Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:22 AM GMT

PDB ID	:	3HQP
Title	:	Crystal structure of Leishmania mexicana pyruvate kinase (LmPYK) in complex with ATP, Oxalate and fructose 2,6 bisphosphate
Authors	:	Morgan, H.P.; Walkinshaw, M.D.
Deposited on	:	2009-06-08
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
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:

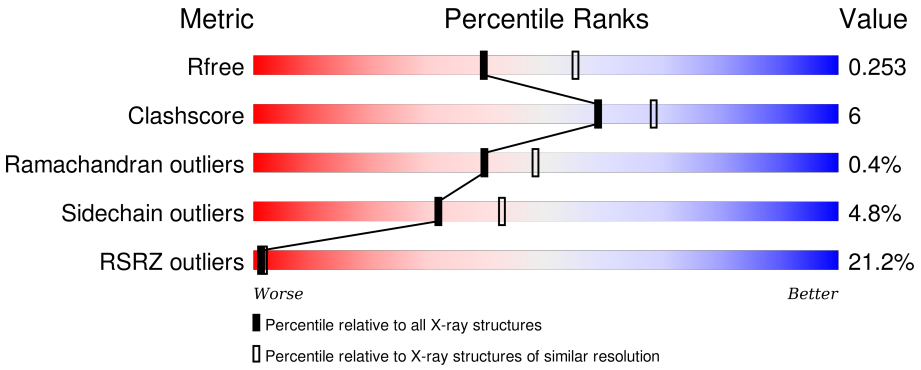
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	499	25% 86% 12% •
1	B	499	8% 82% 15% •
1	C	499	11% 85% 14% •
1	D	499	11% 85% 13% •
1	E	499	14% 87% 12% •

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Mol	Chain	Length	Quality of chain
1	F	499	16% 86% 13%
1	G	499	29% 85% 13%
1	H	499	17% 84% 14%
1	I	499	10% 85% 13%
1	J	499	8% 84% 15%
1	K	499	6% 83% 16%
1	L	499	13% 88% 11%
1	M	499	26% 85% 14%
1	N	499	41% 85% 13%
1	O	499	52% 89% 10%
1	P	499	51% 86% 13%

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	O	501	-	-	-	X
7	GOL	O	499	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 65997 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	2	0
			3818	2379	674	739	26			
1	B	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	C	498	Total	C	N	O	S	0	2	0
			3815	2378	672	739	26			
1	D	498	Total	C	N	O	S	0	1	0
			3809	2374	673	736	26			
1	E	498	Total	C	N	O	S	0	1	0
			3808	2373	672	737	26			
1	F	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	G	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	H	498	Total	C	N	O	S	0	2	0
			3817	2379	675	737	26			
1	I	498	Total	C	N	O	S	0	2	0
			3816	2379	674	737	26			
1	J	498	Total	C	N	O	S	0	3	0
			3824	2383	676	739	26			
1	K	498	Total	C	N	O	S	0	2	0
			3816	2377	673	740	26			
1	L	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	M	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	N	498	Total	C	N	O	S	0	1	0
			3808	2373	671	738	26			
1	O	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			
1	P	498	Total	C	N	O	S	0	0	0
			3799	2368	670	735	26			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	382	SER	GLY	SEE REMARK 999	UNP Q27686
A	389	TYR	SER	SEE REMARK 999	UNP Q27686
A	404	ARG	ALA	SEE REMARK 999	UNP Q27686
A	405	SER	GLY	SEE REMARK 999	UNP Q27686
B	382	SER	GLY	SEE REMARK 999	UNP Q27686
B	389	TYR	SER	SEE REMARK 999	UNP Q27686
B	404	ARG	ALA	SEE REMARK 999	UNP Q27686
B	405	SER	GLY	SEE REMARK 999	UNP Q27686
C	382	SER	GLY	SEE REMARK 999	UNP Q27686
C	389	TYR	SER	SEE REMARK 999	UNP Q27686
C	404	ARG	ALA	SEE REMARK 999	UNP Q27686
C	405	SER	GLY	SEE REMARK 999	UNP Q27686
D	382	SER	GLY	SEE REMARK 999	UNP Q27686
D	389	TYR	SER	SEE REMARK 999	UNP Q27686
D	404	ARG	ALA	SEE REMARK 999	UNP Q27686
D	405	SER	GLY	SEE REMARK 999	UNP Q27686
E	382	SER	GLY	SEE REMARK 999	UNP Q27686
E	389	TYR	SER	SEE REMARK 999	UNP Q27686
E	404	ARG	ALA	SEE REMARK 999	UNP Q27686
E	405	SER	GLY	SEE REMARK 999	UNP Q27686
F	382	SER	GLY	SEE REMARK 999	UNP Q27686
F	389	TYR	SER	SEE REMARK 999	UNP Q27686
F	404	ARG	ALA	SEE REMARK 999	UNP Q27686
F	405	SER	GLY	SEE REMARK 999	UNP Q27686
G	382	SER	GLY	SEE REMARK 999	UNP Q27686
G	389	TYR	SER	SEE REMARK 999	UNP Q27686
G	404	ARG	ALA	SEE REMARK 999	UNP Q27686
G	405	SER	GLY	SEE REMARK 999	UNP Q27686
H	382	SER	GLY	SEE REMARK 999	UNP Q27686
H	389	TYR	SER	SEE REMARK 999	UNP Q27686
H	404	ARG	ALA	SEE REMARK 999	UNP Q27686
H	405	SER	GLY	SEE REMARK 999	UNP Q27686
I	382	SER	GLY	SEE REMARK 999	UNP Q27686
I	389	TYR	SER	SEE REMARK 999	UNP Q27686
I	404	ARG	ALA	SEE REMARK 999	UNP Q27686
I	405	SER	GLY	SEE REMARK 999	UNP Q27686
J	382	SER	GLY	SEE REMARK 999	UNP Q27686
J	389	TYR	SER	SEE REMARK 999	UNP Q27686
J	404	ARG	ALA	SEE REMARK 999	UNP Q27686
J	405	SER	GLY	SEE REMARK 999	UNP Q27686
K	382	SER	GLY	SEE REMARK 999	UNP Q27686
K	389	TYR	SER	SEE REMARK 999	UNP Q27686

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Chain	Residue	Modelled	Actual	Comment	Reference
K	404	ARG	ALA	SEE REMARK 999	UNP Q27686
K	405	SER	GLY	SEE REMARK 999	UNP Q27686
L	382	SER	GLY	SEE REMARK 999	UNP Q27686
L	389	TYR	SER	SEE REMARK 999	UNP Q27686
L	404	ARG	ALA	SEE REMARK 999	UNP Q27686
L	405	SER	GLY	SEE REMARK 999	UNP Q27686
M	382	SER	GLY	SEE REMARK 999	UNP Q27686
M	389	TYR	SER	SEE REMARK 999	UNP Q27686
M	404	ARG	ALA	SEE REMARK 999	UNP Q27686
M	405	SER	GLY	SEE REMARK 999	UNP Q27686
N	382	SER	GLY	SEE REMARK 999	UNP Q27686
N	389	TYR	SER	SEE REMARK 999	UNP Q27686
N	404	ARG	ALA	SEE REMARK 999	UNP Q27686
N	405	SER	GLY	SEE REMARK 999	UNP Q27686
O	382	SER	GLY	SEE REMARK 999	UNP Q27686
O	389	TYR	SER	SEE REMARK 999	UNP Q27686
O	404	ARG	ALA	SEE REMARK 999	UNP Q27686
O	405	SER	GLY	SEE REMARK 999	UNP Q27686
P	382	SER	GLY	SEE REMARK 999	UNP Q27686
P	389	TYR	SER	SEE REMARK 999	UNP Q27686
P	404	ARG	ALA	SEE REMARK 999	UNP Q27686
P	405	SER	GLY	SEE REMARK 999	UNP Q27686

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	2	Total Mg 2 2	0	0
2	G	2	Total Mg 2 2	0	0
2	J	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	K	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	H	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	A	2	Total Mg 2 2	0	0
2	N	2	Total Mg 2 2	0	0
2	L	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0
2	M	2	Total Mg 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	2	Total K 2 2	0	0
3	G	2	Total K 2 2	0	0
3	J	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	K	2	Total K 2 2	0	0
3	E	2	Total K 2 2	0	0
3	H	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	I	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	N	2	Total K 2 2	0	0

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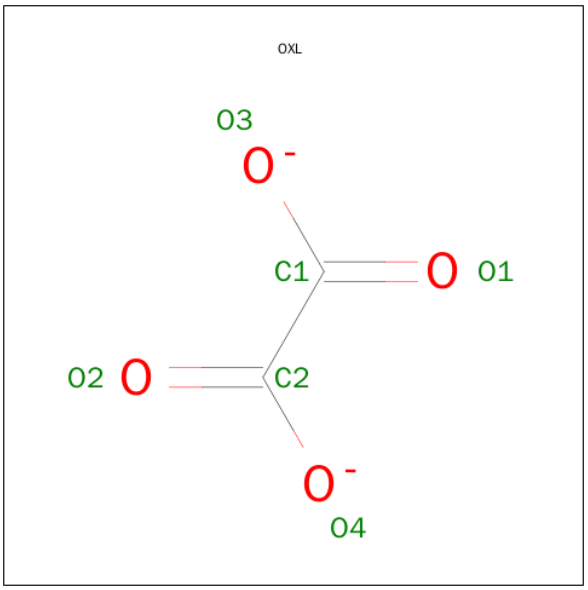
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	2	Total K 2 2	0	0
3	L	2	Total K 2 2	0	0
3	F	2	Total K 2 2	0	0
3	M	2	Total K 2 2	0	0

- Molecule 4 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 2 4	0	0
4	B	1	Total C O 6 2 4	0	0
4	C	1	Total C O 6 2 4	0	0
4	D	1	Total C O 6 2 4	0	0
4	E	1	Total C O 6 2 4	0	0
4	F	1	Total C O 6 2 4	0	0
4	G	1	Total C O 6 2 4	0	0

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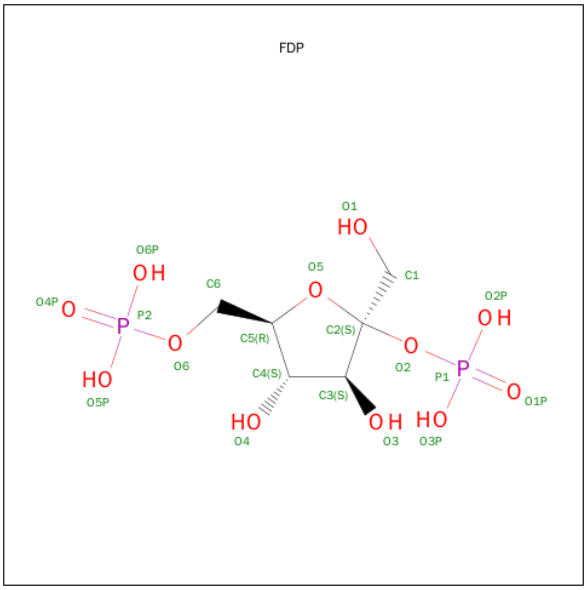
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 2 4	0	0
4	I	1	Total C O 6 2 4	0	0
4	J	1	Total C O 6 2 4	0	0
4	K	1	Total C O 6 2 4	0	0
4	L	1	Total C O 6 2 4	0	0
4	M	1	Total C O 6 2 4	0	0
4	N	1	Total C O 6 2 4	0	0
4	P	1	Total C O 6 2 4	0	0

- Molecule 5 is SUGAR (FRUCTOSE-2,6-DIPHOSPHATE) (three-letter code: FDP) (formula: $C_6H_{14}O_{12}P_2$).



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

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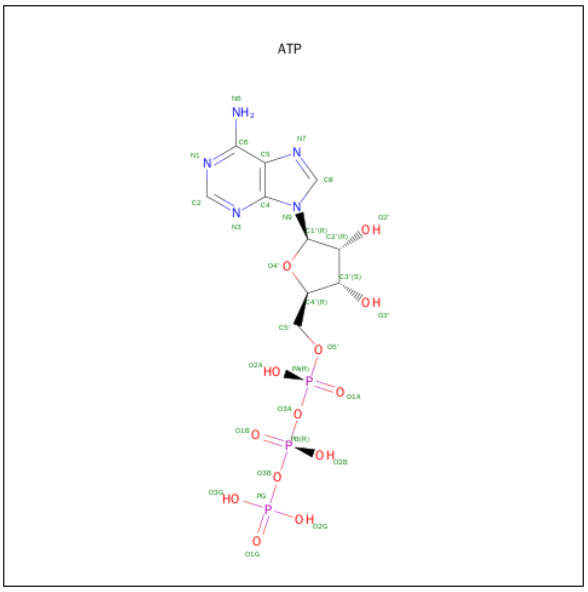
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	P	0	0
			20	6	12	2		
5	E	1	Total	C	O	P	0	0
			20	6	12	2		
5	F	1	Total	C	O	P	0	0
			20	6	12	2		
5	G	1	Total	C	O	P	0	0
			20	6	12	2		
5	H	1	Total	C	O	P	0	0
			20	6	12	2		
5	I	1	Total	C	O	P	0	0
			20	6	12	2		
5	J	1	Total	C	O	P	0	0
			20	6	12	2		
5	K	1	Total	C	O	P	0	0
			20	6	12	2		
5	L	1	Total	C	O	P	0	0
			20	6	12	2		
5	M	1	Total	C	O	P	0	0
			20	6	12	2		
5	N	1	Total	C	O	P	0	0
			20	6	12	2		
5	O	1	Total	C	O	P	0	0
			20	6	12	2		
5	P	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	M	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
6	N	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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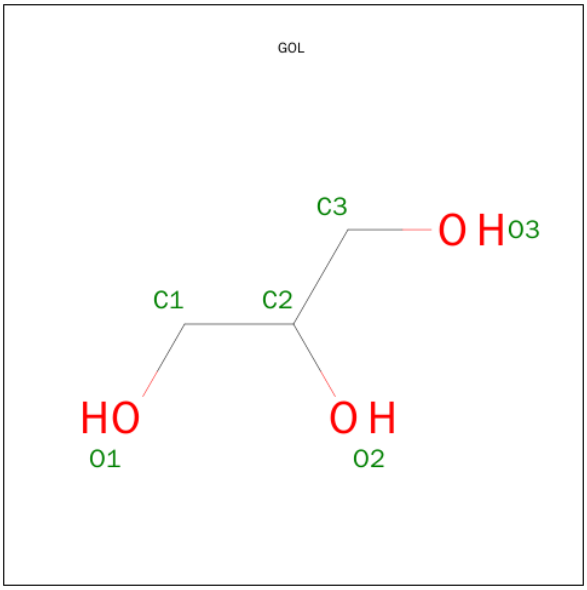
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	P	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	O		0	0
			6	3	3			
7	G	1	Total	C	O		0	0
			6	3	3			
7	I	1	Total	C	O		0	0
			6	3	3			
7	I	1	Total	C	O		0	0
			6	3	3			
7	J	1	Total	C	O		0	0
			6	3	3			
7	O	1	Total	C	O		0	0
			6	3	3			

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	167	Total	O	0	0
			167	167		
8	B	379	Total	O	0	0
			379	379		

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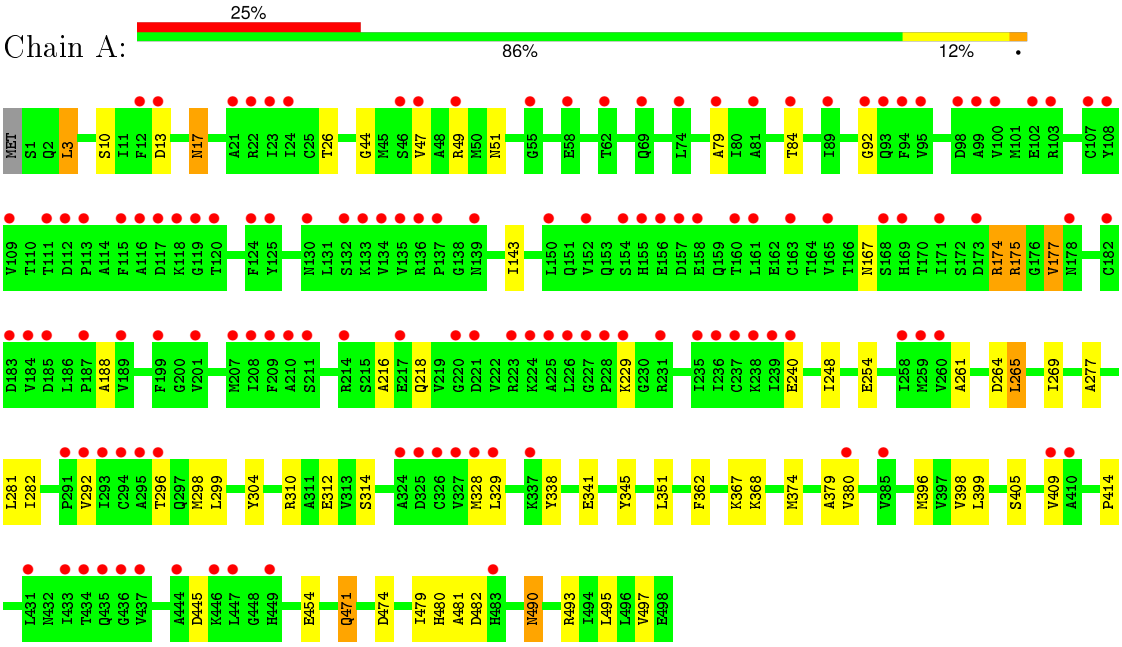
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	305	Total O 305 305	0	0
8	D	400	Total O 400 400	0	0
8	E	232	Total O 232 232	0	0
8	F	187	Total O 187 187	0	0
8	G	139	Total O 139 139	0	0
8	H	215	Total O 215 215	0	0
8	I	415	Total O 415 415	0	0
8	J	499	Total O 499 499	0	0
8	K	462	Total O 462 462	0	0
8	L	316	Total O 316 316	0	0
8	M	140	Total O 140 140	0	0
8	N	103	Total O 103 103	0	0
8	O	69	Total O 69 69	0	0
8	P	72	Total O 72 72	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.

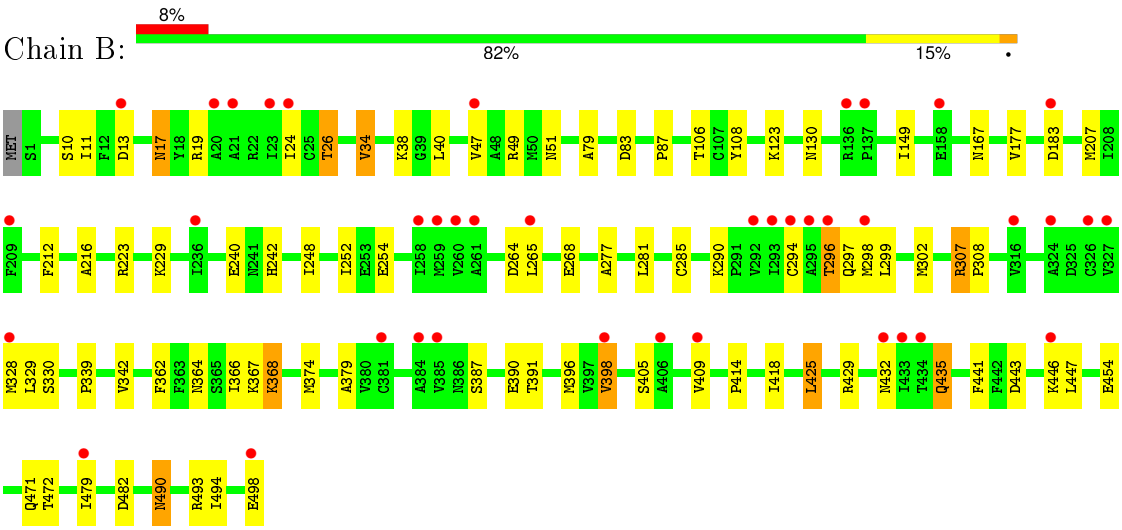
- Molecule 1: Pyruvate kinase

Chain A:



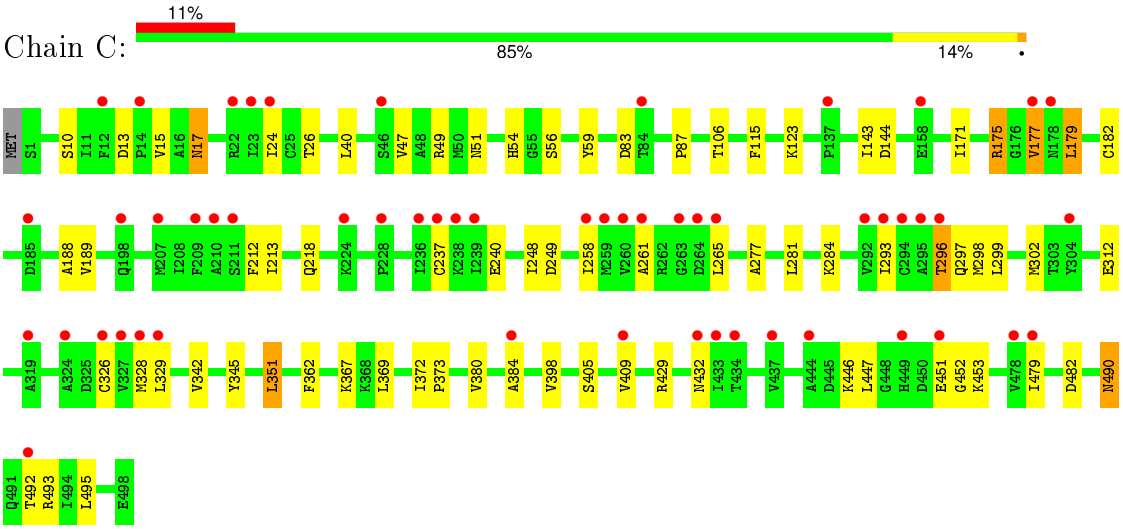
- Molecule 1: Pyruvate kinase

Chain B:



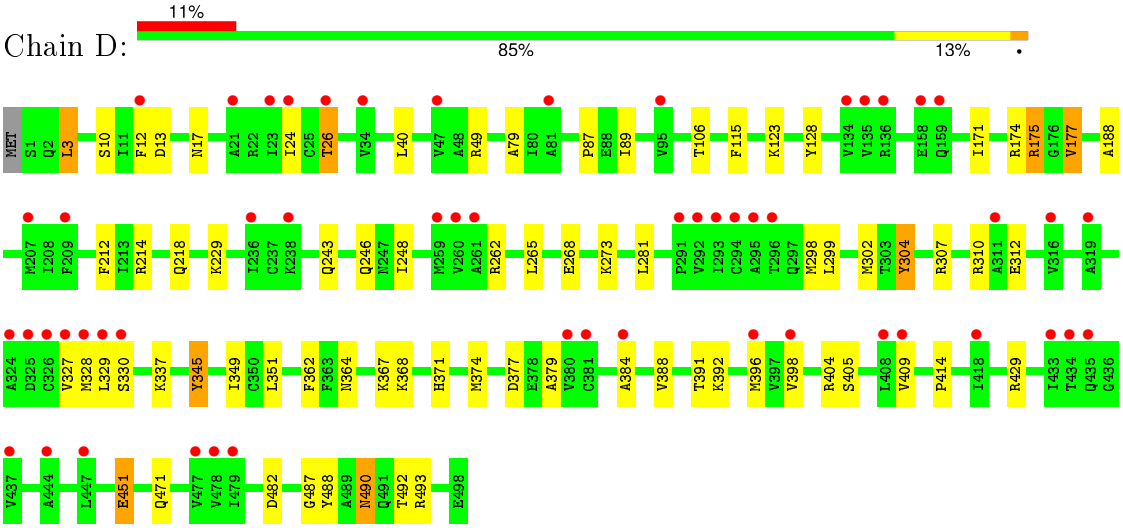
- Molecule 1: Pyruvate kinase

Chain C:



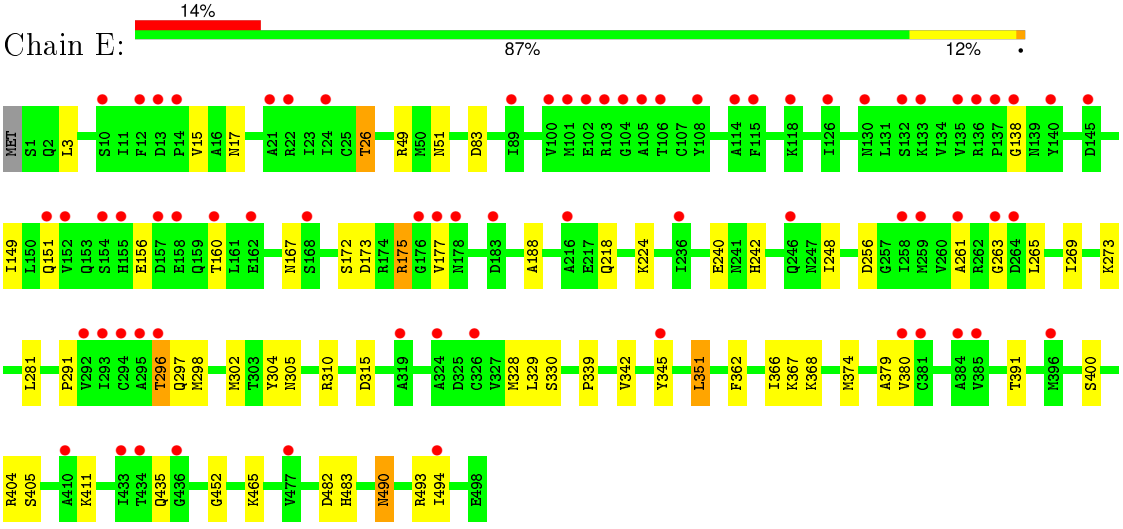
• Molecule 1: Pyruvate kinase

Chain D:



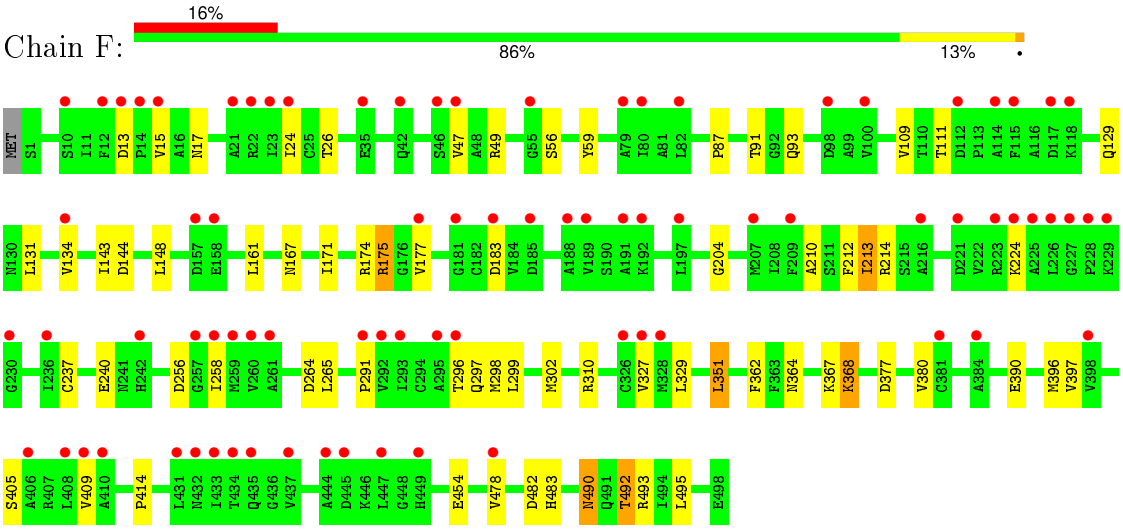
• Molecule 1: Pyruvate kinase

Chain E:



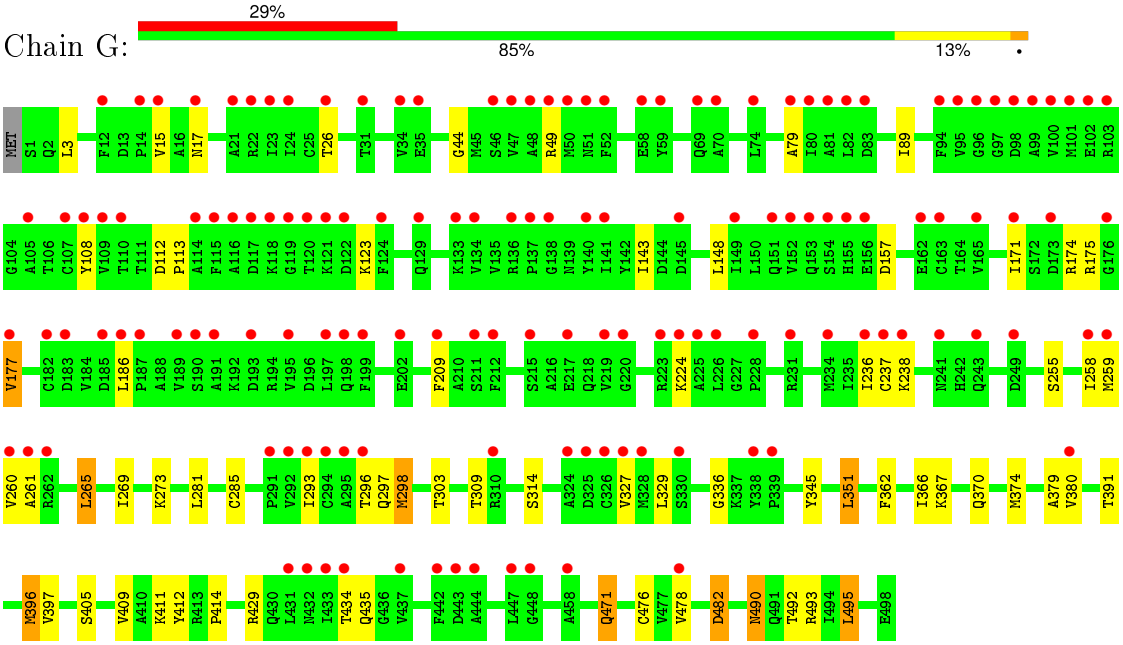
• Molecule 1: Pyruvate kinase

Chain F:



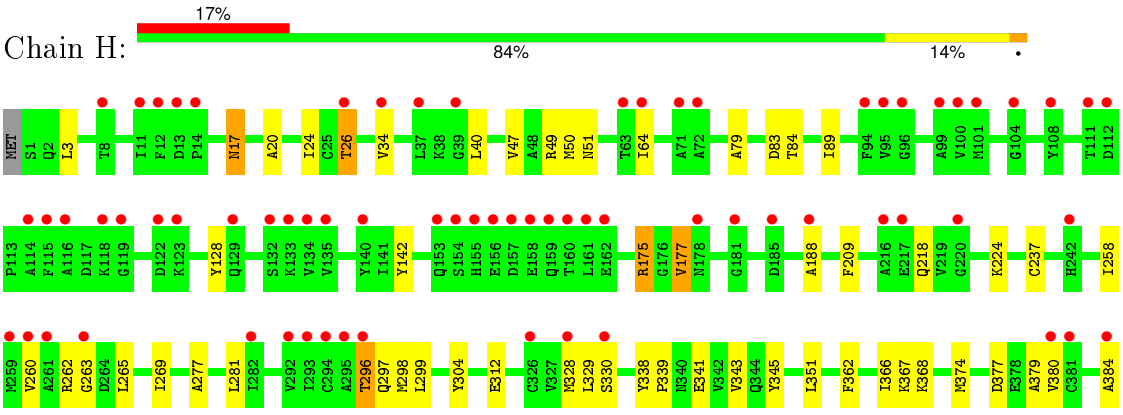
• Molecule 1: Pyruvate kinase

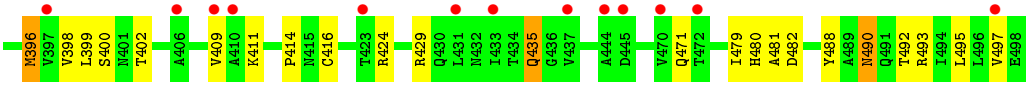
Chain G:



• Molecule 1: Pyruvate kinase

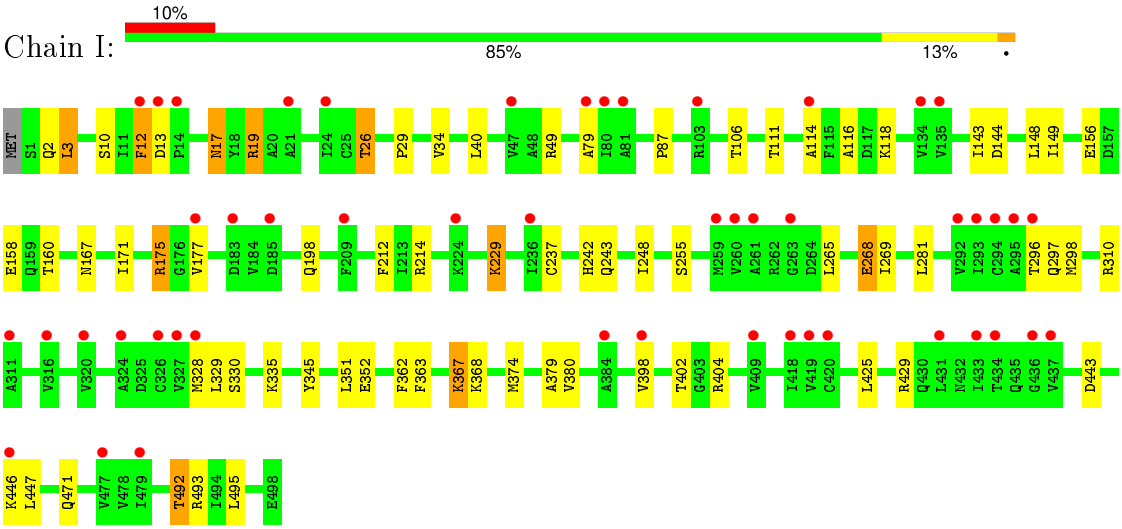
Chain H:





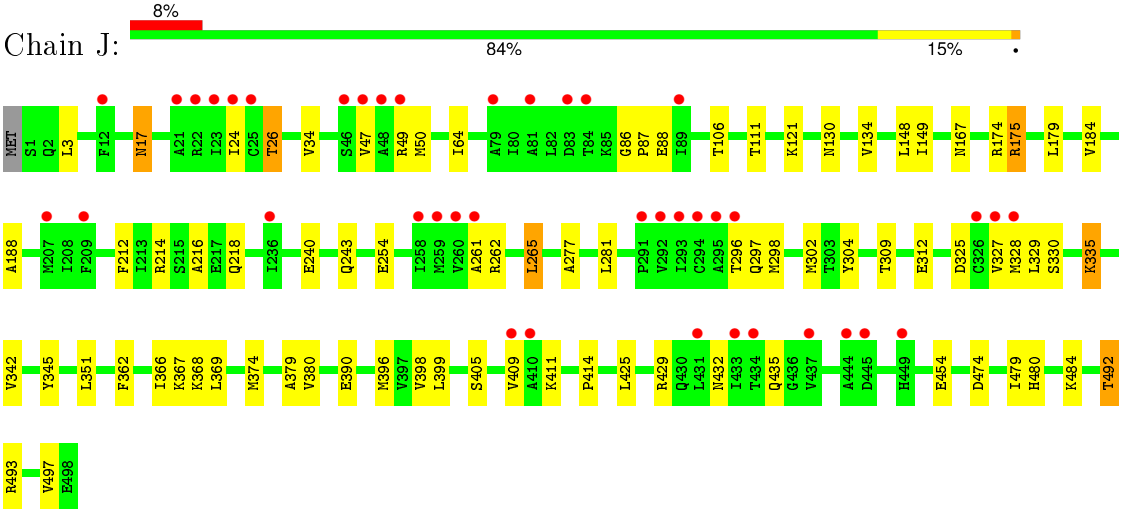
• Molecule 1: Pyruvate kinase

Chain I:



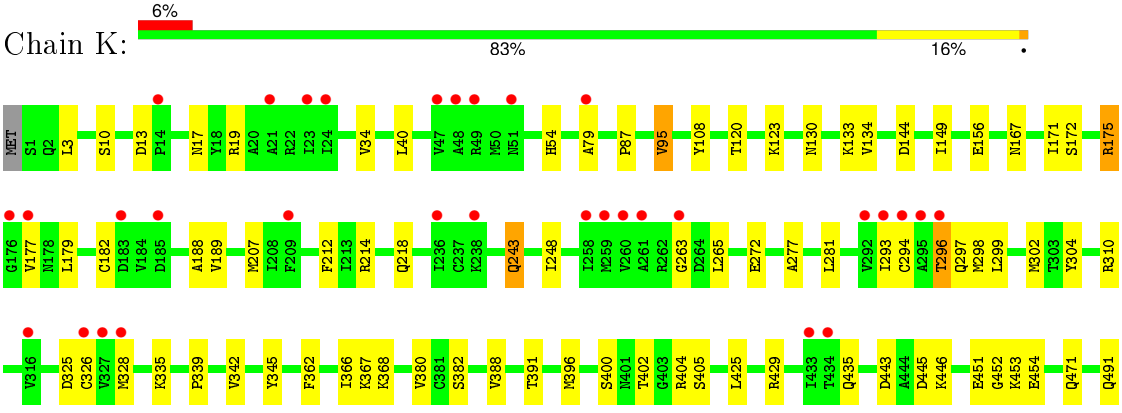
• Molecule 1: Pyruvate kinase

Chain J:



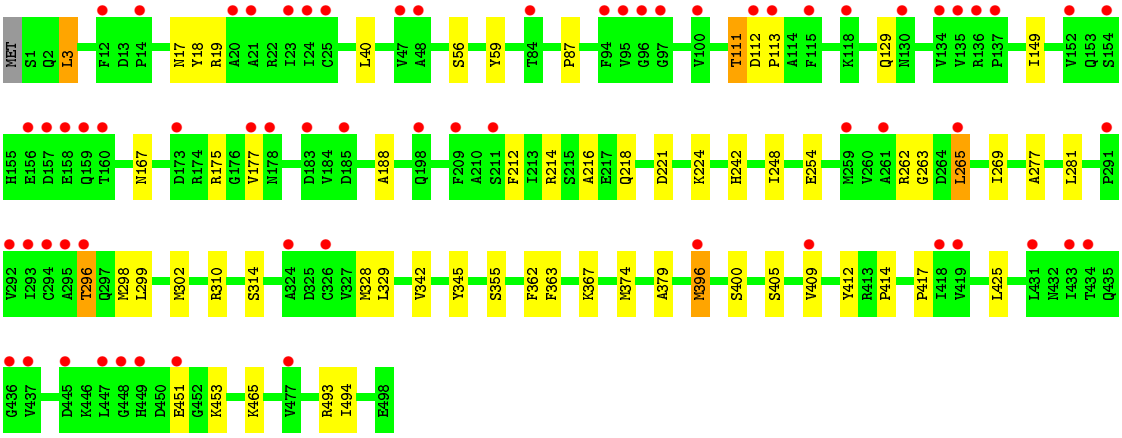
• Molecule 1: Pyruvate kinase

Chain K:



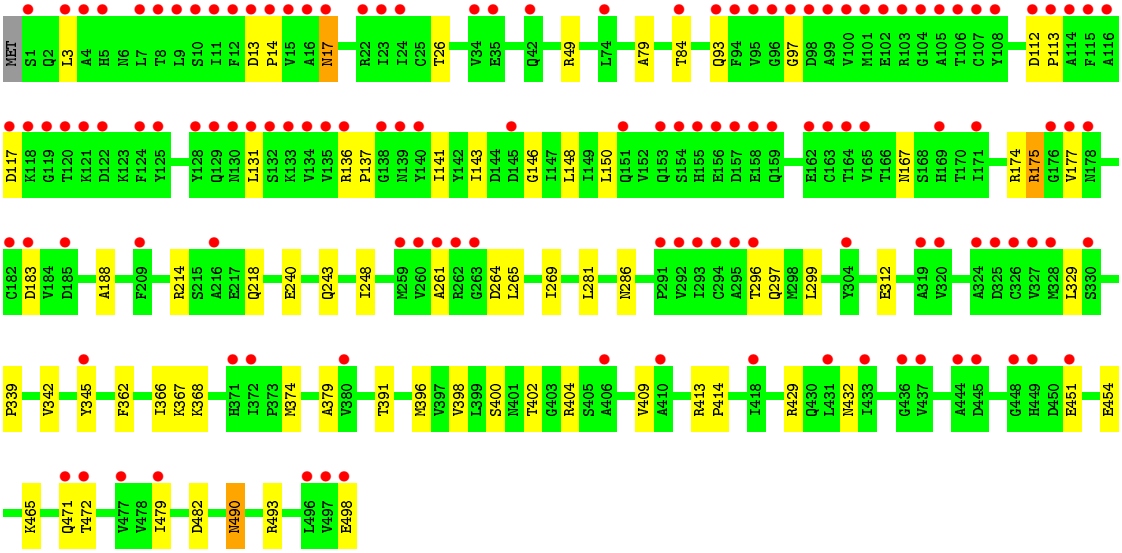
• Molecule 1: Pyruvate kinase

Chain L:



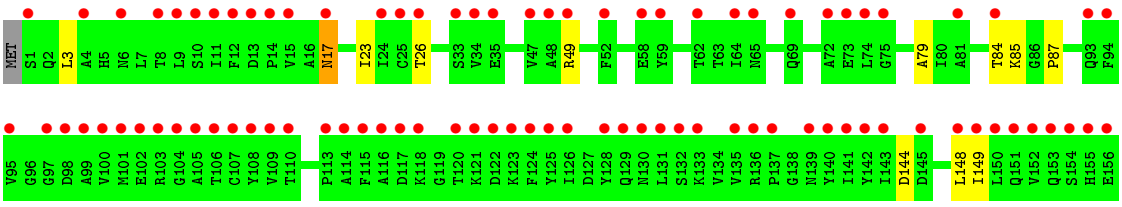
• Molecule 1: Pyruvate kinase

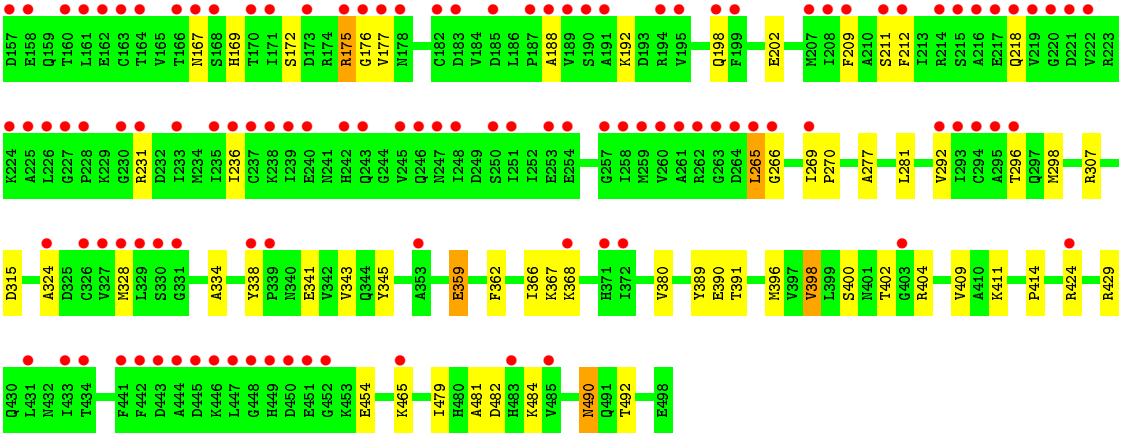
Chain M:



• Molecule 1: Pyruvate kinase

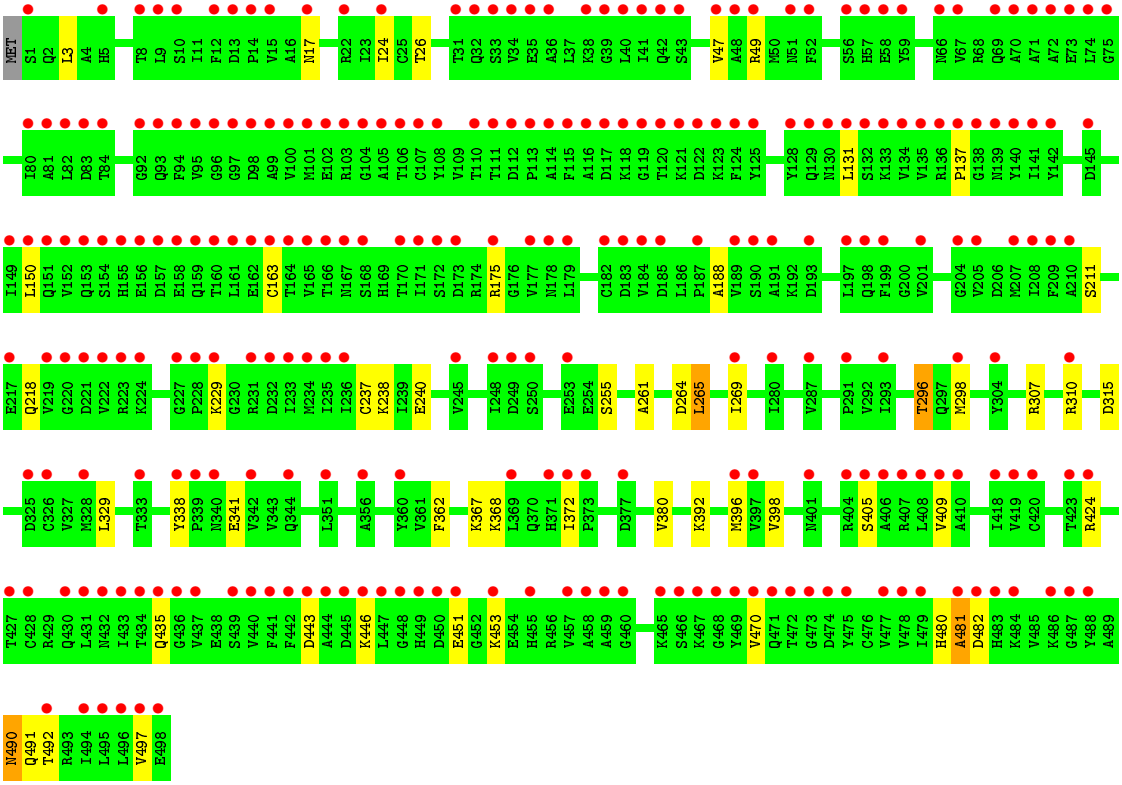
Chain N:





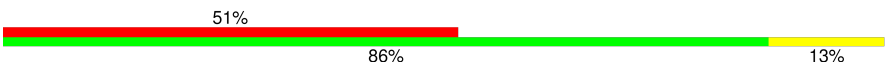
- Molecule 1: Pyruvate kinase

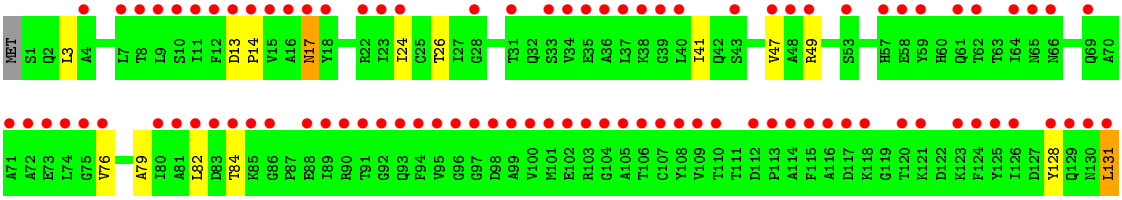
Chain O:

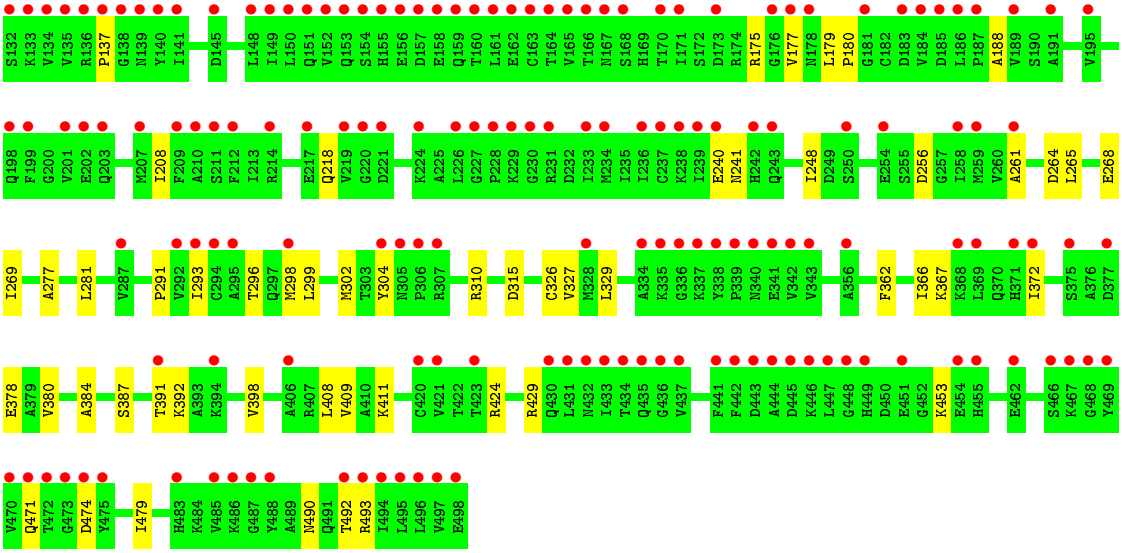


- Molecule 1: Pyruvate kinase

Chain P:






S132 K133 V134 V135 R136 P137 G138 N139 Y140 I141 D145 L148 I149 L150 Q151 V152 Q153 S154 H155 E156 D157 E158 Q159 T160 L161 E162 C163 T164 V165 T166 N167 S168 H169 T170 I171 S172 D173 R174 R175 G176 V177 N178 L179 P180 G181 C182 D183 V184 D185 L186 P187 A188 V189 S190 A191 V195
Q198 F199 G200 V201 E202 Q203 M207 I208 P209 A210 S211 F212 I213 R214 E217 Q218 V219 G220 D221 K224 A225 L226 G227 P228 K229 G230 R231 D232 I233 M234 I235 I236 C237 K238 I239 E240 N241 H242 Q243 I248 D249 S250 E254 S255 D256 G257 I258 M259 V260 A261 D264 L265 E268
I269 A277 L281 V287 P291 V292 I293 C294 A295 T296 Q297 M298 L299 M302 T303 Y304 N305 P306 R307 R310 D315 C326 V327 M328 L329 A334 K335 G336 K337 Y338 P339 N340 E341 V342 V343 A356 F362 I366 K367 K368 L369 Q370 H371 I372 S375 A376 D377
E378 A379 V380 A384 S387 T391 K392 A393 K394 V398 A406 R407 L408 V409 A410 K411 C420 V421 T422 T423 R424 R429 Q430 L431 N432 I433 T434 Q435 G436 V437 F441 F442 D443 A444 D445 K446 L447 G448 H449 D450 E451 G452 K453 E454 H455 E462 S466 K467 G468 Y469
V470 Q471 T472 G473 D474 Y475 I479 H483 K484 V485 K486 G487 Y488 A489 N490 Q491 T492 R493 I494 L495 L496 V497 E498

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	127.49Å 151.14Å 160.32Å 89.73° 80.17° 71.64°	Depositor
Resolution (Å)	34.46 – 2.30 34.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (34.46-2.30) 92.9 (34.09-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.252 0.201 , 0.253	Depositor DCC
R_{free} test set	23579 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 469839 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	65997	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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, MG, K, OXL, FDP, ATP

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	0.34	0/3876	0.50	0/5247
1	B	0.39	0/3856	0.55	0/5220
1	C	0.36	0/3872	0.53	0/5242
1	D	0.40	0/3867	0.55	0/5235
1	E	0.36	0/3865	0.51	0/5232
1	F	0.36	0/3856	0.51	0/5220
1	G	0.33	0/3856	0.49	0/5220
1	H	0.37	0/3874	0.51	0/5244
1	I	0.44	0/3874	0.59	1/5245 (0.0%)
1	J	0.44	0/3882	0.58	0/5256
1	K	0.45	0/3873	0.59	0/5243
1	L	0.41	0/3856	0.56	0/5220
1	M	0.35	0/3856	0.49	0/5220
1	N	0.35	0/3865	0.48	0/5232
1	O	0.34	0/3856	0.47	0/5220
1	P	0.33	0/3856	0.46	0/5220
All	All	0.38	0/61840	0.53	1/83716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	19	ARG	NE-CZ-NH1	-5.07	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3818	0	3813	48	0
1	B	3799	0	3801	66	0
1	C	3815	0	3814	51	0
1	D	3809	0	3807	57	0
1	E	3808	0	3808	38	0
1	F	3799	0	3801	50	0
1	G	3799	0	3801	40	0
1	H	3817	0	3821	46	0
1	I	3816	0	3815	48	0
1	J	3824	0	3820	58	0
1	K	3816	0	3811	49	0
1	L	3799	0	3802	35	0
1	M	3799	0	3802	42	0
1	N	3808	0	3807	39	0
1	O	3799	0	3802	37	0
1	P	3799	0	3802	38	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	P	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	1	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	6	0	0	0	0
4	D	6	0	0	0	0
4	E	6	0	0	0	0
4	F	6	0	0	0	0
4	G	6	0	0	0	0
4	H	6	0	0	0	0
4	I	6	0	0	0	0
4	J	6	0	0	0	0
4	K	6	0	0	0	0
4	L	6	0	0	0	0
4	M	6	0	0	1	0
4	N	6	0	0	0	0
4	P	6	0	0	0	0
5	A	20	0	10	0	0
5	B	20	0	10	0	0
5	C	20	0	10	0	0
5	D	20	0	10	2	0
5	E	20	0	10	0	0
5	F	20	0	10	0	0
5	G	20	0	10	0	0
5	H	20	0	10	0	0
5	I	20	0	9	1	0
5	J	20	0	10	0	0
5	K	20	0	10	0	0
5	L	20	0	10	0	0
5	M	20	0	10	0	0
5	N	20	0	10	2	0
5	O	20	0	10	1	0
5	P	20	0	10	1	0
6	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	31	0	12	0	0
6	C	31	0	12	3	0
6	D	31	0	12	3	0
6	E	31	0	12	1	0
6	F	31	0	12	1	0
6	G	31	0	12	1	0
6	H	31	0	12	1	0
6	I	31	0	12	0	0
6	J	31	0	12	0	0
6	K	31	0	12	2	0
6	L	31	0	12	0	0
6	M	31	0	12	0	0
6	N	31	0	12	0	0
6	P	31	0	12	0	0
7	E	6	0	8	0	0
7	G	6	0	8	0	0
7	I	12	0	16	1	0
7	J	6	0	8	1	0
7	O	6	0	8	0	0
8	A	167	0	0	1	0
8	B	379	0	0	7	0
8	C	305	0	0	0	0
8	D	400	0	0	4	0
8	E	232	0	0	0	0
8	F	187	0	0	1	0
8	G	139	0	0	1	0
8	H	215	0	0	1	0
8	I	415	0	0	6	0
8	J	499	0	0	5	0
8	K	462	0	0	1	0
8	L	316	0	0	2	0
8	M	140	0	0	0	0
8	N	103	0	0	0	0
8	O	69	0	0	0	0
8	P	72	0	0	0	0
All	All	65997	0	61314	710	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 (710) 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:K:388:VAL:HG21	1:K:396:MET:HE1	1.34	1.09
1:C:26:THR:HG22	1:C:49:ARG:HD3	1.40	1.04
1:J:298:MET:HE3	1:J:327:VAL:HB	1.39	1.01
1:K:388:VAL:HG21	1:K:396:MET:CE	1.90	0.99
1:J:398[A]:VAL:HG11	1:J:409:VAL:HG21	1.50	0.92
1:B:396:MET:HE1	1:B:414:PRO:HG3	1.53	0.90
1:J:298:MET:HE1	1:J:328:MET:H	1.35	0.90
1:H:26:THR:CG2	1:H:330:SER:HA	2.02	0.89
1:A:26:THR:HG22	1:A:49:ARG:HD3	1.55	0.89
1:A:396:MET:HE1	1:A:414:PRO:HG3	1.54	0.88
3:I:504:K:K	8:I:678:HOH:O	1.86	0.87
1:F:26:THR:HG22	1:F:49:ARG:HD3	1.55	0.87
1:J:374:MET:CE	1:J:379:ALA:HA	2.05	0.86
1:B:396:MET:CE	1:B:414:PRO:HG3	2.06	0.85
1:C:398[A]:VAL:HG11	1:C:409:VAL:HG21	1.57	0.84
5:N:700:FDP:H11	5:N:700:FDP:O3P	1.75	0.84
1:I:26:THR:HG21	1:I:49:ARG:HH11	1.43	0.83
1:I:26:THR:HG23	1:I:329:LEU:O	1.78	0.83
1:J:111:THR:HG22	8:J:950:HOH:O	1.78	0.82
1:L:248:ILE:HG12	1:L:281:LEU:HD22	1.62	0.82
1:P:453:LYS:NZ	5:P:700:FDP:O1P	2.12	0.81
1:J:380:VAL:HG13	1:J:492:THR:HG22	1.61	0.81
1:J:26:THR:HG23	1:J:329:LEU:O	1.80	0.80
1:A:17:ASN:HD22	1:A:17:ASN:H	1.28	0.80
1:D:26:THR:HG21	1:D:49:ARG:HH11	1.47	0.80
1:F:210:ALA:HB1	1:F:213:ILE:HD11	1.64	0.79
1:H:26:THR:HG23	1:H:330:SER:HA	1.61	0.79
1:G:26:THR:HG22	1:G:49:ARG:HD3	1.63	0.79
1:I:19:ARG:NH1	8:I:507:HOH:O	2.13	0.79
1:B:297:GLN:HE21	1:D:310:ARG:H	1.31	0.78
1:L:374:MET:CE	1:L:379:ALA:HA	2.13	0.78
1:I:10:SER:HB3	1:I:13:ASP:OD1	1.82	0.78
1:A:497:VAL:HB	8:A:748:HOH:O	1.84	0.76
1:F:210:ALA:CB	1:F:213:ILE:CD1	2.62	0.76
1:A:482:ASP:H	1:A:490:ASN:HD21	1.34	0.76
1:F:26:THR:HG21	1:F:49:ARG:HH11	1.49	0.76
1:O:26:THR:HG21	1:O:49:ARG:HH11	1.48	0.76
1:M:26:THR:HG21	1:M:49:ARG:HH11	1.51	0.76
1:A:175:ARG:HE	1:A:175:ARG:HA	1.49	0.75
1:F:210:ALA:CB	1:F:213:ILE:HD11	2.15	0.75
1:E:374:MET:HE2	1:F:390:GLU:HB3	1.69	0.75
1:B:396:MET:HE3	1:B:418:ILE:HG12	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398[A]:VAL:HG12	1:C:479:ILE:HB	1.70	0.74
1:E:26:THR:HG22	1:E:49:ARG:HD3	1.67	0.74
1:B:297:GLN:NE2	1:D:310:ARG:H	1.86	0.73
1:I:374:MET:CE	1:I:379:ALA:HA	2.18	0.73
1:D:364:ASN:O	1:D:368:LYS:HD3	1.89	0.72
1:F:210:ALA:HB3	1:F:213:ILE:CD1	2.19	0.72
1:G:171:ILE:HB	1:G:175:ARG:HG3	1.72	0.72
1:M:398:VAL:HG11	1:M:409:VAL:HG21	1.72	0.72
1:K:298:MET:CE	1:K:328:MET:H	2.03	0.71
1:D:214:ARG:HB2	1:D:243:GLN:HG3	1.73	0.70
1:H:398[A]:VAL:HG11	1:H:409:VAL:HG21	1.72	0.70
1:L:302:MET:HE1	1:L:342:VAL:HA	1.73	0.70
1:D:248:ILE:HG12	1:D:281:LEU:HD22	1.71	0.70
1:D:87:PRO:HD2	1:D:212:PHE:HB2	1.73	0.70
1:N:269:ILE:HG13	1:N:270:PRO:HD2	1.74	0.70
1:I:374:MET:HE2	1:I:379:ALA:HA	1.73	0.69
1:C:384:ALA:HB2	1:C:492:THR:HG21	1.74	0.69
1:A:396:MET:HE1	1:A:414:PRO:CG	2.21	0.69
1:I:297:GLN:HE21	1:K:310:ARG:H	1.41	0.69
1:M:214:ARG:HB2	1:M:243:GLN:HG3	1.74	0.69
1:B:398:VAL:HG11	1:B:409:VAL:HG21	1.75	0.69
1:O:480:HIS:CB	1:O:481:ALA:HB3	2.23	0.69
1:D:298:MET:HE3	1:D:327:VAL:HB	1.74	0.69
1:J:297:GLN:HE21	1:L:310:ARG:H	1.39	0.68
1:C:405:SER:O	1:C:409:VAL:HG23	1.93	0.68
1:J:277:ALA:O	1:J:281:LEU:HG	1.93	0.68
1:I:26:THR:HG21	1:I:49:ARG:NH1	2.07	0.68
1:B:298:MET:CE	1:B:328:MET:H	2.05	0.68
1:D:374:MET:CE	1:D:379:ALA:HA	2.24	0.68
1:G:26:THR:HG21	1:G:49:ARG:HH11	1.59	0.68
1:L:302:MET:HE3	1:L:342:VAL:HG23	1.76	0.68
1:D:487:GLY:HA2	1:I:229:LYS:HG3	1.74	0.68
1:A:398:VAL:HG11	1:A:409:VAL:HG21	1.74	0.68
1:K:188:ALA:HB1	1:K:218:GLN:HG3	1.77	0.67
1:I:87:PRO:HD2	1:I:212:PHE:HB2	1.76	0.67
1:J:26:THR:CG2	1:J:330:SER:HA	2.24	0.67
1:D:451:GLU:CD	1:D:451:GLU:H	1.98	0.67
1:C:26:THR:CG2	1:C:49:ARG:HD3	2.22	0.67
6:D:1001:ATP:H8	6:D:1001:ATP:H5'1	1.59	0.67
1:B:26:THR:HG21	1:B:49:ARG:HH11	1.60	0.66
1:A:17:ASN:N	1:A:17:ASN:HD22	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:THR:HG23	1:D:330:SER:HA	1.77	0.66
1:J:298:MET:CE	1:J:327:VAL:HB	2.23	0.66
1:M:26:THR:HG23	1:M:329:LEU:O	1.96	0.66
1:J:398[A]:VAL:HG12	1:J:479:ILE:HB	1.76	0.65
1:F:310:ARG:H	1:H:297:GLN:HE21	1.45	0.65
1:B:298:MET:HE1	1:B:328:MET:H	1.59	0.65
1:N:398:VAL:HG11	1:N:409:VAL:HG21	1.79	0.65
1:E:26:THR:HG23	1:E:329:LEU:O	1.97	0.65
1:J:297:GLN:NE2	1:L:310:ARG:H	1.94	0.65
1:P:398:VAL:HG11	1:P:409:VAL:HG21	1.77	0.65
1:I:380:VAL:HG13	1:I:492:THR:HG22	1.78	0.65
1:I:26:THR:CG2	1:I:49:ARG:HH11	2.08	0.65
1:F:210:ALA:HB1	1:F:213:ILE:CD1	2.25	0.65
1:O:480:HIS:CA	1:O:481:ALA:HB3	2.26	0.64
1:J:374:MET:HE2	1:J:379:ALA:HA	1.79	0.64
1:E:298:MET:HE1	1:E:328:MET:H	1.61	0.64
1:M:175:ARG:HE	1:M:175:ARG:HA	1.62	0.64
1:O:398:VAL:HG11	1:O:409:VAL:HG21	1.78	0.64
1:E:482:ASP:H	1:E:490:ASN:HD21	1.43	0.64
1:J:26:THR:HG23	1:J:330:SER:HA	1.77	0.64
1:L:19:ARG:NH1	8:L:527:HOH:O	2.30	0.64
1:A:482:ASP:H	1:A:490:ASN:ND2	1.95	0.64
1:I:297:GLN:NE2	1:K:310:ARG:H	1.95	0.64
1:O:480:HIS:HB3	1:O:482:ASP:H	1.63	0.64
1:D:482:ASP:H	1:D:490:ASN:HD21	1.45	0.64
1:B:87:PRO:HD2	1:B:212:PHE:HB2	1.79	0.63
1:B:26:THR:HG23	1:B:329:LEU:O	1.98	0.63
1:O:480:HIS:HA	1:O:481:ALA:HB3	1.79	0.63
1:D:388:VAL:HG21	1:D:396:MET:CE	2.27	0.63
1:A:398:VAL:HG12	1:A:479:ILE:HB	1.81	0.63
1:I:352:GLU:HG2	1:K:272:GLU:O	1.98	0.63
1:J:240:GLU:HB3	1:J:261:ALA:HB3	1.79	0.63
1:I:446:LYS:HG3	1:I:447:LEU:HG	1.81	0.63
1:B:49:ARG:NH2	1:B:83:ASP:OD2	2.32	0.62
1:D:26:THR:HG23	1:D:329:LEU:O	2.00	0.62
1:E:26:THR:HG21	1:E:49:ARG:HH11	1.64	0.62
1:O:480:HIS:HA	1:O:481:ALA:CB	2.30	0.62
1:K:19:ARG:NH1	8:K:519:HOH:O	2.33	0.62
1:J:298:MET:HE1	1:J:328:MET:N	2.11	0.62
1:B:277:ALA:O	1:B:281:LEU:HG	1.99	0.62
1:C:26:THR:HG21	1:C:49:ARG:HH11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:380:VAL:HG13	1:H:492:THR:HG23	1.82	0.61
1:H:262:ARG:NH2	1:H:298:MET:HG2	2.14	0.61
1:M:143:ILE:HB	1:M:148:LEU:HB3	1.81	0.61
1:O:480:HIS:HB3	1:O:481:ALA:HB3	1.82	0.61
1:E:242:HIS:HA	1:E:269:ILE:HD11	1.81	0.61
1:D:299:LEU:HD13	1:D:302:MET:HE3	1.81	0.61
1:A:277:ALA:O	1:A:281:LEU:HG	2.00	0.61
1:H:482:ASP:H	1:H:490:ASN:HD21	1.46	0.61
1:E:298:MET:CE	1:E:328:MET:H	2.14	0.61
1:F:26:THR:CG2	1:F:49:ARG:HH11	2.12	0.61
1:H:396:MET:HE1	1:H:414:PRO:CB	2.31	0.61
1:B:248:ILE:HG12	1:B:281:LEU:HD22	1.81	0.60
1:J:396:MET:HE1	1:J:414:PRO:CB	2.31	0.60
1:A:17:ASN:H	1:A:17:ASN:ND2	1.99	0.60
1:B:26:THR:HG23	1:B:330:SER:HA	1.83	0.60
1:G:366:ILE:HD13	1:G:411:LYS:O	2.01	0.60
1:B:26:THR:HG22	1:B:49:ARG:HE	1.66	0.60
1:H:398[A]:VAL:HG12	1:H:479:ILE:HB	1.84	0.60
1:O:26:THR:HG22	1:O:49:ARG:HD3	1.84	0.59
1:D:298:MET:HE1	1:D:328:MET:H	1.67	0.59
1:J:174:ARG:HD2	7:J:499:GOL:H11	1.85	0.59
1:B:17:ASN:HD22	1:B:17:ASN:H	1.50	0.59
1:H:479:ILE:HG12	1:H:492:THR:HG22	1.84	0.59
1:F:240:GLU:HB2	1:F:264:ASP:HB2	1.84	0.59
1:D:345:TYR:O	1:D:349:ILE:HG13	2.02	0.59
1:F:144:ASP:HB2	1:F:175:ARG:HG3	1.85	0.59
1:B:482:ASP:H	1:B:490:ASN:HD21	1.51	0.59
1:A:474:ASP:O	1:A:497:VAL:HG22	2.03	0.58
1:M:26:THR:HG21	1:M:49:ARG:NH1	2.18	0.58
1:A:3:LEU:HD13	1:C:369:LEU:HD12	1.85	0.58
1:A:405:SER:O	1:A:409:VAL:HG23	2.04	0.58
1:K:325:ASP:HA	1:K:435:GLN:HB2	1.86	0.58
1:N:175:ARG:NE	1:N:175:ARG:HA	2.18	0.58
1:B:398:VAL:HG12	1:B:479:ILE:HB	1.85	0.58
1:H:277:ALA:O	1:H:281:LEU:HG	2.04	0.58
1:A:26:THR:HG21	1:A:49:ARG:HH11	1.68	0.58
1:E:188:ALA:HB1	1:E:218:GLN:HG3	1.86	0.58
1:K:175:ARG:NH2	6:K:1001:ATP:O3'	2.36	0.58
1:D:371:HIS:ND1	8:D:706:HOH:O	2.33	0.57
1:F:482:ASP:H	1:F:490:ASN:HD21	1.51	0.57
1:E:175:ARG:NH2	6:E:1001:ATP:O3'	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:108:TYR:CE1	1:K:156:GLU:HG3	2.38	0.57
1:J:216:ALA:HB1	1:J:254:GLU:HG3	1.84	0.57
1:D:487:GLY:CA	1:I:229:LYS:HG3	2.35	0.57
1:K:388:VAL:HG21	1:K:396:MET:HE2	1.83	0.57
1:J:398[A]:VAL:CG1	1:J:409:VAL:HG21	2.31	0.57
1:C:302:MET:HE3	1:C:342:VAL:HA	1.87	0.57
1:N:188:ALA:HB1	1:N:218:GLN:HG3	1.87	0.57
1:A:374:MET:HE3	1:A:379:ALA:HA	1.87	0.57
1:J:26:THR:HG21	1:J:49:ARG:HH11	1.69	0.56
1:H:396:MET:HE2	1:H:416:CYS:SG	2.45	0.56
1:K:248:ILE:HG12	1:K:281:LEU:HD22	1.87	0.56
1:F:87:PRO:HD2	1:F:212:PHE:HB2	1.87	0.56
1:K:380:VAL:HG23	1:L:494:ILE:HD12	1.86	0.56
1:O:480:HIS:CA	1:O:481:ALA:CB	2.84	0.56
1:L:405:SER:O	1:L:409:VAL:HG23	2.06	0.56
1:A:310:ARG:H	1:C:297:GLN:HE21	1.54	0.56
1:H:384:ALA:CB	1:H:479:ILE:HD11	2.35	0.56
1:M:482:ASP:H	1:M:490:ASN:HD21	1.53	0.56
1:D:490:ASN:HD22	1:D:490:ASN:H	1.53	0.56
1:C:175:ARG:HH22	6:C:1001:ATP:HO3'	1.49	0.56
1:O:26:THR:CG2	1:O:49:ARG:HH11	2.17	0.56
1:M:398:VAL:HG12	1:M:479:ILE:HB	1.88	0.56
1:F:93:GLN:HE21	1:F:174:ARG:HH21	1.54	0.56
1:I:10:SER:OG	1:I:12:PHE:HD2	1.89	0.55
1:B:26:THR:CG2	1:B:49:ARG:HE	2.18	0.55
1:N:400:SER:OG	1:N:402:THR:O	2.19	0.55
1:I:3:LEU:HD11	1:K:366:ILE:HG13	1.87	0.55
1:B:19:ARG:NH1	8:B:513:HOH:O	2.39	0.55
1:J:335:LYS:HE2	8:J:634:HOH:O	2.05	0.55
1:E:366:ILE:HD13	1:E:411:LYS:O	2.05	0.55
1:I:79:ALA:HB2	1:I:429:ARG:O	2.07	0.55
1:I:363:PHE:CZ	1:I:367:LYS:HE3	2.42	0.55
1:J:369:LEU:HD12	1:L:3:LEU:HD13	1.89	0.55
1:P:24:ILE:HG12	1:P:47:VAL:HB	1.89	0.55
1:F:364:ASN:O	1:F:368:LYS:HD3	2.07	0.55
1:P:26:THR:HG21	1:P:49:ARG:HH11	1.70	0.55
1:F:210:ALA:HB3	1:F:213:ILE:HD13	1.88	0.55
1:B:364:ASN:O	1:B:368:LYS:HD3	2.06	0.55
1:N:84:THR:HB	1:N:211:SER:H	1.72	0.55
1:F:396:MET:HE1	1:F:414:PRO:CB	2.37	0.55
1:I:298:MET:CE	1:I:328:MET:H	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:148:LEU:HD13	1:N:169:HIS:HB3	1.89	0.55
1:A:26:THR:CG2	1:A:49:ARG:HH11	2.20	0.54
1:O:26:THR:HG21	1:O:49:ARG:NH1	2.20	0.54
1:B:374:MET:CE	1:B:379:ALA:HA	2.36	0.54
1:M:490:ASN:H	1:M:490:ASN:HD22	1.56	0.54
1:F:175:ARG:NH2	6:F:1001:ATP:O3'	2.41	0.54
1:P:248:ILE:HG12	1:P:281:LEU:HD22	1.89	0.54
1:N:149:ILE:H	1:N:167:ASN:HD21	1.55	0.54
1:C:188:ALA:HB1	1:C:218:GLN:HG3	1.89	0.54
1:C:87:PRO:HD2	1:C:212:PHE:HB2	1.87	0.54
1:C:277:ALA:O	1:C:281:LEU:HG	2.07	0.54
1:H:374:MET:CE	1:H:379:ALA:HA	2.37	0.54
1:K:214:ARG:HB2	1:K:243:GLN:HG3	1.89	0.54
1:J:405:SER:O	1:J:409:VAL:HG23	2.08	0.54
1:G:26:THR:CG2	1:G:49:ARG:HH11	2.21	0.54
1:K:294:CYS:O	1:K:298:MET:HE1	2.08	0.54
1:D:79:ALA:HB2	1:D:429:ARG:O	2.08	0.54
1:H:51:ASN:HA	1:H:83:ASP:HB3	1.87	0.54
1:M:374:MET:CE	1:M:379:ALA:HA	2.38	0.54
1:I:443:ASP:HB3	1:I:446:LYS:HG2	1.90	0.54
1:C:240:GLU:HB3	1:C:261:ALA:HB3	1.88	0.54
1:C:10:SER:HB3	1:C:13:ASP:OD2	2.08	0.54
1:M:79:ALA:HB2	1:M:429:ARG:O	2.07	0.54
1:I:116:ALA:HB3	7:I:499:GOL:H11	1.89	0.54
1:F:143:ILE:HB	1:F:148:LEU:HB3	1.88	0.54
1:D:298:MET:CE	1:D:327:VAL:HB	2.35	0.53
1:N:380:VAL:HG13	1:N:492:THR:HG23	1.90	0.53
1:M:188:ALA:HB1	1:M:218:GLN:HG3	1.90	0.53
1:L:262:ARG:NH2	1:L:298:MET:HG2	2.24	0.53
1:D:188:ALA:HB1	1:D:218:GLN:HG3	1.89	0.53
1:D:246:GLN:HG3	8:D:1886:HOH:O	2.07	0.53
1:O:380:VAL:HG13	1:O:492:THR:HG23	1.89	0.53
1:C:179:LEU:HB3	1:C:182:CYS:HB2	1.91	0.53
1:N:482:ASP:H	1:N:490:ASN:HD21	1.56	0.53
1:P:240:GLU:HB3	1:P:261:ALA:HB3	1.92	0.52
1:I:248:ILE:HG12	1:I:281:LEU:HD22	1.90	0.52
1:D:298:MET:CE	1:D:328:MET:H	2.21	0.52
1:A:374:MET:CE	1:A:379:ALA:HA	2.39	0.52
1:A:47:VAL:HG22	1:A:79:ALA:HB3	1.92	0.52
1:C:298:MET:CE	1:C:328:MET:H	2.23	0.52
1:E:374:MET:CE	1:E:379:ALA:HA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ARG:NH2	6:C:1001:ATP:O3'	2.32	0.52
1:L:87:PRO:HD2	1:L:212:PHE:HB2	1.91	0.52
1:I:298:MET:HE1	1:I:328:MET:H	1.75	0.52
1:D:268:GLU:HG3	8:D:610:HOH:O	2.09	0.52
1:G:303:THR:HG23	1:G:336:GLY:HA2	1.91	0.52
1:A:310:ARG:H	1:C:297:GLN:NE2	2.07	0.52
1:M:297:GLN:HE21	1:O:310:ARG:H	1.58	0.52
1:G:482:ASP:H	1:G:490:ASN:HD21	1.58	0.52
1:M:17:ASN:H	1:M:17:ASN:HD22	1.57	0.52
1:P:17:ASN:HD22	1:P:17:ASN:H	1.57	0.52
1:H:188:ALA:HB1	1:H:218:GLN:HG3	1.91	0.52
1:A:175:ARG:NH2	6:A:1001:ATP:O3'	2.42	0.52
1:K:298:MET:HE1	1:K:328:MET:H	1.75	0.52
1:C:296:THR:HG22	1:C:297:GLN:HG3	1.91	0.52
1:B:472:THR:HG23	1:B:498:GLU:HA	1.92	0.52
1:A:248:ILE:HG12	1:A:281:LEU:HD22	1.91	0.52
1:B:149:ILE:H	1:B:167:ASN:HD21	1.57	0.52
1:A:396:MET:CE	1:A:414:PRO:HG3	2.34	0.52
1:H:298:MET:CE	1:H:328:MET:H	2.22	0.52
1:B:366:ILE:HG13	1:D:3:LEU:HD11	1.92	0.52
1:K:10:SER:HB3	1:K:13:ASP:OD1	2.10	0.52
1:B:17:ASN:HD22	1:B:17:ASN:N	2.08	0.51
1:P:128:TYR:HB3	1:P:131:LEU:HD22	1.92	0.51
1:P:366:ILE:HD13	1:P:411:LYS:O	2.10	0.51
1:N:26:THR:HG23	1:N:334:ALA:HB2	1.92	0.51
1:C:17:ASN:HD22	1:C:17:ASN:N	2.07	0.51
1:L:149:ILE:H	1:L:167:ASN:HD21	1.59	0.51
1:J:184:VAL:HG23	1:J:184:VAL:O	2.11	0.51
1:M:136:ARG:HB3	1:M:137:PRO:HD2	1.91	0.51
1:E:298:MET:HG2	1:E:315:ASP:OD2	2.11	0.51
1:O:443:ASP:HB3	1:O:446:LYS:HG2	1.93	0.51
1:G:108:TYR:HB2	1:G:123:LYS:HG3	1.92	0.51
1:K:299:LEU:HD13	1:K:302:MET:CE	2.41	0.51
1:C:429:ARG:O	1:C:432:ASN:HB2	2.11	0.51
1:P:298:MET:HG2	1:P:315:ASP:OD2	2.10	0.51
1:O:24:ILE:HG12	1:O:47:VAL:HB	1.92	0.51
1:B:387:SER:O	1:B:391:THR:HG22	2.11	0.51
1:B:297:GLN:NE2	1:D:310:ARG:HG2	2.25	0.51
1:L:263:GLY:CA	1:L:296:THR:HG21	2.41	0.51
5:N:700:FDP:C1	5:N:700:FDP:O3P	2.55	0.51
1:C:380:VAL:HG13	1:C:492:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:396:MET:HE3	1:F:414:PRO:HG3	1.93	0.51
1:L:298:MET:CE	1:L:328:MET:H	2.24	0.51
1:O:188:ALA:HB1	1:O:218:GLN:HG3	1.92	0.51
1:B:294:CYS:O	1:B:298:MET:HE1	2.10	0.50
1:B:446:LYS:HG3	1:B:447:LEU:HG	1.92	0.50
1:N:17:ASN:H	1:N:17:ASN:ND2	2.09	0.50
1:F:26:THR:HG23	1:F:329:LEU:O	2.11	0.50
1:J:374:MET:CE	1:J:379:ALA:CA	2.84	0.50
1:G:237:CYS:SG	1:G:255:SER:HB3	2.50	0.50
1:C:144:ASP:HB2	1:C:175:ARG:HG3	1.92	0.50
1:P:277:ALA:O	1:P:281:LEU:HG	2.10	0.50
1:K:79:ALA:HB1	1:K:207:MET:HE3	1.92	0.50
1:C:26:THR:HG21	1:C:49:ARG:NH1	2.27	0.50
1:J:297:GLN:NE2	1:L:310:ARG:HG2	2.26	0.50
1:B:268:GLU:HG3	8:B:615:HOH:O	2.10	0.50
1:K:277:ALA:O	1:K:281:LEU:HG	2.12	0.50
1:I:3:LEU:CD1	1:K:366:ILE:HG13	2.41	0.50
1:O:405:SER:HB2	5:O:700:FDP:O4P	2.12	0.50
1:A:338:TYR:HB3	1:A:341:GLU:HB2	1.92	0.50
1:N:266:GLY:HA3	1:P:310:ARG:HE	1.76	0.50
1:I:268:GLU:HG3	8:I:568:HOH:O	2.12	0.50
1:B:299:LEU:HD13	1:B:302:MET:HE3	1.94	0.50
1:C:26:THR:HG23	1:C:329:LEU:O	2.11	0.50
1:B:396:MET:CE	1:B:418:ILE:HG12	2.38	0.50
1:D:388:VAL:HG21	1:D:396:MET:HE1	1.93	0.50
1:H:481:ALA:HA	1:H:490:ASN:HD22	1.76	0.50
1:O:380:VAL:HG21	1:O:490:ASN:HA	1.94	0.50
1:N:396:MET:CE	1:N:414:PRO:HG3	2.42	0.50
1:O:480:HIS:HB3	1:O:482:ASP:N	2.25	0.50
1:P:380:VAL:HG21	1:P:490:ASN:HA	1.94	0.50
1:E:452:GLY:HA2	1:E:483:HIS:CE1	2.47	0.50
1:F:405:SER:O	1:F:409:VAL:HG23	2.11	0.50
1:O:372:ILE:HG22	1:P:392:LYS:HE2	1.94	0.49
1:M:131:LEU:HD23	1:M:131:LEU:H	1.76	0.49
1:M:93:GLN:HB2	1:M:117:ASP:HA	1.94	0.49
1:P:240:GLU:HB2	1:P:264:ASP:HB2	1.94	0.49
1:C:17:ASN:ND2	1:C:17:ASN:H	2.10	0.49
1:C:372:ILE:HG22	1:D:392:LYS:HE2	1.94	0.49
1:E:15:VAL:HB	1:E:351:LEU:HD22	1.94	0.49
1:A:471:GLN:O	1:A:497:VAL:HG23	2.13	0.49
1:M:26:THR:HG22	1:M:49:ARG:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:THR:CG2	1:B:330:SER:HA	2.43	0.49
1:D:26:THR:HG21	1:D:49:ARG:NH1	2.21	0.49
1:E:156:GLU:HB2	1:E:160:THR:HB	1.94	0.49
1:G:396:MET:HE1	1:G:414:PRO:CB	2.42	0.49
1:H:83:ASP:HA	1:H:209:PHE:HB2	1.94	0.49
1:N:277:ALA:O	1:N:281:LEU:HG	2.13	0.49
1:A:380:VAL:HG23	1:B:494:ILE:HD12	1.94	0.49
1:J:87:PRO:HD2	1:J:212:PHE:HB2	1.95	0.49
1:J:262:ARG:NH2	1:J:298:MET:HG2	2.27	0.49
1:J:366:ILE:HD13	1:J:411:LYS:O	2.12	0.49
1:J:374:MET:HE1	1:J:379:ALA:HA	1.93	0.48
1:F:240:GLU:HA	1:F:265:LEU:HB2	1.93	0.48
1:N:17:ASN:H	1:N:17:ASN:HD22	1.61	0.48
1:A:240:GLU:HB3	1:A:261:ALA:HB3	1.94	0.48
1:F:26:THR:HG21	1:F:49:ARG:NH1	2.24	0.48
1:O:26:THR:HG23	1:O:329:LEU:O	2.12	0.48
1:O:338:TYR:HB3	1:O:341:GLU:HB2	1.94	0.48
1:K:130:ASN:HD21	1:K:133:LYS:HD3	1.77	0.48
1:J:429:ARG:O	1:J:432:ASN:HB2	2.13	0.48
1:I:26:THR:CG2	1:I:330:SER:HA	2.44	0.48
1:A:175:ARG:NE	1:A:175:ARG:HA	2.23	0.48
1:N:298:MET:HG2	1:N:315:ASP:OD2	2.14	0.48
1:K:149:ILE:H	1:K:167:ASN:HD21	1.61	0.48
1:L:374:MET:HE3	1:L:379:ALA:HA	1.95	0.48
1:B:490:ASN:HD22	1:B:490:ASN:H	1.62	0.48
1:M:26:THR:CG2	1:M:49:ARG:HH11	2.21	0.48
1:P:378:GLU:HG3	1:P:408:LEU:HD11	1.95	0.48
1:O:453:LYS:HG3	1:O:480:HIS:HD2	1.78	0.48
1:P:387:SER:O	1:P:391:THR:HG22	2.14	0.48
1:K:491:GLN:OE1	1:K:493:ARG:HD2	2.13	0.48
1:B:396:MET:HE2	1:B:414:PRO:HG3	1.92	0.48
1:P:398:VAL:HG12	1:P:479:ILE:HB	1.96	0.48
1:C:54:HIS:HE1	6:C:1001:ATP:O2B	1.97	0.48
1:I:149:ILE:H	1:I:167:ASN:HD21	1.60	0.48
1:D:26:THR:CG2	1:D:49:ARG:HH11	2.23	0.48
1:N:366:ILE:HD13	1:N:411:LYS:O	2.13	0.48
1:A:396:MET:HE1	1:A:414:PRO:CB	2.42	0.48
1:J:26:THR:CG2	1:J:329:LEU:O	2.58	0.48
1:D:374:MET:HE2	1:D:379:ALA:HA	1.96	0.47
1:D:388:VAL:HG21	1:D:396:MET:HE2	1.96	0.47
1:E:26:THR:HG21	1:E:49:ARG:NH1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:SER:O	1:K:175:ARG:CD	2.62	0.47
1:C:171:ILE:HB	1:C:175:ARG:HG2	1.95	0.47
1:J:26:THR:HG21	1:J:330:SER:HA	1.95	0.47
1:O:150:LEU:HB3	1:O:163:CYS:HB3	1.96	0.47
1:H:34:VAL:HG12	8:H:829:HOH:O	2.15	0.47
1:O:240:GLU:HB3	1:O:261:ALA:HB3	1.96	0.47
1:P:384:ALA:HB2	1:P:492:THR:HG21	1.95	0.47
1:I:310:ARG:HG2	1:K:297:GLN:OE1	2.14	0.47
1:G:476:CYS:HB3	1:G:495:LEU:HD12	1.96	0.47
1:D:26:THR:CG2	1:D:330:SER:HA	2.42	0.47
1:G:79:ALA:HB2	1:G:429:ARG:O	2.13	0.47
1:I:156:GLU:HB2	1:I:160:THR:HB	1.96	0.47
1:N:396:MET:HE1	1:N:414:PRO:CB	2.44	0.47
1:K:263:GLY:CA	1:K:296:THR:HG21	2.44	0.47
1:J:130[B]:ASN:ND2	8:J:694:HOH:O	2.47	0.47
1:K:95:VAL:HG13	1:K:120:THR:HG22	1.97	0.47
1:G:405:SER:O	1:G:409:VAL:HG23	2.15	0.47
1:E:490:ASN:HD22	1:E:490:ASN:H	1.62	0.47
1:H:24:ILE:HB	1:H:328:MET:HG3	1.95	0.47
1:E:269:ILE:HG23	1:E:273:LYS:HB2	1.97	0.47
1:P:26:THR:CG2	1:P:49:ARG:HH11	2.28	0.47
1:A:240:GLU:HB2	1:A:264:ASP:HB2	1.95	0.47
1:N:338:TYR:HB3	1:N:341:GLU:HB2	1.97	0.47
1:J:17:ASN:C	1:J:17:ASN:HD22	2.18	0.47
1:O:453:LYS:HE3	1:O:481:ALA:HB1	1.96	0.47
1:P:299:LEU:HD12	1:P:329:LEU:HD21	1.97	0.47
1:H:299:LEU:HD23	1:H:312:GLU:HB3	1.96	0.47
1:N:198:GLN:HE21	1:N:202:GLU:HG3	1.80	0.47
1:E:263:GLY:CA	1:E:296:THR:HG21	2.45	0.47
1:A:26:THR:HG23	1:A:329:LEU:O	2.14	0.47
1:H:79:ALA:HB2	1:H:429:ARG:O	2.15	0.47
1:C:17:ASN:H	1:C:17:ASN:HD22	1.63	0.47
1:G:186:LEU:HB3	8:G:611:HOH:O	2.15	0.47
1:F:396:MET:HB2	1:F:396:MET:HE2	1.49	0.46
1:F:397:VAL:HB	1:F:478:VAL:HG22	1.97	0.46
1:I:402:THR:OG1	1:I:404:ARG:HB2	2.14	0.46
1:H:26:THR:HG21	1:H:49:ARG:HH11	1.79	0.46
1:C:299:LEU:HB3	1:C:302:MET:HE2	1.98	0.46
1:P:256:ASP:O	1:P:291:PRO:HD2	2.14	0.46
1:N:79:ALA:HB2	1:N:429:ARG:O	2.16	0.46
1:C:248:ILE:HG12	1:C:281:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ALA:O	1:G:265:LEU:HB2	2.16	0.46
1:D:89:ILE:HG22	1:D:177:VAL:HG13	1.97	0.46
1:D:404:ARG:HD3	8:D:628:HOH:O	2.14	0.46
1:H:142:TYR:O	1:H:177:VAL:HA	2.15	0.46
1:A:216:ALA:HB1	1:A:254:GLU:HG3	1.97	0.46
1:M:396:MET:HE1	1:M:414:PRO:HG3	1.96	0.46
1:G:143:ILE:HB	1:G:148:LEU:HB3	1.97	0.46
1:F:56:SER:H	1:F:59:TYR:HB3	1.81	0.46
1:G:374:MET:CE	1:G:379:ALA:HA	2.45	0.46
1:I:144:ASP:HB2	1:I:175:ARG:HG3	1.98	0.46
1:K:172:SER:O	1:K:175:ARG:HD3	2.16	0.46
1:E:310:ARG:H	1:G:297:GLN:NE2	2.12	0.46
1:D:10:SER:HB3	1:D:13:ASP:OD1	2.15	0.46
1:M:374:MET:HE1	1:M:379:ALA:HA	1.98	0.46
1:E:297:GLN:HE21	1:G:309:THR:HB	1.81	0.46
1:G:260:VAL:HG22	1:G:281:LEU:HD12	1.96	0.46
1:E:494:ILE:HD12	1:F:380:VAL:HG23	1.98	0.46
1:C:51:ASN:HA	1:C:83:ASP:HB3	1.97	0.46
1:D:384:ALA:HB2	1:D:492:THR:HG21	1.98	0.46
1:A:188:ALA:HB1	1:A:218:GLN:HG3	1.98	0.46
1:F:131:LEU:HA	1:F:134:VAL:HB	1.98	0.46
1:B:405:SER:O	1:B:409:VAL:HG23	2.16	0.46
1:D:396:MET:HE1	1:D:414:PRO:CB	2.46	0.46
1:E:172:SER:O	1:E:175:ARG:HD3	2.16	0.46
1:K:299:LEU:HD13	1:K:302:MET:HE3	1.98	0.46
1:O:392:LYS:HE2	1:P:372:ILE:HG22	1.98	0.46
1:H:47:VAL:HG22	1:H:79:ALA:HB3	1.98	0.46
1:K:443:ASP:OD2	1:K:446:LYS:HE2	2.16	0.46
1:C:249:ASP:OD1	1:C:284:LYS:NZ	2.45	0.45
1:M:17:ASN:N	1:M:17:ASN:HD22	2.13	0.45
1:E:138:GLY:HA2	1:E:151:GLN:HE21	1.81	0.45
1:L:242:HIS:HD2	8:L:662:HOH:O	1.99	0.45
1:I:26:THR:HG23	1:I:330:SER:HA	1.98	0.45
1:D:396:MET:HE2	1:D:396:MET:HB2	1.78	0.45
1:J:396:MET:HB2	1:J:396:MET:HE2	1.55	0.45
1:P:79:ALA:HB2	1:P:429:ARG:O	2.17	0.45
1:P:293:ILE:HG12	1:P:326:CYS:HB2	1.98	0.45
1:M:141:ILE:HB	1:M:150:LEU:HB2	1.97	0.45
1:N:292:VAL:HG13	1:N:324:ALA:HA	1.98	0.45
1:K:452:GLY:C	1:K:453:LYS:HG2	2.37	0.45
1:G:26:THR:HG23	1:G:329:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:396:MET:HE1	1:J:414:PRO:HB3	1.97	0.45
1:I:143:ILE:HB	1:I:148:LEU:HB3	1.98	0.45
1:K:339:PRO:O	1:K:342:VAL:HG12	2.15	0.45
1:M:299:LEU:HD23	1:M:312:GLU:HB3	1.98	0.45
1:D:304:TYR:HA	1:D:337:LYS:HD3	1.97	0.45
1:H:17:ASN:N	1:H:17:ASN:HD22	2.12	0.45
1:B:374:MET:HE3	1:B:379:ALA:HA	1.97	0.45
1:G:209:PHE:HB3	1:G:238:LYS:HD2	1.98	0.45
1:I:171:ILE:HB	1:I:175:ARG:HG2	1.98	0.45
1:P:82:LEU:HB3	1:P:208:ILE:HD13	1.99	0.45
1:H:338:TYR:HB3	1:H:341:GLU:HB2	1.97	0.45
1:H:175:ARG:NH2	6:H:1001:ATP:O3'	2.48	0.45
1:A:299:LEU:HD23	1:A:312:GLU:HB3	1.97	0.45
1:N:398:VAL:HG12	1:N:479:ILE:HB	1.99	0.45
1:B:443:ASP:HB3	1:B:446:LYS:HG2	1.99	0.45
1:P:188:ALA:HB1	1:P:218:GLN:HG3	1.98	0.45
1:D:487:GLY:HA2	1:I:229:LYS:CG	2.45	0.45
1:F:171:ILE:HB	1:F:175:ARG:HG2	1.99	0.45
1:J:50:MET:SD	1:J:64:ILE:HG13	2.57	0.45
1:N:398:VAL:CG1	1:N:409:VAL:HG21	2.45	0.45
1:A:265:LEU:HD22	1:A:269:ILE:HG12	1.99	0.45
1:E:339:PRO:O	1:E:342:VAL:HG12	2.17	0.45
1:N:481:ALA:HA	1:N:490:ASN:HD22	1.82	0.44
1:B:264:ASP:O	1:B:268:GLU:HB2	2.17	0.44
1:J:214:ARG:HG2	1:J:218:GLN:OE1	2.17	0.44
1:F:299:LEU:HD13	1:F:302:MET:HE3	1.98	0.44
1:F:310:ARG:HG2	1:H:297:GLN:NE2	2.32	0.44
1:F:380:VAL:HG13	1:F:492:THR:HG22	2.00	0.44
1:L:400:SER:HB2	1:L:405:SER:HB2	1.98	0.44
1:C:482:ASP:H	1:C:490:ASN:HD21	1.64	0.44
1:J:309:THR:OG1	1:J:312:GLU:HG3	2.17	0.44
1:G:269:ILE:HG23	1:G:273:LYS:HB2	1.99	0.44
1:G:112:ASP:HA	1:G:113:PRO:HD3	1.81	0.44
1:G:370:GLN:HG3	1:G:412:TYR:OH	2.16	0.44
1:M:374:MET:HE2	1:N:390:GLU:CD	2.37	0.44
1:J:24:ILE:HG12	1:J:47:VAL:HB	1.98	0.44
1:M:429:ARG:O	1:M:432:ASN:HB2	2.17	0.44
1:A:92:GLY:H	1:A:174:ARG:HA	1.83	0.44
1:C:15:VAL:HB	1:C:351:LEU:HD22	1.99	0.44
1:L:221:ASP:HA	1:L:224:LYS:HE2	1.98	0.44
1:L:396:MET:HE1	1:L:414:PRO:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:26:THR:HG21	1:P:49:ARG:NH1	2.31	0.44
1:F:129:GLN:CD	1:F:129:GLN:H	2.20	0.44
1:P:299:LEU:HB3	1:P:302:MET:HE3	1.99	0.44
1:D:405:SER:O	1:D:409:VAL:HG23	2.18	0.44
1:L:277:ALA:O	1:L:281:LEU:HG	2.17	0.44
1:B:296:THR:HG22	1:B:297:GLN:HG3	1.98	0.44
1:P:479:ILE:HG12	1:P:492:THR:HG22	1.99	0.44
1:L:18:TYR:CD2	1:L:417:PRO:HG3	2.52	0.44
1:L:265:LEU:HD22	1:L:269:ILE:HG12	1.99	0.44
1:L:188:ALA:HB1	1:L:218:GLN:HG3	2.00	0.44
1:H:339:PRO:O	1:H:343:VAL:HG23	2.18	0.44
1:E:51:ASN:HA	1:E:83:ASP:HB3	2.00	0.44
1:G:380:VAL:HG13	1:G:492:THR:CG2	2.48	0.44
1:E:26:THR:CG2	1:E:49:ARG:HD3	2.42	0.44
1:F:240:GLU:HB2	1:F:264:ASP:CB	2.47	0.44
1:M:240:GLU:HB2	1:M:264:ASP:HB2	1.99	0.44
1:M:286:ASN:HB3	1:M:366:ILE:HD11	2.00	0.44
1:F:204:GLY:HA3	8:F:711:HOH:O	2.18	0.44
1:J:398[A]:VAL:HG11	1:J:409:VAL:CG2	2.36	0.43
1:O:482:ASP:HB3	1:O:491:GLN:NE2	2.33	0.43
1:D:396:MET:HE1	1:D:414:PRO:HB3	2.00	0.43
1:J:261:ALA:O	1:J:265:LEU:HB2	2.18	0.43
1:C:298:MET:HE3	1:C:328:MET:H	1.82	0.43
1:L:214:ARG:HG2	1:L:218:GLN:OE1	2.18	0.43
1:C:115:PHE:CE2	1:C:123:LYS:HD3	2.53	0.43
1:N:23:ILE:HG21	1:N:343:VAL:HG13	1.99	0.43
1:A:51:ASN:ND2	6:A:1001:ATP:O3A	2.51	0.43
1:B:49:ARG:NH1	8:B:1882:HOH:O	2.48	0.43
1:F:380:VAL:HG21	1:F:490:ASN:HA	2.00	0.43
1:M:339:PRO:O	1:M:342:VAL:HG12	2.18	0.43
1:K:400:SER:HB2	1:K:405:SER:HB2	2.00	0.43
1:E:149:ILE:H	1:E:167:ASN:HD21	1.66	0.43
1:I:404:ARG:NH2	5:I:700:FDP:O6P	2.51	0.43
1:F:256:ASP:O	1:F:291:PRO:HD2	2.17	0.43
1:M:13:ASP:HA	1:M:14:PRO:HD3	1.89	0.43
1:G:15:VAL:HB	1:G:351:LEU:HD22	1.99	0.43
1:J:149:ILE:H	1:J:167:ASN:HD21	1.65	0.43
1:I:198:GLN:HA	1:I:198:GLN:OE1	2.18	0.43
1:B:79:ALA:HB1	1:B:207:MET:HE3	1.99	0.43
1:A:17:ASN:N	1:A:17:ASN:ND2	2.64	0.43
1:L:396:MET:HE2	1:L:396:MET:HB2	1.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:248:ILE:HG12	1:M:281:LEU:HD22	2.00	0.43
1:F:296:THR:HG22	1:F:297:GLN:HG3	2.00	0.43
1:P:47:VAL:HG13	1:P:79:ALA:HB3	2.00	0.43
1:I:214:ARG:HB2	1:I:243:GLN:HG3	2.00	0.43
1:K:293:ILE:HG12	1:K:326:CYS:HB2	2.00	0.43
1:B:339:PRO:O	1:B:342:VAL:HG12	2.18	0.43
1:B:24:ILE:HG12	1:B:47:VAL:HB	2.00	0.43
1:K:175:ARG:N	1:K:175:ARG:HD2	2.34	0.43
1:F:396:MET:CE	1:F:414:PRO:HG3	2.48	0.43
1:N:209:PHE:HD1	1:N:236:ILE:HB	1.84	0.43
1:L:112:ASP:HA	1:L:113:PRO:HD3	1.80	0.43
1:P:241:ASN:HA	1:P:268:GLU:HG2	2.01	0.43
1:C:446:LYS:HG3	1:C:447:LEU:HG	2.01	0.43
1:B:51:ASN:HA	1:B:83:ASP:HB3	2.01	0.43
1:A:374:MET:HE1	1:B:390:GLU:CD	2.39	0.43
1:J:214:ARG:HB2	1:J:243:GLN:HG3	2.01	0.43
1:B:79:ALA:HB2	1:B:429:ARG:O	2.18	0.43
1:I:29:PRO:HA	8:I:637:HOH:O	2.18	0.43
1:J:325:ASP:HA	1:J:435:GLN:HB2	2.01	0.43
5:D:700:FDP:O3P	5:D:700:FDP:O1	2.30	0.43
1:L:216:ALA:HB1	1:L:254:GLU:HG3	1.99	0.43
1:E:26:THR:HG23	1:E:330:SER:HA	2.00	0.43
1:E:380:VAL:HG21	1:E:490:ASN:HA	2.01	0.43
1:B:108:TYR:O	1:B:123:LYS:HA	2.19	0.43
1:A:143:ILE:HD13	1:A:177:VAL:HB	2.01	0.43
1:B:242:HIS:CE1	1:D:12:PHE:HE1	2.37	0.43
1:P:380:VAL:HG13	1:P:492:THR:HG23	2.02	0.42
1:H:299:LEU:HD12	1:H:329:LEU:HD21	2.01	0.42
1:F:478:VAL:HG21	1:F:495:LEU:HD22	2.01	0.42
1:F:237:CYS:HB2	1:F:258:ILE:HD13	2.00	0.42
1:I:374:MET:CE	1:I:379:ALA:CA	2.94	0.42
1:G:175:ARG:NH1	6:G:1001:ATP:O3'	2.52	0.42
1:C:299:LEU:HD23	1:C:312:GLU:HB3	2.01	0.42
1:N:396:MET:HE1	1:N:414:PRO:HG3	2.01	0.42
1:B:223:ARG:NH1	8:B:982:HOH:O	2.52	0.42
1:K:402:THR:OG1	1:K:404:ARG:HB2	2.19	0.42
1:B:216:ALA:HB1	1:B:254:GLU:HG3	2.01	0.42
1:B:49:ARG:NH2	8:B:1882:HOH:O	2.27	0.42
1:G:259:MET:HG3	1:G:293:ILE:HB	2.00	0.42
1:B:285:CYS:HB3	1:B:290:LYS:O	2.19	0.42
1:I:367:LYS:HD3	1:J:390:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:MET:HE1	1:G:414:PRO:HB3	2.01	0.42
1:M:261:ALA:HB1	4:M:510:OXL:C1	2.49	0.42
1:A:10:SER:HB3	1:A:13:ASP:OD1	2.20	0.42
1:B:425:LEU:HD13	1:B:441:PHE:CG	2.54	0.42
1:L:363:PHE:HB2	1:L:412:TYR:O	2.19	0.42
1:B:87:PRO:HB2	8:B:868:HOH:O	2.18	0.42
1:C:237:CYS:HB2	1:C:258:ILE:HD13	2.01	0.42
1:F:91:THR:O	1:F:174:ARG:HA	2.20	0.42
1:P:41:ILE:HG21	1:P:76:VAL:HG21	2.01	0.42
1:L:111:THR:CG2	1:L:129:GLN:HA	2.50	0.42
1:N:359:GLU:HB3	1:N:389:TYR:OH	2.19	0.42
1:K:54:HIS:HE1	6:K:1001:ATP:O2B	2.02	0.42
1:B:299:LEU:HD13	1:B:302:MET:CE	2.50	0.42
1:G:89:ILE:HG22	1:G:177:VAL:HG13	2.01	0.42
1:I:17:ASN:HB3	8:I:798:HOH:O	2.19	0.42
1:C:24:ILE:HG12	1:C:47:VAL:HB	2.01	0.42
1:E:248:ILE:HG12	1:E:281:LEU:HD22	2.01	0.42
1:M:175:ARG:CA	1:M:175:ARG:HE	2.32	0.42
1:O:240:GLU:HB2	1:O:264:ASP:HB2	2.00	0.42
1:J:399:LEU:HG	1:J:480:HIS:HB3	2.02	0.42
1:E:240:GLU:HB3	1:E:261:ALA:HB3	2.01	0.42
1:E:256:ASP:O	1:E:291:PRO:HD2	2.20	0.42
1:G:471:GLN:HB2	1:G:471:GLN:HE21	1.69	0.42
1:D:451:GLU:CD	1:D:451:GLU:N	2.71	0.42
1:E:173:ASP:O	1:E:175:ARG:NH1	2.52	0.42
1:N:144:ASP:N	1:N:176:GLY:O	2.52	0.42
1:H:20:ALA:HB1	1:H:435:GLN:HG2	2.02	0.42
1:G:258:ILE:HB	1:G:285:CYS:SG	2.59	0.42
1:M:400:SER:OG	1:M:402:THR:O	2.25	0.42
1:D:171:ILE:HB	1:D:175:ARG:HG2	2.02	0.42
1:K:171:ILE:HB	1:K:175:ARG:HG2	2.02	0.41
1:K:144:ASP:HB2	1:K:175:ARG:HG3	2.03	0.41
1:C:17:ASN:ND2	1:C:17:ASN:N	2.67	0.41
1:B:307:ARG:HB2	1:B:308:PRO:HD2	2.02	0.41
1:L:374:MET:CE	1:L:379:ALA:CA	2.94	0.41
1:A:481:ALA:HA	1:A:490:ASN:HD22	1.85	0.41
1:D:299:LEU:HD23	1:D:312:GLU:HB3	2.02	0.41
1:D:89:ILE:HG12	1:D:128:TYR:HB2	2.02	0.41
1:B:429:ARG:O	1:B:432:ASN:HB2	2.19	0.41
1:H:377:ASP:HB3	1:H:488:TYR:HB2	2.02	0.41
1:B:10:SER:HB3	1:B:13:ASP:CG	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:298:MET:HE3	1:K:328:MET:H	1.80	0.41
6:D:1001:ATP:H5'1	6:D:1001:ATP:C8	2.48	0.41
1:K:79:ALA:HB2	1:K:429:ARG:O	2.20	0.41
1:H:89:ILE:HG23	1:H:128:TYR:HB2	2.02	0.41
1:H:366:ILE:HD13	1:H:411:LYS:O	2.20	0.41
1:F:109:VAL:HG23	1:F:161:LEU:HB2	2.01	0.41
1:C:143:ILE:HD13	1:C:177:VAL:HB	2.02	0.41
1:J:130[B]:ASN:H	1:J:130[B]:ASN:HD22	1.68	0.41
1:G:380:VAL:HG13	1:G:492:THR:HG23	2.02	0.41
1:I:237:CYS:SG	1:I:255:SER:HB3	2.60	0.41
1:P:179:LEU:HA	1:P:180:PRO:HD3	1.89	0.41
1:H:50:MET:SD	1:H:64:ILE:HG13	2.60	0.41
1:A:298:MET:CE	1:A:328:MET:H	2.34	0.41
1:J:302:MET:CE	1:J:342:VAL:HG23	2.50	0.41
1:M:472:THR:HG23	1:M:498:GLU:HA	2.02	0.41
1:N:87:PRO:HD2	1:N:212:PHE:HB2	2.03	0.41
1:G:26:THR:HG22	1:G:49:ARG:HB3	2.03	0.41
1:O:298:MET:HG2	1:O:315:ASP:OD2	2.20	0.41
1:J:86:GLY:O	1:J:88:GLU:N	2.53	0.41
1:A:282:ILE:HA	1:A:292:VAL:HG21	2.02	0.41
1:N:265:LEU:O	1:N:269:ILE:HG22	2.21	0.41
1:H:24:ILE:HG12	1:H:47:VAL:HB	2.02	0.41
1:F:396:MET:HE1	1:F:414:PRO:HB2	2.03	0.41
1:C:372:ILE:HG23	1:C:373:PRO:HA	2.03	0.41
1:B:435:GLN:NE2	8:B:1233:HOH:O	2.41	0.41
1:G:298:MET:HE1	1:G:327:VAL:HG12	2.01	0.41
1:I:242:HIS:ND1	1:I:269:ILE:HG22	2.35	0.41
1:I:2:GLN:NE2	8:I:683:HOH:O	2.53	0.41
1:H:396:MET:HE1	1:H:414:PRO:HB2	2.01	0.41
1:N:172:SER:HB2	1:N:175:ARG:HH11	1.85	0.41
1:M:240:GLU:HB3	1:M:261:ALA:HB3	2.02	0.41
1:L:451:GLU:O	1:L:453:LYS:HE2	2.20	0.41
1:H:237:CYS:HB2	1:H:258:ILE:HD13	2.03	0.41
1:E:302:MET:HA	1:E:305:ASN:O	2.21	0.41
1:O:470:VAL:HB	1:O:497:VAL:HG21	2.03	0.41
1:B:11:ILE:O	1:D:273:LYS:HD2	2.21	0.41
1:D:24:ILE:HG21	1:D:328:MET:HE2	2.02	0.41
1:N:26:THR:HA	1:N:49:ARG:HB3	2.01	0.41
1:G:209:PHE:HD1	1:G:236:ILE:HB	1.85	0.41
1:K:179:LEU:O	1:K:182:CYS:HB2	2.20	0.41
1:F:15:VAL:HB	1:F:351:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:399:LEU:HG	1:H:480:HIS:HB3	2.03	0.41
1:M:146:GLY:O	1:O:307:ARG:HD2	2.21	0.41
1:O:211:SER:HA	1:O:238:LYS:HB2	2.02	0.41
1:H:263:GLY:CA	1:H:296:THR:HG21	2.51	0.41
1:G:26:THR:CG2	1:G:49:ARG:HD3	2.42	0.41
1:K:294:CYS:O	1:K:298:MET:CE	2.69	0.41
1:G:490:ASN:HD22	1:G:490:ASN:H	1.69	0.41
1:K:87:PRO:HD2	1:K:212:PHE:HB2	2.03	0.41
1:N:85:LYS:HE2	1:N:192:LYS:HD3	2.03	0.41
1:C:452:GLY:C	1:C:453:LYS:HG2	2.41	0.41
1:D:377:ASP:HB3	1:D:488:TYR:CD1	2.56	0.41
1:L:56:SER:H	1:L:59:TYR:HB3	1.85	0.41
1:A:399:LEU:HG	1:A:480:HIS:HB3	2.02	0.41
1:D:262:ARG:NH2	1:D:298:MET:HG2	2.36	0.41
1:K:108:TYR:O	1:K:123:LYS:HA	2.21	0.41
1:J:148:LEU:HA	1:J:167:ASN:HD21	1.84	0.41
5:D:700:FDP:O3P	5:D:700:FDP:C1	2.69	0.41
1:F:298:MET:CE	1:F:327:VAL:HB	2.51	0.41
1:G:397:VAL:HB	1:G:478:VAL:HG22	2.02	0.41
1:P:13:ASP:HA	1:P:14:PRO:HD3	1.94	0.41
1:M:112:ASP:HA	1:M:113:PRO:HD3	1.87	0.41
1:O:229:LYS:HA	1:O:229:LYS:HE2	2.03	0.41
1:C:293:ILE:HG12	1:C:326:CYS:HB2	2.03	0.41
1:M:362:PHE:CD2	1:M:413:ARG:HG3	2.56	0.41
1:D:26:THR:HG22	1:D:49:ARG:HD3	2.03	0.40
1:F:310:ARG:H	1:H:297:GLN:NE2	2.15	0.40
1:B:248:ILE:O	1:B:252:ILE:HG13	2.20	0.40
1:N:298:MET:CE	1:N:328:MET:H	2.34	0.40
1:I:114:ALA:O	1:I:118:LYS:HE2	2.20	0.40
1:J:484:LYS:NZ	8:J:595:HOH:O	2.54	0.40
1:J:474:ASP:O	1:J:497:VAL:HG13	2.20	0.40
1:L:299:LEU:HD12	1:L:329:LEU:HD21	2.02	0.40
1:O:237:CYS:SG	1:O:255:SER:HB3	2.61	0.40
1:E:400:SER:HB2	1:E:405:SER:HB2	2.03	0.40
6:D:1001:ATP:O1G	6:D:1001:ATP:O1A	2.40	0.40
1:H:260:VAL:HG22	1:H:281:LEU:HD12	2.02	0.40
1:P:26:THR:HG22	1:P:49:ARG:HD3	2.03	0.40
1:C:213:ILE:HA	1:C:218:GLN:OE1	2.20	0.40
1:M:136:ARG:HB3	1:M:137:PRO:CD	2.51	0.40
1:P:378:GLU:HA	1:P:408:LEU:HD21	2.02	0.40
1:O:261:ALA:O	1:O:265:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:263:GLY:HA3	1:K:296:THR:HG21	2.02	0.40
1:F:24:ILE:HG12	1:F:47:VAL:HB	2.03	0.40
1:D:115:PHE:CE2	1:D:123:LYS:HD3	2.56	0.40
1:B:34:VAL:O	1:B:38:LYS:HG3	2.21	0.40
1:C:56:SER:H	1:C:59:TYR:HB3	1.86	0.40
1:E:26:THR:CG2	1:E:49:ARG:HH11	2.34	0.40
1:N:396:MET:HE3	1:N:414:PRO:HG3	2.03	0.40
1:M:396:MET:HE1	1:M:414:PRO:CB	2.51	0.40
1:H:402:THR:HG22	1:H:424:ARG:NH2	2.36	0.40
1:J:175:ARG:NH2	8:J:634:HOH:O	2.54	0.40
1:H:17:ASN:H	1:H:17:ASN:HD22	1.67	0.40
1:J:188:ALA:HB1	1:J:218:GLN:HG3	2.04	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	498/499 (100%)	481 (97%)	14 (3%)	3 (1%)	30	36
1	B	496/499 (99%)	486 (98%)	8 (2%)	2 (0%)	39	48
1	C	498/499 (100%)	482 (97%)	15 (3%)	1 (0%)	52	64
1	D	497/499 (100%)	483 (97%)	14 (3%)	0	100	100
1	E	497/499 (100%)	477 (96%)	19 (4%)	1 (0%)	52	64
1	F	496/499 (99%)	480 (97%)	14 (3%)	2 (0%)	39	48
1	G	496/499 (99%)	465 (94%)	27 (5%)	4 (1%)	24	27
1	H	498/499 (100%)	477 (96%)	20 (4%)	1 (0%)	52	64
1	I	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	52	64
1	J	499/499 (100%)	483 (97%)	15 (3%)	1 (0%)	52	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	52	64
1	L	496/499 (99%)	477 (96%)	18 (4%)	1 (0%)	52	64
1	M	496/499 (99%)	472 (95%)	20 (4%)	4 (1%)	24	27
1	N	497/499 (100%)	476 (96%)	20 (4%)	1 (0%)	52	64
1	O	496/499 (99%)	466 (94%)	27 (5%)	3 (1%)	30	36
1	P	496/499 (99%)	469 (95%)	25 (5%)	2 (0%)	39	48
All	All	7952/7984 (100%)	7646 (96%)	278 (4%)	28 (0%)	39	48

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	481	ALA
1	O	296	THR
1	A	174	ARG
1	I	296	THR
1	J	296	THR
1	P	137	PRO
1	B	296	THR
1	F	183	ASP
1	F	377	ASP
1	G	482	ASP
1	M	174	ARG
1	A	296	THR
1	E	296	THR
1	G	174	ARG
1	G	296	THR
1	K	296	THR
1	L	296	THR
1	M	296	THR
1	N	296	THR
1	B	183	ASP
1	C	296	THR
1	H	296	THR
1	M	183	ASP
1	P	296	THR
1	M	97	GLY
1	A	44	GLY
1	O	137	PRO
1	G	44	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	418/417 (100%)	397 (95%)	21 (5%)	30	41
1	B	416/417 (100%)	395 (95%)	21 (5%)	30	41
1	C	418/417 (100%)	401 (96%)	17 (4%)	37	50
1	D	417/417 (100%)	395 (95%)	22 (5%)	28	37
1	E	417/417 (100%)	398 (95%)	19 (5%)	33	44
1	F	416/417 (100%)	398 (96%)	18 (4%)	35	47
1	G	416/417 (100%)	396 (95%)	20 (5%)	31	42
1	H	418/417 (100%)	394 (94%)	24 (6%)	25	34
1	I	418/417 (100%)	391 (94%)	27 (6%)	21	27
1	J	419/417 (100%)	398 (95%)	21 (5%)	30	41
1	K	418/417 (100%)	392 (94%)	26 (6%)	23	30
1	L	416/417 (100%)	400 (96%)	16 (4%)	40	54
1	M	416/417 (100%)	397 (95%)	19 (5%)	33	44
1	N	417/417 (100%)	397 (95%)	20 (5%)	31	42
1	O	416/417 (100%)	401 (96%)	15 (4%)	42	57
1	P	416/417 (100%)	400 (96%)	16 (4%)	40	54
All	All	6672/6672 (100%)	6350 (95%)	322 (5%)	31	42

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	17	ASN
1	A	84	THR
1	A	167	ASN
1	A	175	ARG
1	A	177	VAL
1	A	229	LYS
1	A	265	LEU

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Mol	Chain	Res	Type
1	A	304	TYR
1	A	314	SER
1	A	345	TYR
1	A	351	LEU
1	A	362	PHE
1	A	367	LYS
1	A	368	LYS
1	A	445	ASP
1	A	454	GLU
1	A	471	GLN
1	A	490	ASN
1	A	493	ARG
1	A	495	LEU
1	B	17	ASN
1	B	26	THR
1	B	34	VAL
1	B	40	LEU
1	B	106	THR
1	B	130	ASN
1	B	177	VAL
1	B	229	LYS
1	B	240	GLU
1	B	265	LEU
1	B	307	ARG
1	B	362	PHE
1	B	367	LYS
1	B	368	LYS
1	B	398	VAL
1	B	425	LEU
1	B	435	GLN
1	B	454	GLU
1	B	471	GLN
1	B	490	ASN
1	B	493	ARG
1	C	17	ASN
1	C	40	LEU
1	C	106	THR
1	C	175	ARG
1	C	177	VAL
1	C	179	LEU
1	C	189	VAL
1	C	265	LEU

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Mol	Chain	Res	Type
1	C	345	TYR
1	C	351	LEU
1	C	362	PHE
1	C	367	LYS
1	C	451[A]	GLU
1	C	451[B]	GLU
1	C	490	ASN
1	C	493	ARG
1	C	495	LEU
1	D	3	LEU
1	D	17	ASN
1	D	26	THR
1	D	40	LEU
1	D	106	THR
1	D	174	ARG
1	D	175	ARG
1	D	177	VAL
1	D	229	LYS
1	D	265	LEU
1	D	304	TYR
1	D	307	ARG
1	D	345	TYR
1	D	351	LEU
1	D	362	PHE
1	D	367	LYS
1	D	391	THR
1	D	398	VAL
1	D	451	GLU
1	D	471	GLN
1	D	490	ASN
1	D	493	ARG
1	E	3	LEU
1	E	17	ASN
1	E	26	THR
1	E	175	ARG
1	E	177	VAL
1	E	224	LYS
1	E	265	LEU
1	E	304	TYR
1	E	345	TYR
1	E	351	LEU
1	E	362	PHE

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Mol	Chain	Res	Type
1	E	367	LYS
1	E	368	LYS
1	E	391	THR
1	E	404	ARG
1	E	435	GLN
1	E	465	LYS
1	E	490	ASN
1	E	493	ARG
1	F	13	ASP
1	F	17	ASN
1	F	111	THR
1	F	167	ASN
1	F	175	ARG
1	F	177	VAL
1	F	213	ILE
1	F	214	ARG
1	F	224	LYS
1	F	351	LEU
1	F	362	PHE
1	F	367	LYS
1	F	368	LYS
1	F	454	GLU
1	F	483	HIS
1	F	490	ASN
1	F	492	THR
1	F	493	ARG
1	G	3	LEU
1	G	17	ASN
1	G	157	ASP
1	G	177	VAL
1	G	224	LYS
1	G	265	LEU
1	G	298	MET
1	G	314	SER
1	G	345	TYR
1	G	351	LEU
1	G	362	PHE
1	G	367	LYS
1	G	391	THR
1	G	396	MET
1	G	434	THR
1	G	435	GLN

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Mol	Chain	Res	Type
1	G	471	GLN
1	G	490	ASN
1	G	493	ARG
1	G	495	LEU
1	H	3	LEU
1	H	17	ASN
1	H	26	THR
1	H	40	LEU
1	H	84	THR
1	H	175	ARG
1	H	177	VAL
1	H	224	LYS
1	H	265	LEU
1	H	269	ILE
1	H	304	TYR
1	H	345	TYR
1	H	351	LEU
1	H	362	PHE
1	H	367	LYS
1	H	368	LYS
1	H	396	MET
1	H	400	SER
1	H	435	GLN
1	H	471	GLN
1	H	490	ASN
1	H	493	ARG
1	H	495	LEU
1	H	497	VAL
1	I	3	LEU
1	I	12	PHE
1	I	17	ASN
1	I	26	THR
1	I	34	VAL
1	I	40	LEU
1	I	106	THR
1	I	111	THR
1	I	158	GLU
1	I	175	ARG
1	I	177	VAL
1	I	229	LYS
1	I	265	LEU
1	I	268	GLU

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Mol	Chain	Res	Type
1	I	335	LYS
1	I	345	TYR
1	I	351	LEU
1	I	362	PHE
1	I	367	LYS
1	I	368	LYS
1	I	398[A]	VAL
1	I	398[B]	VAL
1	I	425	LEU
1	I	471	GLN
1	I	492	THR
1	I	493	ARG
1	I	495	LEU
1	J	3	LEU
1	J	17	ASN
1	J	26	THR
1	J	34	VAL
1	J	106	THR
1	J	121	LYS
1	J	134	VAL
1	J	175	ARG
1	J	179	LEU
1	J	265	LEU
1	J	304	TYR
1	J	335	LYS
1	J	345	TYR
1	J	351	LEU
1	J	362	PHE
1	J	367	LYS
1	J	368	LYS
1	J	425	LEU
1	J	454	GLU
1	J	492	THR
1	J	493	ARG
1	K	3	LEU
1	K	17	ASN
1	K	34	VAL
1	K	40	LEU
1	K	95	VAL
1	K	134	VAL
1	K	175	ARG
1	K	177	VAL

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Mol	Chain	Res	Type
1	K	189	VAL
1	K	243	GLN
1	K	265	LEU
1	K	304	TYR
1	K	335	LYS
1	K	345	TYR
1	K	362	PHE
1	K	367	LYS
1	K	368	LYS
1	K	382	SER
1	K	391	THR
1	K	425	LEU
1	K	445	ASP
1	K	451	GLU
1	K	454	GLU
1	K	471	GLN
1	K	495	LEU
1	K	497	VAL
1	L	3	LEU
1	L	17	ASN
1	L	40	LEU
1	L	111	THR
1	L	175	ARG
1	L	177	VAL
1	L	265	LEU
1	L	314	SER
1	L	345	TYR
1	L	355	SER
1	L	362	PHE
1	L	367	LYS
1	L	396	MET
1	L	425	LEU
1	L	465	LYS
1	L	493	ARG
1	M	3	LEU
1	M	17	ASN
1	M	84	THR
1	M	167	ASN
1	M	175	ARG
1	M	177	VAL
1	M	265	LEU
1	M	269	ILE

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Mol	Chain	Res	Type
1	M	345	TYR
1	M	367	LYS
1	M	368	LYS
1	M	391	THR
1	M	404	ARG
1	M	451	GLU
1	M	454	GLU
1	M	465	LYS
1	M	471	GLN
1	M	490	ASN
1	M	493	ARG
1	N	3	LEU
1	N	17	ASN
1	N	175	ARG
1	N	177	VAL
1	N	231	ARG
1	N	265	LEU
1	N	307	ARG
1	N	345	TYR
1	N	359	GLU
1	N	362	PHE
1	N	367	LYS
1	N	368	LYS
1	N	391	THR
1	N	398	VAL
1	N	404	ARG
1	N	424	ARG
1	N	454	GLU
1	N	465	LYS
1	N	484	LYS
1	N	490	ASN
1	O	3	LEU
1	O	17	ASN
1	O	131	LEU
1	O	175	ARG
1	O	265	LEU
1	O	269	ILE
1	O	296	THR
1	O	362	PHE
1	O	367	LYS
1	O	368	LYS
1	O	396	MET

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Mol	Chain	Res	Type
1	O	424	ARG
1	O	435	GLN
1	O	451	GLU
1	O	490	ASN
1	P	3	LEU
1	P	17	ASN
1	P	84	THR
1	P	131	LEU
1	P	175	ARG
1	P	177	VAL
1	P	265	LEU
1	P	269	ILE
1	P	304	TYR
1	P	327	VAL
1	P	362	PHE
1	P	367	LYS
1	P	424	ARG
1	P	471	GLN
1	P	474	ASP
1	P	493	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	17	ASN
1	A	54	HIS
1	A	65	ASN
1	A	167	ASN
1	A	286	ASN
1	A	297	GLN
1	A	322	ASN
1	A	344	GLN
1	A	471	GLN
1	A	490	ASN
1	B	2	GLN
1	B	17	ASN
1	B	42	GLN
1	B	167	ASN
1	B	178	ASN
1	B	242	HIS
1	B	243	GLN

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Mol	Chain	Res	Type
1	B	297	GLN
1	B	305	ASN
1	B	322	ASN
1	B	344	GLN
1	B	490	ASN
1	B	491	GLN
1	C	17	ASN
1	C	54	HIS
1	C	178	ASN
1	C	243	GLN
1	C	286	ASN
1	C	297	GLN
1	C	305	ASN
1	C	322	ASN
1	C	344	GLN
1	C	490	ASN
1	D	2	GLN
1	D	17	ASN
1	D	42	GLN
1	D	167	ASN
1	D	178	ASN
1	D	305	ASN
1	D	344	GLN
1	D	435	GLN
1	D	490	ASN
1	E	17	ASN
1	E	151	GLN
1	E	167	ASN
1	E	178	ASN
1	E	297	GLN
1	E	401	ASN
1	E	483	HIS
1	E	490	ASN
1	E	491	GLN
1	F	17	ASN
1	F	42	GLN
1	F	167	ASN
1	F	278	GLN
1	F	286	ASN
1	F	297	GLN
1	F	322	ASN
1	F	490	ASN

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Mol	Chain	Res	Type
1	G	17	ASN
1	G	57	HIS
1	G	139	ASN
1	G	167	ASN
1	G	243	GLN
1	G	297	GLN
1	G	322	ASN
1	G	386	ASN
1	G	471	GLN
1	G	490	ASN
1	H	17	ASN
1	H	93	GLN
1	H	167	ASN
1	H	297	GLN
1	H	386	ASN
1	H	401	ASN
1	H	490	ASN
1	I	2	GLN
1	I	17	ASN
1	I	167	ASN
1	I	178	ASN
1	I	297	GLN
1	I	305	ASN
1	I	344	GLN
1	I	401	ASN
1	I	435	GLN
1	J	17	ASN
1	J	54	HIS
1	J	93	GLN
1	J	167	ASN
1	J	246	GLN
1	J	297	GLN
1	J	305	ASN
1	J	401	ASN
1	K	17	ASN
1	K	54	HIS
1	K	130	ASN
1	K	167	ASN
1	K	178	ASN
1	K	243	GLN
1	K	305	ASN
1	K	344	GLN

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Mol	Chain	Res	Type
1	K	435	GLN
1	K	471	GLN
1	L	2	GLN
1	L	17	ASN
1	L	42	GLN
1	L	54	HIS
1	L	167	ASN
1	L	178	ASN
1	L	242	HIS
1	L	243	GLN
1	L	318	ASN
1	L	344	GLN
1	L	401	ASN
1	M	17	ASN
1	M	167	ASN
1	M	178	ASN
1	M	278	GLN
1	M	286	ASN
1	M	297	GLN
1	M	322	ASN
1	M	401	ASN
1	M	490	ASN
1	N	17	ASN
1	N	42	GLN
1	N	51	ASN
1	N	54	HIS
1	N	167	ASN
1	N	198	GLN
1	N	242	HIS
1	N	243	GLN
1	N	286	ASN
1	N	344	GLN
1	N	471	GLN
1	N	490	ASN
1	O	17	ASN
1	O	42	GLN
1	O	480	HIS
1	O	490	ASN
1	O	491	GLN
1	P	17	ASN
1	P	318	ASN
1	P	322	ASN

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 114 ligands modelled in this entry, 62 are monoatomic - leaving 52 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	$\#\|Z\| > 2$
6	ATP	A	1001	3,2	24,33,33	1.06	1 (4%)	31,52,52	1.88	6 (19%)
4	OXL	A	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	A	700	-	20,20,20	0.88	0	27,32,32	1.28	3 (11%)
6	ATP	B	1001	3,2	24,33,33	0.97	1 (4%)	31,52,52	2.03	6 (19%)
4	OXL	B	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	B	700	-	20,20,20	1.37	2 (10%)	27,32,32	1.64	5 (18%)
6	ATP	C	1001	3,2	24,33,33	1.10	2 (8%)	31,52,52	1.97	6 (19%)
4	OXL	C	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	C	700	-	20,20,20	0.86	0	27,32,32	1.60	4 (14%)
6	ATP	D	1001	3,2	24,33,33	1.03	1 (4%)	31,52,52	2.14	7 (22%)
4	OXL	D	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	D	700	-	20,20,20	1.31	2 (10%)	27,32,32	1.57	2 (7%)
6	ATP	E	1001	3,2	24,33,33	1.07	2 (8%)	31,52,52	2.05	5 (16%)
7	GOL	E	499	-	5,5,5	0.36	0	5,5,5	0.25	0
4	OXL	E	510	2	0,5,5	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FDP	E	700	-	20,20,20	1.15	2 (10%)	27,32,32	1.09	2 (7%)
6	ATP	F	1001	3,2	24,33,33	1.10	2 (8%)	31,52,52	1.93	5 (16%)
4	OXL	F	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	F	700	-	20,20,20	1.04	0	27,32,32	1.39	4 (14%)
6	ATP	G	1001	2	24,33,33	1.03	1 (4%)	31,52,52	1.98	5 (16%)
7	GOL	G	499	-	5,5,5	0.36	0	5,5,5	0.24	0
4	OXL	G	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	G	700	-	20,20,20	1.20	2 (10%)	27,32,32	1.47	5 (18%)
6	ATP	H	1001	3,2	24,33,33	1.02	1 (4%)	31,52,52	1.92	5 (16%)
4	OXL	H	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	H	700	-	20,20,20	1.03	2 (10%)	27,32,32	1.53	4 (14%)
6	ATP	I	1001	3,2	24,33,33	1.11	2 (8%)	31,52,52	1.97	6 (19%)
7	GOL	I	499	-	5,5,5	0.34	0	5,5,5	0.24	0
7	GOL	I	501	-	5,5,5	0.37	0	5,5,5	0.41	0
4	OXL	I	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	I	700	-	20,20,20	1.89	4 (20%)	27,32,32	1.39	2 (7%)
6	ATP	J	1001	3,2	24,33,33	1.07	2 (8%)	31,52,52	2.05	4 (12%)
7	GOL	J	499	-	5,5,5	0.33	0	5,5,5	0.35	0
4	OXL	J	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	J	700	-	20,20,20	1.12	2 (10%)	27,32,32	1.42	5 (18%)
6	ATP	K	1001	3,2	24,33,33	0.98	1 (4%)	31,52,52	1.93	4 (12%)
4	OXL	K	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	K	700	-	20,20,20	1.02	1 (5%)	27,32,32	1.56	7 (25%)
6	ATP	L	1001	3,2	24,33,33	1.11	2 (8%)	31,52,52	1.99	6 (19%)
4	OXL	L	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	L	700	-	20,20,20	1.16	2 (10%)	27,32,32	1.72	4 (14%)
6	ATP	M	1001	3,2	24,33,33	1.06	2 (8%)	31,52,52	1.91	5 (16%)
4	OXL	M	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	M	700	-	20,20,20	0.69	0	27,32,32	1.18	3 (11%)
6	ATP	N	1001	3,2	24,33,33	1.06	2 (8%)	31,52,52	1.92	5 (16%)
4	OXL	N	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	N	700	-	20,20,20	1.08	2 (10%)	27,32,32	1.33	2 (7%)
7	GOL	O	499	-	5,5,5	0.34	0	5,5,5	0.21	0
5	FDP	O	700	-	20,20,20	1.05	1 (5%)	27,32,32	1.08	2 (7%)
6	ATP	P	1001	3,2	24,33,33	1.04	2 (8%)	31,52,52	1.87	5 (16%)
4	OXL	P	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	P	700	-	20,20,20	1.15	3 (15%)	27,32,32	0.87	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
6	ATP	A	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	A	510	2	-	0/0/4/4	0/0/0/0
5	FDP	A	700	-	-	0/12/34/34	0/1/1/1
6	ATP	B	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	B	510	2	-	0/0/4/4	0/0/0/0
5	FDP	B	700	-	-	0/12/34/34	0/1/1/1
6	ATP	C	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	C	510	2	-	0/0/4/4	0/0/0/0
5	FDP	C	700	-	-	0/12/34/34	0/1/1/1
6	ATP	D	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	D	510	2	-	0/0/4/4	0/0/0/0
5	FDP	D	700	-	-	0/12/34/34	0/1/1/1
6	ATP	E	1001	3,2	-	0/18/38/38	0/3/3/3
7	GOL	E	499	-	-	0/4/4/4	0/0/0/0
4	OXL	E	510	2	-	0/0/4/4	0/0/0/0
5	FDP	E	700	-	-	0/12/34/34	0/1/1/1
6	ATP	F	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	F	510	2	-	0/0/4/4	0/0/0/0
5	FDP	F	700	-	-	0/12/34/34	0/1/1/1
6	ATP	G	1001	2	-	0/18/38/38	0/3/3/3
7	GOL	G	499	-	-	0/4/4/4	0/0/0/0
4	OXL	G	510	2	-	0/0/4/4	0/0/0/0
5	FDP	G	700	-	-	0/12/34/34	0/1/1/1
6	ATP	H	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	H	510	2	-	0/0/4/4	0/0/0/0
5	FDP	H	700	-	-	0/12/34/34	0/1/1/1
6	ATP	I	1001	3,2	-	0/18/38/38	0/3/3/3
7	GOL	I	499	-	-	0/4/4/4	0/0/0/0
7	GOL	I	501	-	-	0/4/4/4	0/0/0/0
4	OXL	I	510	2	-	0/0/4/4	0/0/0/0
5	FDP	I	700	-	-	0/12/34/34	0/1/1/1
6	ATP	J	1001	3,2	-	0/18/38/38	0/3/3/3
7	GOL	J	499	-	-	0/4/4/4	0/0/0/0
4	OXL	J	510	2	-	0/0/4/4	0/0/0/0
5	FDP	J	700	-	-	0/12/34/34	0/1/1/1
6	ATP	K	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	K	510	2	-	0/0/4/4	0/0/0/0
5	FDP	K	700	-	-	0/12/34/34	0/1/1/1
6	ATP	L	1001	3,2	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OXL	L	510	2	-	0/0/4/4	0/0/0/0
5	FDP	L	700	-	-	0/12/34/34	0/1/1/1
6	ATP	M	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	M	510	2	-	0/0/4/4	0/0/0/0
5	FDP	M	700	-	-	0/12/34/34	0/1/1/1
6	ATP	N	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	N	510	2	-	0/0/4/4	0/0/0/0
5	FDP	N	700	-	-	0/12/34/34	0/1/1/1
7	GOL	O	499	-	-	0/4/4/4	0/0/0/0
5	FDP	O	700	-	-	0/12/34/34	0/1/1/1
6	ATP	P	1001	3,2	-	0/18/38/38	0/3/3/3
4	OXL	P	510	2	-	0/0/4/4	0/0/0/0
5	FDP	P	700	-	-	0/12/34/34	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	700	FDP	O2-C2	-4.74	1.35	1.47
5	B	700	FDP	P2-O6	-4.35	1.45	1.60
5	I	700	FDP	P1-O2P	-4.08	1.40	1.54
5	D	700	FDP	O2-C2	-3.50	1.38	1.47
5	I	700	FDP	O3-C3	-3.01	1.36	1.42
5	E	700	FDP	P2-O6	-2.88	1.50	1.60
5	H	700	FDP	O2-C2	-2.75	1.40	1.47
5	L	700	FDP	O2-C2	-2.74	1.40	1.47
5	I	700	FDP	P2-O6	-2.70	1.51	1.60
5	J	700	FDP	O4-C4	-2.39	1.37	1.43
5	J	700	FDP	P2-O5P	-2.34	1.46	1.54
5	K	700	FDP	P1-O2P	-2.25	1.46	1.54
5	L	700	FDP	P2-O6	-2.25	1.52	1.60
5	B	700	FDP	P1-O3P	-2.18	1.46	1.54
5	O	700	FDP	P1-O3P	2.02	1.62	1.54
5	N	700	FDP	P1-O2P	2.03	1.62	1.54
5	P	700	FDP	P2-O5P	2.05	1.62	1.54
6	P	1001	ATP	O4'-C1'	2.07	1.43	1.41
6	N	1001	ATP	O4'-C1'	2.07	1.43	1.41
5	P	700	FDP	P1-O2P	2.15	1.62	1.54
6	M	1001	ATP	O4'-C1'	2.16	1.43	1.41
5	H	700	FDP	P2-O5P	2.18	1.62	1.54
6	E	1001	ATP	O4'-C1'	2.22	1.44	1.41
6	J	1001	ATP	O4'-C1'	2.25	1.44	1.41
6	C	1001	ATP	O4'-C1'	2.26	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	700	FDP	P2-O6P	2.28	1.62	1.54
5	N	700	FDP	P2-O5P	2.30	1.63	1.54
6	F	1001	ATP	O4'-C1'	2.45	1.44	1.41
6	L	1001	ATP	O4'-C1'	2.48	1.44	1.41
5	E	700	FDP	O5-C2	2.48	1.48	1.42
5	P	700	FDP	P1-O3P	2.51	1.63	1.54
6	I	1001	ATP	O4'-C1'	2.52	1.44	1.41
5	G	700	FDP	O5-C2	2.55	1.48	1.42
5	D	700	FDP	O5-C5	2.77	1.50	1.43
6	K	1001	ATP	C5-C4	3.03	1.47	1.40
6	J	1001	ATP	C5-C4	3.14	1.47	1.40
6	B	1001	ATP	C5-C4	3.14	1.47	1.40
6	I	1001	ATP	C5-C4	3.23	1.47	1.40
6	P	1001	ATP	C5-C4	3.26	1.47	1.40
6	E	1001	ATP	C5-C4	3.28	1.47	1.40
6	H	1001	ATP	C5-C4	3.29	1.47	1.40
6	F	1001	ATP	C5-C4	3.29	1.47	1.40
6	G	1001	ATP	C5-C4	3.33	1.48	1.40
6	D	1001	ATP	C5-C4	3.36	1.48	1.40
6	N	1001	ATP	C5-C4	3.39	1.48	1.40
6	A	1001	ATP	C5-C4	3.42	1.48	1.40
6	M	1001	ATP	C5-C4	3.42	1.48	1.40
6	C	1001	ATP	C5-C4	3.44	1.48	1.40
6	L	1001	ATP	C5-C4	3.46	1.48	1.40

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1001	ATP	N3-C2-N1	-8.26	122.57	128.89
6	E	1001	ATP	N3-C2-N1	-7.76	122.95	128.89
6	J	1001	ATP	N3-C2-N1	-7.58	123.09	128.89
6	G	1001	ATP	N3-C2-N1	-7.43	123.20	128.89
6	L	1001	ATP	N3-C2-N1	-7.39	123.23	128.89
6	P	1001	ATP	N3-C2-N1	-7.37	123.25	128.89
6	K	1001	ATP	N3-C2-N1	-7.32	123.29	128.89
6	N	1001	ATP	N3-C2-N1	-7.24	123.35	128.89
6	M	1001	ATP	N3-C2-N1	-7.16	123.41	128.89
6	I	1001	ATP	N3-C2-N1	-7.16	123.41	128.89
6	F	1001	ATP	N3-C2-N1	-7.15	123.42	128.89
6	H	1001	ATP	N3-C2-N1	-6.98	123.55	128.89
6	A	1001	ATP	N3-C2-N1	-6.89	123.62	128.89
6	D	1001	ATP	N3-C2-N1	-6.75	123.73	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1001	ATP	N3-C2-N1	-6.74	123.74	128.89
6	J	1001	ATP	C2'-C1'-N9	-5.45	105.96	114.29
6	K	1001	ATP	C2'-C1'-N9	-5.33	106.14	114.29
6	D	1001	ATP	C2'-C1'-N9	-5.18	106.37	114.29
6	C	1001	ATP	C2'-C1'-N9	-4.97	106.70	114.29
6	B	1001	ATP	C2'-C1'-N9	-4.92	106.78	114.29
6	I	1001	ATP	C2'-C1'-N9	-4.86	106.87	114.29
6	E	1001	ATP	C2'-C1'-N9	-4.73	107.07	114.29
6	F	1001	ATP	C2'-C1'-N9	-4.61	107.25	114.29
6	D	1001	ATP	PA-O3A-PB	-4.12	121.17	132.73
6	M	1001	ATP	C2'-C1'-N9	-4.01	108.17	114.29
6	H	1001	ATP	C2'-C1'-N9	-3.97	108.22	114.29
6	G	1001	ATP	PA-O3A-PB	-3.78	122.11	132.73
6	G	1001	ATP	C2'-C1'-N9	-3.67	108.69	114.29
6	L	1001	ATP	C2'-C1'-N9	-3.61	108.77	114.29
6	A	1001	ATP	C2'-C1'-N9	-3.57	108.84	114.29
5	G	700	FDP	C6-C5-C4	-3.45	101.50	115.21
5	I	700	FDP	O5-C2-C3	-3.40	97.83	105.58
5	H	700	FDP	C6-C5-C4	-3.36	101.88	115.21
6	A	1001	ATP	PA-O3A-PB	-3.35	123.33	132.73
6	H	1001	ATP	PA-O3A-PB	-3.32	123.42	132.73
6	N	1001	ATP	PB-O3B-PG	-3.30	121.60	132.67
6	L	1001	ATP	PA-O3A-PB	-3.26	123.57	132.73
5	B	700	FDP	C6-C5-C4	-3.23	102.39	115.21
6	F	1001	ATP	PB-O3B-PG	-3.20	121.95	132.67
6	C	1001	ATP	C4-C5-N7	-3.19	106.55	109.48
6	N	1001	ATP	C4-C5-N7	-3.14	106.59	109.48
6	J	1001	ATP	C4-C5-N7	-3.13	106.60	109.48
6	I	1001	ATP	C4-C5-N7	-3.09	106.64	109.48
6	E	1001	ATP	PA-O3A-PB	-3.03	124.23	132.73
6	D	1001	ATP	C4-C5-N7	-3.01	106.71	109.48
6	N	1001	ATP	PA-O3A-PB	-3.01	124.29	132.73
6	P	1001	ATP	PB-O3B-PG	-2.99	122.63	132.67
5	B	700	FDP	O5-C2-C3	-2.99	98.77	105.58
6	F	1001	ATP	C4-C5-N7	-2.99	106.73	109.48
6	G	1001	ATP	PB-O3B-PG	-2.96	122.75	132.67
6	M	1001	ATP	C4-C5-N7	-2.95	106.77	109.48
6	M	1001	ATP	PA-O3A-PB	-2.93	124.50	132.73
5	F	700	FDP	O6P-P2-O6	-2.93	98.14	106.56
5	F	700	FDP	O5-C2-C3	-2.92	98.93	105.58
6	P	1001	ATP	C4-C5-N7	-2.91	106.81	109.48
6	M	1001	ATP	PB-O3B-PG	-2.88	123.00	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1001	ATP	C4-C5-N7	-2.88	106.83	109.48
6	H	1001	ATP	C4-C5-N7	-2.85	106.86	109.48
5	K	700	FDP	C6-C5-C4	-2.83	103.96	115.21
6	C	1001	ATP	PB-O3B-PG	-2.80	123.30	132.67
6	A	1001	ATP	C4-C5-N7	-2.79	106.91	109.48
6	L	1001	ATP	PB-O3B-PG	-2.79	123.31	132.67
6	K	1001	ATP	C4-C5-N7	-2.74	106.96	109.48
6	G	1001	ATP	C4-C5-N7	-2.72	106.98	109.48
5	L	700	FDP	C6-C5-C4	-2.67	104.61	115.21
6	N	1001	ATP	C2'-C1'-N9	-2.66	110.23	114.29
6	I	1001	ATP	PA-O3A-PB	-2.63	125.34	132.73
6	L	1001	ATP	C4-C5-N7	-2.60	107.08	109.48
6	P	1001	ATP	PA-O3A-PB	-2.60	125.43	132.73
6	E	1001	ATP	PB-O3B-PG	-2.56	124.10	132.67
6	A	1001	ATP	PB-O3B-PG	-2.54	124.16	132.67
5	J	700	FDP	C6-C5-C4	-2.49	105.34	115.21
6	I	1001	ATP	PB-O3B-PG	-2.49	124.33	132.67
5	C	700	FDP	O5P-P2-O6	-2.48	99.42	106.56
6	P	1001	ATP	C2'-C1'-N9	-2.46	110.53	114.29
5	L	700	FDP	O5-C2-C3	-2.45	100.00	105.58
5	A	700	FDP	C6-C5-C4	-2.45	105.48	115.21
6	D	1001	ATP	PB-O3B-PG	-2.36	124.74	132.67
6	B	1001	ATP	C4-C5-N7	-2.32	107.35	109.48
6	H	1001	ATP	PB-O3B-PG	-2.28	125.01	132.67
5	G	700	FDP	O5P-P2-O4P	-2.27	103.27	110.58
5	E	700	FDP	O5-C2-C3	-2.27	100.42	105.58
5	D	700	FDP	C6-C5-C4	-2.24	106.33	115.21
6	F	1001	ATP	PA-O3A-PB	-2.21	126.51	132.73
5	K	700	FDP	O4-C4-C5	-2.21	104.42	111.05
5	K	700	FDP	C2-C3-C4	-2.13	96.65	102.00
5	O	700	FDP	C5-C4-C3	-2.08	94.46	101.89
6	B	1001	ATP	PA-O3A-PB	-2.05	126.97	132.73
5	M	700	FDP	C6-C5-C4	-2.05	107.07	115.21
5	J	700	FDP	O5-C2-C3	-2.04	100.94	105.58
6	C	1001	ATP	PA-O3A-PB	-2.02	127.05	132.73
6	K	1001	ATP	PB-O3B-PG	-2.02	125.90	132.67
5	H	700	FDP	O2-C2-C3	2.03	115.37	108.17
6	B	1001	ATP	O2G-PG-O1G	2.04	117.16	110.58
6	L	1001	ATP	O4'-C1'-N9	2.05	112.38	108.10
5	G	700	FDP	O5-C5-C6	2.09	114.25	109.49
5	K	700	FDP	O5-C5-C6	2.11	114.29	109.49
6	D	1001	ATP	O3G-PG-O2G	2.11	115.42	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1001	ATP	C4'-O4'-C1'	2.13	112.06	109.72
6	B	1001	ATP	C2-N1-C6	2.14	122.59	118.77
5	E	700	FDP	O6-P2-O4P	2.15	112.60	107.14
5	F	700	FDP	O6-P2-O4P	2.15	112.62	107.14
6	C	1001	ATP	O3G-PG-O2G	2.22	115.83	107.38
5	G	700	FDP	O6-P2-O4P	2.22	112.80	107.14
5	M	700	FDP	O2-P1-O1P	2.27	112.78	107.11
6	I	1001	ATP	O3G-PG-O2G	2.31	116.17	107.38
5	A	700	FDP	O6-P2-O4P	2.36	113.15	107.14
5	B	700	FDP	O6-P2-O4P	2.37	113.16	107.14
6	J	1001	ATP	O4'-C1'-N9	2.40	113.12	108.10
6	D	1001	ATP	O4'-C1'-N9	2.53	113.39	108.10
5	C	700	FDP	O2-P1-O1P	2.57	113.52	107.11
5	N	700	FDP	O6-P2-O4P	2.58	113.70	107.14
5	K	700	FDP	O2-P1-O1P	2.59	113.56	107.11
5	M	700	FDP	O6-P2-O4P	2.66	113.90	107.14
5	K	700	FDP	O2-C2-C3	2.67	117.63	108.17
5	O	700	FDP	O2-P1-O1P	2.73	113.94	107.11
5	K	700	FDP	O6P-P2-O4P	2.78	119.53	110.58
5	J	700	FDP	O2-P1-O1P	2.90	114.36	107.11
5	J	700	FDP	O2-C2-C3	2.91	118.48	108.17
5	J	700	FDP	O6-P2-O4P	3.11	115.06	107.14
5	C	700	FDP	O6P-P2-O4P	3.12	120.61	110.58
5	F	700	FDP	O2-C2-C3	3.14	119.30	108.17
5	H	700	FDP	O2-P1-O1P	3.16	114.99	107.11
5	L	700	FDP	O2-C2-C3	3.46	120.44	108.17
5	B	700	FDP	O2-C2-C3	3.52	120.67	108.17
5	I	700	FDP	O2-C2-C3	3.54	120.74	108.17
5	A	700	FDP	O2-C2-C3	3.59	120.92	108.17
5	G	700	FDP	O2-P1-O1P	3.64	116.19	107.11
5	H	700	FDP	O3P-P1-O1P	3.70	122.49	110.58
5	N	700	FDP	O2-P1-O1P	3.78	116.54	107.11
5	C	700	FDP	O6-P2-O4P	3.88	117.01	107.14
5	B	700	FDP	O2-P1-O1P	4.33	117.92	107.11
5	D	700	FDP	O2-P1-O1P	5.28	120.30	107.11
5	L	700	FDP	O2-P1-O1P	6.46	123.24	107.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	ATP	2	0
6	C	1001	ATP	3	0
6	D	1001	ATP	3	0
5	D	700	FDP	2	0
6	E	1001	ATP	1	0
6	F	1001	ATP	1	0
6	G	1001	ATP	1	0
6	H	1001	ATP	1	0
7	I	499	GOL	1	0
5	I	700	FDP	1	0
7	J	499	GOL	1	0
6	K	1001	ATP	2	0
4	M	510	OXL	1	0
5	N	700	FDP	2	0
5	O	700	FDP	1	0
5	P	700	FDP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	498/499 (99%)	1.20	127 (25%) 1 1	31, 42, 59, 61	0
1	B	498/499 (99%)	0.40	40 (8%) 15 21	15, 25, 34, 42	0
1	C	498/499 (99%)	0.63	54 (10%) 8 11	28, 39, 50, 59	0
1	D	498/499 (99%)	0.54	54 (10%) 8 11	17, 27, 43, 45	0
1	E	498/499 (99%)	0.71	70 (14%) 4 6	30, 42, 52, 56	0
1	F	498/499 (99%)	0.85	81 (16%) 2 4	36, 52, 66, 70	0
1	G	498/499 (99%)	1.48	144 (28%) 1 1	44, 52, 60, 63	0
1	H	498/499 (99%)	0.91	83 (16%) 2 4	38, 46, 52, 55	0
1	I	498/499 (99%)	0.53	49 (9%) 10 14	13, 22, 47, 53	0
1	J	498/499 (99%)	0.41	40 (8%) 15 21	15, 22, 30, 41	0
1	K	498/499 (99%)	0.33	32 (6%) 23 31	13, 22, 31, 40	0
1	L	498/499 (99%)	0.67	65 (13%) 5 7	19, 29, 60, 62	0
1	M	498/499 (99%)	1.23	130 (26%) 1 1	35, 47, 56, 59	0
1	N	498/499 (99%)	1.91	204 (40%) 0 0	45, 60, 69, 71	0
1	O	498/499 (99%)	2.50	260 (52%) 0 0	35, 55, 84, 86	0
1	P	498/499 (99%)	2.37	253 (50%) 0 0	48, 60, 83, 86	0
All	All	7968/7984 (99%)	1.04	1686 (21%) 1 2	13, 43, 65, 86	0

All (1686) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	155	HIS	10.1
1	O	444	ALA	10.0
1	O	100	VAL	9.9
1	O	95	VAL	9.6
1	N	447	LEU	9.4

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Mol	Chain	Res	Type	RSRZ
1	O	431	LEU	9.3
1	N	195	VAL	8.9
1	O	113	PRO	8.7
1	P	496	LEU	8.2
1	O	120	THR	8.0
1	N	259	MET	7.9
1	O	447	LEU	7.9
1	P	444	ALA	7.7
1	O	433	ILE	7.7
1	O	132	SER	7.6
1	N	444	ALA	7.5
1	N	115	PHE	7.4
1	P	446	LYS	7.4
1	O	442	PHE	7.4
1	P	209	PHE	7.2
1	P	135	VAL	7.1
1	N	153	GLN	7.1
1	P	114	ALA	7.1
1	N	74	LEU	7.1
1	P	100	VAL	7.0
1	O	496	LEU	7.0
1	O	163	CYS	7.0
1	O	134	VAL	6.9
1	P	134	VAL	6.9
1	N	163	CYS	6.8
1	P	447	LEU	6.8
1	P	470	VAL	6.8
1	O	140	TYR	6.8
1	G	108	TYR	6.8
1	P	158	GLU	6.8
1	N	14	PRO	6.7
1	P	12	PHE	6.7
1	H	118	LYS	6.7
1	O	488	TYR	6.6
1	P	191	ALA	6.6
1	P	101	MET	6.6
1	M	118	LYS	6.6
1	O	34	VAL	6.6
1	O	156	GLU	6.6
1	M	104	GLY	6.5
1	M	108	TYR	6.5
1	G	198	GLN	6.5

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Mol	Chain	Res	Type	RSRZ
1	P	113	PRO	6.4
1	N	97	GLY	6.4
1	N	260	VAL	6.4
1	O	74	LEU	6.3
1	P	14	PRO	6.3
1	O	119	GLY	6.3
1	P	108	TYR	6.3
1	N	24	ILE	6.3
1	O	108	TYR	6.3
1	O	224	LYS	6.2
1	P	118	LYS	6.2
1	N	108	TYR	6.2
1	P	125	TYR	6.2
1	G	24	ILE	6.2
1	N	105	ALA	6.2
1	P	131	LEU	6.2
1	O	209	PHE	6.2
1	O	449	HIS	6.2
1	O	151	GLN	6.2
1	A	152	VAL	6.2
1	P	472	THR	6.2
1	O	135	VAL	6.2
1	O	472	THR	6.2
1	O	157	ASP	6.1
1	O	105	ALA	6.1
1	P	153	GLN	6.1
1	O	102	GLU	6.0
1	O	455	HIS	6.0
1	O	12	PHE	6.0
1	P	238	LYS	6.0
1	O	99	ALA	6.0
1	A	209	PHE	6.0
1	N	448	GLY	5.9
1	P	154	SER	5.9
1	O	39	GLY	5.9
1	G	189	VAL	5.9
1	P	129	GLN	5.9
1	O	187	PRO	5.9
1	N	449	HIS	5.9
1	N	214	ARG	5.9
1	O	137	PRO	5.9
1	P	150	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	O	448	GLY	5.8
1	P	106	THR	5.8
1	P	498	GLU	5.8
1	P	431	LEU	5.8
1	G	96	GLY	5.8
1	P	107	CYS	5.8
1	N	247	ASN	5.8
1	E	118	LYS	5.8
1	O	38	LYS	5.7
1	P	449	HIS	5.7
1	P	229	LYS	5.7
1	P	137	PRO	5.7
1	N	104	GLY	5.7
1	P	443	ASP	5.7
1	O	481	ALA	5.7
1	G	163	CYS	5.7
1	P	433	ILE	5.6
1	M	120	THR	5.6
1	H	293	ILE	5.6
1	P	227	GLY	5.6
1	P	445	ASP	5.6
1	P	39	GLY	5.6
1	F	293	ILE	5.6
1	O	445	ASP	5.6
1	G	12	PHE	5.5
1	H	115	PHE	5.5
1	N	100	VAL	5.5
1	O	458	ALA	5.5
1	O	31	THR	5.5
1	O	434	THR	5.5
1	P	195	VAL	5.5
1	H	157	ASP	5.4
1	N	187	PRO	5.4
1	G	294	CYS	5.4
1	P	115	PHE	5.4
1	G	327	VAL	5.4
1	O	220	GLY	5.4
1	P	434	THR	5.4
1	M	115	PHE	5.4
1	A	95	VAL	5.4
1	P	165	VAL	5.4
1	O	131	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	P	82	LEU	5.3
1	N	8	THR	5.3
1	H	100	VAL	5.3
1	P	132	SER	5.3
1	I	134	VAL	5.3
1	O	129	GLN	5.3
1	O	106	THR	5.3
1	M	182	CYS	5.3
1	N	216	ALA	5.3
1	P	451	GLU	5.3
1	H	497	VAL	5.2
1	N	107	CYS	5.2
1	N	148	LEU	5.2
1	E	177	VAL	5.2
1	A	108	TYR	5.2
1	O	133	LYS	5.2
1	N	225	ALA	5.2
1	O	124	PHE	5.2
1	G	120	THR	5.2
1	G	124	PHE	5.2
1	P	110	THR	5.2
1	M	100	VAL	5.2
1	M	294	CYS	5.2
1	O	441	PHE	5.1
1	A	24	ILE	5.1
1	O	436	GLY	5.1
1	N	166	THR	5.1
1	N	251	ILE	5.1
1	M	156	GLU	5.1
1	G	118	LYS	5.1
1	M	293	ILE	5.1
1	P	105	ALA	5.1
1	O	125	TYR	5.1
1	P	128	TYR	5.1
1	G	293	ILE	5.1
1	A	293	ILE	5.1
1	P	228	PRO	5.0
1	H	12	PHE	5.0
1	K	293	ILE	5.0
1	G	47	VAL	5.0
1	O	221	ASP	5.0
1	O	139	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	N	154	SER	5.0
1	O	154	SER	5.0
1	O	118	LYS	5.0
1	O	471	GLN	5.0
1	N	258	ILE	5.0
1	P	83	ASP	5.0
1	N	103	ARG	5.0
1	P	72	ALA	5.0
1	N	185	ASP	4.9
1	O	182	CYS	4.9
1	P	95	VAL	4.9
1	P	199	PHE	4.9
1	A	158	GLU	4.9
1	N	176	GLY	4.9
1	P	306	PRO	4.9
1	N	12	PHE	4.9
1	N	209	PHE	4.9
1	P	11	ILE	4.9
1	N	164	THR	4.9
1	G	116	ALA	4.9
1	P	187	PRO	4.9
1	O	443	ASP	4.9
1	N	102	GLU	4.9
1	C	293	ILE	4.9
1	F	433	ILE	4.9
1	O	130	ASN	4.8
1	O	469	TYR	4.8
1	P	471	GLN	4.8
1	G	228	PRO	4.8
1	M	295	ALA	4.8
1	O	70	ALA	4.8
1	O	468	GLY	4.8
1	G	48	ALA	4.8
1	E	176	GLY	4.8
1	G	107	CYS	4.8
1	N	329	LEU	4.8
1	P	10	SER	4.8
1	P	24	ILE	4.8
1	P	448	GLY	4.8
1	M	135	VAL	4.8
1	N	95	VAL	4.8
1	P	37	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	155	HIS	4.8
1	O	14	PRO	4.8
1	O	13	ASP	4.8
1	P	207	MET	4.8
1	P	466	SER	4.8
1	G	152	VAL	4.7
1	E	12	PHE	4.7
1	N	293	ILE	4.7
1	O	107	CYS	4.7
1	N	98	ASP	4.7
1	P	136	ARG	4.7
1	O	114	ALA	4.7
1	G	326	CYS	4.7
1	M	158	GLU	4.7
1	N	145	ASP	4.7
1	P	74	LEU	4.7
1	L	115	PHE	4.7
1	O	67	VAL	4.7
1	N	129	GLN	4.7
1	G	115	PHE	4.7
1	P	483	HIS	4.7
1	N	160	THR	4.7
1	N	189	VAL	4.6
1	O	152	VAL	4.6
1	N	188	ALA	4.6
1	O	35	GLU	4.6
1	P	124	PHE	4.6
1	M	96	GLY	4.6
1	P	17	ASN	4.6
1	P	103	ARG	4.6
1	P	293	ILE	4.6
1	N	94	PHE	4.6
1	H	160	THR	4.6
1	M	292	VAL	4.6
1	N	139	ASN	4.6
1	O	404	ARG	4.6
1	O	94	PHE	4.6
1	G	95	VAL	4.6
1	M	95	VAL	4.6
1	M	121	LYS	4.6
1	O	164	THR	4.6
1	O	228	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	M	12	PHE	4.5
1	M	185	ASP	4.5
1	O	446	LYS	4.5
1	O	136	ARG	4.5
1	A	133	LYS	4.5
1	P	75	GLY	4.5
1	G	292	VAL	4.5
1	G	137	PRO	4.5
1	A	118	LYS	4.5
1	M	433	ILE	4.5
1	N	372	ILE	4.5
1	P	236	ILE	4.5
1	A	449	HIS	4.5
1	E	108	TYR	4.5
1	C	433	ILE	4.5
1	D	293	ILE	4.5
1	G	74	LEU	4.5
1	G	224	LYS	4.5
1	M	328	MET	4.5
1	N	133	LYS	4.5
1	N	162	GLU	4.5
1	A	228	PRO	4.5
1	E	14	PRO	4.5
1	O	470	VAL	4.5
1	M	326	CYS	4.5
1	O	236	ILE	4.5
1	F	12	PHE	4.5
1	J	295	ALA	4.5
1	O	287	VAL	4.5
1	P	102	GLU	4.4
1	G	94	PHE	4.4
1	G	259	MET	4.4
1	N	226	LEU	4.4
1	N	69	GLN	4.4
1	P	198	GLN	4.4
1	P	394	LYS	4.4
1	F	326	CYS	4.4
1	F	112	ASP	4.4
1	F	24	ILE	4.4
1	L	12	PHE	4.4
1	G	295	ALA	4.4
1	G	258	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	K	433	ILE	4.4
1	A	94	PHE	4.4
1	A	156	GLU	4.4
1	O	81	ALA	4.4
1	O	92	GLY	4.4
1	P	120	THR	4.3
1	A	183	ASP	4.3
1	N	261	ALA	4.3
1	G	153	GLN	4.3
1	P	99	ALA	4.3
1	N	132	SER	4.3
1	M	134	VAL	4.3
1	C	259	MET	4.3
1	A	434	THR	4.3
1	O	435	GLN	4.3
1	O	165	VAL	4.3
1	P	89	ILE	4.3
1	O	451	GLU	4.3
1	N	124	PHE	4.3
1	N	140	TYR	4.3
1	P	488	TYR	4.3
1	M	145	ASP	4.3
1	N	217	GLU	4.3
1	O	371	HIS	4.2
1	O	173	ASP	4.2
1	P	295	ALA	4.2
1	G	209	PHE	4.2
1	A	326	CYS	4.2
1	F	47	VAL	4.2
1	P	168	SER	4.2
1	O	73	GLU	4.2
1	A	433	ILE	4.2
1	A	259	MET	4.2
1	N	328	MET	4.2
1	O	483	HIS	4.2
1	N	330	SER	4.2
1	N	264	ASP	4.2
1	P	155	HIS	4.2
1	O	227	GLY	4.2
1	H	123	LYS	4.2
1	N	246	GLN	4.2
1	G	262	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	N	228	PRO	4.2
1	P	441	PHE	4.2
1	O	204	GLY	4.2
1	P	130	ASN	4.2
1	G	223	ARG	4.2
1	J	293	ILE	4.2
1	N	433	ILE	4.2
1	M	437	VAL	4.1
1	G	226	LEU	4.1
1	O	158	GLU	4.1
1	G	296	THR	4.1
1	N	135	VAL	4.1
1	P	372	ILE	4.1
1	O	168	SER	4.1
1	P	96	GLY	4.1
1	N	295	ALA	4.1
1	O	72	ALA	4.1
1	M	103	ARG	4.1
1	O	207	MET	4.1
1	P	475	TYR	4.1
1	O	110	THR	4.1
1	O	111	THR	4.1
1	O	487	GLY	4.1
1	C	260	VAL	4.1
1	O	98	ASP	4.1
1	N	294	CYS	4.1
1	O	304	TYR	4.1
1	A	327	VAL	4.1
1	C	327	VAL	4.1
1	M	372	ILE	4.1
1	P	152	VAL	4.1
1	N	465	LYS	4.1
1	G	260	VAL	4.0
1	M	34	VAL	4.0
1	N	327	VAL	4.0
1	A	328	MET	4.0
1	H	108	TYR	4.0
1	N	125	TYR	4.0
1	N	151	GLN	4.0
1	O	59	TYR	4.0
1	P	22	ARG	4.0
1	M	165	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	P	473	GLY	4.0
1	E	115	PHE	4.0
1	F	291	PRO	4.0
1	H	470	VAL	4.0
1	J	24	ILE	4.0
1	J	294	CYS	4.0
1	M	9	LEU	4.0
1	N	219	VAL	4.0
1	N	240	GLU	4.0
1	N	451	GLU	4.0
1	A	236	ILE	4.0
1	J	260	VAL	4.0
1	N	161	LEU	4.0
1	P	181	GLY	4.0
1	P	487	GLY	4.0
1	B	326	CYS	4.0
1	A	120	THR	4.0
1	L	449	HIS	4.0
1	P	432	ASN	4.0
1	P	455	HIS	4.0
1	A	292	VAL	4.0
1	C	24	ILE	4.0
1	C	294	CYS	4.0
1	N	114	ALA	4.0
1	P	176	GLY	4.0
1	O	369	LEU	4.0
1	A	12	PHE	3.9
1	A	93	GLN	3.9
1	F	221	ASP	3.9
1	H	156	GLU	3.9
1	O	161	LEU	3.9
1	E	295	ALA	3.9
1	F	191	ALA	3.9
1	G	49	ARG	3.9
1	M	410	ALA	3.9
1	O	191	ALA	3.9
1	O	112	ASP	3.9
1	P	156	GLU	3.9
1	O	432	ASN	3.9
1	D	292	VAL	3.9
1	P	84	THR	3.9
1	E	136	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	326	CYS	3.9
1	H	294	CYS	3.9
1	G	433	ILE	3.9
1	N	47	VAL	3.9
1	N	120	THR	3.9
1	P	160	THR	3.9
1	N	263	GLY	3.9
1	N	446	LYS	3.9
1	P	161	LEU	3.9
1	M	11	ILE	3.9
1	N	109	VAL	3.9
1	O	32	GLN	3.9
1	P	133	LYS	3.9
1	G	185	ASP	3.9
1	C	238	LYS	3.9
1	O	170	THR	3.9
1	G	109	VAL	3.9
1	N	199	PHE	3.8
1	G	187	PRO	3.8
1	P	93	GLN	3.8
1	P	468	GLY	3.8
1	H	132	SER	3.8
1	J	47	VAL	3.8
1	M	183	ASP	3.8
1	O	123	LYS	3.8
1	M	159	GLN	3.8
1	P	9	LEU	3.8
1	L	158	GLU	3.8
1	O	326	CYS	3.8
1	M	418	ILE	3.8
1	M	155	HIS	3.8
1	E	158	GLU	3.8
1	A	294	CYS	3.8
1	E	326	CYS	3.8
1	N	106	THR	3.8
1	H	129	GLN	3.8
1	P	210	ALA	3.8
1	N	224	LYS	3.8
1	O	409	VAL	3.8
1	P	73	GLU	3.8
1	M	304	TYR	3.8
1	O	115	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	160	THR	3.8
1	O	198	GLN	3.8
1	G	447	LEU	3.8
1	N	121	LYS	3.8
1	P	178	ASN	3.8
1	G	238	LYS	3.7
1	C	210	ALA	3.7
1	M	4	ALA	3.7
1	M	114	ALA	3.7
1	N	178	ASN	3.7
1	F	228	PRO	3.7
1	H	159	GLN	3.7
1	O	219	VAL	3.7
1	O	142	TYR	3.7
1	P	162	GLU	3.7
1	G	114	ALA	3.7
1	P	36	ALA	3.7
1	F	226	LEU	3.7
1	N	13	ASP	3.7
1	A	291	PRO	3.7
1	E	293	ILE	3.7
1	O	56	SER	3.7
1	H	445	ASP	3.7
1	P	85	LYS	3.7
1	C	328	MET	3.7
1	M	496	LEU	3.7
1	N	64	ILE	3.7
1	J	326	CYS	3.7
1	A	98	ASP	3.7
1	N	59	TYR	3.7
1	N	183	ASP	3.7
1	O	103	ARG	3.7
1	P	173	ASP	3.7
1	P	242	HIS	3.7
1	O	408	LEU	3.7
1	O	479	ILE	3.7
1	M	498	GLU	3.7
1	M	153	GLN	3.7
1	G	155	HIS	3.7
1	F	261	ALA	3.7
1	H	259	MET	3.7
1	O	82	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	N	118	LYS	3.7
1	P	76	VAL	3.7
1	O	75	GLY	3.7
1	G	261	ALA	3.7
1	G	98	ASP	3.6
1	E	89	ILE	3.6
1	O	372	ILE	3.6
1	A	135	VAL	3.6
1	F	181	GLY	3.6
1	M	436	GLY	3.6
1	E	160	THR	3.6
1	O	231	ARG	3.6
1	I	295	ALA	3.6
1	J	48	ALA	3.6
1	K	295	ALA	3.6
1	O	338	TYR	3.6
1	O	475	TYR	3.6
1	G	237	CYS	3.6
1	N	117	ASP	3.6
1	O	122	ASP	3.6
1	O	339	PRO	3.6
1	P	117	ASP	3.6
1	N	238	LYS	3.6
1	D	24	ILE	3.6
1	G	236	ILE	3.6
1	J	433	ILE	3.6
1	O	418	ILE	3.6
1	P	8	THR	3.6
1	H	295	ALA	3.6
1	J	81	ALA	3.6
1	P	259	MET	3.6
1	P	34	VAL	3.6
1	D	324	ALA	3.6
1	M	324	ALA	3.6
1	O	128	TYR	3.6
1	F	197	LEU	3.6
1	P	49	ARG	3.6
1	H	292	VAL	3.6
1	A	444	ALA	3.6
1	O	373	PRO	3.6
1	A	103	ARG	3.6
1	A	92	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	431	LEU	3.6
1	N	156	GLU	3.6
1	P	371	HIS	3.6
1	D	296	THR	3.6
1	C	261	ALA	3.6
1	L	95	VAL	3.6
1	N	168	SER	3.6
1	P	13	ASP	3.6
1	K	259	MET	3.6
1	O	234	MET	3.6
1	P	304	TYR	3.6
1	O	340	ASN	3.6
1	D	294	CYS	3.5
1	P	123	LYS	3.5
1	B	409	VAL	3.5
1	C	295	ALA	3.5
1	M	105	ALA	3.5
1	P	145	ASP	3.5
1	N	338	TYR	3.5
1	O	229	LYS	3.5
1	O	8	THR	3.5
1	O	149	ILE	3.5
1	N	443	ASP	3.5
1	O	474	ASP	3.5
1	F	134	VAL	3.5
1	G	138	GLY	3.5
1	M	15	VAL	3.5
1	N	177	VAL	3.5
1	N	25	CYS	3.5
1	N	194	ARG	3.5
1	O	162	GLU	3.5
1	M	259	MET	3.5
1	N	150	LEU	3.5
1	P	212	PHE	3.5
1	G	434	THR	3.5
1	O	117	ASP	3.5
1	C	258	ILE	3.5
1	A	47	VAL	3.5
1	H	95	VAL	3.5
1	L	118	LYS	3.5
1	P	43	SER	3.5
1	G	162	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	M	176	GLY	3.5
1	E	324	ALA	3.5
1	P	4	ALA	3.5
1	O	457	VAL	3.5
1	A	447	LEU	3.5
1	O	150	LEU	3.5
1	G	182	CYS	3.5
1	N	326	CYS	3.5
1	E	137	PRO	3.5
1	E	140	TYR	3.5
1	G	119	GLY	3.5
1	G	171	ILE	3.5
1	O	437	VAL	3.5
1	O	450	ASP	3.5
1	O	33	SER	3.5
1	P	104	GLY	3.5
1	A	258	ILE	3.5
1	B	24	ILE	3.5
1	F	225	ALA	3.5
1	N	72	ALA	3.5
1	P	185	ASP	3.4
1	O	97	GLY	3.4
1	O	104	GLY	3.4
1	P	391	THR	3.4
1	P	88	GLU	3.4
1	P	163	CYS	3.4
1	O	424	ARG	3.4
1	O	47	VAL	3.4
1	D	158	GLU	3.4
1	G	176	GLY	3.4
1	A	229	LYS	3.4
1	E	296	THR	3.4
1	M	164	THR	3.4
1	I	13	ASP	3.4
1	N	424	ARG	3.4
1	A	81	ALA	3.4
1	P	116	ALA	3.4
1	D	433	ILE	3.4
1	D	326	CYS	3.4
1	E	154	SER	3.4
1	M	327	VAL	3.4
1	P	497	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	431	LEU	3.4
1	N	155	HIS	3.4
1	O	160	THR	3.4
1	O	325	ASP	3.4
1	I	12	PHE	3.4
1	A	21	ALA	3.4
1	F	295	ALA	3.4
1	G	59	TYR	3.4
1	N	483	HIS	3.4
1	O	419	VAL	3.4
1	A	207	MET	3.4
1	M	3	LEU	3.4
1	L	159	GLN	3.4
1	I	324	ALA	3.4
1	G	23	ILE	3.4
1	N	211	SER	3.4
1	M	102	GLU	3.4
1	P	462	GLU	3.4
1	A	163	CYS	3.4
1	E	133	LYS	3.4
1	E	292	VAL	3.4
1	G	165	VAL	3.4
1	O	201	VAL	3.4
1	O	495	LEU	3.4
1	N	250	SER	3.4
1	O	183	ASP	3.4
1	P	338	TYR	3.4
1	A	109	VAL	3.3
1	P	15	VAL	3.3
1	O	420	CYS	3.3
1	O	405	SER	3.3
1	O	171	ILE	3.3
1	D	260	VAL	3.3
1	G	100	VAL	3.3
1	M	157	ASP	3.3
1	G	52	PHE	3.3
1	M	471	GLN	3.3
1	C	449	HIS	3.3
1	C	236	ILE	3.3
1	D	479	ILE	3.3
1	F	14	PRO	3.3
1	A	130	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	380	VAL	3.3
1	F	409	VAL	3.3
1	N	245	VAL	3.3
1	P	177	VAL	3.3
1	N	1	SER	3.3
1	P	211	SER	3.3
1	C	12	PHE	3.3
1	H	94	PHE	3.3
1	L	433	ILE	3.3
1	O	430	GLN	3.3
1	N	131	LEU	3.3
1	L	295	ALA	3.3
1	O	406	ALA	3.3
1	P	81	ALA	3.3
1	N	262	ARG	3.3
1	F	209	PHE	3.3
1	P	442	PHE	3.3
1	F	183	ASP	3.3
1	M	17	ASN	3.3
1	F	23	ILE	3.3
1	P	58	GLU	3.3
1	P	138	GLY	3.3
1	A	224	LYS	3.3
1	D	409	VAL	3.3
1	I	183	ASP	3.3
1	N	65	ASN	3.3
1	O	93	GLN	3.3
1	N	254	GLU	3.3
1	J	23	ILE	3.3
1	E	434	THR	3.3
1	N	170	THR	3.3
1	B	260	VAL	3.3
1	O	9	LEU	3.3
1	P	186	LEU	3.3
1	P	189	VAL	3.3
1	A	137	PRO	3.2
1	A	238	LYS	3.2
1	N	113	PRO	3.2
1	J	89	ILE	3.2
1	J	236	ILE	3.2
1	P	336	GLY	3.2
1	M	169	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	152	VAL	3.2
1	G	195	VAL	3.2
1	G	154	SER	3.2
1	N	10	SER	3.2
1	N	445	ASP	3.2
1	P	183	ASP	3.2
1	P	18	TYR	3.2
1	B	327	VAL	3.2
1	C	292	VAL	3.2
1	N	222	VAL	3.2
1	O	189	VAL	3.2
1	O	477	VAL	3.2
1	P	90	ARG	3.2
1	G	129	GLN	3.2
1	H	384	ALA	3.2
1	L	177	VAL	3.2
1	O	185	ASP	3.2
1	G	31	THR	3.2
1	N	371	HIS	3.2
1	N	235	ILE	3.2
1	P	494	ILE	3.2
1	G	82	LEU	3.2
1	P	298	MET	3.2
1	N	230	GLY	3.2
1	N	257	GLY	3.2
1	N	215	SER	3.2
1	F	434	THR	3.2
1	H	155	HIS	3.2
1	O	49	ARG	3.2
1	D	236	ILE	3.2
1	F	224	LYS	3.2
1	O	486	LYS	3.2
1	G	186	LEU	3.2
1	G	249	ASP	3.2
1	H	39	GLY	3.2
1	N	157	ASP	3.2
1	P	436	GLY	3.2
1	G	102	GLU	3.2
1	O	57	HIS	3.2
1	D	209	PHE	3.1
1	H	326	CYS	3.1
1	O	190	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	7	LEU	3.1
1	O	205	VAL	3.1
1	G	243	GLN	3.1
1	N	143	ILE	3.1
1	E	168	SER	3.1
1	D	329	LEU	3.1
1	F	207	MET	3.1
1	F	449	HIS	3.1
1	I	177	VAL	3.1
1	K	292	VAL	3.1
1	N	152	VAL	3.1
1	O	253	GLU	3.1
1	A	157	ASP	3.1
1	P	170	THR	3.1
1	H	119	GLY	3.1
1	A	295	ALA	3.1
1	D	295	ALA	3.1
1	O	36	ALA	3.1
1	A	231	ARG	3.1
1	D	437	VAL	3.1
1	G	121	LYS	3.1
1	J	292	VAL	3.1
1	M	133	LYS	3.1
1	N	34	VAL	3.1
1	O	465	LYS	3.1
1	D	434	THR	3.1
1	M	296	THR	3.1
1	L	97	GLY	3.1
1	O	52	PHE	3.1
1	M	14	PRO	3.1
1	A	235	ILE	3.1
1	B	479	ILE	3.1
1	I	185	ASP	3.1
1	C	237	CYS	3.1
1	A	184	VAL	3.1
1	L	156	GLU	3.1
1	P	94	PHE	3.1
1	E	261	ALA	3.1
1	F	227	GLY	3.1
1	I	294	CYS	3.1
1	K	294	CYS	3.1
1	B	47	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	184	VAL	3.1
1	L	183	ASP	3.1
1	M	261	ALA	3.0
1	O	58	GLU	3.0
1	P	40	LEU	3.0
1	A	436	GLY	3.0
1	P	423	THR	3.0
1	D	95	VAL	3.0
1	G	437	VAL	3.0
1	I	326	CYS	3.0
1	F	406	ALA	3.0
1	H	11	ILE	3.0
1	H	114	ALA	3.0
1	I	293	ILE	3.0
1	O	293	ILE	3.0
1	O	66	ASN	3.0
1	P	430	GLN	3.0
1	A	431	LEU	3.0
1	M	101	MET	3.0
1	P	339	PRO	3.0
1	A	124	PHE	3.0
1	F	114	ALA	3.0
1	F	188	ALA	3.0
1	M	99	ALA	3.0
1	O	401	ASN	3.0
1	C	265	LEU	3.0
1	P	157	ASP	3.0
1	G	339	PRO	3.0
1	P	38	LYS	3.0
1	A	69	GLN	3.0
1	F	100	VAL	3.0
1	A	237	CYS	3.0
1	N	11	ILE	3.0
1	O	141	ILE	3.0
1	F	13	ASP	3.0
1	D	328	MET	3.0
1	H	154	SER	3.0
1	M	472	THR	3.0
1	F	292	VAL	3.0
1	M	380	VAL	3.0
1	F	223	ARG	3.0
1	N	35[A]	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	O	498	GLU	3.0
1	P	220	GLY	3.0
1	C	209	PHE	3.0
1	N	123	LYS	3.0
1	H	433	ILE	3.0
1	P	141	ILE	3.0
1	G	211	SER	3.0
1	G	17	ASN	3.0
1	D	135	VAL	3.0
1	G	15	VAL	3.0
1	G	177	VAL	3.0
1	I	327	VAL	3.0
1	L	134	VAL	3.0
1	O	15	VAL	3.0
1	O	121	LYS	3.0
1	O	138	GLY	3.0
1	I	81	ALA	3.0
1	N	191	ALA	3.0
1	H	64	ILE	3.0
1	N	136	ARG	3.0
1	O	423	THR	3.0
1	N	182	CYS	2.9
1	K	263	GLY	2.9
1	P	230	GLY	2.9
1	D	261	ALA	2.9
1	L	21	ALA	2.9
1	M	140	TYR	2.9
1	P	59	TYR	2.9
1	E	126	ILE	2.9
1	F	296	THR	2.9
1	N	101	MET	2.9
1	G	173	ASP	2.9
1	H	158	GLU	2.9
1	M	319	ALA	2.9
1	O	43	SER	2.9
1	D	12	PHE	2.9
1	J	12	PHE	2.9
1	B	433	ILE	2.9
1	F	158	GLU	2.9
1	P	454	GLU	2.9
1	G	105	ALA	2.9
1	K	260	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	84	THR	2.9
1	G	26	THR	2.9
1	P	243	GLN	2.9
1	L	96	GLY	2.9
1	N	9	LEU	2.9
1	E	102	GLU	2.9
1	L	47	VAL	2.9
1	P	69	GLN	2.9
1	A	84	THR	2.9
1	G	291	PRO	2.9
1	L	113	PRO	2.9
1	I	433	ILE	2.9
1	L	293	ILE	2.9
1	N	49	ARG	2.9
1	O	248	ILE	2.9
1	P	171	ILE	2.9
1	A	161	LEU	2.9
1	B	259	MET	2.9
1	J	259	MET	2.9
1	C	185	ASP	2.9
1	O	83	ASP	2.9
1	G	70	ALA	2.9
1	G	191	ALA	2.9
1	D	327	VAL	2.9
1	A	62	THR	2.9
1	O	492	THR	2.9
1	I	209	PHE	2.9
1	P	305	ASN	2.9
1	P	340	ASN	2.9
1	A	324	ALA	2.8
1	H	72	ALA	2.8
1	I	261	ALA	2.8
1	K	261	ALA	2.8
1	F	327	VAL	2.8
1	J	327	VAL	2.8
1	L	437	VAL	2.8
1	M	291	PRO	2.8
1	N	58	GLU	2.8
1	N	227	GLY	2.8
1	O	222	VAL	2.8
1	P	201	VAL	2.8
1	F	118	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	258	ILE	2.8
1	O	24	ILE	2.8
1	H	112	ASP	2.8
1	N	207	MET	2.8
1	G	46	SER	2.8
1	J	49	ARG	2.8
1	P	16	ALA	2.8
1	C	434	THR	2.8
1	D	134	VAL	2.8
1	I	296	THR	2.8
1	K	177	VAL	2.8
1	N	110	THR	2.8
1	P	287	VAL	2.8
1	E	130	ASN	2.8
1	G	443	ASP	2.8
1	P	435	GLN	2.8
1	G	80	ILE	2.8
1	H	162	GLU	2.8
1	M	107	CYS	2.8
1	O	172	SER	2.8
1	F	257	GLY	2.8
1	C	228	PRO	2.8
1	P	237	CYS	2.8
1	A	116	ALA	2.8
1	I	384	ALA	2.8
1	M	113	PRO	2.8
1	N	450	ASP	2.8
1	E	135	VAL	2.8
1	P	33	SER	2.8
1	P	148	LEU	2.8
1	O	159	GLN	2.8
1	A	102	GLU	2.8
1	M	97	GLY	2.8
1	B	13	ASP	2.8
1	F	98	ASP	2.8
1	G	81	ALA	2.8
1	H	116	ALA	2.8
1	L	326	CYS	2.8
1	P	91	THR	2.8
1	A	134	VAL	2.8
1	F	15	VAL	2.8
1	I	292	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	10	SER	2.8
1	P	421	VAL	2.8
1	P	202	GLU	2.8
1	G	328	MET	2.8
1	P	226	LEU	2.8
1	P	234	MET	2.8
1	D	319	ALA	2.8
1	O	210	ALA	2.8
1	A	100	VAL	2.7
1	D	316	VAL	2.7
1	E	100	VAL	2.7
1	F	177	VAL	2.7
1	P	485	VAL	2.7
1	N	175	ARG	2.7
1	O	145	ASP	2.7
1	F	258	ILE	2.7
1	N	442	PHE	2.7
1	B	295	ALA	2.7
1	H	71	ALA	2.7
1	J	21	ALA	2.7
1	O	48	ALA	2.7
1	A	111	THR	2.7
1	H	330	SER	2.7
1	O	439	SER	2.7
1	M	449	HIS	2.7
1	O	232	ASP	2.7
1	P	112	ASP	2.7
1	G	51	ASN	2.7
1	I	135	VAL	2.7
1	I	437	VAL	2.7
1	K	326	CYS	2.7
1	N	237	CYS	2.7
1	A	119	GLY	2.7
1	F	55	GLY	2.7
1	P	109	VAL	2.7
1	A	150	LEU	2.7
1	A	115	PHE	2.7
1	B	158	GLU	2.7
1	C	23	ILE	2.7
1	M	209	PHE	2.7
1	N	149	ILE	2.7
1	N	265	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	384	ALA	2.7
1	G	190	SER	2.7
1	N	434	THR	2.7
1	G	202	GLU	2.7
1	H	409	VAL	2.7
1	O	440	VAL	2.7
1	A	182	CYS	2.7
1	D	418	ILE	2.7
1	J	328	MET	2.7
1	N	198	GLN	2.7
1	M	94	PHE	2.7
1	N	137	PRO	2.7
1	G	324	ALA	2.7
1	A	168	SER	2.7
1	E	106	THR	2.7
1	I	434	THR	2.7
1	N	296	THR	2.7
1	P	164	THR	2.7
1	N	75	GLY	2.7
1	P	92	GLY	2.7
1	G	133	LYS	2.7
1	P	219	VAL	2.7
1	O	407	ARG	2.7
1	A	74	LEU	2.7
1	A	239	ILE	2.7
1	B	236	ILE	2.7
1	B	294	CYS	2.7
1	F	236	ILE	2.7
1	O	179	LEU	2.7
1	O	197	LEU	2.7
1	P	64	ILE	2.7
1	P	495	LEU	2.7
1	J	25	CYS	2.7
1	N	122	ASP	2.7
1	D	384	ALA	2.7
1	P	250	SER	2.7
1	L	160	THR	2.7
1	N	167	ASN	2.7
1	G	219	VAL	2.7
1	L	292	VAL	2.7
1	L	137	PRO	2.7
1	M	122	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	447	LEU	2.7
1	M	131	LEU	2.7
1	I	418	ILE	2.7
1	M	171	ILE	2.7
1	A	220	GLY	2.7
1	P	61	GLN	2.7
1	P	159	GLN	2.7
1	G	338	TYR	2.7
1	A	187	PRO	2.7
1	P	437	VAL	2.7
1	E	259	MET	2.6
1	I	431	LEU	2.6
1	B	261	ALA	2.6
1	C	384	ALA	2.6
1	J	444	ALA	2.6
1	L	24	ILE	2.6
1	M	10	SER	2.6
1	O	1	SER	2.6
1	O	41	ILE	2.6
1	O	466	SER	2.6
1	N	212	PHE	2.6
1	O	96	GLY	2.6
1	O	223	ARG	2.6
1	P	97	GLY	2.6
1	N	62	THR	2.6
1	O	360	TYR	2.6
1	M	130	ASN	2.6
1	N	130	ASN	2.6
1	A	132	SER	2.6
1	D	398	VAL	2.6
1	O	184	VAL	2.6
1	F	328	MET	2.6
1	P	369	LEU	2.6
1	H	104	GLY	2.6
1	N	48	ALA	2.6
1	N	126	ILE	2.6
1	P	239	ILE	2.6
1	K	209	PHE	2.6
1	K	296	THR	2.6
1	M	117	ASP	2.6
1	M	325	ASP	2.6
1	P	486	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	223	ARG	2.6
1	M	35	GLU	2.6
1	P	35	GLU	2.6
1	G	330	SER	2.6
1	A	165	VAL	2.6
1	L	477	VAL	2.6
1	M	116	ALA	2.6
1	M	13	ASP	2.6
1	M	479	ILE	2.6
1	P	31	THR	2.6
1	P	166	THR	2.6
1	J	291	PRO	2.6
1	E	132	SER	2.6
1	O	428	CYS	2.6
1	P	53	SER	2.6
1	H	263	GLY	2.6
1	L	448	GLY	2.6
1	F	437	VAL	2.6
1	K	47	VAL	2.6
1	L	157	ASP	2.6
1	B	434	THR	2.6
1	E	433	ILE	2.6
1	P	62	THR	2.6
1	N	441	PHE	2.6
1	P	341	GLU	2.6
1	E	345	TYR	2.6
1	I	14	PRO	2.6
1	K	14	PRO	2.6
1	A	483[A]	HIS	2.6
1	M	445	ASP	2.6
1	O	217	GLU	2.6
1	G	444	ALA	2.6
1	H	34	VAL	2.6
1	I	259	MET	2.6
1	G	231	ARG	2.6
1	L	418	ILE	2.6
1	N	171	ILE	2.6
1	P	167	ASN	2.6
1	A	117	ASP	2.6
1	E	436	GLY	2.6
1	G	136	ARG	2.6
1	G	21	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	225	ALA	2.6
1	L	261	ALA	2.6
1	O	356	ALA	2.6
1	N	15	VAL	2.6
1	I	236	ILE	2.6
1	I	479	ILE	2.6
1	N	236	ILE	2.6
1	A	154	SER	2.5
1	C	211	SER	2.5
1	M	112	ASP	2.5
1	J	449	HIS	2.5
1	M	129	GLN	2.5
1	K	49	ARG	2.5
1	N	142	TYR	2.5
1	M	216	ALA	2.5
1	N	4	ALA	2.5
1	O	51	ASN	2.5
1	C	437	VAL	2.5
1	H	397	VAL	2.5
1	I	316	VAL	2.5
1	M	177	VAL	2.5
1	A	112	ASP	2.5
1	M	98	ASP	2.5
1	O	249	ASP	2.5
1	P	126	ILE	2.5
1	A	22	ARG	2.5
1	A	446	LYS	2.5
1	G	14	PRO	2.5
1	P	86	GLY	2.5
1	E	155	HIS	2.5
1	G	217	GLU	2.5
1	E	264	ASP	2.5
1	H	296	THR	2.5
1	A	409	VAL	2.5
1	F	260	VAL	2.5
1	N	292	VAL	2.5
1	O	478	VAL	2.5
1	A	171	ILE	2.5
1	M	154	SER	2.5
1	L	291	PRO	2.5
1	P	469	TYR	2.5
1	C	296	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	447	LEU	2.5
1	G	197	LEU	2.5
1	L	259	MET	2.5
1	O	101	MET	2.5
1	D	34	VAL	2.5
1	F	10	SER	2.5
1	I	260	VAL	2.5
1	L	152	VAL	2.5
1	C	239	ILE	2.5
1	E	183	ASP	2.5
1	O	42	GLN	2.5
1	P	307	ARG	2.5
1	C	444	ALA	2.5
1	M	128	TYR	2.5
1	A	211	SER	2.5
1	M	74	LEU	2.5
1	M	263	GLY	2.5
1	P	328	MET	2.5
1	C	177	VAL	2.5
1	E	477	VAL	2.5
1	P	292	VAL	2.5
1	N	141	ILE	2.5
1	O	484	LYS	2.5
1	J	209	PHE	2.5
1	M	22	ARG	2.5
1	C	324	ALA	2.5
1	F	410	ALA	2.5
1	E	138	GLY	2.5
1	E	263	GLY	2.5
1	N	220	GLY	2.5
1	I	446	LYS	2.5
1	M	7	LEU	2.5
1	N	128	TYR	2.5
1	E	178	ASN	2.5
1	H	178	ASN	2.5
1	O	17	ASN	2.5
1	H	122	ASP	2.5
1	I	24	ILE	2.5
1	O	344	GLN	2.5
1	P	98	ASP	2.5
1	P	258	ILE	2.5
1	H	99	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	26	THR	2.4
1	J	46	SER	2.4
1	J	296	THR	2.4
1	G	241	ASN	2.4
1	A	113	PRO	2.4
1	A	329	LEU	2.4
1	B	498	GLU	2.4
1	F	259	MET	2.4
1	N	93	GLN	2.4
1	P	224	LYS	2.4
1	G	220	GLY	2.4
1	I	263	GLY	2.4
1	K	176	GLY	2.4
1	A	225	ALA	2.4
1	C	432	ASN	2.4
1	D	330	SER	2.4
1	E	105	ALA	2.4
1	F	22	ARG	2.4
1	G	103	ARG	2.4
1	G	183	ASP	2.4
1	G	193	ASP	2.4
1	F	82	LEU	2.4
1	G	50	MET	2.4
1	G	149	ILE	2.4
1	I	398[A]	VAL	2.4
1	M	260	VAL	2.4
1	O	397	VAL	2.4
1	N	452	GLY	2.4
1	G	22	ARG	2.4
1	A	169	HIS	2.4
1	O	482	ASP	2.4
1	B	328	MET	2.4
1	D	259	MET	2.4
1	B	23	ILE	2.4
1	M	163	CYS	2.4
1	M	477	VAL	2.4
1	O	494	ILE	2.4
1	P	342	VAL	2.4
1	N	173	ASP	2.4
1	P	474	ASP	2.4
1	D	26	THR	2.4
1	O	459	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	158	GLU	2.4
1	J	431	LEU	2.4
1	D	159	GLN	2.4
1	O	22	ARG	2.4
1	P	493	ARG	2.4
1	A	13	ASP	2.4
1	G	97	GLY	2.4
1	H	181	GLY	2.4
1	I	47	VAL	2.4
1	I	80	ILE	2.4
1	K	316	VAL	2.4
1	M	24	ILE	2.4
1	B	381	CYS	2.4
1	L	294	CYS	2.4
1	B	209	PHE	2.4
1	G	156	GLU	2.4
1	H	423	THR	2.4
1	J	410	ALA	2.4
1	M	8	THR	2.4
1	N	99	ALA	2.4
1	D	238	LYS	2.4
1	D	396	MET	2.4
1	E	157	ASP	2.4
1	N	266	GLY	2.4
1	O	167	ASN	2.4
1	A	23	ILE	2.4
1	L	451	GLU	2.4
1	M	132	SER	2.4
1	M	497	VAL	2.4
1	O	269	ILE	2.4
1	L	209	PHE	2.4
1	B	21	ALA	2.4
1	G	110	THR	2.4
1	J	434	THR	2.4
1	O	410	ALA	2.4
1	C	22	ARG	2.4
1	N	231	ARG	2.4
1	F	445	ASP	2.3
1	G	117	ASP	2.3
1	N	17	ASN	2.3
1	A	227	GLY	2.3
1	P	217	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	292	VAL	2.3
1	C	478	VAL	2.3
1	A	337	LYS	2.3
1	C	198	GLN	2.3
1	I	311	ALA	2.3
1	E	13	ASP	2.3
1	A	178	ASN	2.3
1	B	265	LEU	2.3
1	H	101	MET	2.3
1	M	431	LEU	2.3
1	O	351	LEU	2.3
1	C	224	LYS	2.3
1	B	398	VAL	2.3
1	H	437	VAL	2.3
1	N	208	ILE	2.3
1	P	80	ILE	2.3
1	P	233	ILE	2.3
1	A	173	ASP	2.3
1	B	137	PRO	2.3
1	N	158	GLU	2.3
1	E	145	ASP	2.3
1	F	21	ALA	2.3
1	F	117	ASP	2.3
1	I	21	ALA	2.3
1	L	185	ASP	2.3
1	M	444	ALA	2.3
1	C	178	ASN	2.3
1	M	178	ASN	2.3
1	P	139	ASN	2.3
1	F	408	LEU	2.3
1	G	234	MET	2.3
1	J	22	ARG	2.3
1	N	243	GLN	2.3
1	G	58	GLU	2.3
1	A	325	ASP	2.3
1	F	189	VAL	2.3
1	O	235	ILE	2.3
1	L	14	PRO	2.3
1	B	324	ALA	2.3
1	B	406	ALA	2.3
1	D	81	ALA	2.3
1	L	324	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	434	THR	2.3
1	N	84	THR	2.3
1	P	28	GLY	2.3
1	D	435	GLN	2.3
1	M	162	GLU	2.3
1	N	253	GLU	2.3
1	G	101	MET	2.3
1	L	431	LEU	2.3
1	N	431	LEU	2.3
1	P	294	CYS	2.3
1	M	139	ASN	2.3
1	A	125	TYR	2.3
1	D	477	VAL	2.3
1	K	236	ILE	2.3
1	N	339	PRO	2.3
1	P	23	ILE	2.3
1	G	79	ALA	2.3
1	J	79	ALA	2.3
1	N	324	ALA	2.3
1	O	71	ALA	2.3
1	M	448	GLY	2.3
1	F	115	PHE	2.3
1	G	35	GLU	2.3
1	G	69	GLN	2.3
1	G	199	PHE	2.3
1	G	122	ASP	2.3
1	O	453	LYS	2.3
1	P	368	LYS	2.3
1	E	381	CYS	2.3
1	F	80	ILE	2.3
1	K	23	ILE	2.3
1	A	210	ALA	2.3
1	F	216	ALA	2.3
1	I	79	ALA	2.3
1	K	327	VAL	2.3
1	O	460	GLY	2.3
1	P	48	ALA	2.3
1	A	199	PHE	2.3
1	F	46	SER	2.3
1	A	185	ASP	2.3
1	N	221	ASP	2.3
1	D	447	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	51	ASN	2.3
1	C	14	PRO	2.2
1	L	198	GLN	2.2
1	F	230	GLY	2.2
1	B	296	THR	2.2
1	K	258	ILE	2.2
1	L	84	THR	2.2
1	A	385	VAL	2.2
1	E	385	VAL	2.2
1	H	134	VAL	2.2
1	I	477	VAL	2.2
1	M	1	SER	2.2
1	G	432	ASN	2.2
1	O	178	ASN	2.2
1	K	328	MET	2.2
1	I	436	GLY	2.2
1	K	434	THR	2.2
1	E	410	ALA	2.2
1	F	444	ALA	2.2
1	H	444	ALA	2.2
1	K	21	ALA	2.2
1	K	183	ASP	2.2
1	N	116	ALA	2.2
1	O	377	ASP	2.2
1	A	240	GLU	2.2
1	E	380	VAL	2.2
1	G	34	VAL	2.2
1	N	73	GLU	2.2
1	P	214	ARG	2.2
1	O	69	GLN	2.2
1	F	229	LYS	2.2
1	I	328	MET	2.2
1	A	217	GLU	2.2
1	E	162	GLU	2.2
1	M	451	GLU	2.2
1	P	254	GLU	2.2
1	H	8	THR	2.2
1	N	26	THR	2.2
1	A	46	SER	2.2
1	D	21	ALA	2.2
1	E	10	SER	2.2
1	E	384	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	188	ALA	2.2
1	H	406	ALA	2.2
1	B	293	ILE	2.2
1	M	5	HIS	2.2
1	G	134	VAL	2.2
1	H	135	VAL	2.2
1	H	380	VAL	2.2
1	L	130	ASN	2.2
1	M	42	GLN	2.2
1	M	93	GLN	2.2
1	N	6	ASN	2.2
1	O	153	GLN	2.2
1	O	177	VAL	2.2
1	F	192	LYS	2.2
1	H	140	TYR	2.2
1	P	140	TYR	2.2
1	A	107	CYS	2.2
1	D	381	CYS	2.2
1	I	420	CYS	2.2
1	L	94	PHE	2.2
1	B	298	MET	2.2
1	A	49	ARG	2.2
1	E	22	ARG	2.2
1	H	472	THR	2.2
1	L	296	THR	2.2
1	M	262	ARG	2.2
1	B	20	ALA	2.2
1	H	242	HIS	2.2
1	K	79	ALA	2.2
1	M	16	ALA	2.2
1	N	81	ALA	2.2
1	O	116	ALA	2.2
1	P	334	ALA	2.2
1	B	316	VAL	2.2
1	D	478	VAL	2.2
1	I	409	VAL	2.2
1	L	409	VAL	2.2
1	M	320	VAL	2.2
1	P	47	VAL	2.2
1	E	104	GLY	2.2
1	G	325	ASP	2.2
1	G	448	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	138	GLY	2.2
1	H	431	LEU	2.2
1	L	136	ARG	2.2
1	P	231	ARG	2.2
1	E	246	GLN	2.2
1	O	467	LYS	2.2
1	F	242	HIS	2.2
1	O	250	SER	2.2
1	A	58	GLU	2.2
1	A	410	ALA	2.2
1	F	79	ALA	2.2
1	H	261	ALA	2.2
1	K	48	ALA	2.2
1	P	406	ALA	2.2
1	E	24	ILE	2.2
1	E	236	ILE	2.2
1	G	478	VAL	2.2
1	O	245	VAL	2.2
1	D	136	ARG	2.2
1	H	96	GLY	2.2
1	G	212	PHE	2.2
1	I	103	ARG	2.2
1	F	435	GLN	2.2
1	E	101	MET	2.2
1	C	46	SER	2.2
1	F	432	ASN	2.2
1	H	161	LEU	2.2
1	O	40	LEU	2.2
1	C	492	THR	2.2
1	E	294	CYS	2.2
1	L	154	SER	2.2
1	J	84	THR	2.2
1	M	106	THR	2.2
1	P	420	CYS	2.2
1	A	79	ALA	2.2
1	E	21	ALA	2.2
1	A	89	ILE	2.1
1	H	13	ASP	2.1
1	K	185	ASP	2.1
1	M	136	ARG	2.1
1	O	208	ILE	2.1
1	P	467	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	100	VAL	2.1
1	L	419	VAL	2.1
1	M	371	HIS	2.1
1	A	296	THR	2.1
1	M	84	THR	2.1
1	O	427	THR	2.1
1	A	221	ASP	2.1
1	B	183	ASP	2.1
1	D	325	ASP	2.1
1	J	445	ASP	2.1
1	O	175	ARG	2.1
1	O	193	ASP	2.1
1	P	335	LYS	2.1
1	C	479	ILE	2.1
1	F	42	GLN	2.1
1	O	233	ILE	2.1
1	A	189	VAL	2.1
1	C	409	VAL	2.1
1	F	398	VAL	2.1
1	G	380	VAL	2.1
1	H	260	VAL	2.1
1	L	178	ASN	2.1
1	M	124	PHE	2.1
1	M	330	SER	2.1
1	O	199	PHE	2.1
1	J	207	MET	2.1
1	H	63	THR	2.1
1	H	185	ASP	2.1
1	C	451[A]	GLU	2.1
1	F	35	GLU	2.1
1	G	151	GLN	2.1
1	G	458	ALA	2.1
1	H	216	ALA	2.1
1	H	410	ALA	2.1
1	N	218	GLN	2.1
1	L	436	GLY	2.1
1	O	473	GLY	2.1
1	A	139	ASN	2.1
1	K	238	LYS	2.1
1	O	342	VAL	2.1
1	N	190	SER	2.1
1	G	145	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	217	GLU	2.1
1	L	445	ASP	2.1
1	O	310	ARG	2.1
1	M	125	TYR	2.1
1	M	345	TYR	2.1
1	A	435	GLN	2.1
1	H	328	MET	2.1
1	L	396	MET	2.1
1	M	151	GLN	2.1
1	O	166	THR	2.1
1	O	396	MET	2.1
1	A	55	GLY	2.1
1	E	114	ALA	2.1
1	I	114	ALA	2.1
1	P	261	ALA	2.1
1	C	137	PRO	2.1
1	K	24	ILE	2.1
1	L	23	ILE	2.1
1	N	239	ILE	2.1
1	A	380	VAL	2.1
1	J	409	VAL	2.1
1	L	135	VAL	2.1
1	P	221	ASP	2.1
1	G	442	PHE	2.1
1	C	207	MET	2.1
1	H	111	THR	2.1
1	O	84	THR	2.1
1	O	298	MET	2.1
1	C	263	GLY	2.1
1	D	311	ALA	2.1
1	H	133	LYS	2.1
1	H	220	GLY	2.1
1	I	224	LYS	2.1
1	N	331	GLY	2.1
1	P	71	ALA	2.1
1	B	432	ASN	2.1
1	B	136	ARG	2.1
1	A	208	ILE	2.1
1	B	258	ILE	2.1
1	D	23	ILE	2.1
1	N	33	SER	2.1
1	N	233	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	5	HIS	2.1
1	O	280	ILE	2.1
1	P	149	ILE	2.1
1	P	375	SER	2.1
1	D	47	VAL	2.1
1	F	381	CYS	2.1
1	L	265	LEU	2.1
1	P	492	THR	2.1
1	P	66	ASN	2.1
1	L	48	ALA	2.1
1	E	151	GLN	2.1
1	G	83	ASP	2.1
1	J	83	ASP	2.1
1	P	151	GLN	2.1
1	H	14	PRO	2.1
1	E	258	ILE	2.1
1	O	80	ILE	2.1
1	P	121	LYS	2.1
1	A	260	VAL	2.1
1	P	343	VAL	2.1
1	A	214	ARG	2.0
1	E	103	ARG	2.0
1	N	52	PHE	2.0
1	O	333	THR	2.0
1	D	408	LEU	2.0
1	E	396	MET	2.0
1	C	319	ALA	2.0
1	E	216	ALA	2.0
1	E	319	ALA	2.0
1	N	353	ALA	2.0
1	F	185	ASP	2.0
1	L	173	ASP	2.0
1	P	203	GLN	2.0
1	L	211	SER	2.0
1	E	494	ILE	2.0
1	M	23	ILE	2.0
1	A	136	ARG	2.0
1	A	201	VAL	2.0
1	A	437	VAL	2.0
1	I	320	VAL	2.0
1	I	419	VAL	2.0
1	J	437	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	403	GLY	2.0
1	P	65	ASN	2.0
1	F	157	ASP	2.0
1	H	153	GLN	2.0
1	L	112	ASP	2.0
1	P	337	LYS	2.0
1	P	377	ASP	2.0
1	A	99	ALA	2.0
1	B	384	ALA	2.0
1	D	207	MET	2.0
1	D	444	ALA	2.0
1	H	37	LEU	2.0
1	M	406	ALA	2.0
1	O	328	MET	2.0
1	P	356	ALA	2.0
1	C	304	TYR	2.0
1	L	25	CYS	2.0
1	G	215	SER	2.0
1	N	242	HIS	2.0
1	P	57	HIS	2.0
1	P	240	GLU	2.0
1	G	141	ILE	2.0
1	H	282	ILE	2.0
1	M	119	GLY	2.0
1	N	248	ILE	2.0
1	N	269	ILE	2.0
1	B	446	LYS	2.0
1	N	368	LYS	2.0
1	B	385	VAL	2.0
1	C	264	ASP	2.0
1	F	478	VAL	2.0
1	N	485	VAL	2.0
1	O	497	VAL	2.0
1	A	226	LEU	2.0
1	C	329	LEU	2.0
1	G	99	ALA	2.0
1	J	261	ALA	2.0
1	L	20	ALA	2.0
1	D	291	PRO	2.0
1	G	140	TYR	2.0
1	G	310	ARG	2.0
1	O	291	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	381	CYS	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 (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
3	K	O	501	1/1	0.96	0.42	2.48	30,30,30,30	0
7	GOL	O	499	6/6	0.85	0.41	2.09	74,75,75,75	0
3	K	K	499	1/1	0.97	0.13	1.11	52,52,52,52	0
4	OXL	F	510	6/6	0.91	0.26	0.44	83,83,83,83	0
3	K	A	504	1/1	0.68	0.28	0.12	106,106,106,106	0
7	GOL	E	499	6/6	0.91	0.15	-0.13	78,79,80,80	0
6	ATP	K	1001	31/31	0.98	0.14	-0.78	28,31,37,38	0
3	K	N	504	1/1	0.90	0.20	-0.86	84,84,84,84	0
5	FDP	N	700	20/20	0.97	0.12	-0.94	76,78,81,82	0
6	ATP	G	1001	31/31	0.90	0.17	-0.95	77,97,101,101	0
6	ATP	P	1001	31/31	0.86	0.20	-0.98	132,134,134,134	0
6	ATP	A	1001	31/31	0.94	0.15	-1.02	70,85,87,87	0
4	OXL	P	510	6/6	0.83	0.19	-1.08	85,85,85,86	0
5	FDP	P	700	20/20	0.89	0.16	-1.08	110,115,119,119	0
5	FDP	A	700	20/20	0.96	0.11	-1.09	53,58,61,64	0
6	ATP	C	1001	31/31	0.95	0.11	-1.21	43,52,54,54	0
6	ATP	J	1001	31/31	0.98	0.11	-1.23	26,34,36,36	0
6	ATP	N	1001	31/31	0.92	0.12	-1.26	83,94,95,95	0
6	ATP	E	1001	31/31	0.96	0.10	-1.33	52,58,63,63	0
6	ATP	M	1001	31/31	0.95	0.10	-1.34	66,73,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	ATP	H	1001	31/31	0.94	0.12	-1.37	62,69,72,72	0
5	FDP	L	700	20/20	0.98	0.08	-1.37	37,41,43,43	0
6	ATP	D	1001	31/31	0.98	0.10	-1.37	35,42,44,44	0
6	ATP	I	1001	31/31	0.97	0.10	-1.41	36,37,39,40	0
6	ATP	L	1001	31/31	0.96	0.11	-1.43	44,55,59,59	0
5	FDP	C	700	20/20	0.98	0.09	-1.46	36,45,48,50	0
5	FDP	B	700	20/20	0.98	0.08	-1.52	37,40,45,46	0
6	ATP	B	1001	31/31	0.98	0.10	-1.55	31,35,39,40	0
6	ATP	F	1001	31/31	0.95	0.12	-1.58	64,73,76,76	0
5	FDP	F	700	20/20	0.98	0.07	-1.59	48,53,55,56	0
4	OXL	A	510	6/6	0.92	0.14	-1.79	63,65,66,66	0
5	FDP	O	700	20/20	0.91	0.13	-1.82	118,119,121,121	0
5	FDP	M	700	20/20	0.98	0.07	-1.84	55,59,62,64	0
3	K	G	504	1/1	0.84	0.15	-1.87	82,82,82,82	0
4	OXL	M	510	6/6	0.90	0.16	-1.87	64,66,67,67	0
3	K	C	504	1/1	0.94	0.13	-1.88	56,56,56,56	0
3	K	P	504	1/1	0.79	0.19	-1.94	98,98,98,98	0
5	FDP	D	700	20/20	0.98	0.07	-1.94	32,40,43,45	0
4	OXL	C	510	6/6	0.95	0.17	-1.98	39,40,41,41	0
4	OXL	G	510	6/6	0.91	0.15	-2.02	71,74,75,75	0
5	FDP	E	700	20/20	0.99	0.07	-2.04	38,41,46,47	0
5	FDP	G	700	20/20	0.97	0.08	-2.08	69,74,75,75	0
5	FDP	H	700	20/20	0.98	0.10	-2.13	54,57,59,60	0
2	MG	C	502	1/1	0.97	0.14	-2.20	38,38,38,38	0
2	MG	P	502	1/1	0.88	0.07	-2.23	64,64,64,64	0
5	FDP	I	700	20/20	0.99	0.07	-2.24	29,32,34,35	0
4	OXL	E	510	6/6	0.98	0.15	-2.32	48,49,49,50	0
5	FDP	K	700	20/20	0.98	0.07	-2.46	36,38,42,43	0
4	OXL	I	510	6/6	0.99	0.14	-2.51	32,33,34,35	0
3	K	E	504	1/1	0.99	0.07	-2.71	48,48,48,48	0
3	K	K	504	1/1	1.00	0.10	-2.74	29,29,29,29	0
4	OXL	N	510	6/6	0.90	0.15	-2.75	77,79,80,80	0
4	OXL	H	510	6/6	0.95	0.10	-2.87	54,54,55,55	0
4	OXL	J	510	6/6	0.99	0.11	-2.90	30,31,32,33	0
3	K	D	504	1/1	0.99	0.08	-2.98	33,33,33,33	0
4	OXL	D	510	6/6	0.99	0.10	-3.00	37,38,39,39	0
5	FDP	J	700	20/20	0.99	0.05	-3.06	25,32,34,35	0
4	OXL	K	510	6/6	0.98	0.12	-3.27	25,27,28,28	0
3	K	H	504	1/1	0.97	0.06	-3.37	59,59,59,59	0
3	K	F	504	1/1	0.94	0.07	-3.40	69,69,69,69	0
3	K	M	504	1/1	0.98	0.04	-3.41	61,61,61,61	0
3	K	B	504	1/1	0.99	0.05	-3.84	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	K	J	504	1/1	0.99	0.07	-4.37	35,35,35,35	0
4	OXL	L	510	6/6	0.97	0.10	-4.54	37,38,38,39	0
3	K	I	504	1/1	0.99	0.05	-4.87	36,36,36,36	0
3	K	L	504	1/1	0.97	0.06	-4.91	52,52,52,52	0
2	MG	L	502	1/1	0.98	0.12	-5.96	37,37,37,37	0
4	OXL	B	510	6/6	0.99	0.06	-7.55	30,32,33,33	0
2	MG	J	500	1/1	0.99	0.12	-	27,27,27,27	0
2	MG	I	500	1/1	0.91	0.12	-	36,36,36,36	0
2	MG	H	502	1/1	0.96	0.31	-	61,61,61,61	0
2	MG	A	500	1/1	0.98	0.20	-	77,77,77,77	0
2	MG	P	500	1/1	0.87	0.39	-	94,94,94,94	0
2	MG	M	502	1/1	0.96	0.14	-	60,60,60,60	0
2	MG	K	500	1/1	0.98	0.11	-	29,29,29,29	0
3	K	J	501	1/1	0.99	0.09	-	50,50,50,50	0
7	GOL	I	499	6/6	0.82	0.44	-	91,91,91,92	0
7	GOL	I	501	6/6	0.85	0.47	-	85,85,85,85	0
2	MG	D	502	1/1	0.98	0.12	-	34,34,34,34	0
3	K	O	500	1/1	0.65	0.31	-	122,122,122,122	0
2	MG	C	500	1/1	0.97	0.18	-	45,45,45,45	0
3	K	D	499	1/1	0.98	0.07	-	53,53,53,53	0
2	MG	I	502	1/1	0.91	0.12	-	30,30,30,30	0
3	K	G	501	1/1	0.74	0.36	-	137,137,137,137	0
2	MG	A	502	1/1	0.97	0.15	-	58,58,58,58	0
2	MG	D	500	1/1	0.96	0.10	-	37,37,37,37	0
2	MG	G	500	1/1	0.95	0.36	-	81,81,81,81	0
3	K	N	499	1/1	0.70	0.28	-	107,107,107,107	0
2	MG	N	502	1/1	0.91	0.20	-	76,76,76,76	0
2	MG	F	502	1/1	0.86	0.10	-	60,60,60,60	0
2	MG	L	500	1/1	0.95	0.07	-	46,46,46,46	0
7	GOL	G	499	6/6	0.88	0.16	-	97,97,97,97	0
2	MG	G	502	1/1	0.97	0.20	-	66,66,66,66	0
3	K	C	499	1/1	0.95	0.09	-	68,68,68,68	0
3	K	P	499	1/1	0.78	0.22	-	119,119,119,119	0
2	MG	E	502	1/1	0.96	0.13	-	48,48,48,48	0
3	K	H	499	1/1	0.96	0.06	-	76,76,76,76	0
3	K	I	503	1/1	0.99	0.12	-	47,47,47,47	0
2	MG	H	500	1/1	0.93	0.14	-	63,63,63,63	0
2	MG	B	502	1/1	0.97	0.10	-	28,28,28,28	0
2	MG	M	500	1/1	0.96	0.14	-	69,69,69,69	0
2	MG	K	502	1/1	0.97	0.10	-	28,28,28,28	0
2	MG	J	502	1/1	0.97	0.07	-	26,26,26,26	0
7	GOL	J	499	6/6	0.66	0.37	-	69,71,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	K	M	499	1/1	0.80	0.15	-	106,106,106,106	0
2	MG	F	500	1/1	0.98	0.24	-	67,67,67,67	0
3	K	E	501	1/1	0.95	0.10	-	75,75,75,75	0
3	K	F	499	1/1	0.90	0.09	-	85,85,85,85	0
2	MG	E	500	1/1	0.92	0.08	-	55,55,55,55	0
3	K	A	499	1/1	0.99	0.12	-	60,60,60,60	0
3	K	L	499	1/1	0.99	0.04	-	47,47,47,47	0
2	MG	B	500	1/1	0.99	0.08	-	35,35,35,35	0
3	K	B	499	1/1	0.97	0.04	-	60,60,60,60	0
2	MG	N	500	1/1	0.89	0.43	-	88,88,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.