1600:PRO:HG3	2.08	0.53
1:E:13[B]:GLN:CD	1:E:13[B]:GLN:H	2.10	0.53
1:G:330:LEU:HD12	1:G:360:LEU:HD21	1.90	0.53
7:F:6010:GOL:H31	1:H:338:ARG:HB2	1.92	0.52
1:E:465:TYR:HB2	1:E:468:ILE:HD12	1.92	0.52
1:H:73:MET:HE1	1:H:109:VAL:HG13	1.92	0.52
1:D:74:ASN:HD22	8:D:6017:EDO:H21	1.75	0.51
1:H:390:HIS:CE1	1:H:446:ARG:HB3	2.45	0.51
1:C:60:LEU:HD13	1:C:90:VAL:HA	1.92	0.51
1:A:310:LYS:HB3	1:C:29:LYS:CG	2.40	0.51
1:H:215:VAL:HG12	9:H:964:HOH:O	2.09	0.51
1:H:25[A]:PHE:CE2	1:H:392:LYS:HG3	2.45	0.51
1:B:252:GLU:O	1:B:256:ILE:HG12	2.11	0.51
1:H:403:GLN:HB3	9:H:1659:HOH:O	2.11	0.51
1:G:509:ILE:CD1	1:G:526:VAL:HG12	2.40	0.51
1:H:118:ILE:HG23	1:H:160:TYR:HB2	1.93	0.51
1:A:436:SER:O	1:A:440:VAL:HG23	2.11	0.51
1:H:55:ARG:NH2	1:H:85:GLU:HB3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ASP:HB3	1:A:36:SER:HB2	1.92	0.51
1:H:186:GLN:HB3	1:H:193:VAL:CG1	2.41	0.50
1:A:399[A]:ARG:CZ	1:B:391[A]:ARG:HH12	2.24	0.50
1:A:42:ARG:HE	1:A:378:HIS:CD2	2.26	0.50
1:D:43:ASN:O	2:D:1600:PRO:HG3	2.11	0.50
1:F:25:PHE:CZ	1:H:25[A]:PHE:CD2	2.99	0.50
1:D:131:VAL:HG11	1:D:152:ASP:HA	1.92	0.50
1:C:28:HIS:HD2	9:C:1651:HOH:O	1.94	0.50
1:F:330:LEU:HD12	1:F:360:LEU:HD21	1.94	0.50
1:H:430:LEU:HD22	1:H:512:THR:HG22	1.94	0.50
1:F:148:MET:HG3	1:F:149:GLU:HG3	1.94	0.50
1:H:141:ILE:HB	1:H:192:LEU:HB2	1.94	0.50
1:F:292:ALA:HB1	4:F:1500:PYR:C1	2.41	0.50
1:G:292:ALA:HB1	4:G:1500:PYR:C1	2.41	0.50
1:H:47:ILE:HB	1:H:359:MET:HG3	1.92	0.50
1:A:369:TYR:HB3	1:A:372[B]:GLU:CG	2.41	0.49
1:A:271:GLU:HB3	1:A:292:ALA:HB3	1.92	0.49
1:C:430:LEU:HD22	1:C:512:THR:HG22	1.94	0.49
1:C:59:THR:O	1:C:63[B]:MET:HG3	2.12	0.49
1:B:249:ASP:O	1:B:253:VAL:HG23	2.13	0.49
1:A:429:VAL:O	1:A:451:ALA:HA	2.12	0.49
1:H:156:LEU:HD13	1:H:202:LEU:HD21	1.93	0.49
1:H:159:ASP:OD1	9:H:1652:HOH:O	2.20	0.49
1:F:287:ASP:O	1:F:322:PRO:HD2	2.13	0.48
1:B:49:THR:OG1	1:B:72:ARG:HD3	2.12	0.48
1:H:47:ILE:HD12	1:H:324:ILE:HD13	1.95	0.48
1:E:54:SER:HA	1:E:59:THR:HG21	1.95	0.48
1:B:455:ASN:HB3	1:B:458:THR:HB	1.95	0.48
1:A:23:ASP:OD1	1:B:399[A]:ARG:NH2	2.45	0.48
4:A:1000:PYR:H33	9:A:1214:HOH:O	2.13	0.48
1:A:456:HIS:HB3	1:A:460:ARG:HH12	1.77	0.48
1:D:417:GLU:OE1	1:D:417:GLU:HA	2.14	0.48
1:C:412:ALA:O	1:C:416:VAL:HG23	2.13	0.48
1:B:465:TYR:HB2	1:B:468:ILE:HD12	1.95	0.48
1:C:528:PRO:HG2	9:C:1628:HOH:O	2.13	0.48
1:G:140:LYS:HE3	1:G:191:PHE:HB2	1.95	0.48
1:E:518:SER:HA	9:E:647:HOH:O	2.14	0.48
1:G:524[A]:MET:CE	1:H:524[A]:MET:CE	2.91	0.48
1:C:271:GLU:HB3	1:C:292:ALA:HB3	1.94	0.48
1:F:367:GLY:HA3	9:F:1636:HOH:O	2.14	0.47
1:E:525:ARG:HD3	1:F:514:TRP:CE3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:PRO:O	1:D:374:VAL:HG23	2.15	0.47
1:E:187:LYS:NZ	9:E:974:HOH:O	2.40	0.47
1:C:22:ALA:HB1	1:C:27[B]:GLU:HB3	1.96	0.47
1:E:49:THR:HA	1:E:72:ARG:HB3	1.97	0.47
1:A:143[A]:LEU:HD11	1:A:163:ILE:HG22	1.97	0.47
1:G:327:THR:HG22	1:G:328[B]:GLN:HG3	1.97	0.47
1:A:524[B]:MET:SD	1:B:524[B]:MET:HE1	2.55	0.47
1:C:439[A]:GLN:OE1	1:C:442:ARG:HD3	2.15	0.47
1:C:59:THR:O	1:C:63[A]:MET:HG2	2.14	0.47
1:C:382:ARG:HB2	9:C:599:HOH:O	2.15	0.47
1:A:430:LEU:HD22	1:A:512:THR:HG22	1.97	0.47
1:F:330:LEU:HD11	1:F:377:GLN:HG3	1.97	0.46
1:A:265:LYS:CE	9:A:1210:HOH:O	2.63	0.46
1:B:73:MET:CE	1:B:109:VAL:HG13	2.45	0.46
1:F:186:GLN:HG2	1:F:187:LYS:H	1.80	0.46
1:B:519:GLY:O	1:B:520:PHE:HB3	2.16	0.46
1:H:252:GLU:O	1:H:256:ILE:HG12	2.15	0.46
1:B:376:MET:HG3	1:B:380:ILE:HD11	1.97	0.46
1:F:436:SER:O	1:F:440:VAL:HG23	2.15	0.46
1:E:111:LEU:HD23	1:E:111:LEU:C	2.36	0.46
1:A:524[B]:MET:CE	1:B:524[B]:MET:CB	2.90	0.46
1:E:25:PHE:CD2	1:E:389:PHE:HD1	2.33	0.46
1:A:117:GLU:HG2	7:A:6301:GOL:H32	1.97	0.46
1:H:412:ALA:O	1:H:416:VAL:HG23	2.16	0.46
1:G:524[A]:MET:HE2	1:H:524[A]:MET:CE	2.46	0.45
1:G:265:LYS:HA	1:G:287:ASP:OD1	2.15	0.45
1:A:322:PRO:HB3	1:A:464:LEU:O	2.16	0.45
1:H:230:PHE:CZ	1:H:234:GLN:HG3	2.51	0.45
1:F:47:ILE:HG12	1:F:70:VAL:HB	1.98	0.45
1:B:469:PHE:HE2	1:B:499:ARG:CZ	2.30	0.45
1:G:252:GLU:O	1:G:256:ILE:HG12	2.16	0.45
1:H:133:LEU:HD11	1:H:202:LEU:HD22	1.98	0.45
1:E:392:LYS:O	1:E:396:GLU:HG3	2.16	0.45
1:B:267:ILE:HD12	1:B:288:GLY:HA3	1.97	0.45
1:B:29[A]:LYS:HA	1:B:29[A]:LYS:HD3	1.59	0.45
1:F:144:ASP:HB3	1:F:147:TYR:HD2	1.82	0.45
1:C:369:TYR:HB3	1:C:372:GLU:HB2	1.99	0.45
1:B:241:ALA:O	1:B:244:ILE:HG12	2.16	0.45
1:H:455:ASN:HB3	1:H:458:THR:HB	1.98	0.45
1:G:116:PRO:HD2	1:G:243:PHE:HB2	1.98	0.45
1:A:287:ASP:O	1:A:322:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:LEU:O	1:D:495:VAL:HG23	2.17	0.45
1:B:267:ILE:HG21	1:B:324:ILE:HD12	1.99	0.45
1:C:322:PRO:HB3	1:C:464:LEU:O	2.16	0.45
1:H:49:THR:OG1	1:H:72:ARG:HD3	2.16	0.45
1:A:273:HIS:CE1	1:A:277:ARG:NH2	2.85	0.44
1:A:421:LYS:NZ	1:B:401:SER:O	2.50	0.44
1:H:329:MET:HE2	1:H:347:VAL:HG22	1.99	0.44
1:B:245[B]:ARG:NH2	7:B:6202:GOL:O1	2.45	0.44
1:D:369:TYR:HB3	1:D:372:GLU:HB2	1.99	0.44
1:G:429:VAL:O	1:G:451:ALA:HA	2.17	0.44
1:B:65:LYS:HA	1:B:105:ARG:HH12	1.82	0.44
1:C:122:LEU:HD22	1:C:149:GLU:HG2	1.99	0.44
1:A:310:LYS:HB3	1:C:29:LYS:HG2	1.99	0.44
1:C:415:SER:HA	1:C:524[A]:MET:SD	2.58	0.44
1:G:43:ASN:H	1:G:385:GLU:CD	2.20	0.44
1:G:526:VAL:O	1:G:526:VAL:HG23	2.17	0.44
1:F:186:GLN:HB3	1:F:193:VAL:CG1	2.48	0.44
1:F:112:ASP:HA	1:F:240:PHE:HB2	1.99	0.44
1:F:75:PHE:CE1	1:F:111:LEU:HG	2.52	0.44
1:H:295:ASP:OD2	7:H:6308:GOL:H31	2.18	0.44
1:H:55:ARG:HD2	1:H:82:TYR:OH	2.17	0.44
1:A:265:LYS:HD2	1:A:287:ASP:CG	2.37	0.44
1:E:322:PRO:HB3	1:E:464:LEU:O	2.18	0.44
1:F:139:LEU:HD21	1:F:156:LEU:HD22	2.00	0.44
1:B:173:VAL:HG13	1:B:182:LEU:HB2	2.00	0.44
1:B:102:ILE:O	1:B:499:ARG:NH2	2.51	0.43
1:D:322:PRO:HB3	1:D:464:LEU:O	2.17	0.43
1:G:54:SER:HA	1:G:59:THR:HG21	1.99	0.43
1:A:333:MET:HA	1:A:336:LYS:O	2.18	0.43
1:A:399[A]:ARG:CZ	1:B:391[A]:ARG:NH1	2.82	0.43
1:H:515:ARG:HB3	1:H:516:PRO:HD2	1.98	0.43
1:A:99:SER:O	1:A:101:PRO:HD3	2.18	0.43
1:B:84:ALA:HB2	1:B:230:PHE:HZ	1.83	0.43
1:G:509:ILE:HD12	1:G:526:VAL:HG12	2.00	0.43
1:A:510:VAL:HG12	1:A:512:THR:HG23	2.00	0.43
1:B:376:MET:HG3	1:B:380:ILE:CD1	2.48	0.43
1:D:162[A]:ASN:OD1	1:D:165:LYS:HD2	2.18	0.43
1:A:327:THR:HG22	1:A:328:GLN:HG3	2.00	0.43
1:A:339:PRO:HG3	1:A:376:MET:HG2	1.99	0.43
1:G:122:LEU:HD13	1:G:149:GLU:HG2	2.00	0.43
1:C:55[B]:ARG:CZ	1:C:82[B]:TYR:CE1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:HG11	1:A:184:VAL:HG21	2.00	0.43
1:E:160:TYR:OH	1:E:216:ASP:OD1	2.28	0.43
1:C:47:ILE:HG12	1:C:70:VAL:HB	2.00	0.43
1:H:117:GLU:HG2	7:H:6308:GOL:H11	1.99	0.43
1:D:122:LEU:HB2	1:D:149:GLU:HA	1.99	0.43
1:C:137:ALA:O	1:C:196:VAL:HG23	2.18	0.43
1:H:496:GLY:HA3	1:H:502:PHE:CZ	2.53	0.43
1:G:72:ARG:NH2	9:G:651:HOH:O	2.52	0.43
1:H:493:MET:CG	1:H:530:PRO:HD2	2.44	0.43
1:A:106:PRO:HG2	1:A:470:PRO:HG2	1.99	0.43
1:A:249:ASP:O	1:A:253:VAL:HG23	2.18	0.43
1:C:409:GLU:HG2	1:C:439[A]:GLN:OE1	2.19	0.43
1:G:28:HIS:HE1	9:G:1620:HOH:O	2.02	0.43
1:F:243:PHE:HZ	7:F:6306:GOL:H32	1.83	0.43
1:F:24:THR:HB	1:H:396:GLU:CD	2.39	0.43
1:H:277[B]:ARG:HH21	1:H:278:ARG:HH11	1.67	0.43
1:H:390:HIS:HD2	9:H:758:HOH:O	2.02	0.43
1:F:265:LYS:HA	1:F:265:LYS:HD3	1.81	0.43
1:C:327:THR:HG22	1:C:328[A]:GLN:HG3	2.01	0.42
1:E:63[B]:MET:HG3	1:E:371:LEU:HD23	2.01	0.42
1:B:141:ILE:HB	1:B:192:LEU:HB2	2.01	0.42
1:B:330:LEU:HD23	1:B:343:GLU:HB3	2.01	0.42
1:E:173:VAL:HB	1:E:182:LEU:HB2	2.00	0.42
1:H:43:ASN:O	2:H:1600:PRO:HG3	2.19	0.42
1:F:271:GLU:HB3	1:F:292:ALA:HB3	2.00	0.42
1:H:277[B]:ARG:HH21	1:H:278:ARG:HD2	1.84	0.42
1:H:450[B]:ILE:HD13	1:H:469:PHE:HB3	2.01	0.42
1:F:328:GLN:OE1	1:H:341:ARG:HG2	2.19	0.42
1:G:64:ILE:HG12	1:G:107:VAL:HG21	2.00	0.42
1:A:526[A]:VAL:HG23	1:B:411:MET:SD	2.59	0.42
1:C:220:VAL:HG12	1:C:225:ILE:HG13	2.01	0.42
1:H:66:SER:HB3	1:H:375:ARG:HG3	2.01	0.42
1:C:69:ASN:OD1	2:C:1600:PRO:HA	2.20	0.42
1:A:525:ARG:HD3	1:B:514:TRP:CE3	2.55	0.42
1:C:470:PRO:HD2	2:C:1600:PRO:OXT	2.20	0.42
1:H:84:ALA:HB2	1:H:230:PHE:HZ	1.85	0.42
1:C:235:ASP:OD1	9:C:1653:HOH:O	2.22	0.42
1:D:313:ILE:HA	1:D:323:VAL:HG11	2.02	0.42
1:H:22:ALA:HB1	1:H:27[A]:GLU:HB3	2.01	0.42
1:F:315:ARG:HG2	1:F:318:ARG:HH21	1.84	0.42
1:B:496:GLY:HA3	1:B:502:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ALA:O	1:D:269:LYS:HB2	2.20	0.42
1:G:141:ILE:HG12	1:G:156:LEU:HD23	2.02	0.42
1:H:116:PRO:HG3	9:H:994:HOH:O	2.18	0.42
1:A:524[B]:MET:SD	1:B:524[B]:MET:CE	3.08	0.42
1:B:295:ASP:OD2	8:B:6048:EDO:H12	2.20	0.41
1:E:271:GLU:HB3	1:E:292:ALA:HB3	2.02	0.41
1:B:37:ALA:HA	1:B:38:PRO:HD2	1.90	0.41
1:D:433:SER:OG	1:D:435:ARG:HG2	2.20	0.41
1:C:47:ILE:CD1	1:C:324:ILE:HD13	2.51	0.41
1:B:408:MET:HG3	1:B:439[B]:GLN:HG3	2.02	0.41
1:E:403:GLN:NE2	9:E:1048:HOH:O	2.53	0.41
1:A:47:ILE:HG23	1:A:70:VAL:HB	2.01	0.41
1:B:18:HIS:CE1	1:B:31:ARG:HD3	2.55	0.41
1:D:13:GLN:O	1:D:36:SER:OG	2.27	0.41
1:F:392:LYS:HE2	1:F:395:GLU:OE2	2.20	0.41
1:B:114:LYS:HD3	1:B:223:LYS:HD2	2.03	0.41
1:E:47:ILE:HG12	1:E:70:VAL:HB	2.02	0.41
1:B:395:GLU:O	1:B:399[A]:ARG:HG3	2.20	0.41
1:C:242:SER:HA	1:C:269:LYS:HD3	2.02	0.41
1:G:471:VAL:HG11	1:G:495:VAL:HG21	2.01	0.41
1:E:246:LYS:O	1:E:249:ASP:HB2	2.21	0.41
1:E:273:HIS:CE1	1:G:35:ASP:OD2	2.73	0.41
1:A:295:ASP:OD1	7:A:6301:GOL:H12	2.21	0.41
1:H:299:GLU:OE2	9:H:806:HOH:O	2.22	0.41
1:E:403:GLN:H	1:E:403:GLN:CD	2.24	0.41
1:E:514:TRP:CE3	1:F:525:ARG:HD3	2.56	0.41
1:H:330:LEU:HD11	1:H:377:GLN:HG3	2.03	0.41
1:F:316:CYS:SG	1:F:323:VAL:HB	2.61	0.41
1:F:123:ILE:O	1:F:124:LYS:C	2.58	0.41
9:A:1155:HOH:O	1:B:403:GLN:HG3	2.21	0.41
1:B:399[B]:ARG:NH1	9:B:929:HOH:O	2.54	0.41
1:D:42:ARG:HB2	1:D:378:HIS:CE1	2.56	0.41
1:B:293:ARG:NH2	1:B:329:MET:HG2	2.36	0.41
1:D:72:ARG:HH12	8:D:6017:EDO:H22	1.85	0.40
1:G:525:ARG:HD3	1:H:514:TRP:CE3	2.56	0.40
1:B:391[A]:ARG:NH2	1:B:392:LYS:NZ	2.69	0.40
4:G:1500:PYR:H33	9:G:1081:HOH:O	2.21	0.40
1:C:27[A]:GLU:OE1	1:C:27[A]:GLU:HA	2.22	0.40
1:B:182:LEU:HD22	1:B:196:VAL:HG22	2.03	0.40
1:F:439:GLN:NE2	9:F:721:HOH:O	2.50	0.40
1:A:330:LEU:HD23	1:A:343:GLU:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LEU:HD13	1:B:90:VAL:HA	2.02	0.40
1:B:396:GLU:CD	1:D:24:THR:HB	2.41	0.40
1:E:496:GLY:HA3	1:E:502:PHE:CZ	2.57	0.40
1:A:174:TYR:O	1:A:208:VAL:HA	2.21	0.40
1:E:287:ASP:O	1:E:322:PRO:HD2	2.22	0.40
1:D:122:LEU:HD12	1:D:204:SER:HB3	2.02	0.40
1:A:245[B]:ARG:HD3	1:A:274:GLU:OE1	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	531/531 (100%)	518 (98%)	13 (2%)	0	100	100
1	B	513/531 (97%)	497 (97%)	14 (3%)	2 (0%)	39	54
1	C	520/531 (98%)	502 (96%)	17 (3%)	1 (0%)	52	69
1	D	528/531 (99%)	516 (98%)	11 (2%)	1 (0%)	52	69
1	E	527/531 (99%)	510 (97%)	15 (3%)	2 (0%)	39	54
1	F	517/531 (97%)	497 (96%)	20 (4%)	0	100	100
1	G	510/531 (96%)	494 (97%)	14 (3%)	2 (0%)	39	54
1	H	529/531 (100%)	510 (96%)	19 (4%)	0	100	100
All	All	4175/4248 (98%)	4044 (97%)	123 (3%)	8 (0%)	52	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	177	ASP
1	D	327	THR
1	B	327	THR

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Mol	Chain	Res	Type
1	C	327	THR
1	G	327	THR
1	B	176	ASP
1	E	176	ASP
1	G	169	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	439/434 (101%)	434 (99%)	5 (1%)	80 91
1	B	429/434 (99%)	422 (98%)	7 (2%)	70 85
1	C	435/434 (100%)	433 (100%)	2 (0%)	92 97
1	D	435/434 (100%)	430 (99%)	5 (1%)	80 91
1	E	434/434 (100%)	431 (99%)	3 (1%)	88 95
1	F	432/434 (100%)	425 (98%)	7 (2%)	70 85
1	G	426/434 (98%)	420 (99%)	6 (1%)	74 88
1	H	439/434 (101%)	431 (98%)	8 (2%)	66 83
All	All	3469/3472 (100%)	3426 (99%)	43 (1%)	78 90

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	SER
1	A	126	SER
1	A	171	SER
1	A	389	PHE
1	A	515	ARG
1	B	81	GLU
1	B	138	THR
1	B	158	LEU
1	B	202	LEU
1	B	335	LYS

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Mol	Chain	Res	Type
1	B	389	PHE
1	B	403	GLN
1	C	155	ILE
1	C	389	PHE
1	D	25	PHE
1	D	122	LEU
1	D	165	LYS
1	D	345	SER
1	D	389	PHE
1	E	162	ASN
1	E	345	SER
1	E	389	PHE
1	F	122	LEU
1	F	132	GLU
1	F	167	VAL
1	F	246	LYS
1	F	317	ASN
1	F	358	ILE
1	F	389	PHE
1	G	138	THR
1	G	139	LEU
1	G	205	LYS
1	G	257	LEU
1	G	389	PHE
1	G	503	LYS
1	H	145	ASN
1	H	168	ASP
1	H	193	VAL
1	H	259[A]	GLU
1	H	259[B]	GLU
1	H	389	PHE
1	H	432[A]	GLU
1	H	432[B]	GLU

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	378	HIS
1	A	390	HIS
1	A	456	HIS
1	B	273	HIS
1	B	378	HIS

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Mol	Chain	Res	Type
1	E	390	HIS
1	F	390	HIS
1	G	198	ASN
1	G	209	ASN
1	G	494	ASN
1	H	145	ASN
1	H	209	ASN
1	H	390	HIS

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)

Of 78 ligands modelled in this entry, 28 are monoatomic - leaving 50 for Mogul analysis.

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	$\#\|Z\| > 2$
4	PYR	A	1000	3	2,5,5	1.98	1 (50%)	2,6,6	0.68	0
2	PRO	A	1200	-	4,8,8	0.49	0	5,10,10	1.17	0
7	GOL	A	6002	-	5,5,5	0.32	0	5,5,5	0.55	0
8	EDO	A	6043	-	3,3,3	0.52	0	2,2,2	0.38	0
8	EDO	A	6050	-	3,3,3	0.49	0	2,2,2	0.51	0
8	EDO	A	6051	-	3,3,3	0.43	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	A	6201	-	5,5,5	0.31	0	5,5,5	0.48	0
7	GOL	A	6301	-	5,5,5	0.34	0	5,5,5	0.31	0
4	PYR	B	1500	3	2,5,5	1.74	1 (50%)	2,6,6	0.26	0
2	PRO	B	1600	-	4,8,8	0.72	0	5,10,10	1.12	0
7	GOL	B	6007	-	5,5,5	0.26	0	5,5,5	0.37	0
8	EDO	B	6013	-	3,3,3	0.46	0	2,2,2	0.47	0
8	EDO	B	6048	-	3,3,3	0.48	0	2,2,2	0.36	0
7	GOL	B	6202	-	5,5,5	0.30	0	5,5,5	0.33	0
7	GOL	B	6302	-	5,5,5	0.33	0	5,5,5	0.48	0
4	PYR	C	1500	3	2,5,5	1.67	1 (50%)	2,6,6	0.68	0
2	PRO	C	1600	-	4,8,8	0.63	0	5,10,10	0.99	0
8	EDO	C	6014	-	3,3,3	0.47	0	2,2,2	0.45	0
7	GOL	C	6055	-	5,5,5	0.32	0	5,5,5	0.22	0
7	GOL	C	6303	-	5,5,5	0.36	0	5,5,5	0.33	0
4	PYR	D	1500	3	2,5,5	1.56	1 (50%)	2,6,6	1.01	0
2	PRO	D	1600	-	4,8,8	0.49	0	5,10,10	1.11	0
8	EDO	D	6011	-	3,3,3	0.48	0	2,2,2	0.53	0
8	EDO	D	6017	-	3,3,3	0.52	0	2,2,2	0.36	0
8	EDO	D	6033	-	3,3,3	0.51	0	2,2,2	0.31	0
7	GOL	D	6056	-	5,5,5	0.39	0	5,5,5	0.29	0
7	GOL	D	6204	-	5,5,5	0.32	0	5,5,5	0.33	0
7	GOL	D	6304	-	5,5,5	0.29	0	5,5,5	0.50	0
4	PYR	E	1500	3	2,5,5	1.75	1 (50%)	2,6,6	0.24	0
2	PRO	E	1600	-	4,8,8	0.67	0	5,10,10	1.09	0
8	EDO	E	6015	-	3,3,3	0.54	0	2,2,2	0.40	0
8	EDO	E	6039	-	3,3,3	0.54	0	2,2,2	0.30	0
8	EDO	E	6046	-	3,3,3	0.49	0	2,2,2	0.47	0
8	EDO	E	6049	-	3,3,3	0.56	0	2,2,2	0.34	0
7	GOL	E	6205	-	5,5,5	0.36	0	5,5,5	0.30	0
7	GOL	E	6305	-	5,5,5	0.25	0	5,5,5	0.68	0
4	PYR	F	1500	3	2,5,5	1.83	1 (50%)	2,6,6	0.82	0
2	PRO	F	1600	-	4,8,8	0.63	0	5,10,10	1.02	0
7	GOL	F	6010	-	5,5,5	0.32	0	5,5,5	0.29	0
8	EDO	F	6012	-	3,3,3	0.49	0	2,2,2	0.50	0
7	GOL	F	6206	-	5,5,5	0.45	0	5,5,5	0.35	0
7	GOL	F	6306	-	5,5,5	0.28	0	5,5,5	0.51	0
4	PYR	G	1500	3	2,5,5	1.74	1 (50%)	2,6,6	0.71	0
2	PRO	G	1600	-	4,8,8	0.61	0	5,10,10	1.11	0
7	GOL	G	6207	-	5,5,5	0.35	0	5,5,5	0.28	0
7	GOL	G	6307	-	5,5,5	0.32	0	5,5,5	0.27	0
4	PYR	H	1500	3	2,5,5	1.75	1 (50%)	2,6,6	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PRO	H	1600	-	4,8,8	0.69	0	5,10,10	1.12	0
8	EDO	H	6037	-	3,3,3	0.58	0	2,2,2	0.31	0
7	GOL	H	6308	-	5,5,5	0.27	0	5,5,5	0.48	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
4	PYR	A	1000	3	-	0/0/4/4	0/0/0/0
2	PRO	A	1200	-	-	0/0/11/11	0/1/1/1
7	GOL	A	6002	-	-	0/4/4/4	0/0/0/0
8	EDO	A	6043	-	-	0/1/1/1	0/0/0/0
8	EDO	A	6050	-	-	0/1/1/1	0/0/0/0
8	EDO	A	6051	-	-	0/1/1/1	0/0/0/0
7	GOL	A	6201	-	-	0/4/4/4	0/0/0/0
7	GOL	A	6301	-	-	0/4/4/4	0/0/0/0
4	PYR	B	1500	3	-	0/0/4/4	0/0/0/0
2	PRO	B	1600	-	-	0/0/11/11	0/1/1/1
7	GOL	B	6007	-	-	0/4/4/4	0/0/0/0
8	EDO	B	6013	-	-	0/1/1/1	0/0/0/0
8	EDO	B	6048	-	-	0/1/1/1	0/0/0/0
7	GOL	B	6202	-	-	0/4/4/4	0/0/0/0
7	GOL	B	6302	-	-	0/4/4/4	0/0/0/0
4	PYR	C	1500	3	-	0/0/4/4	0/0/0/0
2	PRO	C	1600	-	-	0/0/11/11	0/1/1/1
8	EDO	C	6014	-	-	0/1/1/1	0/0/0/0
7	GOL	C	6055	-	-	0/4/4/4	0/0/0/0
7	GOL	C	6303	-	-	0/4/4/4	0/0/0/0
4	PYR	D	1500	3	-	0/0/4/4	0/0/0/0
2	PRO	D	1600	-	-	0/0/11/11	0/1/1/1
8	EDO	D	6011	-	-	0/1/1/1	0/0/0/0
8	EDO	D	6017	-	-	0/1/1/1	0/0/0/0
8	EDO	D	6033	-	-	0/1/1/1	0/0/0/0
7	GOL	D	6056	-	-	0/4/4/4	0/0/0/0
7	GOL	D	6204	-	-	0/4/4/4	0/0/0/0
7	GOL	D	6304	-	-	0/4/4/4	0/0/0/0
4	PYR	E	1500	3	-	0/0/4/4	0/0/0/0
2	PRO	E	1600	-	-	0/0/11/11	0/1/1/1
8	EDO	E	6015	-	-	0/1/1/1	0/0/0/0
8	EDO	E	6039	-	-	0/1/1/1	0/0/0/0
8	EDO	E	6046	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	E	6049	-	-	0/1/1/1	0/0/0/0
7	GOL	E	6205	-	-	0/4/4/4	0/0/0/0
7	GOL	E	6305	-	-	0/4/4/4	0/0/0/0
4	PYR	F	1500	3	-	0/0/4/4	0/0/0/0
2	PRO	F	1600	-	-	0/0/11/11	0/1/1/1
7	GOL	F	6010	-	-	0/4/4/4	0/0/0/0
8	EDO	F	6012	-	-	0/1/1/1	0/0/0/0
7	GOL	F	6206	-	-	0/4/4/4	0/0/0/0
7	GOL	F	6306	-	-	0/4/4/4	0/0/0/0
4	PYR	G	1500	3	-	0/0/4/4	0/0/0/0
2	PRO	G	1600	-	-	0/0/11/11	0/1/1/1
7	GOL	G	6207	-	-	0/4/4/4	0/0/0/0
7	GOL	G	6307	-	-	0/4/4/4	0/0/0/0
4	PYR	H	1500	3	-	0/0/4/4	0/0/0/0
2	PRO	H	1600	-	-	0/0/11/11	0/1/1/1
8	EDO	H	6037	-	-	0/1/1/1	0/0/0/0
7	GOL	H	6308	-	-	0/4/4/4	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1500	PYR	O3-C2	2.18	1.30	1.22
4	C	1500	PYR	O3-C2	2.31	1.30	1.22
4	G	1500	PYR	O3-C2	2.45	1.31	1.22
4	B	1500	PYR	O3-C2	2.45	1.31	1.22
4	H	1500	PYR	O3-C2	2.46	1.31	1.22
4	E	1500	PYR	O3-C2	2.47	1.31	1.22
4	F	1500	PYR	O3-C2	2.56	1.31	1.22
4	A	1000	PYR	O3-C2	2.79	1.32	1.22

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	PYR	1	0
7	A	6301	GOL	2	0
4	B	1500	PYR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1600	PRO	1	0
8	B	6048	EDO	1	0
7	B	6202	GOL	1	0
7	B	6302	GOL	1	0
2	C	1600	PRO	3	0
4	D	1500	PYR	1	0
2	D	1600	PRO	2	0
8	D	6017	EDO	2	0
7	D	6304	GOL	2	0
2	E	1600	PRO	1	0
4	F	1500	PYR	2	0
7	F	6010	GOL	2	0
7	F	6306	GOL	1	0
4	G	1500	PYR	2	0
2	G	1600	PRO	1	0
7	G	6207	GOL	1	0
2	H	1600	PRO	2	0
7	H	6308	GOL	2	0

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, 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	519/531 (97%)	-0.70	2 (0%) 93 93	2, 5, 11, 18	1 (0%)
1	B	508/531 (95%)	-0.45	0 100 100	2, 5, 10, 16	0
1	C	512/531 (96%)	-0.74	0 100 100	2, 4, 9, 18	0
1	D	521/531 (98%)	-0.71	2 (0%) 93 93	2, 5, 11, 16	0
1	E	521/531 (98%)	-0.74	0 100 100	2, 4, 11, 18	0
1	F	515/531 (96%)	-0.68	2 (0%) 93 93	2, 3, 8, 19	0
1	G	510/531 (96%)	-0.47	2 (0%) 93 93	2, 3, 9, 13	0
1	H	519/531 (97%)	-0.67	3 (0%) 90 90	2, 4, 9, 14	0
All	All	4125/4248 (97%)	-0.65	11 (0%) 94 94	2, 4, 10, 19	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	155	ILE	3.4
1	A	128	THR	2.8
1	H	128	THR	2.8
1	D	127	GLY	2.4
1	G	201	PHE	2.3
1	G	169	VAL	2.3
1	A	190	ASP	2.2
1	H	127	GLY	2.2
1	F	201	PHE	2.1
1	D	201	PHE	2.0
1	H	214	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
8	EDO	D	6017	4/4	0.81	0.40	18.50	48,49,50,50	0
8	EDO	E	6046	4/4	0.93	0.20	9.16	27,30,31,33	0
7	GOL	C	6055	6/6	0.87	0.21	7.85	53,54,54,54	0
7	GOL	A	6301	6/6	0.78	0.19	6.79	46,47,48,49	0
8	EDO	A	6043	4/4	0.89	0.19	6.40	64,65,66,66	0
7	GOL	C	6303	6/6	0.94	0.15	3.26	28,30,31,31	0
7	GOL	F	6306	6/6	0.90	0.16	3.16	38,39,40,40	0
8	EDO	E	6049	4/4	0.90	0.16	2.65	38,40,41,42	0
7	GOL	A	6002	6/6	0.96	0.14	2.46	28,30,31,32	0
7	GOL	H	6308	6/6	0.94	0.14	2.10	22,22,24,26	0
7	GOL	F	6206	6/6	0.96	0.15	1.72	34,36,36,36	0
2	PRO	C	1600	8/8	0.97	0.12	1.59	20,20,21,21	0
7	GOL	B	6302	6/6	0.89	0.17	1.53	34,36,37,37	0
7	GOL	G	6307	6/6	0.90	0.17	1.36	44,45,45,46	0
7	GOL	F	6010	6/6	0.89	0.14	1.34	53,53,53,53	0
8	EDO	A	6050	4/4	0.94	0.12	1.33	43,44,44,44	0
7	GOL	B	6007	6/6	0.91	0.18	1.30	48,48,49,49	0
4	PYR	D	1500	6/6	0.97	0.11	0.99	13,15,17,20	0
7	GOL	B	6202	6/6	0.91	0.16	0.95	62,63,63,64	0
8	EDO	H	6037	4/4	0.87	0.12	0.94	40,41,41,41	0
7	GOL	A	6201	6/6	0.94	0.12	0.85	29,30,30,32	0
7	GOL	D	6304	6/6	0.98	0.11	0.83	29,30,31,33	0
6	NA	A	2100	1/1	0.98	0.13	0.77	29,29,29,29	0
2	PRO	F	1600	8/8	0.97	0.11	0.77	17,18,18,19	0
8	EDO	A	6051	4/4	0.85	0.16	0.72	49,50,50,51	0
4	PYR	A	1000	6/6	0.98	0.10	0.67	22,24,25,27	0
2	PRO	D	1600	8/8	0.95	0.11	0.65	23,23,24,24	0
7	GOL	D	6204	6/6	0.94	0.12	0.53	36,36,36,37	0
7	GOL	D	6056	6/6	0.94	0.11	0.46	35,37,38,39	0
6	NA	F	2000	1/1	0.95	0.12	0.24	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PRO	E	1600	8/8	0.96	0.10	0.17	24,24,24,24	0
5	K	H	1700	1/1	0.98	0.11	0.02	26,26,26,26	0
2	PRO	A	1200	8/8	0.94	0.11	-0.09	21,21,22,23	0
4	PYR	B	1500	6/6	0.97	0.10	-0.11	32,33,33,34	0
8	EDO	B	6048	4/4	0.97	0.10	-0.16	28,28,28,28	0
5	K	E	1700	1/1	0.98	0.10	-0.28	25,25,25,25	0
4	PYR	H	1500	6/6	0.98	0.09	-0.31	17,18,18,19	0
7	GOL	G	6207	6/6	0.92	0.12	-0.54	39,40,40,40	0
2	PRO	H	1600	8/8	0.98	0.09	-0.57	17,18,18,18	0
6	NA	E	2100	1/1	0.99	0.10	-0.65	13,13,13,13	0
4	PYR	F	1500	6/6	0.98	0.08	-0.96	6,7,7,9	0
5	K	A	1100	1/1	0.99	0.09	-0.98	23,23,23,23	0
7	GOL	E	6305	6/6	0.97	0.09	-1.07	21,21,21,22	0
6	NA	D	2100	1/1	0.98	0.08	-1.07	21,21,21,21	0
7	GOL	E	6205	6/6	0.93	0.09	-1.09	28,29,31,31	0
6	NA	H	2100	1/1	0.95	0.08	-1.11	32,32,32,32	0
2	PRO	G	1600	8/8	0.96	0.09	-1.18	38,38,38,38	0
6	NA	B	2000	1/1	0.95	0.10	-1.21	48,48,48,48	0
6	NA	E	2000	1/1	0.97	0.10	-1.42	31,31,31,31	0
6	NA	A	1300	1/1	0.93	0.08	-1.47	40,40,40,40	0
4	PYR	G	1500	6/6	0.98	0.08	-1.48	21,22,24,25	0
5	K	G	1700	1/1	0.99	0.07	-1.54	42,42,42,42	0
6	NA	H	2000	1/1	0.96	0.07	-1.60	40,40,40,40	0
6	NA	G	2000	1/1	0.92	0.08	-1.62	41,41,41,41	0
6	NA	D	2000	1/1	0.94	0.06	-1.72	35,35,35,35	0
6	NA	C	2000	1/1	0.98	0.07	-1.74	22,22,22,22	0
2	PRO	B	1600	8/8	0.97	0.09	-1.79	26,26,26,27	0
4	PYR	C	1500	6/6	0.99	0.08	-1.99	11,12,12,13	0
5	K	C	1700	1/1	1.00	0.08	-2.06	20,20,20,20	0
4	PYR	E	1500	6/6	0.99	0.08	-2.09	10,12,14,14	0
5	K	F	1700	1/1	0.99	0.07	-2.62	17,17,17,17	0
8	EDO	E	6039	4/4	0.98	0.07	-3.00	33,34,34,34	0
5	K	B	1700	1/1	0.97	0.05	-3.18	38,38,38,38	0
5	K	D	1700	1/1	0.99	0.05	-3.64	22,22,22,22	0
8	EDO	F	6012	4/4	0.94	0.11	-	33,33,33,34	0
3	MN	E	640	1/1	0.99	0.10	-	21,21,21,21	0
3	MN	G	640	1/1	0.99	0.05	-	26,26,26,26	0
8	EDO	D	6033	4/4	0.96	0.11	-	33,34,35,36	0
3	MN	C	640	1/1	0.99	0.07	-	15,15,15,15	0
3	MN	D	640	1/1	1.00	0.09	-	20,20,20,20	0
3	MN	B	640	1/1	0.99	0.06	-	33,33,33,33	0
8	EDO	B	6013	4/4	0.93	0.18	-	54,54,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MN	A	640	1/1	1.00	0.07	-	17,17,17,17	0
8	EDO	C	6014	4/4	0.93	0.11	-	37,37,38,38	0
3	MN	H	640	1/1	0.99	0.09	-	16,16,16,16	0
8	EDO	D	6011	4/4	0.93	0.13	-	46,46,46,46	0
3	MN	F	640	1/1	1.00	0.05	-	18,18,18,18	0
8	EDO	E	6015	4/4	0.96	0.12	-	35,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.