



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:24 am GMT

PDB ID : 3SRF
Title : Human M1 pyruvate kinase
Authors : Morgan, H.P.; O'Reilly, F.; Palmer, R.; McNae, I.W.; Nowicki, M.W.; Wear, M.A.; Fothergill-Gilmore, L.A.; Walkinshaw, M.D.
Deposited on : 2011-07-07
Resolution : 2.85 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

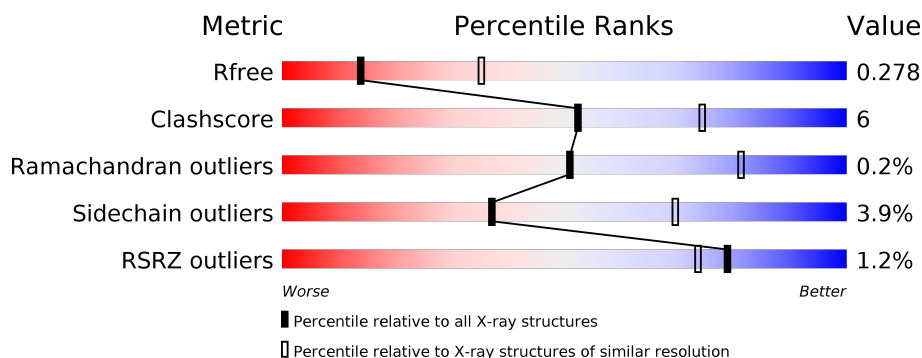
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3466 (2.88-2.80)
Clashscore	112137	3975 (2.88-2.80)
Ramachandran outliers	110173	3902 (2.88-2.80)
Sidechain outliers	110143	3905 (2.88-2.80)
RSRZ outliers	101464	3501 (2.88-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 5%, yellow 12%, green 80%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 80% 12% 6% </div> </div>
1	B	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 78%, yellow 15%, orange 5%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 78% 15% 6% </div> </div>
1	C	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 76%, yellow 16%, orange 5%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 76% 16% 6% </div> </div>
1	D	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 79%, yellow 13%, orange 5%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 79% 13% 7% </div> </div>
1	E	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, green 79%, yellow 13%, orange 5%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 79% 13% 7% </div> </div>
1	F	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 79%, yellow 14%, orange 5%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 79% 14% 6% </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	551	 2% 80% 12% • 7%
1	H	551	 % 76% 17% • 6%

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
3	K	B	532	-	-	-	X
5	PYR	B	534	-	-	-	X
5	PYR	H	534	-	-	-	X
6	GOL	A	535	-	-	-	X
6	GOL	F	535	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 32320 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	C	517	Total	C	N	O	S	0	0	0
			3968	2493	704	743	28			
1	A	517	Total	C	N	O	S	0	0	0
			3968	2493	704	743	28			
1	B	517	Total	C	N	O	S	0	0	0
			3966	2490	704	744	28			
1	D	515	Total	C	N	O	S	0	0	0
			3957	2487	702	740	28			
1	E	514	Total	C	N	O	S	0	0	0
			3949	2481	701	739	28			
1	F	516	Total	C	N	O	S	0	0	0
			3960	2487	703	742	28			
1	G	513	Total	C	N	O	S	0	0	0
			3944	2478	700	738	28			
1	H	519	Total	C	N	O	S	0	0	0
			3978	2498	706	746	28			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	MET	-	EXPRESSION TAG	UNP P14618
C	-19	GLY	-	EXPRESSION TAG	UNP P14618
C	-18	SER	-	EXPRESSION TAG	UNP P14618
C	-17	SER	-	EXPRESSION TAG	UNP P14618
C	-16	HIS	-	EXPRESSION TAG	UNP P14618
C	-15	HIS	-	EXPRESSION TAG	UNP P14618
C	-14	HIS	-	EXPRESSION TAG	UNP P14618
C	-13	HIS	-	EXPRESSION TAG	UNP P14618
C	-12	HIS	-	EXPRESSION TAG	UNP P14618
C	-11	HIS	-	EXPRESSION TAG	UNP P14618
C	-10	SER	-	EXPRESSION TAG	UNP P14618
C	-9	SER	-	EXPRESSION TAG	UNP P14618
C	-8	GLY	-	EXPRESSION TAG	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	EXPRESSION TAG	UNP P14618
C	-6	VAL	-	EXPRESSION TAG	UNP P14618
C	-5	PRO	-	EXPRESSION TAG	UNP P14618
C	-4	ARG	-	EXPRESSION TAG	UNP P14618
C	-3	GLY	-	EXPRESSION TAG	UNP P14618
C	-2	SER	-	EXPRESSION TAG	UNP P14618
C	-1	HIS	-	EXPRESSION TAG	UNP P14618
A	-20	MET	-	EXPRESSION TAG	UNP P14618
A	-19	GLY	-	EXPRESSION TAG	UNP P14618
A	-18	SER	-	EXPRESSION TAG	UNP P14618
A	-17	SER	-	EXPRESSION TAG	UNP P14618
A	-16	HIS	-	EXPRESSION TAG	UNP P14618
A	-15	HIS	-	EXPRESSION TAG	UNP P14618
A	-14	HIS	-	EXPRESSION TAG	UNP P14618
A	-13	HIS	-	EXPRESSION TAG	UNP P14618
A	-12	HIS	-	EXPRESSION TAG	UNP P14618
A	-11	HIS	-	EXPRESSION TAG	UNP P14618
A	-10	SER	-	EXPRESSION TAG	UNP P14618
A	-9	SER	-	EXPRESSION TAG	UNP P14618
A	-8	GLY	-	EXPRESSION TAG	UNP P14618
A	-7	LEU	-	EXPRESSION TAG	UNP P14618
A	-6	VAL	-	EXPRESSION TAG	UNP P14618
A	-5	PRO	-	EXPRESSION TAG	UNP P14618
A	-4	ARG	-	EXPRESSION TAG	UNP P14618
A	-3	GLY	-	EXPRESSION TAG	UNP P14618
A	-2	SER	-	EXPRESSION TAG	UNP P14618
A	-1	HIS	-	EXPRESSION TAG	UNP P14618
B	-20	MET	-	EXPRESSION TAG	UNP P14618
B	-19	GLY	-	EXPRESSION TAG	UNP P14618
B	-18	SER	-	EXPRESSION TAG	UNP P14618
B	-17	SER	-	EXPRESSION TAG	UNP P14618
B	-16	HIS	-	EXPRESSION TAG	UNP P14618
B	-15	HIS	-	EXPRESSION TAG	UNP P14618
B	-14	HIS	-	EXPRESSION TAG	UNP P14618
B	-13	HIS	-	EXPRESSION TAG	UNP P14618
B	-12	HIS	-	EXPRESSION TAG	UNP P14618
B	-11	HIS	-	EXPRESSION TAG	UNP P14618
B	-10	SER	-	EXPRESSION TAG	UNP P14618
B	-9	SER	-	EXPRESSION TAG	UNP P14618
B	-8	GLY	-	EXPRESSION TAG	UNP P14618
B	-7	LEU	-	EXPRESSION TAG	UNP P14618
B	-6	VAL	-	EXPRESSION TAG	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	PRO	-	EXPRESSION TAG	UNP P14618
B	-4	ARG	-	EXPRESSION TAG	UNP P14618
B	-3	GLY	-	EXPRESSION TAG	UNP P14618
B	-2	SER	-	EXPRESSION TAG	UNP P14618
B	-1	HIS	-	EXPRESSION TAG	UNP P14618
D	-20	MET	-	EXPRESSION TAG	UNP P14618
D	-19	GLY	-	EXPRESSION TAG	UNP P14618
D	-18	SER	-	EXPRESSION TAG	UNP P14618
D	-17	SER	-	EXPRESSION TAG	UNP P14618
D	-16	HIS	-	EXPRESSION TAG	UNP P14618
D	-15	HIS	-	EXPRESSION TAG	UNP P14618
D	-14	HIS	-	EXPRESSION TAG	UNP P14618
D	-13	HIS	-	EXPRESSION TAG	UNP P14618
D	-12	HIS	-	EXPRESSION TAG	UNP P14618
D	-11	HIS	-	EXPRESSION TAG	UNP P14618
D	-10	SER	-	EXPRESSION TAG	UNP P14618
D	-9	SER	-	EXPRESSION TAG	UNP P14618
D	-8	GLY	-	EXPRESSION TAG	UNP P14618
D	-7	LEU	-	EXPRESSION TAG	UNP P14618
D	-6	VAL	-	EXPRESSION TAG	UNP P14618
D	-5	PRO	-	EXPRESSION TAG	UNP P14618
D	-4	ARG	-	EXPRESSION TAG	UNP P14618
D	-3	GLY	-	EXPRESSION TAG	UNP P14618
D	-2	SER	-	EXPRESSION TAG	UNP P14618
D	-1	HIS	-	EXPRESSION TAG	UNP P14618
E	-20	MET	-	EXPRESSION TAG	UNP P14618
E	-19	GLY	-	EXPRESSION TAG	UNP P14618
E	-18	SER	-	EXPRESSION TAG	UNP P14618
E	-17	SER	-	EXPRESSION TAG	UNP P14618
E	-16	HIS	-	EXPRESSION TAG	UNP P14618
E	-15	HIS	-	EXPRESSION TAG	UNP P14618
E	-14	HIS	-	EXPRESSION TAG	UNP P14618
E	-13	HIS	-	EXPRESSION TAG	UNP P14618
E	-12	HIS	-	EXPRESSION TAG	UNP P14618
E	-11	HIS	-	EXPRESSION TAG	UNP P14618
E	-10	SER	-	EXPRESSION TAG	UNP P14618
E	-9	SER	-	EXPRESSION TAG	UNP P14618
E	-8	GLY	-	EXPRESSION TAG	UNP P14618
E	-7	LEU	-	EXPRESSION TAG	UNP P14618
E	-6	VAL	-	EXPRESSION TAG	UNP P14618
E	-5	PRO	-	EXPRESSION TAG	UNP P14618
E	-4	ARG	-	EXPRESSION TAG	UNP P14618

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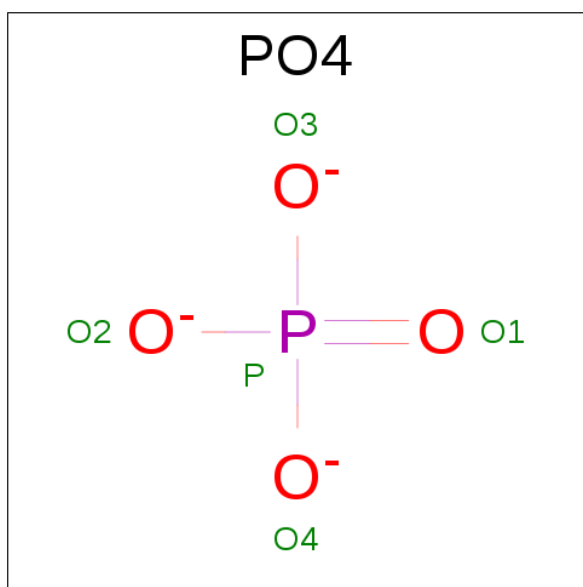
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP P14618
E	-2	SER	-	EXPRESSION TAG	UNP P14618
E	-1	HIS	-	EXPRESSION TAG	UNP P14618
F	-20	MET	-	EXPRESSION TAG	UNP P14618
F	-19	GLY	-	EXPRESSION TAG	UNP P14618
F	-18	SER	-	EXPRESSION TAG	UNP P14618
F	-17	SER	-	EXPRESSION TAG	UNP P14618
F	-16	HIS	-	EXPRESSION TAG	UNP P14618
F	-15	HIS	-	EXPRESSION TAG	UNP P14618
F	-14	HIS	-	EXPRESSION TAG	UNP P14618
F	-13	HIS	-	EXPRESSION TAG	UNP P14618
F	-12	HIS	-	EXPRESSION TAG	UNP P14618
F	-11	HIS	-	EXPRESSION TAG	UNP P14618
F	-10	SER	-	EXPRESSION TAG	UNP P14618
F	-9	SER	-	EXPRESSION TAG	UNP P14618
F	-8	GLY	-	EXPRESSION TAG	UNP P14618
F	-7	LEU	-	EXPRESSION TAG	UNP P14618
F	-6	VAL	-	EXPRESSION TAG	UNP P14618
F	-5	PRO	-	EXPRESSION TAG	UNP P14618
F	-4	ARG	-	EXPRESSION TAG	UNP P14618
F	-3	GLY	-	EXPRESSION TAG	UNP P14618
F	-2	SER	-	EXPRESSION TAG	UNP P14618
F	-1	HIS	-	EXPRESSION TAG	UNP P14618
G	-20	MET	-	EXPRESSION TAG	UNP P14618
G	-19	GLY	-	EXPRESSION TAG	UNP P14618
G	-18	SER	-	EXPRESSION TAG	UNP P14618
G	-17	SER	-	EXPRESSION TAG	UNP P14618
G	-16	HIS	-	EXPRESSION TAG	UNP P14618
G	-15	HIS	-	EXPRESSION TAG	UNP P14618
G	-14	HIS	-	EXPRESSION TAG	UNP P14618
G	-13	HIS	-	EXPRESSION TAG	UNP P14618
G	-12	HIS	-	EXPRESSION TAG	UNP P14618
G	-11	HIS	-	EXPRESSION TAG	UNP P14618
G	-10	SER	-	EXPRESSION TAG	UNP P14618
G	-9	SER	-	EXPRESSION TAG	UNP P14618
G	-8	GLY	-	EXPRESSION TAG	UNP P14618
G	-7	LEU	-	EXPRESSION TAG	UNP P14618
G	-6	VAL	-	EXPRESSION TAG	UNP P14618
G	-5	PRO	-	EXPRESSION TAG	UNP P14618
G	-4	ARG	-	EXPRESSION TAG	UNP P14618
G	-3	GLY	-	EXPRESSION TAG	UNP P14618
G	-2	SER	-	EXPRESSION TAG	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	HIS	-	EXPRESSION TAG	UNP P14618
H	-20	MET	-	EXPRESSION TAG	UNP P14618
H	-19	GLY	-	EXPRESSION TAG	UNP P14618
H	-18	SER	-	EXPRESSION TAG	UNP P14618
H	-17	SER	-	EXPRESSION TAG	UNP P14618
H	-16	HIS	-	EXPRESSION TAG	UNP P14618
H	-15	HIS	-	EXPRESSION TAG	UNP P14618
H	-14	HIS	-	EXPRESSION TAG	UNP P14618
H	-13	HIS	-	EXPRESSION TAG	UNP P14618
H	-12	HIS	-	EXPRESSION TAG	UNP P14618
H	-11	HIS	-	EXPRESSION TAG	UNP P14618
H	-10	SER	-	EXPRESSION TAG	UNP P14618
H	-9	SER	-	EXPRESSION TAG	UNP P14618
H	-8	GLY	-	EXPRESSION TAG	UNP P14618
H	-7	LEU	-	EXPRESSION TAG	UNP P14618
H	-6	VAL	-	EXPRESSION TAG	UNP P14618
H	-5	PRO	-	EXPRESSION TAG	UNP P14618
H	-4	ARG	-	EXPRESSION TAG	UNP P14618
H	-3	GLY	-	EXPRESSION TAG	UNP P14618
H	-2	SER	-	EXPRESSION TAG	UNP P14618
H	-1	HIS	-	EXPRESSION TAG	UNP P14618

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

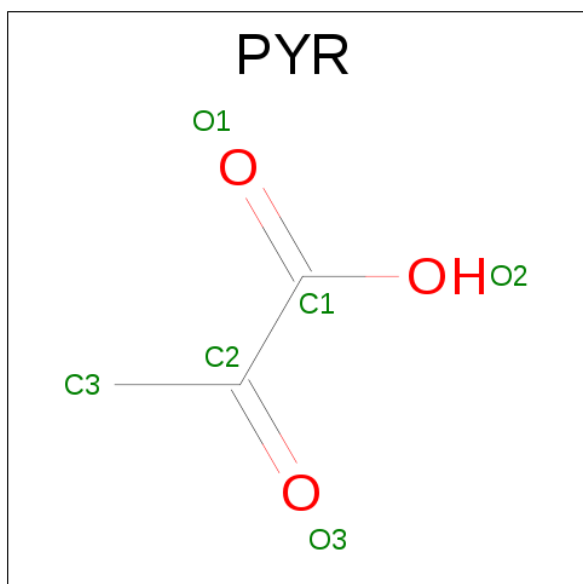
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



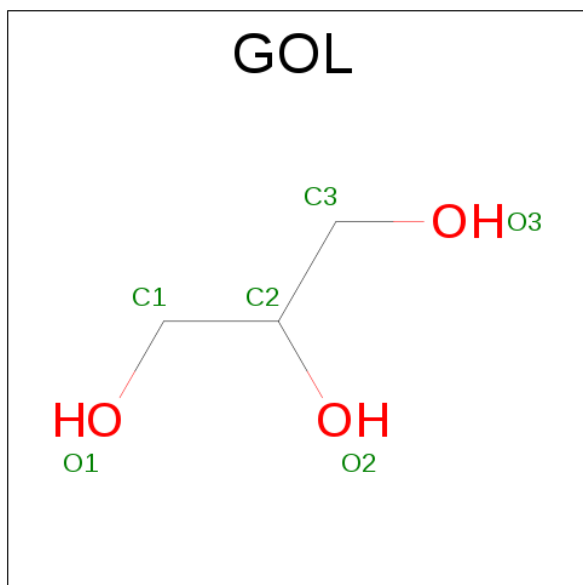
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

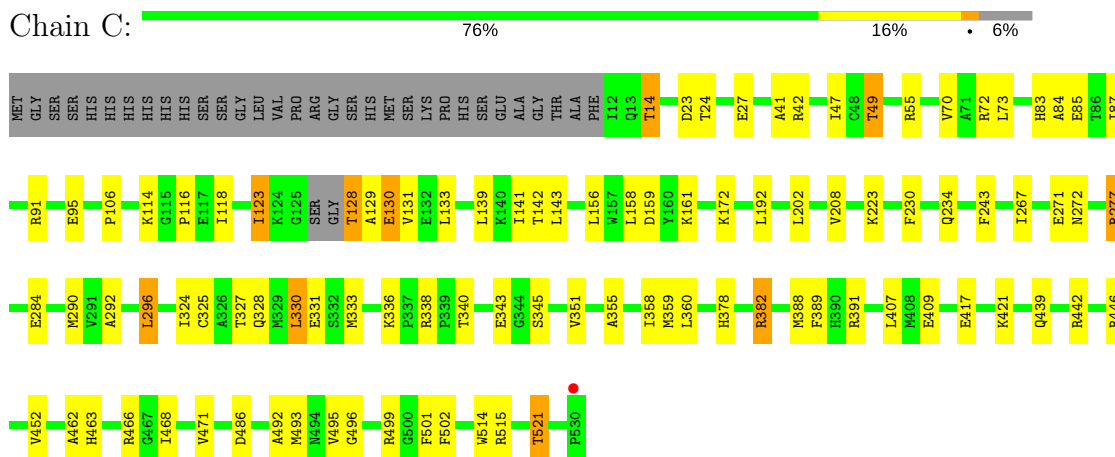
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	59	Total 59	O 59	0	0
7	A	67	Total 67	O 67	0	0
7	B	71	Total 71	O 71	0	0
7	D	76	Total 76	O 76	0	0
7	E	42	Total 42	O 42	0	0
7	F	62	Total 62	O 62	0	0
7	G	50	Total 50	O 50	0	0
7	H	51	Total 51	O 51	0	0

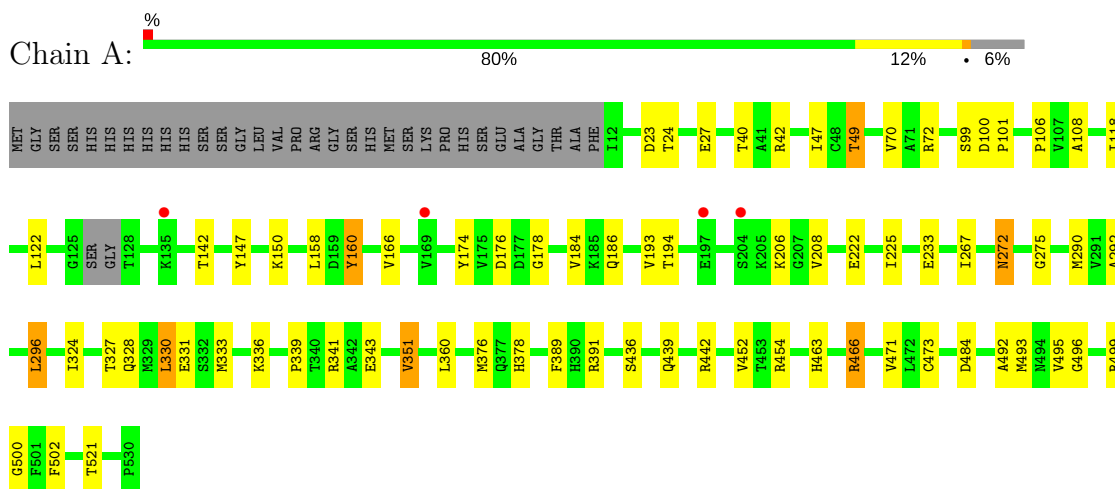
3 Residue-property plots

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

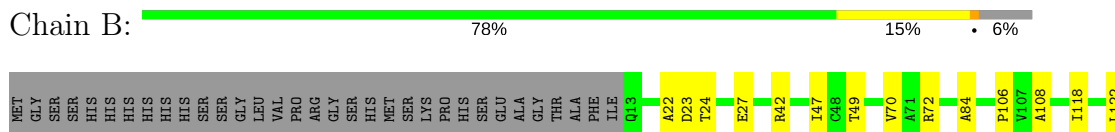
• Molecule 1: Pyruvate kinase isozymes M1/M2

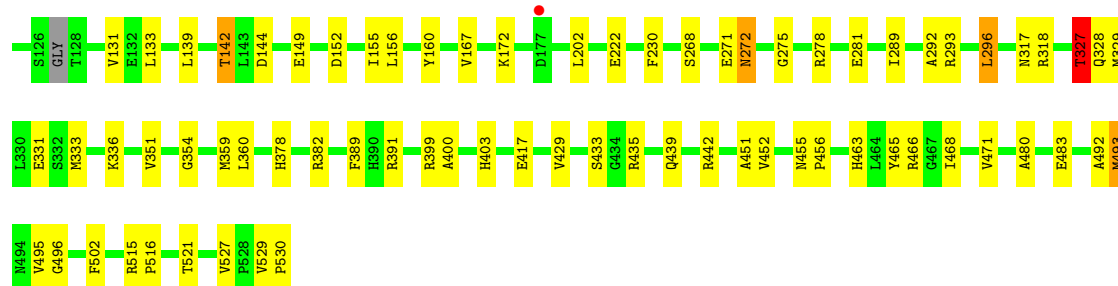


• Molecule 1: Pyruvate kinase isozymes M1/M2



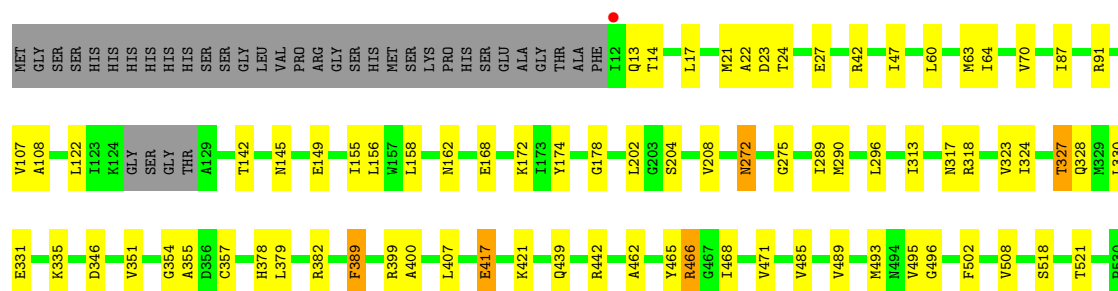
• Molecule 1: Pyruvate kinase isozymes M1/M2





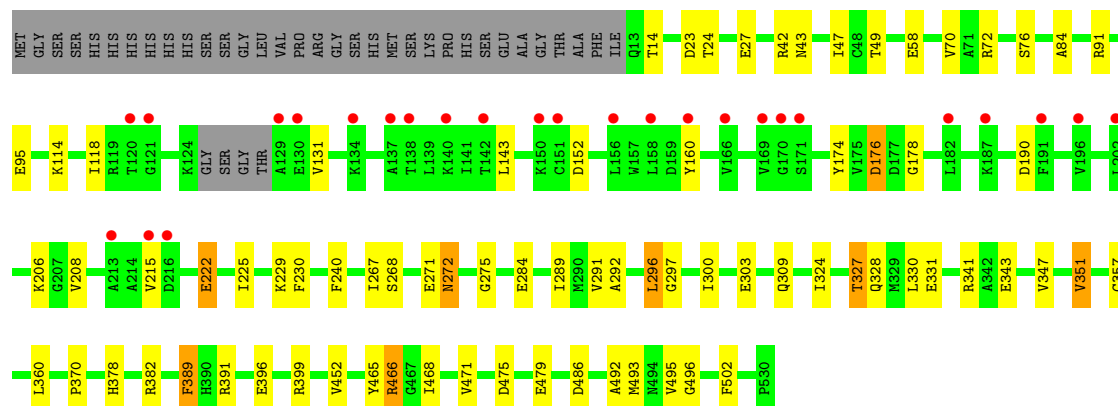
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain D: 79% 13% 7%



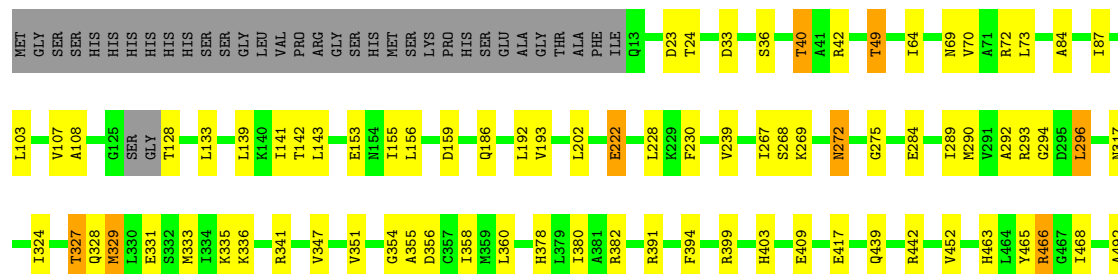
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain E: 5% 79% 13% 7%



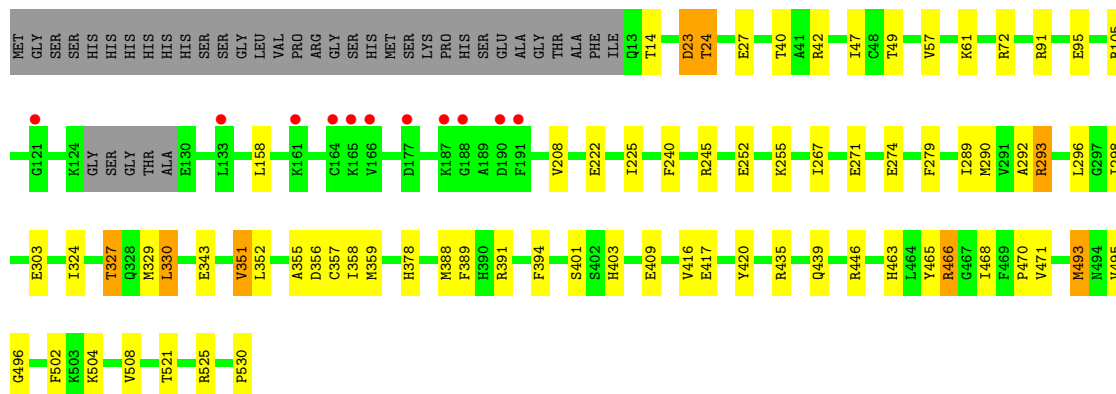
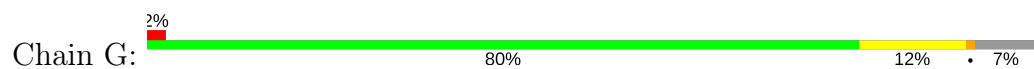
- Molecule 1: Pyruvate kinase isozymes M1/M2

Chain F: 79% 14% 6%

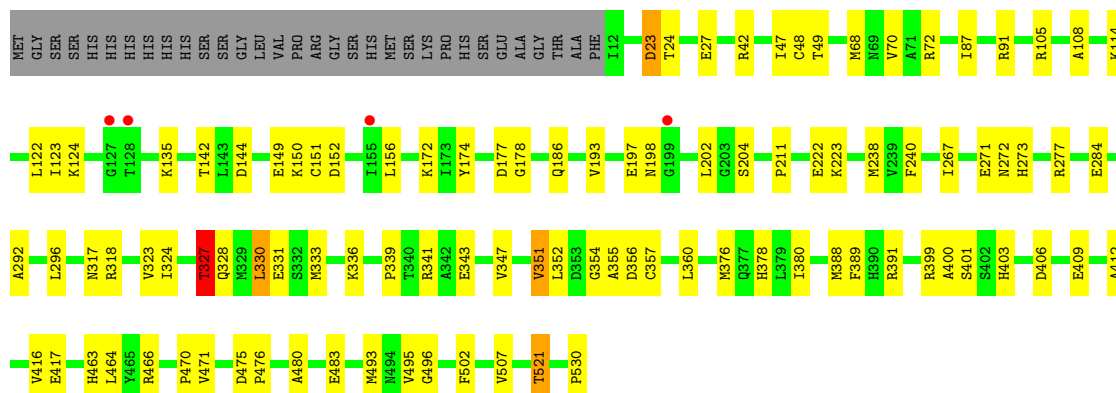
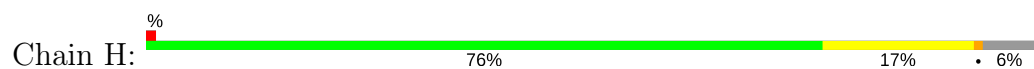




• Molecule 1: Pyruvate kinase isozymes M1/M2



• Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	238.00Å 192.22Å 109.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.85 38.21 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.85) 93.5 (38.21-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.280 0.221 , 0.278	Depositor DCC
R_{free} test set	5346 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 5.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.129 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32320	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.8839e-03.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, GOL, MG, PO4, 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	0.33	0/4030	0.49	0/5435
1	B	0.33	0/4028	0.50	0/5432
1	C	0.33	0/4030	0.50	0/5435
1	D	0.33	0/4019	0.48	0/5420
1	E	0.32	0/4011	0.48	1/5409 (0.0%)
1	F	0.32	0/4022	0.49	0/5424
1	G	0.33	0/4006	0.48	0/5402
1	H	0.33	0/4041	0.49	0/5451
All	All	0.33	0/32187	0.49	1/43408 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	176	ASP	N-CA-C	5.32	125.37	111.00

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	3968	0	4049	51	0
1	B	3966	0	4043	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3968	0	4048	66	0
1	D	3957	0	4038	46	0
1	E	3949	0	4028	47	0
1	F	3960	0	4037	53	0
1	G	3944	0	4023	47	0
1	H	3978	0	4057	63	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	6	0	3	0	0
5	B	6	0	3	0	0
5	C	6	0	3	0	0
5	D	6	0	3	0	0
5	E	6	0	3	0	0
5	F	6	0	3	0	0
5	G	6	0	3	0	0
5	H	6	0	3	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	1	0
6	D	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	6	0	8	0	0
6	F	12	0	16	1	0
6	G	6	0	8	1	0
7	A	67	0	0	1	0
7	B	71	0	0	0	0
7	C	59	0	0	3	0
7	D	76	0	0	1	0
7	E	42	0	0	1	0
7	F	62	0	0	1	0
7	G	50	0	0	2	0
7	H	51	0	0	0	0
All	All	32320	0	32411	406	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 6.

All (406) 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:G:23:ASP:HA	1:G:391:ARG:HH12	1.40	0.84
1:C:128:THR:N	1:C:129:ALA:HA	1.92	0.84
1:G:42:ARG:HE	1:G:378:HIS:HD2	1.29	0.80
1:F:49:THR:HG23	1:F:360:LEU:O	1.81	0.80
1:C:49:THR:HG21	1:C:72:ARG:HH11	1.45	0.80
1:A:49:THR:HG22	1:A:72:ARG:HD3	1.65	0.78
1:F:42:ARG:HE	1:F:378:HIS:HD2	1.34	0.76
1:H:49:THR:HG22	1:H:72:ARG:HD3	1.69	0.75
1:B:49:THR:HG22	1:B:72:ARG:HD3	1.68	0.75
1:C:271:GLU:HG2	1:C:292:ALA:HB3	1.69	0.75
1:E:24:THR:HG22	1:E:27:GLU:H	1.52	0.74
1:F:49:THR:HG21	1:F:72:ARG:HH11	1.54	0.73
1:D:24:THR:HG22	1:D:27:GLU:H	1.54	0.73
1:B:23:ASP:OD2	1:B:23:ASP:C	2.27	0.72
1:C:23:ASP:H	1:C:391:ARG:HH22	1.37	0.71
1:C:23:ASP:HA	1:C:391:ARG:HH12	1.55	0.71
1:A:42:ARG:HE	1:A:378:HIS:HD2	1.37	0.71
1:G:493:MET:HE1	1:G:508:VAL:HG21	1.73	0.70
1:A:70:VAL:HG22	1:A:108:ALA:HB3	1.73	0.69
1:G:24:THR:HG22	1:G:27:GLU:H	1.57	0.69
1:E:49:THR:HG22	1:E:72:ARG:HD3	1.75	0.69
1:H:23:ASP:HA	1:H:391:ARG:HH12	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ILE:HD12	1:C:130:GLU:HA	1.76	0.68
1:D:417:GLU:HG3	1:H:417:GLU:HG3	1.76	0.68
1:H:42:ARG:HE	1:H:378:HIS:HD2	1.42	0.68
1:B:24:THR:HG22	1:B:27:GLU:H	1.59	0.68
1:E:49:THR:HG21	1:E:72:ARG:HH11	1.59	0.67
1:B:42:ARG:HE	1:B:378:HIS:HD2	1.43	0.66
1:A:42:ARG:HE	1:A:378:HIS:CD2	2.13	0.66
1:D:324:ILE:HG12	1:D:357:CYS:HB2	1.79	0.65
1:C:495:VAL:O	1:C:499:ARG:HG2	1.97	0.65
1:A:328:GLN:HG2	1:A:331:GLU:HG3	1.80	0.64
1:A:49:THR:HG21	1:A:72:ARG:HH11	1.61	0.64
1:B:42:ARG:HE	1:B:378:HIS:CD2	2.14	0.64
1:C:521:THR:HG23	1:C:521:THR:O	1.98	0.64
1:A:521:THR:O	1:A:521:THR:HG23	1.97	0.64
1:B:318:ARG:HG3	1:B:400:ALA:HB1	1.80	0.64
1:H:124:LYS:HB3	1:H:150:LYS:HA	1.80	0.63
1:C:14:THR:HB	7:C:553:HOH:O	1.98	0.63
1:E:327:THR:HG22	1:E:328:GLN:HG3	1.80	0.63
1:G:23:ASP:H	1:G:391:ARG:HH22	1.46	0.63
1:G:49:THR:HG22	1:G:72:ARG:HD3	1.81	0.62
1:H:317:ASN:HD21	1:H:354:GLY:HA3	1.64	0.62
1:F:23:ASP:HA	1:F:391:ARG:HH12	1.65	0.62
1:E:143:LEU:HB2	1:E:190:ASP:HB2	1.82	0.62
1:G:521:THR:HG23	1:G:521:THR:O	1.99	0.61
1:A:49:THR:CG2	1:A:72:ARG:HD3	2.30	0.61
1:D:379:LEU:HD23	1:D:382:ARG:HH12	1.64	0.61
1:G:471:VAL:HG11	1:G:495:VAL:HG11	1.83	0.61
1:B:49:THR:HG21	1:B:72:ARG:HH11	1.66	0.61
1:A:351:VAL:O	1:A:466:ARG:NH2	2.31	0.61
1:B:327:THR:HG22	1:B:328:GLN:HG3	1.82	0.60
1:F:33:ASP:HB3	1:F:36:SER:HB2	1.83	0.60
1:C:49:THR:HG23	1:C:360:LEU:O	2.02	0.60
1:C:496:GLY:HA3	1:C:502:PHE:CZ	2.36	0.60
1:E:23:ASP:H	1:E:389:PHE:HZ	1.49	0.59
1:D:317:ASN:HD21	1:D:354:GLY:HA3	1.68	0.59
1:G:49:THR:HG21	1:G:72:ARG:HH11	1.66	0.59
1:D:328:GLN:HA	1:D:331:GLU:HG2	1.85	0.59
1:H:327:THR:HG22	1:H:328:GLN:HG3	1.85	0.59
1:H:122:LEU:HD12	1:H:149:GLU:HG2	1.83	0.59
1:C:417:GLU:HG3	1:G:417:GLU:HG3	1.85	0.59
1:H:49:THR:HG21	1:H:72:ARG:HH11	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ARG:HE	1:C:378:HIS:CD2	2.20	0.58
1:D:471:VAL:HG11	1:D:495:VAL:HG11	1.85	0.58
1:F:49:THR:HG22	1:F:72:ARG:HD3	1.85	0.58
1:A:24:THR:HG22	1:A:27:GLU:H	1.69	0.58
1:E:452:VAL:CG2	1:E:492:ALA:HB2	2.33	0.58
1:H:122:LEU:HD23	1:H:204:SER:HB3	1.84	0.58
1:E:176:ASP:HB2	1:E:206:LYS:HB3	1.86	0.58
1:D:156:LEU:HD13	1:D:202:LEU:HD21	1.85	0.58
1:G:47:ILE:HB	1:G:359:MET:HG3	1.85	0.58
1:H:271:GLU:HG2	1:H:292:ALA:HB3	1.86	0.58
1:A:436:SER:HB2	2:A:531:PO4:O2	2.04	0.57
1:F:159:ASP:HB2	7:F:580:HOH:O	2.03	0.57
1:G:496:GLY:HA3	1:G:502:PHE:CZ	2.38	0.57
1:E:91:ARG:O	1:E:95:GLU:HG2	2.05	0.57
1:F:317:ASN:HD21	1:F:354:GLY:HA3	1.70	0.57
1:F:186:GLN:HB2	1:F:193:VAL:HB	1.86	0.57
1:E:174:TYR:HB3	1:E:178:GLY:HA2	1.87	0.56
1:F:465:TYR:HB2	1:F:468:ILE:HD12	1.87	0.56
1:A:471:VAL:HG11	1:A:495:VAL:HG11	1.85	0.56
1:H:42:ARG:HE	1:H:378:HIS:CD2	2.23	0.56
1:H:521:THR:CG2	1:H:521:THR:O	2.53	0.56
1:H:521:THR:O	1:H:521:THR:HG23	2.05	0.56
1:B:49:THR:HG23	1:B:360:LEU:O	2.06	0.56
1:G:463:HIS:ND1	6:G:535:GOL:H31	2.20	0.56
1:D:70:VAL:HG22	1:D:108:ALA:HB3	1.88	0.56
1:C:49:THR:HG22	1:C:72:ARG:HD3	1.86	0.56
1:D:465:TYR:HB2	1:D:468:ILE:HD12	1.88	0.56
1:C:330:LEU:HD12	1:C:343:GLU:HB3	1.88	0.55
1:C:446:ARG:HD3	7:C:547:HOH:O	2.05	0.55
1:A:47:ILE:HG12	1:A:70:VAL:HB	1.88	0.55
1:B:272:ASN:HD22	1:B:275:GLY:H	1.55	0.55
1:A:49:THR:HG23	1:A:360:LEU:O	2.06	0.55
1:B:47:ILE:HG12	1:B:70:VAL:HB	1.89	0.55
1:F:521:THR:HG23	1:F:521:THR:O	2.07	0.55
1:A:40:THR:HG21	1:A:500:GLY:O	2.06	0.54
1:H:124:LYS:HE3	1:H:152:ASP:HB3	1.88	0.54
1:C:452:VAL:CG2	1:C:492:ALA:HB2	2.38	0.54
1:G:330:LEU:HD12	1:G:343:GLU:HB3	1.89	0.54
1:E:296:LEU:HD22	1:E:300:ILE:HG12	1.88	0.54
1:H:412:ALA:O	1:H:416:VAL:HG23	2.06	0.54
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:MET:HE1	1:F:358:ILE:HB	1.89	0.54
1:H:70:VAL:HG22	1:H:108:ALA:HB3	1.88	0.54
1:A:339:PRO:HG3	1:A:376:MET:HG2	1.88	0.54
1:H:24:THR:HG22	1:H:27:GLU:H	1.73	0.53
1:H:318:ARG:HG3	1:H:400:ALA:HB1	1.89	0.53
1:C:141:ILE:HB	1:C:192:LEU:HB2	1.89	0.53
1:C:421:LYS:NZ	1:G:401:SER:O	2.42	0.53
1:C:23:ASP:N	1:C:391:ARG:HH22	2.04	0.53
1:A:292:ALA:O	1:A:296:LEU:HB2	2.09	0.53
1:H:406:ASP:HB3	1:H:409:GLU:HB2	1.91	0.53
1:C:409:GLU:HG2	1:C:439:GLN:HE21	1.75	0.52
1:C:42:ARG:HB2	1:C:382:ARG:HD2	1.91	0.52
1:E:328:GLN:HA	1:E:331:GLU:HG2	1.91	0.52
1:F:355:ALA:O	1:F:466:ARG:NH1	2.43	0.52
1:F:329:MET:HE3	1:F:347:VAL:HG22	1.91	0.52
1:H:333:MET:HA	1:H:336:LYS:O	2.10	0.52
1:C:514:TRP:CE3	1:G:525:ARG:HD3	2.45	0.52
1:D:521:THR:HG23	1:D:521:THR:O	2.08	0.52
1:E:47:ILE:HG12	1:E:70:VAL:HB	1.91	0.52
1:B:70:VAL:HG22	1:B:108:ALA:HB3	1.92	0.52
1:A:233:GLU:HB3	7:A:567:HOH:O	2.08	0.52
1:B:433:SER:OG	1:B:435:ARG:NH1	2.38	0.52
1:D:272:ASN:HD22	1:D:275:GLY:H	1.55	0.52
1:E:131:VAL:HG21	1:E:152:ASP:HA	1.91	0.52
1:E:465:TYR:HB2	1:E:468:ILE:HD12	1.91	0.52
1:B:493:MET:SD	1:B:530:PRO:HD2	2.50	0.52
1:C:156:LEU:HD13	1:C:202:LEU:HD21	1.91	0.52
1:H:47:ILE:HG12	1:H:70:VAL:HB	1.91	0.52
1:E:297:GLY:HA3	1:F:341:ARG:HE	1.74	0.51
1:E:351:VAL:O	1:E:466:ARG:NH2	2.41	0.51
1:B:439:GLN:HE22	1:B:442:ARG:HH11	1.58	0.51
1:C:333:MET:HA	1:C:336:LYS:O	2.10	0.51
1:E:452:VAL:HG21	1:E:492:ALA:HB2	1.92	0.51
1:H:49:THR:HG23	1:H:360:LEU:O	2.10	0.51
1:A:341:ARG:HG3	1:B:293:ARG:HB3	1.93	0.51
1:A:495:VAL:O	1:A:499:ARG:HG2	2.09	0.51
1:D:493:MET:HE1	1:D:508:VAL:HG21	1.93	0.51
1:F:42:ARG:HE	1:F:378:HIS:CD2	2.22	0.51
1:F:328:GLN:HG2	1:F:331:GLU:HG3	1.93	0.51
1:H:186:GLN:HB2	1:H:193:VAL:HB	1.93	0.51
1:F:292:ALA:O	1:F:296:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:PHE:HD1	1:H:267:ILE:HB	1.76	0.51
1:H:330:LEU:HD12	1:H:343:GLU:HB3	1.92	0.51
1:B:465:TYR:HB2	1:B:468:ILE:HD12	1.92	0.51
1:D:17:LEU:O	1:D:21:MET:HG2	2.11	0.51
1:C:471:VAL:HG11	1:C:495:VAL:HG11	1.93	0.50
1:D:22:ALA:HB3	1:D:389:PHE:CZ	2.46	0.50
1:D:355:ALA:O	1:D:466:ARG:NH1	2.43	0.50
1:E:240:PHE:HD1	1:E:267:ILE:HB	1.76	0.50
1:C:514:TRP:HD1	1:C:515:ARG:HE	1.58	0.50
1:D:47:ILE:HG12	1:D:70:VAL:HB	1.93	0.50
1:B:47:ILE:HB	1:B:359:MET:HG3	1.92	0.50
1:C:24:THR:HG22	1:C:27:GLU:H	1.75	0.50
1:C:521:THR:CG2	1:C:521:THR:O	2.59	0.50
1:F:272:ASN:HD22	1:F:275:GLY:H	1.58	0.50
1:D:318:ARG:HG3	1:D:400:ALA:HB1	1.94	0.50
1:B:471:VAL:HG11	1:B:495:VAL:HG11	1.92	0.50
1:C:439:GLN:NE2	1:C:442:ARG:HH11	2.10	0.50
1:H:174:TYR:HB3	1:H:178:GLY:HA2	1.93	0.50
1:A:439:GLN:NE2	1:A:442:ARG:HD3	2.26	0.50
1:F:49:THR:HG21	1:F:72:ARG:NH1	2.26	0.50
1:G:240:PHE:HD1	1:G:267:ILE:HB	1.76	0.50
1:A:439:GLN:NE2	1:A:442:ARG:HH11	2.10	0.50
1:E:351:VAL:HB	1:E:466:ARG:HH12	1.77	0.50
1:F:133:LEU:HD21	1:F:139:LEU:HD22	1.94	0.50
1:D:168:GLU:HG3	1:E:229:LYS:HE3	1.93	0.49
1:H:114:LYS:HD2	1:H:223:LYS:HE2	1.95	0.49
1:A:452:VAL:HG21	1:A:492:ALA:HB2	1.94	0.49
1:C:118:ILE:HB	1:C:208:VAL:HB	1.94	0.49
1:C:42:ARG:HH21	1:C:378:HIS:HD2	1.59	0.49
1:H:172:LYS:HE2	1:H:197:GLU:HG3	1.94	0.49
1:B:333:MET:HA	1:B:336:LYS:O	2.13	0.49
1:B:317:ASN:HD21	1:B:354:GLY:HA3	1.76	0.49
1:C:47:ILE:HB	1:C:359:MET:HG3	1.95	0.49
1:G:49:THR:CG2	1:G:72:ARG:HD3	2.43	0.49
1:F:49:THR:CG2	1:F:72:ARG:HH11	2.22	0.49
1:A:330:LEU:HD12	1:A:343:GLU:HB3	1.93	0.49
1:A:23:ASP:HA	1:A:391:ARG:HH12	1.77	0.49
1:B:84:ALA:HB2	1:B:230:PHE:HZ	1.78	0.49
1:D:122:LEU:HB2	1:D:149:GLU:HA	1.95	0.49
1:B:133:LEU:HD21	1:B:139:LEU:HD22	1.95	0.49
1:B:131:VAL:HG21	1:B:152:ASP:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:ARG:HE	1:D:378:HIS:CD2	2.31	0.49
1:E:222:GLU:HA	1:E:225:ILE:HD12	1.95	0.49
1:A:454:ARG:NH2	1:A:484:ASP:OD1	2.45	0.48
1:C:290:MET:HG3	1:C:324:ILE:HB	1.95	0.48
1:C:328:GLN:HG2	1:C:331:GLU:CG	2.43	0.48
1:F:141:ILE:HB	1:F:192:LEU:HB2	1.95	0.48
1:F:328:GLN:HA	1:F:331:GLU:HG2	1.95	0.48
1:F:333:MET:HA	1:F:336:LYS:O	2.14	0.48
1:C:73:LEU:HD23	1:C:83:HIS:HB3	1.96	0.48
1:E:272:ASN:HD22	1:E:275:GLY:H	1.62	0.48
1:D:174:TYR:HB3	1:D:178:GLY:HA2	1.96	0.48
1:F:452:VAL:CG2	1:F:492:ALA:HB2	2.44	0.48
1:D:158:LEU:HD22	1:D:208:VAL:HG21	1.96	0.48
1:E:23:ASP:N	1:E:391:ARG:HH22	2.11	0.48
1:B:521:THR:HG23	1:B:521:THR:O	2.14	0.48
1:E:49:THR:HG23	1:E:360:LEU:O	2.14	0.48
1:B:49:THR:CG2	1:B:72:ARG:HD3	2.42	0.48
1:A:184:VAL:HA	1:A:194:THR:HG22	1.94	0.47
1:D:23:ASP:HB3	1:H:399:ARG:NH1	2.29	0.47
7:G:550:HOH:O	1:H:24:THR:HG21	2.14	0.47
1:B:328:GLN:HG2	1:B:331:GLU:HG3	1.96	0.47
1:B:439:GLN:NE2	1:B:442:ARG:HH11	2.12	0.47
1:B:403:HIS:CD2	1:B:403:HIS:H	2.32	0.47
1:E:268:SER:HB2	1:E:289:ILE:HD13	1.96	0.47
1:E:271:GLU:HG2	1:E:292:ALA:HB3	1.96	0.47
1:E:23:ASP:H	1:E:391:ARG:HH22	1.63	0.47
1:G:352:LEU:HD23	1:G:388:MET:HG2	1.96	0.47
1:H:352:LEU:HD23	1:H:388:MET:HG2	1.97	0.47
1:A:158:LEU:HD22	1:A:208:VAL:HG21	1.95	0.47
1:D:23:ASP:HA	7:D:544:HOH:O	2.14	0.47
1:D:60:LEU:HA	1:D:63:MET:HG3	1.95	0.47
1:G:293:ARG:HB3	1:H:341:ARG:HG3	1.96	0.47
1:B:272:ASN:ND2	1:B:275:GLY:H	2.12	0.47
1:D:407:LEU:HD11	1:H:507:VAL:HG21	1.97	0.47
1:B:49:THR:CG2	1:B:72:ARG:HH11	2.26	0.47
1:D:399:ARG:NH1	1:H:23:ASP:OD1	2.47	0.47
1:E:471:VAL:HG11	1:E:495:VAL:HG11	1.97	0.47
1:C:128:THR:N	1:C:129:ALA:CA	2.72	0.47
1:C:83:HIS:O	1:C:87:ILE:HG13	2.15	0.47
1:F:403:HIS:CD2	1:F:403:HIS:H	2.32	0.47
1:F:439:GLN:HE22	1:F:442:ARG:HH11	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:ARG:HH22	1:G:470:PRO:HD2	1.79	0.47
1:C:158:LEU:HD22	1:C:208:VAL:HG21	1.96	0.46
1:C:452:VAL:HG21	1:C:492:ALA:HB2	1.97	0.46
1:B:278:ARG:O	1:B:281:GLU:HG2	2.15	0.46
1:F:439:GLN:O	1:F:442:ARG:HG2	2.15	0.46
1:C:49:THR:HG21	1:C:72:ARG:NH1	2.23	0.46
1:C:84:ALA:HB2	1:C:230:PHE:HZ	1.79	0.46
1:H:471:VAL:HG11	1:H:495:VAL:HG11	1.97	0.46
1:G:351:VAL:O	1:G:466:ARG:NH2	2.38	0.46
1:A:106:PRO:O	1:A:463:HIS:NE2	2.48	0.46
1:A:521:THR:O	1:A:521:THR:CG2	2.64	0.46
1:C:267:ILE:HG21	1:C:324:ILE:HD12	1.97	0.46
1:E:343:GLU:O	1:E:347:VAL:HG23	2.16	0.46
1:F:439:GLN:NE2	1:F:442:ARG:HD3	2.31	0.46
1:A:99:SER:HB2	1:H:530:PRO:HB2	1.96	0.46
1:G:23:ASP:HA	1:G:391:ARG:NH1	2.21	0.46
1:G:290:MET:HG3	1:G:324:ILE:HB	1.97	0.46
1:B:118:ILE:HG12	1:B:160:TYR:HB2	1.97	0.46
1:C:355:ALA:O	1:C:466:ARG:NH1	2.49	0.46
1:C:325:CYS:HB3	1:C:358:ILE:HG22	1.98	0.46
1:G:271:GLU:HG2	1:G:292:ALA:HB3	1.98	0.46
1:H:23:ASP:C	1:H:23:ASP:OD2	2.55	0.46
1:F:439:GLN:NE2	1:F:442:ARG:HH11	2.14	0.46
1:E:496:GLY:HA3	1:E:502:PHE:CZ	2.51	0.45
1:G:303:GLU:HB2	1:H:380:ILE:HA	1.99	0.45
1:D:462:ALA:HB1	1:D:468:ILE:HG21	1.97	0.45
1:G:324:ILE:HG12	1:G:357:CYS:HB2	1.97	0.45
1:C:328:GLN:HA	1:C:331:GLU:HG2	1.98	0.45
1:G:222:GLU:HA	1:G:225:ILE:HD12	1.98	0.45
1:G:91:ARG:O	1:G:95:GLU:HG2	2.16	0.45
1:A:439:GLN:HE22	1:A:442:ARG:HH11	1.64	0.45
1:A:452:VAL:CG2	1:A:492:ALA:HB2	2.47	0.45
1:B:122:LEU:HD12	1:B:149:GLU:HG2	1.98	0.45
1:B:23:ASP:HA	1:B:391:ARG:HH12	1.81	0.45
1:B:268:SER:HB2	1:B:289:ILE:HD13	1.98	0.45
1:C:49:THR:CG2	1:C:72:ARG:HD3	2.45	0.45
1:E:84:ALA:HB2	1:E:230:PHE:HZ	1.81	0.45
1:E:76:SER:HA	1:E:114:LYS:HG3	1.98	0.45
1:F:222:GLU:CD	1:F:222:GLU:H	2.20	0.45
1:H:267:ILE:HG21	1:H:324:ILE:HD12	1.99	0.45
1:E:49:THR:HG22	1:E:72:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:THR:CG2	1:H:72:ARG:HH11	2.28	0.45
1:B:23:ASP:O	1:B:23:ASP:OD2	2.35	0.45
1:C:463:HIS:ND1	6:C:535:GOL:H12	2.32	0.45
1:B:156:LEU:HD13	1:B:202:LEU:HD21	1.98	0.45
1:E:42:ARG:HE	1:E:378:HIS:HD2	1.64	0.45
1:H:324:ILE:HG12	1:H:357:CYS:HB2	1.97	0.45
1:E:370:PRO:HD2	7:E:561:HOH:O	2.17	0.45
1:A:290:MET:HG3	1:A:324:ILE:HB	1.99	0.44
1:C:114:LYS:HD2	1:C:223:LYS:HE3	2.00	0.44
1:C:23:ASP:OD2	1:C:24:THR:N	2.50	0.44
1:D:439:GLN:NE2	1:D:442:ARG:HH11	2.15	0.44
1:H:135:LYS:HG3	1:H:198:ASN:HA	2.00	0.44
1:H:480:ALA:HB3	1:H:483:GLU:HG2	1.98	0.44
1:A:118:ILE:HB	1:A:208:VAL:HB	1.98	0.44
1:H:123:ILE:HA	1:H:151:CYS:HB2	1.99	0.44
1:F:294:GLY:HA3	1:F:327:THR:HG21	1.99	0.44
1:G:329:MET:HE3	1:G:358:ILE:HB	1.98	0.44
1:G:493:MET:HA	1:G:493:MET:HE3	1.99	0.44
1:H:156:LEU:HD13	1:H:202:LEU:HD21	1.99	0.44
1:B:106:PRO:O	1:B:463:HIS:NE2	2.50	0.44
1:B:22:ALA:O	1:B:23:ASP:CG	2.55	0.44
1:D:13:GLN:HG3	1:D:14:THR:H	1.83	0.44
1:H:347:VAL:O	1:H:351:VAL:HG12	2.17	0.44
1:A:439:GLN:HE21	1:A:442:ARG:HD3	1.82	0.44
1:D:496:GLY:HA3	1:D:502:PHE:CZ	2.53	0.44
1:G:355:ALA:O	1:G:466:ARG:NH1	2.51	0.44
1:G:57:VAL:HG12	1:G:61:LYS:HE3	2.00	0.44
1:G:49:THR:CG2	1:G:72:ARG:HH11	2.30	0.44
1:C:116:PRO:HD2	1:C:243:PHE:HB2	1.98	0.44
1:E:118:ILE:O	1:E:208:VAL:N	2.48	0.44
1:F:394:PHE:CE1	1:F:417:GLU:HG2	2.53	0.44
1:B:271:GLU:HG2	1:B:292:ALA:HB3	1.98	0.44
1:C:338:ARG:NH1	1:D:178:GLY:O	2.51	0.44
1:G:394:PHE:CE1	1:G:417:GLU:HG2	2.53	0.44
1:H:142:THR:HG22	1:H:144:ASP:H	1.82	0.44
1:F:156:LEU:HD13	1:F:202:LEU:HD21	1.99	0.43
1:F:267:ILE:HG21	1:F:324:ILE:HD12	2.01	0.43
1:G:416:VAL:HG12	1:G:420:TYR:CE2	2.52	0.43
1:H:49:THR:CG2	1:H:72:ARG:HD3	2.45	0.43
1:A:439:GLN:O	1:A:442:ARG:HG2	2.18	0.43
1:G:267:ILE:HG21	1:G:324:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:323:VAL:HG13	1:H:355:ALA:HA	2.01	0.43
1:H:87:ILE:O	1:H:91:ARG:HG3	2.18	0.43
1:B:515:ARG:HB3	1:B:516:PRO:CD	2.48	0.43
1:G:245:ARG:HG2	1:G:274:GLU:HB3	2.00	0.43
1:H:105:ARG:HH22	1:H:470:PRO:HD2	1.83	0.43
1:C:292:ALA:O	1:C:296:LEU:HB2	2.19	0.43
1:H:496:GLY:HA3	1:H:502:PHE:CZ	2.54	0.43
1:A:272:ASN:HD22	1:A:275:GLY:H	1.64	0.43
1:E:303:GLU:HB2	1:F:380:ILE:HA	2.01	0.43
1:H:48:CYS:SG	1:H:68:MET:HG3	2.58	0.43
1:C:41:ALA:HB2	1:C:501:PHE:CE1	2.54	0.43
1:D:272:ASN:ND2	1:D:275:GLY:H	2.16	0.43
1:E:49:THR:CG2	1:E:72:ARG:HH11	2.31	0.43
1:A:454:ARG:HG2	1:A:473:CYS:O	2.19	0.42
1:C:277:ARG:HD2	7:C:560:HOH:O	2.19	0.42
1:D:87:ILE:O	1:D:91:ARG:HG3	2.19	0.42
1:F:268:SER:HB2	1:F:289:ILE:HD13	2.01	0.42
1:G:446:ARG:HD3	7:G:537:HOH:O	2.18	0.42
1:A:49:THR:CG2	1:A:72:ARG:HH11	2.30	0.42
1:C:388:MET:SD	1:C:466:ARG:NH2	2.92	0.42
1:D:42:ARG:HE	1:D:378:HIS:HD2	1.66	0.42
1:E:292:ALA:O	1:E:296:LEU:HB2	2.19	0.42
1:F:73:LEU:HD21	1:F:87:ILE:HG13	2.00	0.42
1:B:142:THR:HG22	1:B:144:ASP:H	1.84	0.42
1:B:452:VAL:CG2	1:B:492:ALA:HB2	2.49	0.42
1:B:480:ALA:HB3	1:B:483:GLU:HG2	2.00	0.42
1:F:468:ILE:O	6:F:536:GOL:H12	2.19	0.42
1:A:186:GLN:HB2	1:A:193:VAL:HB	2.01	0.42
1:C:133:LEU:HD21	1:C:139:LEU:HD22	2.02	0.42
1:G:409:GLU:HG2	1:G:439:GLN:HE21	1.84	0.42
1:H:273:HIS:CE1	1:H:277:ARG:HD2	2.54	0.42
1:H:328:GLN:HG2	1:H:331:GLU:HG3	2.01	0.42
1:B:496:GLY:HA3	1:B:502:PHE:CZ	2.54	0.42
1:H:238:MET:SD	1:H:464:LEU:HD21	2.59	0.42
1:A:222:GLU:HA	1:A:225:ILE:HD12	2.00	0.42
1:D:327:THR:HG22	1:D:328:GLN:HG3	2.01	0.42
1:A:100:ASP:HA	1:A:101:PRO:HD3	1.87	0.42
1:D:122:LEU:HD23	1:D:204:SER:HB3	2.02	0.42
1:C:47:ILE:HG12	1:C:70:VAL:HB	2.02	0.42
1:C:91:ARG:O	1:C:95:GLU:HG2	2.19	0.42
1:D:64:ILE:HG12	1:D:107:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:ILE:HG12	1:E:357:CYS:HB2	2.02	0.42
1:E:341:ARG:HG3	1:F:293:ARG:HB3	2.02	0.42
1:F:290:MET:HG3	1:F:324:ILE:HB	2.02	0.42
1:F:69:ASN:HD22	1:F:463:HIS:CE1	2.37	0.42
1:G:158:LEU:HD22	1:G:208:VAL:HG21	2.02	0.42
1:G:329:MET:CE	1:G:358:ILE:HB	2.49	0.42
1:G:504:LYS:HG3	1:G:530:PRO:OXT	2.20	0.42
1:A:174:TYR:HB3	1:A:178:GLY:HA2	2.02	0.42
1:A:267:ILE:HG21	1:A:324:ILE:HD12	2.02	0.42
1:C:123:ILE:HG12	1:C:123:ILE:H	1.73	0.42
1:D:289:ILE:O	1:D:323:VAL:HA	2.20	0.42
1:F:49:THR:CG2	1:F:72:ARG:HD3	2.48	0.42
1:G:279:PHE:HE1	1:G:289:ILE:HG21	1.85	0.42
1:B:328:GLN:HA	1:B:331:GLU:HG2	2.01	0.41
1:C:345:SER:OG	1:D:346:ASP:OD1	2.36	0.41
1:B:292:ALA:O	1:B:296:LEU:HB2	2.20	0.41
1:B:455:ASN:HA	1:B:456:PRO:HD3	1.94	0.41
1:E:291:VAL:HG11	1:E:309:GLN:HG3	2.01	0.41
1:E:42:ARG:HE	1:E:378:HIS:CD2	2.38	0.41
1:H:339:PRO:HG3	1:H:376:MET:HG2	2.02	0.41
1:C:55:ARG:NH2	1:C:85:GLU:HB3	2.35	0.41
1:A:147:TYR:HA	1:A:150:LYS:HB2	2.03	0.41
1:B:529:VAL:HA	1:B:530:PRO:HD2	1.92	0.41
1:E:23:ASP:HA	1:E:391:ARG:HH12	1.86	0.41
1:A:333:MET:HA	1:A:336:LYS:O	2.21	0.41
1:A:42:ARG:NE	1:A:378:HIS:HD2	2.12	0.41
1:C:230:PHE:CZ	1:C:234:GLN:HG3	2.56	0.41
1:C:106:PRO:O	1:C:463:HIS:NE2	2.54	0.41
1:D:290:MET:HG3	1:D:324:ILE:HB	2.01	0.41
1:F:84:ALA:HB2	1:F:230:PHE:HZ	1.86	0.41
1:A:160:TYR:HE2	1:A:166:VAL:HG21	1.85	0.41
1:C:462:ALA:HB1	1:C:468:ILE:HG21	2.01	0.41
1:C:340:THR:HA	1:D:328:GLN:OE1	2.20	0.41
1:E:396:GLU:HG2	1:F:24:THR:HG23	2.02	0.41
1:H:105:ARG:HH12	1:H:463:HIS:HE1	1.68	0.41
1:D:421:LYS:NZ	1:H:401:SER:O	2.51	0.41
1:F:269:LYS:HE3	1:F:290:MET:HE1	2.03	0.41
1:G:465:TYR:HB2	1:G:468:ILE:HD12	2.03	0.41
1:H:356:ASP:HB3	1:H:464:LEU:O	2.21	0.41
1:F:23:ASP:C	1:F:23:ASP:OD2	2.59	0.41
1:F:40:THR:HG21	1:F:500:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:VAL:HG22	1:F:108:ALA:HB3	2.01	0.41
1:B:22:ALA:O	1:B:23:ASP:CB	2.69	0.40
1:E:43:ASN:HB3	1:E:466:ARG:HG3	2.02	0.40
1:H:222:GLU:H	1:H:222:GLU:CD	2.24	0.40
1:A:176:ASP:HB2	1:A:206:LYS:HB3	2.03	0.40
1:B:42:ARG:NE	1:B:378:HIS:HD2	2.15	0.40
1:D:313:ILE:HA	1:D:323:VAL:HG11	2.04	0.40
1:F:409:GLU:HG2	1:F:439:GLN:HE21	1.86	0.40
1:F:64:ILE:HG12	1:F:107:VAL:HG21	2.03	0.40
1:G:521:THR:O	1:G:521:THR:CG2	2.67	0.40
1:B:429:VAL:O	1:B:451:ALA:HA	2.22	0.40
1:D:485:VAL:O	1:D:489:VAL:HG23	2.21	0.40
1:F:228:LEU:HD21	1:F:239:VAL:HG11	2.03	0.40
1:G:252:GLU:OE2	1:G:255:LYS:HD3	2.22	0.40
1:H:475:ASP:HA	1:H:476:PRO:HD3	1.99	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	513/551 (93%)	493 (96%)	19 (4%)	1 (0%)	51	81
1	B	513/551 (93%)	492 (96%)	20 (4%)	1 (0%)	51	81
1	C	513/551 (93%)	497 (97%)	15 (3%)	1 (0%)	51	81
1	D	511/551 (93%)	494 (97%)	16 (3%)	1 (0%)	51	81
1	E	510/551 (93%)	495 (97%)	14 (3%)	1 (0%)	51	81
1	F	512/551 (93%)	488 (95%)	23 (4%)	1 (0%)	51	81
1	G	509/551 (92%)	490 (96%)	18 (4%)	1 (0%)	51	81
1	H	517/551 (94%)	492 (95%)	24 (5%)	1 (0%)	51	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4098/4408 (93%)	3941 (96%)	149 (4%)	8 (0%)	51 81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	THR
1	G	327	THR
1	C	327	THR
1	B	327	THR
1	D	327	THR
1	E	327	THR
1	F	327	THR
1	H	327	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	426/453 (94%)	415 (97%)	11 (3%)	51 82
1	B	426/453 (94%)	409 (96%)	17 (4%)	36 69
1	C	426/453 (94%)	403 (95%)	23 (5%)	26 56
1	D	425/453 (94%)	411 (97%)	14 (3%)	43 75
1	E	424/453 (94%)	406 (96%)	18 (4%)	34 67
1	F	425/453 (94%)	406 (96%)	19 (4%)	32 64
1	G	424/453 (94%)	408 (96%)	16 (4%)	38 70
1	H	427/453 (94%)	413 (97%)	14 (3%)	43 75
All	All	3403/3624 (94%)	3271 (96%)	132 (4%)	37 69

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	14	THR
1	C	49	THR

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Mol	Chain	Res	Type
1	C	123	ILE
1	C	128	THR
1	C	130	GLU
1	C	131	VAL
1	C	142	THR
1	C	143	LEU
1	C	159	ASP
1	C	161	LYS
1	C	172	LYS
1	C	272	ASN
1	C	277	ARG
1	C	284	GLU
1	C	296	LEU
1	C	330	LEU
1	C	351	VAL
1	C	382	ARG
1	C	389	PHE
1	C	407	LEU
1	C	486	ASP
1	C	493	MET
1	C	521	THR
1	A	49	THR
1	A	122	LEU
1	A	142	THR
1	A	160	TYR
1	A	272	ASN
1	A	296	LEU
1	A	330	LEU
1	A	351	VAL
1	A	389	PHE
1	A	466	ARG
1	A	493	MET
1	B	142	THR
1	B	155	ILE
1	B	167	VAL
1	B	172	LYS
1	B	222	GLU
1	B	272	ASN
1	B	296	LEU
1	B	327	THR
1	B	329	MET
1	B	351	VAL

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Mol	Chain	Res	Type
1	B	382	ARG
1	B	389	PHE
1	B	399	ARG
1	B	417	GLU
1	B	466	ARG
1	B	493	MET
1	B	527	VAL
1	D	142	THR
1	D	145	ASN
1	D	155	ILE
1	D	162	ASN
1	D	172	LYS
1	D	272	ASN
1	D	296	LEU
1	D	330	LEU
1	D	335	LYS
1	D	351	VAL
1	D	389	PHE
1	D	417	GLU
1	D	466	ARG
1	D	518	SER
1	E	14	THR
1	E	58	GLU
1	E	160	TYR
1	E	215	VAL
1	E	222	GLU
1	E	272	ASN
1	E	284	GLU
1	E	296	LEU
1	E	330	LEU
1	E	351	VAL
1	E	382	ARG
1	E	389	PHE
1	E	399	ARG
1	E	466	ARG
1	E	475	ASP
1	E	479	GLU
1	E	486	ASP
1	E	493	MET
1	F	40	THR
1	F	49	THR
1	F	103	LEU

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Mol	Chain	Res	Type
1	F	128	THR
1	F	142	THR
1	F	143	LEU
1	F	153	GLU
1	F	155	ILE
1	F	222	GLU
1	F	272	ASN
1	F	284	GLU
1	F	296	LEU
1	F	329	MET
1	F	335	LYS
1	F	351	VAL
1	F	356	ASP
1	F	382	ARG
1	F	399	ARG
1	F	466	ARG
1	G	14	THR
1	G	23	ASP
1	G	24	THR
1	G	40	THR
1	G	293	ARG
1	G	296	LEU
1	G	298	ILE
1	G	327	THR
1	G	330	LEU
1	G	351	VAL
1	G	356	ASP
1	G	389	PHE
1	G	403	HIS
1	G	435	ARG
1	G	466	ARG
1	G	493	MET
1	H	23	ASP
1	H	177	ASP
1	H	211	PRO
1	H	272	ASN
1	H	284	GLU
1	H	296	LEU
1	H	327	THR
1	H	330	LEU
1	H	351	VAL
1	H	389	PHE

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Mol	Chain	Res	Type
1	H	403	HIS
1	H	466	ARG
1	H	493	MET
1	H	521	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	145	ASN
1	C	272	ASN
1	C	349	ASN
1	C	377	GLN
1	C	378	HIS
1	C	390	HIS
1	C	403	HIS
1	C	439	GLN
1	A	162	ASN
1	A	263	ASN
1	A	272	ASN
1	A	317	ASN
1	A	378	HIS
1	A	439	GLN
1	A	490	ASN
1	B	145	ASN
1	B	263	ASN
1	B	272	ASN
1	B	317	ASN
1	B	378	HIS
1	B	390	HIS
1	B	403	HIS
1	B	439	GLN
1	D	15	GLN
1	D	145	ASN
1	D	272	ASN
1	D	317	ASN
1	D	349	ASN
1	D	378	HIS
1	D	439	GLN
1	E	13	GLN
1	E	74	ASN
1	E	272	ASN
1	E	378	HIS

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Mol	Chain	Res	Type
1	E	439	GLN
1	E	490	ASN
1	F	15	GLN
1	F	145	ASN
1	F	263	ASN
1	F	272	ASN
1	F	317	ASN
1	F	349	ASN
1	F	378	HIS
1	F	403	HIS
1	F	439	GLN
1	F	490	ASN
1	G	145	ASN
1	G	154	ASN
1	G	162	ASN
1	G	272	ASN
1	G	349	ASN
1	G	378	HIS
1	G	403	HIS
1	G	439	GLN
1	G	490	ASN
1	H	15	GLN
1	H	263	ASN
1	H	272	ASN
1	H	317	ASN
1	H	349	ASN
1	H	377	GLN
1	H	378	HIS
1	H	390	HIS
1	H	439	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 16 are monoatomic - leaving 24 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	$\# Z > 2$
2	PO4	A	531	-	4,4,4	0.81	0	6,6,6	0.42	0
5	PYR	A	534	4	2,5,5	1.01	0	2,6,6	0.64	0
6	GOL	A	535	-	5,5,5	0.32	0	5,5,5	0.42	0
2	PO4	B	531	-	4,4,4	0.75	0	6,6,6	0.45	0
5	PYR	B	534	4	2,5,5	0.95	0	2,6,6	0.18	0
6	GOL	B	535	-	5,5,5	0.32	0	5,5,5	0.34	0
2	PO4	C	531	-	4,4,4	0.79	0	6,6,6	0.37	0
5	PYR	C	534	4	2,5,5	1.03	0	2,6,6	0.14	0
6	GOL	C	535	-	5,5,5	0.40	0	5,5,5	0.28	0
2	PO4	D	531	-	4,4,4	0.77	0	6,6,6	0.40	0
5	PYR	D	534	4	2,5,5	1.01	0	2,6,6	0.21	0
6	GOL	D	535	-	5,5,5	0.34	0	5,5,5	0.31	0
2	PO4	E	531	-	4,4,4	0.77	0	6,6,6	0.47	0
5	PYR	E	534	4	2,5,5	1.05	0	2,6,6	0.22	0
6	GOL	E	535	-	5,5,5	0.36	0	5,5,5	0.28	0
2	PO4	F	531	-	4,4,4	0.79	0	6,6,6	0.44	0
5	PYR	F	534	4	2,5,5	1.03	0	2,6,6	0.36	0
6	GOL	F	535	-	5,5,5	0.31	0	5,5,5	0.41	0
6	GOL	F	536	-	5,5,5	0.39	0	5,5,5	0.23	0
2	PO4	G	531	-	4,4,4	0.79	0	6,6,6	0.33	0
5	PYR	G	534	4	2,5,5	0.98	0	2,6,6	0.16	0
6	GOL	G	535	-	5,5,5	0.31	0	5,5,5	0.27	0
2	PO4	H	531	-	4,4,4	0.82	0	6,6,6	0.39	0
5	PYR	H	534	4	2,5,5	1.02	0	2,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	531	-	-	0/0/0/0	0/0/0/0
5	PYR	A	534	4	-	0/0/4/4	0/0/0/0
6	GOL	A	535	-	-	0/4/4/4	0/0/0/0
2	PO4	B	531	-	-	0/0/0/0	0/0/0/0
5	PYR	B	534	4	-	0/0/4/4	0/0/0/0
6	GOL	B	535	-	-	0/4/4/4	0/0/0/0
2	PO4	C	531	-	-	0/0/0/0	0/0/0/0
5	PYR	C	534	4	-	0/0/4/4	0/0/0/0
6	GOL	C	535	-	-	0/4/4/4	0/0/0/0
2	PO4	D	531	-	-	0/0/0/0	0/0/0/0
5	PYR	D	534	4	-	0/0/4/4	0/0/0/0
6	GOL	D	535	-	-	0/4/4/4	0/0/0/0
2	PO4	E	531	-	-	0/0/0/0	0/0/0/0
5	PYR	E	534	4	-	0/0/4/4	0/0/0/0
6	GOL	E	535	-	-	0/4/4/4	0/0/0/0
2	PO4	F	531	-	-	0/0/0/0	0/0/0/0
5	PYR	F	534	4	-	0/0/4/4	0/0/0/0
6	GOL	F	535	-	-	0/4/4/4	0/0/0/0
6	GOL	F	536	-	-	0/4/4/4	0/0/0/0
2	PO4	G	531	-	-	0/0/0/0	0/0/0/0
5	PYR	G	534	4	-	0/0/4/4	0/0/0/0
6	GOL	G	535	-	-	0/4/4/4	0/0/0/0
2	PO4	H	531	-	-	0/0/0/0	0/0/0/0
5	PYR	H	534	4	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	531	PO4	1	0
6	C	535	GOL	1	0
6	F	536	GOL	1	0
6	G	535	GOL	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	517/551 (93%)	-0.02	4 (0%) 86 82	23, 33, 67, 78	0
1	B	517/551 (93%)	-0.06	1 (0%) 94 94	24, 33, 58, 70	0
1	C	517/551 (93%)	-0.08	1 (0%) 94 94	25, 35, 48, 59	0
1	D	515/551 (93%)	-0.06	1 (0%) 94 94	27, 36, 50, 55	0
1	E	514/551 (93%)	0.39	26 (5%) 29 20	34, 51, 95, 101	0
1	F	516/551 (93%)	-0.05	0 100 100	27, 40, 50, 59	0
1	G	513/551 (93%)	0.13	11 (2%) 64 56	26, 42, 81, 84	0
1	H	519/551 (94%)	0.02	4 (0%) 86 82	28, 38, 60, 66	0
All	All	4128/4408 (93%)	0.03	48 (1%) 79 73	23, 38, 67, 101	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	138	THR	5.1
1	H	128	THR	4.9
1	E	129	ALA	4.8
1	E	170	GLY	4.7
1	E	137	ALA	3.9
1	G	164	CYS	3.7
1	E	187	LYS	3.5
1	E	160	TYR	3.5
1	E	120	THR	3.4
1	E	140	LYS	3.3
1	E	171	SER	3.3
1	E	150	LYS	3.3
1	E	156	LEU	3.2
1	A	204	SER	3.1
1	E	216	ASP	3.1
1	G	165	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	130	GLU	2.8
1	D	12	ILE	2.7
1	E	158	LEU	2.7
1	H	127	GLY	2.7
1	G	187	LYS	2.7
1	G	188	GLY	2.5
1	A	135	LYS	2.5
1	E	202	LEU	2.5
1	H	155	ILE	2.4
1	E	166	VAL	2.4
1	G	133	LEU	2.4
1	E	196	VAL	2.4
1	A	197	GLU	2.3
1	E	121	GLY	2.3
1	H	199	GLY	2.3
1	A	169	VAL	2.3
1	G	191	PHE	2.3
1	G	177	ASP	2.2
1	E	213	ALA	2.2
1	E	182	LEU	2.2
1	E	191	PHE	2.2
1	G	121	GLY	2.2
1	G	161	LYS	2.2
1	E	142	THR	2.2
1	B	177	ASP	2.2
1	E	169	VAL	2.2
1	G	166	VAL	2.1
1	G	190	ASP	2.1
1	E	134	LYS	2.1
1	C	530	PRO	2.1
1	E	151	CYS	2.0
1	E	215	VAL	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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	PYR	H	534	6/6	0.66	0.38	6.08	69,70,70,70	0
6	GOL	F	535	6/6	0.92	0.29	5.13	50,50,50,50	0
6	GOL	A	535	6/6	0.93	0.29	4.67	58,58,59,60	0
3	K	B	532	1/1	0.20	0.32	4.13	94,94,94,94	0
5	PYR	B	534	6/6	0.89	0.21	2.21	42,43,43,43	0
6	GOL	C	535	6/6	0.95	0.21	1.65	32,32,33,33	0
6	GOL	G	535	6/6	0.94	0.21	0.80	34,34,34,34	0
6	GOL	B	535	6/6	0.96	0.22	0.74	46,46,47,47	0
2	PO4	F	531	5/5	0.97	0.21	0.28	45,46,46,46	0
2	PO4	A	531	5/5	0.98	0.18	0.00	41,41,41,41	0
6	GOL	E	535	6/6	0.95	0.19	-0.04	41,42,42,43	0
5	PYR	C	534	6/6	0.94	0.16	-0.07	46,46,46,46	0
2	PO4	B	531	5/5	0.97	0.17	-0.41	37,38,38,38	0
5	PYR	E	534	6/6	0.86	0.17	-0.52	62,63,63,63	0
5	PYR	D	534	6/6	0.92	0.16	-0.55	51,51,52,52	0
2	PO4	D	531	5/5	0.97	0.17	-0.58	47,47,47,47	0
5	PYR	F	534	6/6	0.93	0.15	-0.63	38,38,38,39	0
3	K	E	532	1/1	0.63	0.17	-0.89	85,85,85,85	0
6	GOL	F	536	6/6	0.95	0.15	-0.93	43,44,44,44	0
3	K	F	532	1/1	0.90	0.15	-0.94	46,46,46,46	0
5	PYR	A	534	6/6	0.92	0.13	-1.02	38,38,39,39	0
2	PO4	G	531	5/5	0.98	0.14	-1.10	45,45,46,46	0
6	GOL	D	535	6/6	0.98	0.15	-1.11	31,31,31,31	0
5	PYR	G	534	6/6	0.89	0.12	-1.33	66,67,67,67	0
3	K	D	532	1/1	0.90	0.15	-1.42	48,48,48,48	0
3	K	G	532	1/1	0.76	0.15	-1.47	60,60,60,60	0
2	PO4	C	531	5/5	0.98	0.14	-1.57	40,40,40,41	0
2	PO4	E	531	5/5	0.98	0.12	-1.92	45,45,45,45	0
2	PO4	H	531	5/5	0.98	0.14	-2.39	36,36,36,36	0
3	K	A	532	1/1	0.94	0.09	-3.11	37,37,37,37	0
3	K	H	532	1/1	0.78	0.12	-3.67	48,48,48,48	0
3	K	C	532	1/1	0.94	0.11	-4.03	58,58,58,58	0
4	MG	H	533	1/1	0.94	0.18	-	14,14,14,14	0
4	MG	F	533	1/1	0.91	0.11	-	21,21,21,21	0
4	MG	G	533	1/1	0.96	0.15	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	A	533	1/1	0.91	0.16	-	26,26,26,26	0
4	MG	E	533	1/1	0.96	0.10	-	58,58,58,58	0
4	MG	B	533	1/1	0.94	0.12	-	26,26,26,26	0
4	MG	D	533	1/1	0.92	0.17	-	51,51,51,51	0
4	MG	C	533	1/1	0.97	0.18	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.