



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:47 PM 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 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/ValidationPDFNotes.html>

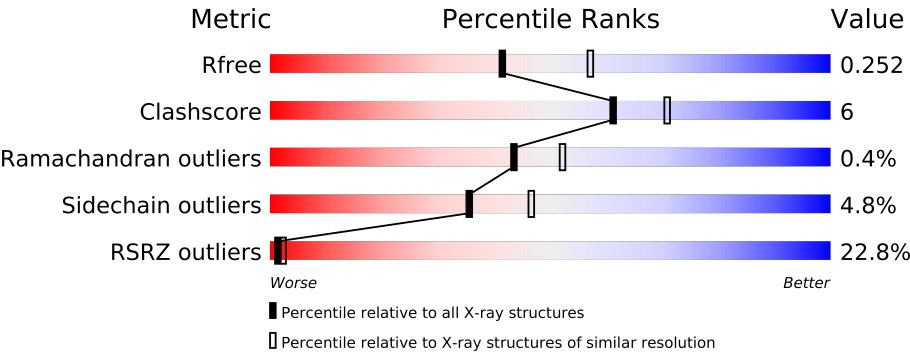
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance i

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	499	<div><div></div><div></div></div>
1	B	499	<div><div></div><div></div></div>
1	C	499	<div><div></div><div></div></div>
1	D	499	<div><div></div><div></div></div>
1	E	499	<div><div></div><div></div></div>
1	F	499	<div><div></div><div></div></div>
1	G	499	<div><div></div><div></div></div>
1	H	499	<div><div></div><div></div></div>
1	I	499	<div><div></div><div></div></div>
1	J	499	<div><div></div><div></div></div>
1	K	499	<div><div></div><div></div></div>
1	L	499	<div><div></div><div></div></div>
1	M	499	<div><div></div><div></div></div>
1	N	499	<div><div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	O	499	
1	P	499	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	500	-	X
2	MG	A	502	-	X
2	MG	B	502	-	X
2	MG	C	500	-	X
2	MG	F	500	-	X
2	MG	F	502	-	X
2	MG	G	500	-	X
2	MG	G	502	-	X
2	MG	H	502	-	X
2	MG	I	500	-	X
2	MG	K	500	-	X
2	MG	M	500	-	X
2	MG	M	502	-	X
2	MG	N	500	-	X
2	MG	N	502	-	X
2	MG	P	500	-	X
3	K	A	504	-	X
3	K	B	499	-	X
3	K	F	504	-	X
3	K	G	501	-	X
3	K	G	504	-	X
3	K	M	504	-	X
3	K	N	499	-	X
3	K	N	504	-	X
3	K	O	501	-	X
3	K	P	504	-	X
4	OXL	A	510	-	X
4	OXL	F	510	-	X
4	OXL	M	510	-	X
4	OXL	N	510	-	X
4	OXL	P	510	-	X
7	GOL	E	499	-	X
7	GOL	I	499	-	X
7	GOL	I	501	-	X
7	GOL	J	499	-	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 hydrogen and 0 are deuterium.

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 2	Mg 2	0	0
2	C	2	Total 2	Mg 2	0	0
2	A	2	Total 2	Mg 2	0	0
2	N	2	Total 2	Mg 2	0	0
2	L	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0
2	M	2	Total 2	Mg 2	0	0

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

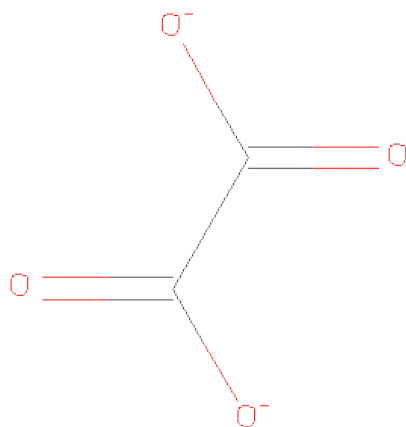
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	2	Total 2	K 2	0	0
3	G	2	Total 2	K 2	0	0
3	J	2	Total 2	K 2	0	0
3	D	2	Total 2	K 2	0	0
3	K	2	Total 2	K 2	0	0
3	E	2	Total 2	K 2	0	0
3	H	2	Total 2	K 2	0	0
3	B	2	Total 2	K 2	0	0
3	I	2	Total 2	K 2	0	0
3	C	2	Total 2	K 2	0	0
3	A	2	Total 2	K 2	0	0
3	N	2	Total 2	K 2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

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

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



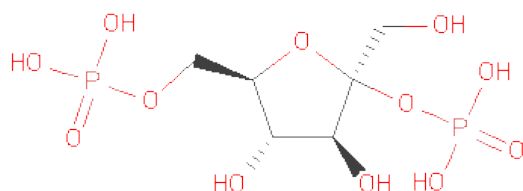
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	2	4		
4	B	1	Total	C	O	0	0
			6	2	4		
4	C	1	Total	C	O	0	0
			6	2	4		
4	D	1	Total	C	O	0	0
			6	2	4		
4	E	1	Total	C	O	0	0
			6	2	4		
4	F	1	Total	C	O	0	0
			6	2	4		
4	G	1	Total	C	O	0	0
			6	2	4		

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

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



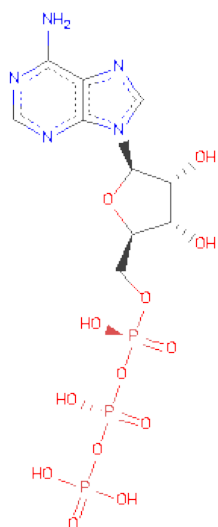
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			20	6	12	2		
5	B	1	Total	C	O	P	0	0
			20	6	12	2		
5	C	1	Total	C	O	P	0	0
			20	6	12	2		

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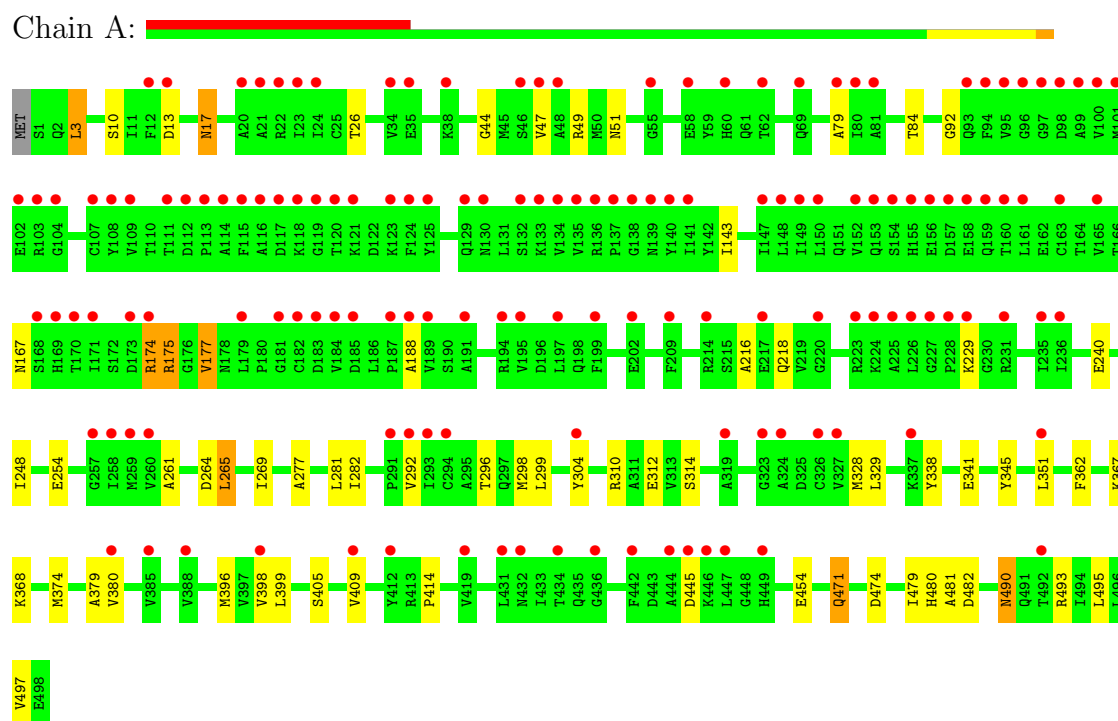
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	305	Total 305	O 305	0	0
8	D	400	Total 400	O 400	0	0
8	E	232	Total 232	O 232	0	0
8	F	187	Total 187	O 187	0	0
8	G	139	Total 139	O 139	0	0
8	H	215	Total 215	O 215	0	0
8	I	415	Total 415	O 415	0	0
8	J	499	Total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

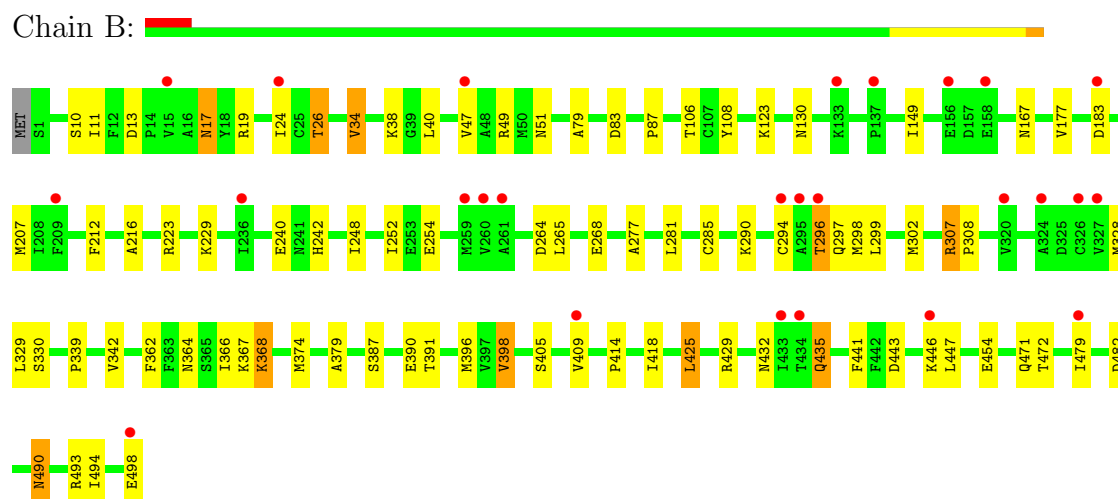
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

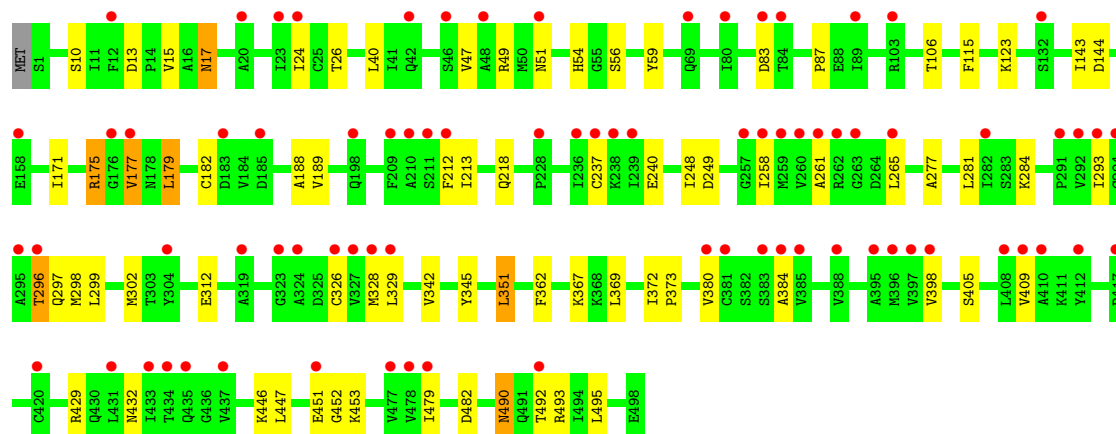
- Molecule 1: Pyruvate kinase



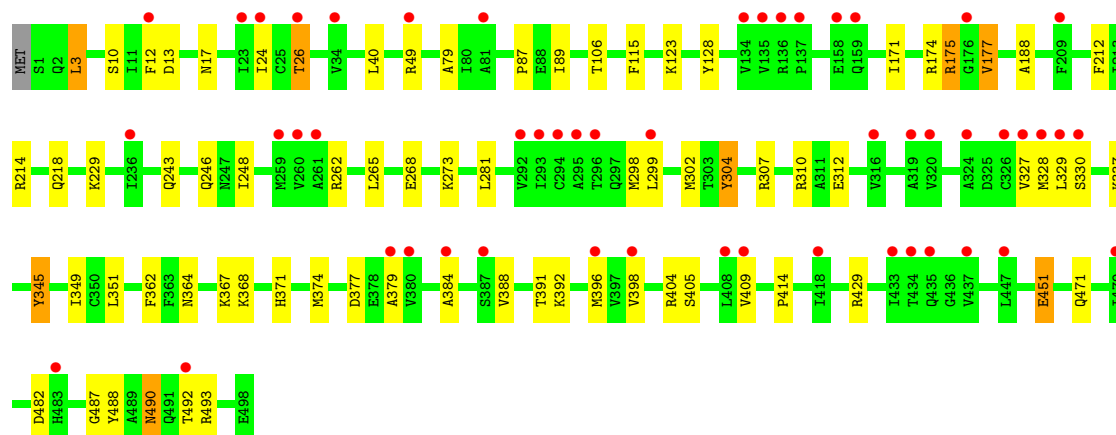
- Molecule 1: Pyruvate kinase



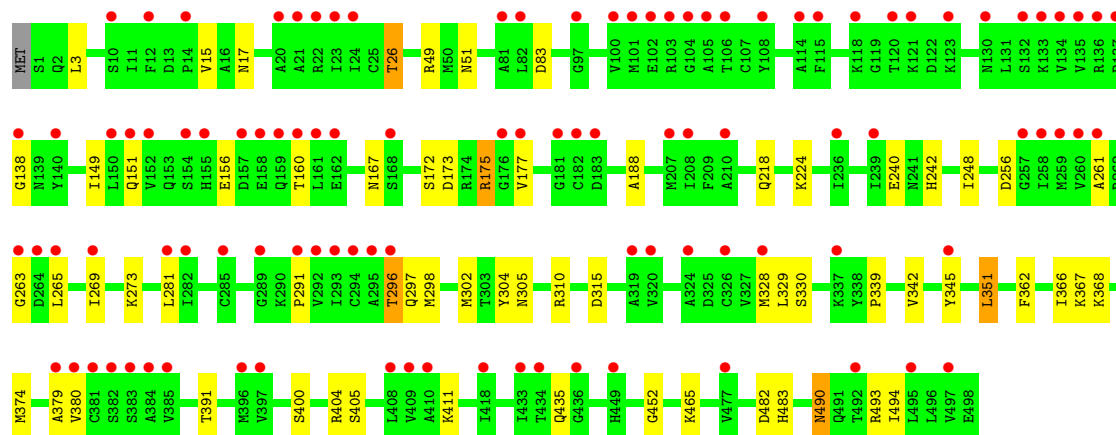
- Molecule 1: Pyruvate kinase

Chain C: 

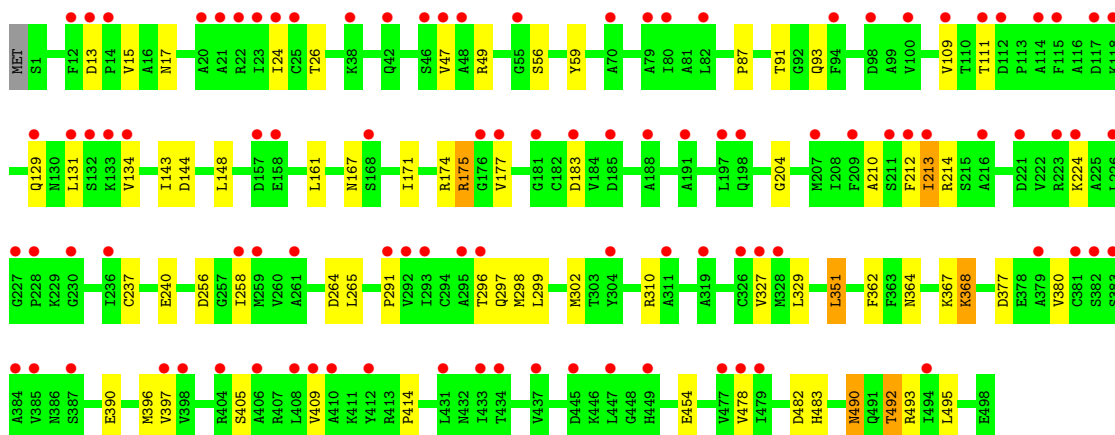
- Molecule 1: Pyruvate kinase

Chain D: 

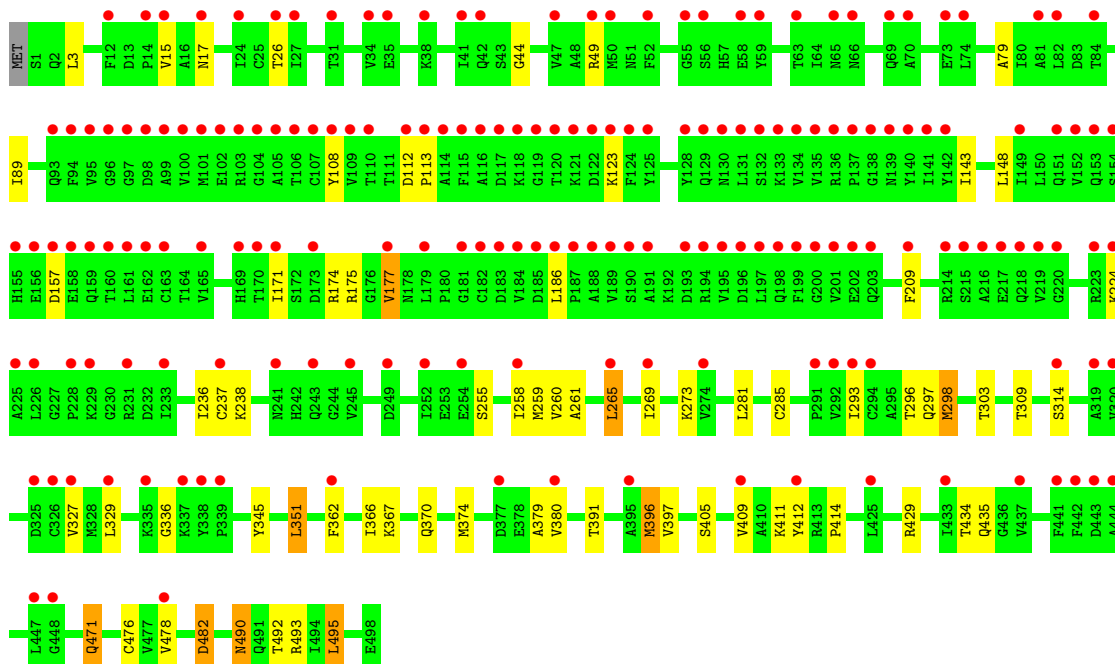
- Molecule 1: Pyruvate kinase

Chain E: 

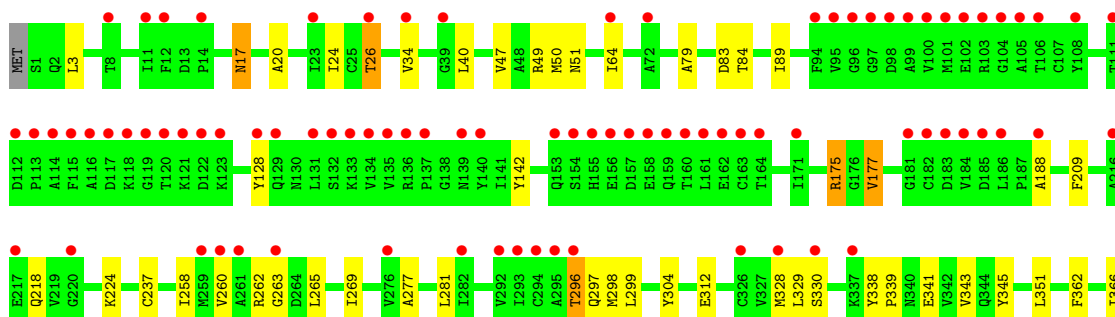
- Molecule 1: Pyruvate kinase

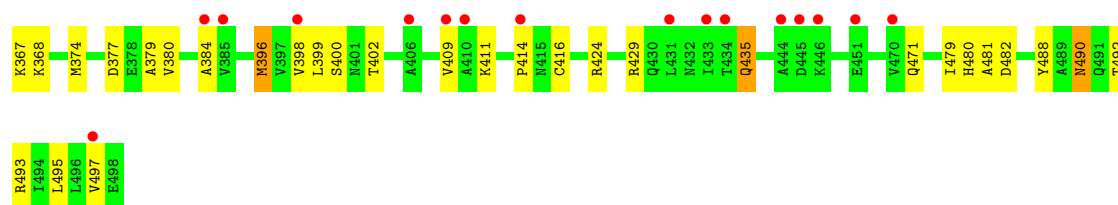
Chain F: 

- Molecule 1: Pyruvate kinase

Chain G: 

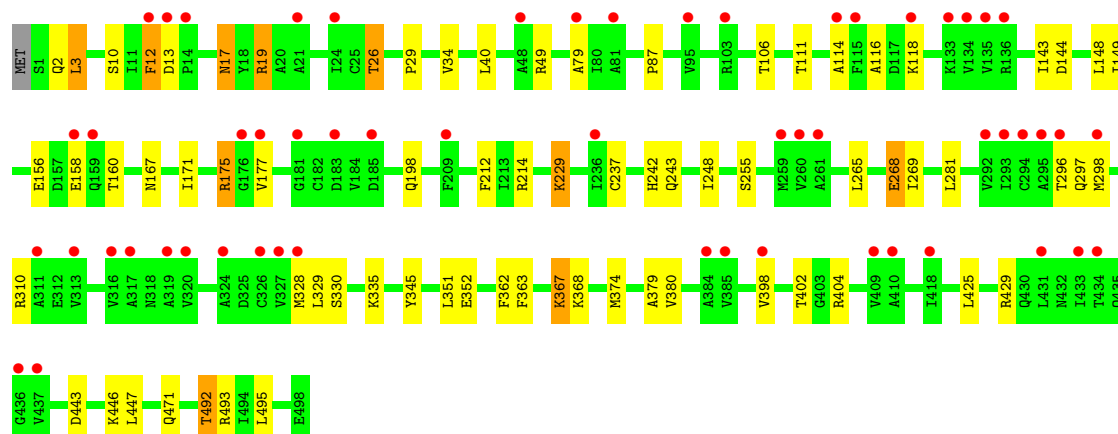
- Molecule 1: Pyruvate kinase

Chain H: 



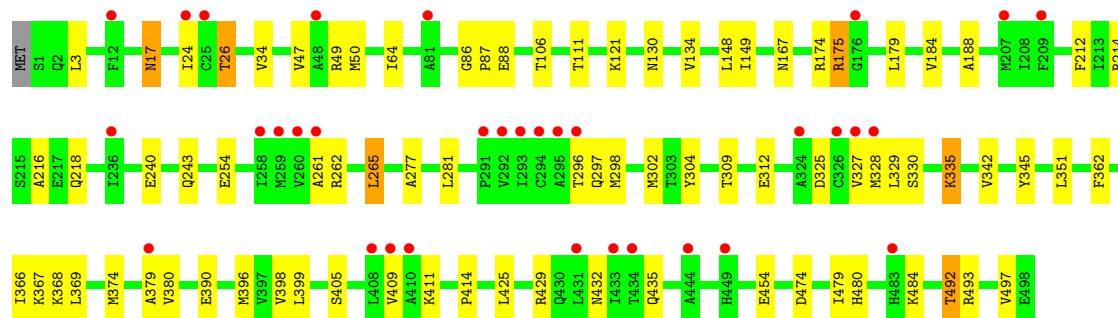
• Molecule 1: Pyruvate kinase

Chain I:



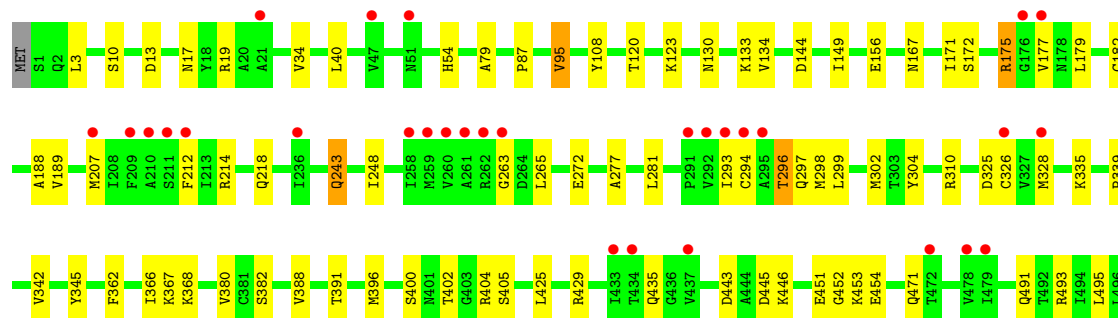
• Molecule 1: Pyruvate kinase

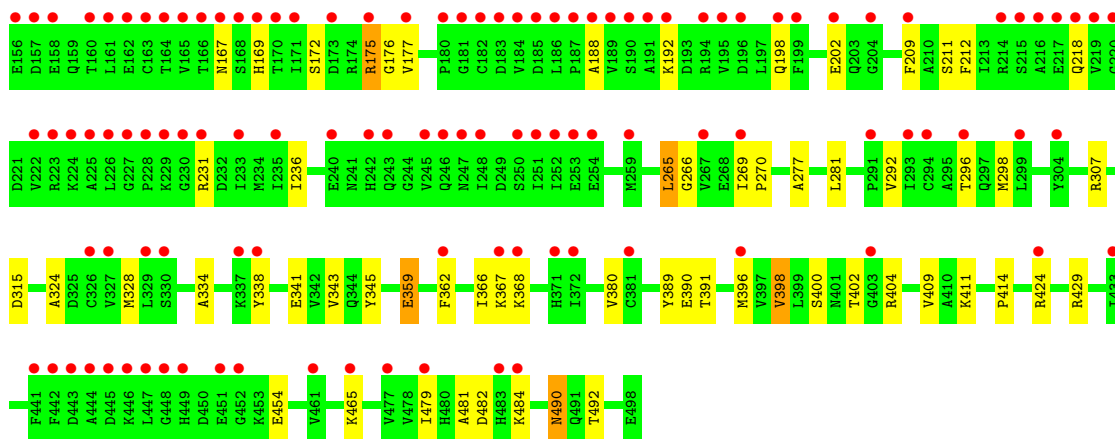
Chain J:



• Molecule 1: Pyruvate kinase

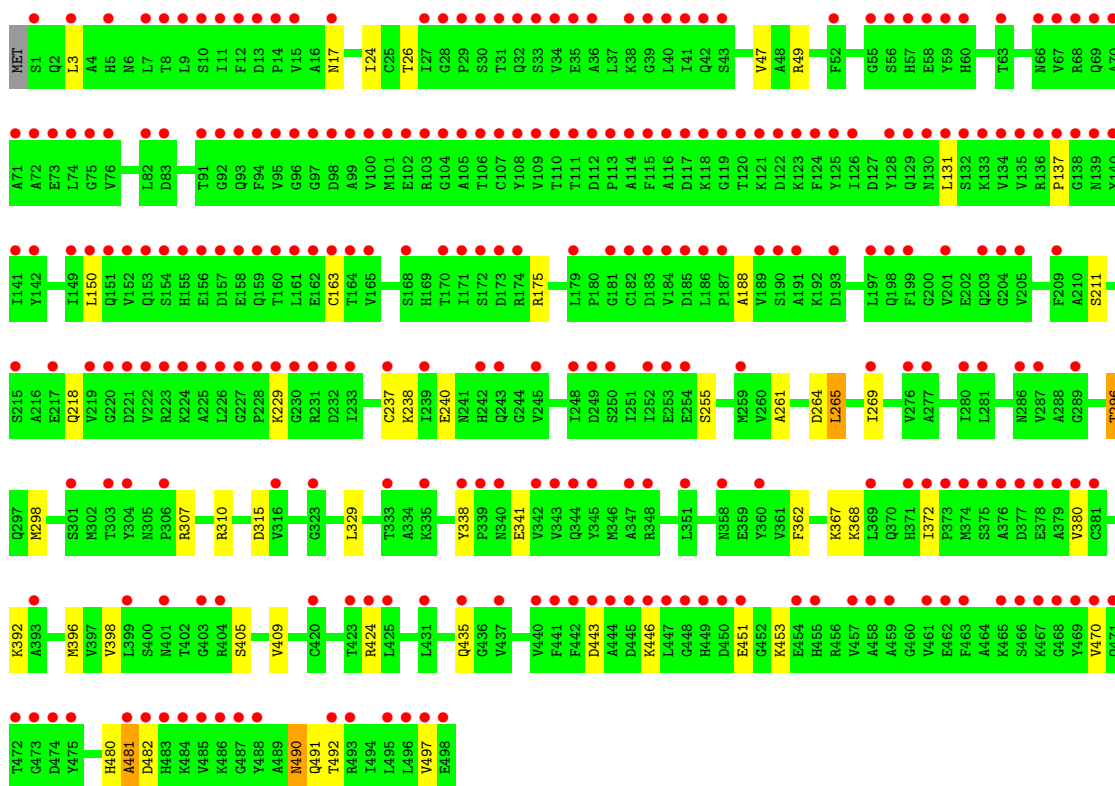
Chain K:





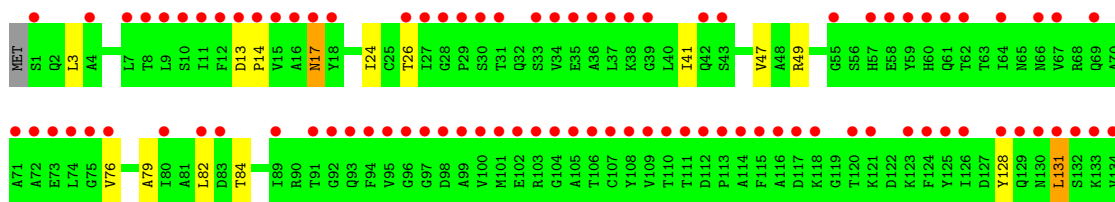
• Molecule 1: Pyruvate kinase

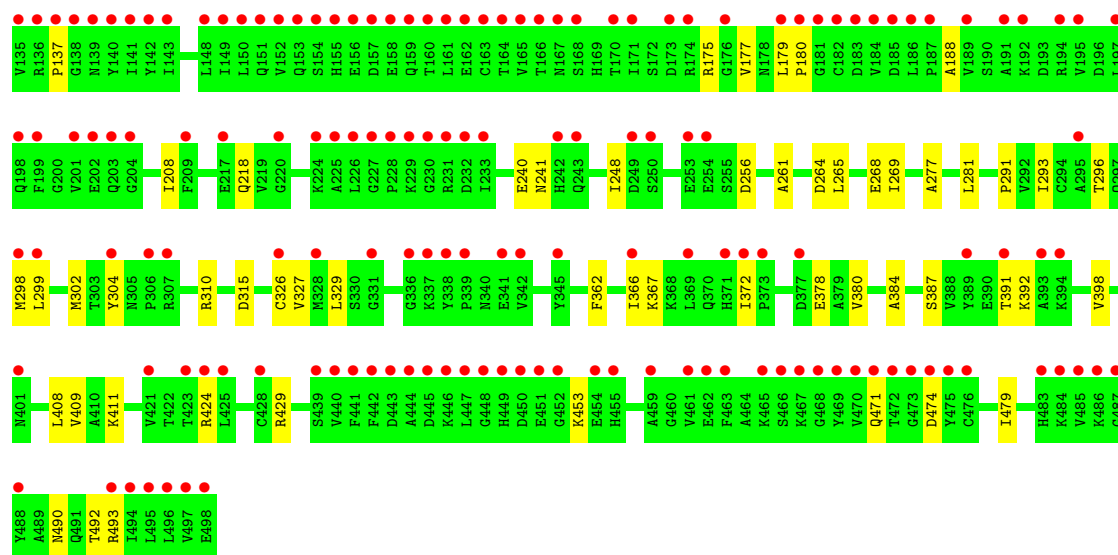
Chain O:



• Molecule 1: Pyruvate kinase

Chain P:





4 Data and refinement statistics

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) 94.6 (34.09-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.252 0.201 , 0.252	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)	0.34 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 469839 reflections	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2	0	0	0	0
3	F	2	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	20	0	10	1	0
6	A	31	0	12	2	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (710) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:C:398[A]:VAL:HG12	1:C:479:ILE:HB	1.70	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

5.3.1 Protein backbone ⓘ

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%)	33	39
1	B	496/499 (99%)	486 (98%)	8 (2%)	2 (0%)	43	52
1	C	498/499 (100%)	482 (97%)	15 (3%)	1 (0%)	56	68
1	D	497/499 (100%)	483 (97%)	14 (3%)	0	100	100
1	E	497/499 (100%)	477 (96%)	19 (4%)	1 (0%)	56	68
1	F	496/499 (99%)	480 (97%)	14 (3%)	2 (0%)	43	52
1	G	496/499 (99%)	465 (94%)	27 (5%)	4 (1%)	27	30
1	H	498/499 (100%)	477 (96%)	20 (4%)	1 (0%)	56	68
1	I	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	56	68
1	J	499/499 (100%)	483 (97%)	15 (3%)	1 (0%)	56	68
1	K	498/499 (100%)	486 (98%)	11 (2%)	1 (0%)	56	68
1	L	496/499 (99%)	477 (96%)	18 (4%)	1 (0%)	56	68
1	M	496/499 (99%)	472 (95%)	20 (4%)	4 (1%)	27	30
1	N	497/499 (100%)	476 (96%)	20 (4%)	1 (0%)	56	68
1	O	496/499 (99%)	466 (94%)	27 (5%)	3 (1%)	33	39
1	P	496/499 (99%)	469 (95%)	25 (5%)	2 (0%)	43	52
All	All	7952/7984 (100%)	7646 (96%)	278 (4%)	28 (0%)	43	52

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	34	45
1	B	416/417 (100%)	395 (95%)	21 (5%)	34	45
1	C	418/417 (100%)	401 (96%)	17 (4%)	41	55
1	D	417/417 (100%)	395 (95%)	22 (5%)	32	41
1	E	417/417 (100%)	398 (95%)	19 (5%)	37	48
1	F	416/417 (100%)	398 (96%)	18 (4%)	40	52
1	G	416/417 (100%)	396 (95%)	20 (5%)	35	46
1	H	418/417 (100%)	394 (94%)	24 (6%)	29	37
1	I	418/417 (100%)	391 (94%)	27 (6%)	24	30
1	J	419/417 (100%)	398 (95%)	21 (5%)	34	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	418/417 (100%)	392 (94%)	26 (6%)	26	33
1	L	416/417 (100%)	400 (96%)	16 (4%)	44	59
1	M	416/417 (100%)	397 (95%)	19 (5%)	37	48
1	N	417/417 (100%)	397 (95%)	20 (5%)	35	46
1	O	416/417 (100%)	401 (96%)	15 (4%)	47	61
1	P	416/417 (100%)	400 (96%)	16 (4%)	44	59
All	All	6672/6672 (100%)	6350 (95%)	322 (5%)	35	46

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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	33,33,33	1.08	2 (6%)	52,52,52	1.74	10 (19%)
4	OXL	A	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	A	700	-	20,20,20	0.87	0	32,32,32	1.30	5 (15%)
6	ATP	B	1001	3,2	33,33,33	1.07	2 (6%)	52,52,52	1.73	9 (17%)
4	OXL	B	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	B	700	-	20,20,20	1.33	2 (10%)	32,32,32	1.59	6 (18%)
6	ATP	C	1001	3,2	33,33,33	1.11	2 (6%)	52,52,52	1.73	9 (17%)
4	OXL	C	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	C	700	-	20,20,20	0.83	0	32,32,32	1.53	5 (15%)
6	ATP	D	1001	3,2	33,33,33	1.14	3 (9%)	52,52,52	1.88	10 (19%)
4	OXL	D	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	D	700	-	20,20,20	1.26	2 (10%)	32,32,32	1.60	3 (9%)
6	ATP	E	1001	3,2	33,33,33	1.06	2 (6%)	52,52,52	1.78	9 (17%)
7	GOL	E	499	-	5,5,5	0.35	0	5,5,5	0.27	0
4	OXL	E	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	E	700	-	20,20,20	1.11	2 (10%)	32,32,32	1.03	2 (6%)
6	ATP	F	1001	3,2	33,33,33	1.12	2 (6%)	52,52,52	1.73	8 (15%)
4	OXL	F	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	F	700	-	20,20,20	1.02	0	32,32,32	1.25	4 (12%)
6	ATP	G	1001	2	33,33,33	1.05	2 (6%)	52,52,52	1.74	8 (15%)
7	GOL	G	499	-	5,5,5	0.34	0	5,5,5	0.27	0
4	OXL	G	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	G	700	-	20,20,20	1.18	2 (10%)	32,32,32	1.41	4 (12%)
6	ATP	H	1001	3,2	33,33,33	1.06	2 (6%)	52,52,52	1.73	8 (15%)
4	OXL	H	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	H	700	-	20,20,20	0.99	2 (10%)	32,32,32	1.47	4 (12%)
6	ATP	I	1001	3,2	33,33,33	1.10	1 (3%)	52,52,52	1.76	11 (21%)
7	GOL	I	499	-	5,5,5	0.33	0	5,5,5	0.26	0
7	GOL	I	501	-	5,5,5	0.35	0	5,5,5	0.46	0
4	OXL	I	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	I	700	-	20,20,20	1.82	4 (20%)	32,32,32	1.40	4 (12%)
6	ATP	J	1001	3,2	33,33,33	1.13	2 (6%)	52,52,52	1.87	8 (15%)
7	GOL	J	499	-	5,5,5	0.32	0	5,5,5	0.39	0
4	OXL	J	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	J	700	-	20,20,20	1.09	2 (10%)	32,32,32	1.33	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ATP	K	1001	3,2	33,33,33	1.20	4 (12%)	52,52,52	1.67	8 (15%)
4	OXL	K	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	K	700	-	20,20,20	1.00	1 (5%)	32,32,32	1.43	6 (18%)
6	ATP	L	1001	3,2	33,33,33	1.13	2 (6%)	52,52,52	1.76	8 (15%)
4	OXL	L	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	L	700	-	20,20,20	1.11	2 (10%)	32,32,32	1.54	5 (15%)
6	ATP	M	1001	3,2	33,33,33	1.06	2 (6%)	52,52,52	1.70	8 (15%)
4	OXL	M	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	M	700	-	20,20,20	0.67	0	32,32,32	1.13	4 (12%)
6	ATP	N	1001	3,2	33,33,33	1.09	2 (6%)	52,52,52	1.79	9 (17%)
4	OXL	N	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	N	700	-	20,20,20	1.06	1 (5%)	32,32,32	1.28	3 (9%)
7	GOL	O	499	-	5,5,5	0.32	0	5,5,5	0.26	0
5	FDP	O	700	-	20,20,20	1.03	0	32,32,32	1.04	2 (6%)
6	ATP	P	1001	3,2	33,33,33	1.04	2 (6%)	52,52,52	1.78	9 (17%)
4	OXL	P	510	2	0,5,5	0.00	-	0,6,6	0.00	-
5	FDP	P	700	-	20,20,20	1.13	3 (15%)	32,32,32	0.82	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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	F	1001	3,2	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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 (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	700	FDP	O2-C2	-4.39	1.35	1.47
5	B	700	FDP	P2-O6	-4.17	1.45	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	700	FDP	P1-O2P	-4.01	1.40	1.54
6	L	1001	ATP	C5-C4	3.46	1.48	1.40
6	C	1001	ATP	C5-C4	3.44	1.48	1.40
6	M	1001	ATP	C5-C4	3.42	1.48	1.40
6	A	1001	ATP	C5-C4	3.42	1.48	1.40
6	N	1001	ATP	C5-C4	3.39	1.48	1.40
6	D	1001	ATP	C5-C4	3.36	1.48	1.40
6	G	1001	ATP	C5-C4	3.33	1.48	1.40
6	F	1001	ATP	C5-C4	3.29	1.47	1.40
6	H	1001	ATP	C5-C4	3.29	1.47	1.40
6	E	1001	ATP	C5-C4	3.28	1.47	1.40
6	P	1001	ATP	C5-C4	3.26	1.47	1.40
6	I	1001	ATP	C5-C4	3.23	1.47	1.40
5	D	700	FDP	O2-C2	-3.23	1.38	1.47
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	K	1001	ATP	C5-C4	3.03	1.47	1.40
5	I	700	FDP	O3-C3	-2.94	1.36	1.42
6	K	1001	ATP	PG-O3B	2.74	1.65	1.60
5	E	700	FDP	P2-O6	-2.74	1.50	1.60
5	D	700	FDP	O5-C5	2.68	1.50	1.43
6	K	1001	ATP	C4-N9	-2.62	1.33	1.37
5	I	700	FDP	P2-O6	-2.57	1.51	1.60
6	J	1001	ATP	C4-N9	-2.53	1.34	1.37
5	H	700	FDP	O2-C2	-2.51	1.40	1.47
5	L	700	FDP	O2-C2	-2.50	1.40	1.47
6	B	1001	ATP	C4-N9	-2.49	1.34	1.37
5	G	700	FDP	O5-C2	2.48	1.48	1.42
5	P	700	FDP	P1-O3P	2.46	1.63	1.54
6	A	1001	ATP	C4-N9	-2.43	1.34	1.37
6	G	1001	ATP	C4-N9	-2.43	1.34	1.37
6	D	1001	ATP	C4-N9	-2.41	1.34	1.37
6	L	1001	ATP	C4-N9	-2.41	1.34	1.37
5	E	700	FDP	O5-C2	2.41	1.48	1.42
6	H	1001	ATP	C4-N9	-2.40	1.34	1.37
5	J	700	FDP	O4-C4	-2.37	1.37	1.43
5	J	700	FDP	P2-O5P	-2.30	1.46	1.54
6	M	1001	ATP	C4-N9	-2.29	1.34	1.37
6	N	1001	ATP	C4-N9	-2.27	1.34	1.37
6	F	1001	ATP	C4-N9	-2.26	1.34	1.37
5	N	700	FDP	P2-O5P	2.26	1.63	1.54
5	G	700	FDP	P2-O6P	2.24	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1001	ATP	C4-N9	-2.24	1.34	1.37
5	K	700	FDP	P1-O2P	-2.21	1.46	1.54
6	P	1001	ATP	C4-N9	-2.17	1.34	1.37
5	B	700	FDP	P1-O3P	-2.14	1.46	1.54
5	H	700	FDP	P2-O5P	2.14	1.62	1.54
6	K	1001	ATP	PB-O3B	2.13	1.63	1.59
5	L	700	FDP	P2-O6	-2.13	1.52	1.60
5	P	700	FDP	P1-O2P	2.11	1.62	1.54
6	E	1001	ATP	C4-N9	-2.10	1.34	1.37
6	D	1001	ATP	PG-O3B	2.07	1.63	1.60
5	P	700	FDP	P2-O5P	2.02	1.62	1.54

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1001	ATP	N3-C2-N1	-7.34	122.57	128.71
6	E	1001	ATP	N3-C2-N1	-6.88	122.95	128.71
6	J	1001	ATP	N3-C2-N1	-6.72	123.09	128.71
6	G	1001	ATP	N3-C2-N1	-6.59	123.20	128.71
6	L	1001	ATP	N3-C2-N1	-6.55	123.23	128.71
6	P	1001	ATP	N3-C2-N1	-6.53	123.25	128.71
6	K	1001	ATP	N3-C2-N1	-6.48	123.29	128.71
6	N	1001	ATP	N3-C2-N1	-6.41	123.35	128.71
6	M	1001	ATP	N3-C2-N1	-6.34	123.41	128.71
6	I	1001	ATP	N3-C2-N1	-6.34	123.41	128.71
6	F	1001	ATP	N3-C2-N1	-6.33	123.42	128.71
6	H	1001	ATP	N3-C2-N1	-6.17	123.55	128.71
6	A	1001	ATP	N3-C2-N1	-6.08	123.62	128.71
6	D	1001	ATP	N3-C2-N1	-5.96	123.73	128.71
6	C	1001	ATP	N3-C2-N1	-5.95	123.74	128.71
5	L	700	FDP	O2-P1-O1P	5.89	123.24	106.79
6	F	1001	ATP	N3-C4-N9	5.52	135.39	125.43
6	P	1001	ATP	N3-C4-N9	5.47	135.30	125.43
6	I	1001	ATP	N3-C4-N9	5.43	135.24	125.43
6	A	1001	ATP	N3-C4-N9	5.38	135.14	125.43
6	E	1001	ATP	N3-C4-N9	5.38	135.14	125.43
6	N	1001	ATP	N3-C4-N9	5.37	135.12	125.43
6	D	1001	ATP	O4'-C1'-N9	5.33	113.39	108.44
6	G	1001	ATP	N3-C4-N9	5.29	134.99	125.43
6	C	1001	ATP	N3-C4-N9	5.29	134.99	125.43
6	B	1001	ATP	N3-C4-N9	5.28	134.97	125.43
6	M	1001	ATP	N3-C4-N9	5.27	134.95	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1001	ATP	N3-C4-N9	5.26	134.93	125.43
6	H	1001	ATP	N3-C4-N9	5.23	134.88	125.43
6	L	1001	ATP	N3-C4-N9	5.14	134.72	125.43
6	J	1001	ATP	N3-C4-N9	5.10	134.63	125.43
6	J	1001	ATP	O4'-C1'-N9	5.03	113.12	108.44
6	D	1001	ATP	N3-C4-N9	4.99	134.44	125.43
5	D	700	FDP	O2-P1-O1P	4.84	120.30	106.79
5	D	700	FDP	O3P-P1-O2	-4.42	94.36	107.09
6	L	1001	ATP	O4'-C1'-N9	4.24	112.38	108.44
5	B	700	FDP	O3P-P1-O2	-4.03	95.49	107.09
5	B	700	FDP	O2-P1-O1P	3.99	117.92	106.79
6	H	1001	ATP	O4'-C1'-N9	3.91	112.08	108.44
6	C	1001	ATP	O4'-C1'-N9	3.73	111.91	108.44
5	H	700	FDP	O3P-P1-O1P	3.69	122.49	110.44
6	I	1001	ATP	O4'-C1'-N9	3.67	111.86	108.44
6	D	1001	ATP	PA-O3A-PB	-3.58	121.17	131.68
6	J	1001	ATP	O3A-PB-O3B	3.58	108.93	101.66
6	A	1001	ATP	O4'-C1'-N9	3.55	111.74	108.44
5	C	700	FDP	O6-P2-O4P	3.51	117.01	106.71
5	N	700	FDP	O2-P1-O1P	3.49	116.54	106.79
6	C	1001	ATP	C4-C5-N7	-3.47	106.55	109.52
6	I	1001	ATP	C5-C4-N3	-3.46	118.17	125.70
6	N	1001	ATP	PB-O3B-PG	-3.44	121.60	131.68
5	G	700	FDP	C6-C5-C4	-3.42	101.50	115.21
6	N	1001	ATP	C4-C5-N7	-3.42	106.59	109.52
6	J	1001	ATP	C4-C5-N7	-3.41	106.60	109.52
6	F	1001	ATP	C5-C4-N3	-3.38	118.35	125.70
6	I	1001	ATP	C4-C5-N7	-3.37	106.64	109.52
5	G	700	FDP	O2-P1-O1P	3.37	116.19	106.79
6	P	1001	ATP	C3'-C2'-C1'	3.34	106.13	100.91
6	P	1001	ATP	C5-C4-N3	-3.33	118.46	125.70
5	H	700	FDP	C6-C5-C4	-3.33	101.88	115.21
6	F	1001	ATP	PB-O3B-PG	-3.32	121.95	131.68
6	F	1001	ATP	O4'-C1'-N9	3.31	111.52	108.44
5	I	700	FDP	O5-C2-C3	-3.31	97.83	105.54
6	A	1001	ATP	C5-C4-N3	-3.31	118.50	125.70
6	D	1001	ATP	C4-C5-N7	-3.29	106.71	109.52
6	C	1001	ATP	C5-C4-N3	-3.27	118.58	125.70
6	F	1001	ATP	C4-C5-N7	-3.26	106.73	109.52
6	G	1001	ATP	PA-O3A-PB	-3.26	122.11	131.68
6	N	1001	ATP	C5-C4-N3	-3.26	118.61	125.70
6	E	1001	ATP	O4'-C1'-N9	3.25	111.46	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1001	ATP	C4-C5-N7	-3.22	106.77	109.52
6	E	1001	ATP	C5-C4-N3	-3.21	118.72	125.70
5	B	700	FDP	C6-C5-C4	-3.20	102.39	115.21
6	H	1001	ATP	C5-C4-N3	-3.19	118.76	125.70
6	P	1001	ATP	C4-C5-N7	-3.17	106.81	109.52
6	N	1001	ATP	C3'-C2'-C1'	3.16	105.86	100.91
6	M	1001	ATP	C5-C4-N3	-3.15	118.85	125.70
6	J	1001	ATP	C5-C4-N3	-3.14	118.86	125.70
6	E	1001	ATP	C4-C5-N7	-3.14	106.83	109.52
6	K	1001	ATP	C5-C4-N3	-3.14	118.86	125.70
6	G	1001	ATP	C5-C4-N3	-3.13	118.88	125.70
5	C	700	FDP	O6P-P2-O4P	3.11	120.61	110.44
6	H	1001	ATP	C4-C5-N7	-3.11	106.86	109.52
6	P	1001	ATP	PB-O3B-PG	-3.09	122.63	131.68
5	F	700	FDP	O6P-P2-O6	-3.08	98.14	106.65
6	D	1001	ATP	C5-C4-N3	-3.07	119.01	125.70
6	B	1001	ATP	C5-C4-N3	-3.06	119.05	125.70
6	A	1001	ATP	C4-C5-N7	-3.05	106.91	109.52
6	G	1001	ATP	PB-O3B-PG	-3.05	122.75	131.68
6	L	1001	ATP	C5-C4-N3	-3.04	119.09	125.70
5	A	700	FDP	P1-O2-C2	3.01	132.63	125.77
6	K	1001	ATP	C4-C5-N7	-2.99	106.96	109.52
6	G	1001	ATP	C4-C5-N7	-2.97	106.98	109.52
6	M	1001	ATP	PB-O3B-PG	-2.96	123.00	131.68
5	H	700	FDP	O2-P1-O1P	2.94	114.99	106.79
6	P	1001	ATP	O4'-C1'-N9	2.93	111.17	108.44
6	M	1001	ATP	O4'-C1'-N9	2.92	111.15	108.44
5	B	700	FDP	O5-C2-C3	-2.91	98.77	105.54
5	A	700	FDP	O2-C2-C3	2.88	120.92	108.39
6	C	1001	ATP	PB-O3B-PG	-2.86	123.30	131.68
6	L	1001	ATP	PB-O3B-PG	-2.85	123.31	131.68
5	J	700	FDP	O6-P2-O4P	2.85	115.06	106.71
6	L	1001	ATP	C4-C5-N7	-2.85	107.08	109.52
6	A	1001	ATP	PA-O3A-PB	-2.85	123.33	131.68
6	J	1001	ATP	C2'-C1'-N9	-2.85	105.96	113.27
5	F	700	FDP	O5-C2-C3	-2.84	98.93	105.54
5	I	700	FDP	O2-C2-C3	2.84	120.74	108.39
5	B	700	FDP	O2-C2-C3	2.82	120.67	108.39
6	H	1001	ATP	PA-O3A-PB	-2.82	123.42	131.68
5	K	700	FDP	C6-C5-C4	-2.81	103.96	115.21
5	K	700	FDP	O6P-P2-O4P	2.78	119.53	110.44
6	K	1001	ATP	C2'-C1'-N9	-2.77	106.14	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	700	FDP	O2-C2-C3	2.77	120.44	108.39
6	L	1001	ATP	PA-O3A-PB	-2.77	123.57	131.68
5	J	700	FDP	O2-P1-O1P	2.71	114.36	106.79
6	D	1001	ATP	C2'-C1'-N9	-2.68	106.37	113.27
5	L	700	FDP	C6-C5-C4	-2.65	104.61	115.21
6	I	1001	ATP	C2-N3-C4	2.62	121.47	114.01
6	E	1001	ATP	C2-N3-C4	2.62	121.46	114.01
5	C	700	FDP	O5P-P2-O6	-2.62	99.42	106.65
6	E	1001	ATP	PB-O3B-PG	-2.59	124.10	131.68
6	F	1001	ATP	C2-N3-C4	2.58	121.36	114.01
6	P	1001	ATP	C2-N3-C4	2.58	121.35	114.01
6	A	1001	ATP	PB-O3B-PG	-2.57	124.16	131.68
5	O	700	FDP	O2-P1-O1P	2.56	113.94	106.79
6	C	1001	ATP	C2'-C1'-N9	-2.56	106.70	113.27
5	I	700	FDP	O3P-P1-O2	2.56	114.45	107.09
6	B	1001	ATP	C2-N3-C4	2.55	121.27	114.01
6	E	1001	ATP	PA-O3A-PB	-2.54	124.23	131.68
6	J	1001	ATP	C2-N3-C4	2.54	121.24	114.01
6	B	1001	ATP	C4-C5-N7	-2.54	107.35	109.52
6	B	1001	ATP	C2'-C1'-N9	-2.53	106.78	113.27
6	N	1001	ATP	C2-N3-C4	2.52	121.20	114.01
6	N	1001	ATP	PA-O3A-PB	-2.52	124.29	131.68
6	I	1001	ATP	PB-O3B-PG	-2.51	124.33	131.68
5	F	700	FDP	O2-C2-C3	2.50	119.30	108.39
6	I	1001	ATP	C2'-C1'-N9	-2.49	106.87	113.27
6	K	1001	ATP	C2-N3-C4	2.49	121.11	114.01
6	G	1001	ATP	C2-N3-C4	2.48	121.08	114.01
6	A	1001	ATP	C2-N3-C4	2.47	121.05	114.01
6	B	1001	ATP	C3'-C2'-C1'	2.47	104.77	100.91
5	N	700	FDP	P1-O2-C2	-2.47	120.14	125.77
5	J	700	FDP	C6-C5-C4	-2.47	105.34	115.21
5	M	700	FDP	O6-P2-O4P	2.46	113.90	106.71
6	M	1001	ATP	PA-O3A-PB	-2.45	124.50	131.68
6	H	1001	ATP	C2-N3-C4	2.44	120.95	114.01
6	M	1001	ATP	C2-N3-C4	2.44	120.94	114.01
5	A	700	FDP	C6-C5-C4	-2.43	105.48	115.21
5	K	700	FDP	O2-P1-O1P	2.43	113.56	106.79
6	A	1001	ATP	C3'-C2'-C1'	2.42	104.69	100.91
6	E	1001	ATP	C2'-C1'-N9	-2.41	107.07	113.27
5	C	700	FDP	O2-P1-O1P	2.41	113.52	106.79
6	L	1001	ATP	C2-N3-C4	2.41	120.87	114.01
5	A	700	FDP	O3P-P1-O2	2.40	114.00	107.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	1001	ATP	O4'-C1'-N9	2.39	110.67	108.44
5	J	700	FDP	O2P-P1-O2	-2.38	100.22	107.09
5	N	700	FDP	O6-P2-O4P	2.39	113.70	106.71
5	L	700	FDP	O5-C2-C3	-2.38	100.00	105.54
6	D	1001	ATP	PB-O3B-PG	-2.37	124.74	131.68
6	C	1001	ATP	C2-N3-C4	2.34	120.69	114.01
6	F	1001	ATP	C2'-C1'-N9	-2.34	107.25	113.27
5	I	700	FDP	O2P-P1-O2	-2.33	100.38	107.09
5	J	700	FDP	O2-C2-C3	2.32	118.48	108.39
6	D	1001	ATP	C2-N3-C4	2.30	120.55	114.01
6	H	1001	ATP	PB-O3B-PG	-2.27	125.01	131.68
5	K	700	FDP	O4-C4-C5	-2.26	104.42	111.08
5	D	700	FDP	C6-C5-C4	-2.22	106.33	115.21
5	C	700	FDP	O2P-P1-O2	-2.21	100.73	107.09
6	G	1001	ATP	O4'-C1'-N9	2.21	110.49	108.44
5	E	700	FDP	O5-C2-C3	-2.20	100.42	105.54
5	B	700	FDP	O6-P2-O4P	2.20	113.16	106.71
6	I	1001	ATP	O3G-PG-O2G	2.20	116.17	107.61
5	A	700	FDP	O6-P2-O4P	2.20	113.15	106.71
5	G	700	FDP	O5P-P2-O4P	-2.20	103.27	110.44
5	L	700	FDP	O3P-P1-O2	-2.19	100.78	107.09
6	K	1001	ATP	O4'-C1'-N9	2.18	110.47	108.44
6	I	1001	ATP	PA-O3A-PB	-2.16	125.34	131.68
5	M	700	FDP	O2-P1-O1P	2.15	112.78	106.79
5	K	700	FDP	C2-C3-C4	-2.14	96.65	102.15
5	M	700	FDP	P1-O2-C2	2.13	130.64	125.77
6	P	1001	ATP	PA-O3A-PB	-2.13	125.43	131.68
6	A	1001	ATP	C4'-O4'-C1'	2.12	112.06	109.75
5	K	700	FDP	O2-C2-C3	2.12	117.63	108.39
6	B	1001	ATP	C2-N1-C6	2.11	122.59	118.77
6	C	1001	ATP	O3G-PG-O2G	2.11	115.83	107.61
5	G	700	FDP	O6-P2-O4P	2.08	112.80	106.71
5	O	700	FDP	C5-C4-C3	-2.07	94.46	101.89
6	B	1001	ATP	O2G-PG-O1G	2.06	117.16	110.44
6	K	1001	ATP	C8-N9-C4	2.05	108.47	106.90
5	M	700	FDP	C6-C5-C4	-2.03	107.07	115.21
5	F	700	FDP	O6-P2-O4P	2.02	112.62	106.71
6	I	1001	ATP	C3'-C2'-C1'	2.02	104.06	100.91
5	E	700	FDP	O6-P2-O4P	2.01	112.60	106.71
6	D	1001	ATP	O3G-PG-O2G	2.01	115.42	107.61
5	H	700	FDP	O3P-P1-O2	-2.00	101.33	107.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	498/499 (99%)	1.45	147 (29%) 1 1	31, 42, 59, 61	0
1	B	498/499 (99%)	0.45	26 (5%) 26 36	15, 25, 34, 42	0
1	C	498/499 (99%)	1.02	79 (15%) 3 4	28, 39, 50, 59	0
1	D	498/499 (99%)	0.68	51 (10%) 7 12	17, 27, 43, 45	0
1	E	498/499 (99%)	1.05	103 (20%) 1 3	30, 42, 52, 56	0
1	F	498/499 (99%)	1.13	100 (20%) 2 3	36, 52, 66, 70	0
1	G	498/499 (99%)	1.78	179 (35%) 1 1	44, 52, 60, 63	0
1	H	498/499 (99%)	1.07	102 (20%) 1 3	38, 46, 52, 55	0
1	I	498/499 (99%)	0.71	56 (11%) 6 9	13, 22, 47, 53	0
1	J	498/499 (99%)	0.43	33 (6%) 18 26	15, 22, 30, 41	0
1	K	498/499 (99%)	0.49	30 (6%) 21 30	13, 22, 31, 40	0
1	L	498/499 (99%)	0.88	75 (15%) 3 5	19, 29, 60, 62	0
1	M	498/499 (99%)	1.22	123 (24%) 1 2	35, 47, 56, 59	0
1	N	498/499 (99%)	1.91	198 (39%) 1 1	45, 60, 69, 71	0
1	O	498/499 (99%)	2.61	270 (54%) 0 0	35, 55, 84, 86	0
1	P	498/499 (99%)	2.35	242 (48%) 1 0	48, 60, 83, 86	0
All	All	7968/7984 (99%)	1.20	1814 (22%) 1 2	13, 43, 65, 86	0

All (1814) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	100	VAL	9.7
1	O	444	ALA	9.3
1	O	113	PRO	9.1
1	P	496	LEU	8.9
1	O	140	TYR	8.8

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Mol	Chain	Res	Type	RSRZ
1	O	155	HIS	8.8
1	M	115	PHE	8.6
1	O	182	CYS	8.4
1	M	118	LYS	8.4
1	P	134	VAL	8.3
1	N	115	PHE	8.3
1	O	472	THR	8.3
1	O	135	VAL	7.9
1	P	135	VAL	7.9
1	O	496	LEU	7.9
1	N	195	VAL	7.8
1	P	118	LYS	7.8
1	P	455	HIS	7.8
1	O	95	VAL	7.8
1	N	447	LEU	7.8
1	P	131	LEU	7.6
1	P	472	THR	7.4
1	M	182	CYS	7.4
1	P	150	LEU	7.4
1	O	447	LEU	7.2
1	O	105	ALA	7.2
1	P	191	ALA	7.2
1	O	100	VAL	7.1
1	O	163	CYS	7.1
1	O	157	ASP	7.0
1	O	134	VAL	7.0
1	O	74	LEU	6.9
1	N	97	GLY	6.9
1	O	39	GLY	6.8
1	P	444	ALA	6.8
1	P	96	GLY	6.8
1	O	442	PHE	6.7
1	P	124	PHE	6.7
1	O	131	LEU	6.7
1	G	108	TYR	6.7
1	P	171	ILE	6.7
1	M	120	THR	6.6
1	N	448	GLY	6.6
1	P	470	VAL	6.6
1	G	96	GLY	6.6
1	P	95	VAL	6.6
1	G	95	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	P	114	ALA	6.5
1	O	487	GLY	6.5
1	P	229	LYS	6.5
1	P	11	ILE	6.4
1	P	449	HIS	6.4
1	P	184	VAL	6.4
1	P	451	GLU	6.4
1	O	137	PRO	6.4
1	O	475	TYR	6.3
1	M	135	VAL	6.3
1	O	132	SER	6.3
1	O	481	ALA	6.3
1	P	74	LEU	6.2
1	A	108	TYR	6.2
1	P	494	ILE	6.2
1	O	124	PHE	6.2
1	G	137	PRO	6.1
1	P	187	PRO	6.1
1	P	158	GLU	6.1
1	N	100	VAL	6.1
1	G	187	PRO	6.1
1	N	132	SER	6.1
1	O	191	ALA	6.1
1	O	448	GLY	6.1
1	P	12	PHE	6.0
1	O	38	LYS	6.0
1	M	100	VAL	6.0
1	O	108	TYR	6.0
1	O	125	TYR	6.0
1	O	488	TYR	6.0
1	G	138	GLY	6.0
1	A	95	VAL	6.0
1	O	130	ASN	6.0
1	H	100	VAL	6.0
1	M	304	TYR	6.0
1	N	108	TYR	6.0
1	N	161	LEU	5.9
1	O	129	GLN	5.9
1	L	115	PHE	5.9
1	O	31	THR	5.9
1	P	446	LYS	5.9
1	H	497	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	N	139	ASN	5.9
1	N	187	PRO	5.9
1	P	498	GLU	5.9
1	P	181	GLY	5.9
1	O	445	ASP	5.9
1	N	189	VAL	5.9
1	P	107	CYS	5.9
1	O	187	PRO	5.9
1	P	115	PHE	5.9
1	P	154	SER	5.9
1	O	12	PHE	5.9
1	G	189	VAL	5.8
1	N	160	THR	5.8
1	N	124	PHE	5.8
1	P	447	LEU	5.8
1	O	220	GLY	5.8
1	P	113	PRO	5.8
1	H	118	LYS	5.7
1	E	118	LYS	5.7
1	G	59	TYR	5.7
1	G	228	PRO	5.7
1	G	191	ALA	5.7
1	P	448	GLY	5.7
1	N	155	HIS	5.7
1	O	67	VAL	5.7
1	A	96	GLY	5.7
1	N	95	VAL	5.7
1	P	132	SER	5.7
1	P	483	HIS	5.6
1	O	154	SER	5.6
1	O	151	GLN	5.6
1	G	124	PHE	5.6
1	M	114	ALA	5.6
1	O	120	THR	5.6
1	P	306	PRO	5.6
1	G	155	HIS	5.6
1	E	108	TYR	5.6
1	O	156	GLU	5.6
1	P	445	ASP	5.6
1	N	141	ILE	5.6
1	P	125	TYR	5.6
1	P	128	TYR	5.6

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Mol	Chain	Res	Type	RSRZ
1	O	119	GLY	5.6
1	P	473	GLY	5.5
1	O	139	ASN	5.5
1	N	449	HIS	5.5
1	N	216	ALA	5.5
1	N	140	TYR	5.5
1	O	449	HIS	5.5
1	N	226	LEU	5.5
1	N	104	GLY	5.5
1	G	118	LYS	5.5
1	A	94	PHE	5.5
1	H	115	PHE	5.5
1	M	108	TYR	5.5
1	P	108	TYR	5.5
1	G	195	VAL	5.4
1	N	214	ARG	5.4
1	O	471	GLN	5.4
1	P	155	HIS	5.4
1	P	423	THR	5.4
1	O	128	TYR	5.4
1	P	338	TYR	5.4
1	G	198	GLN	5.4
1	N	133	LYS	5.4
1	N	12	PHE	5.4
1	N	74	LEU	5.4
1	N	251	ILE	5.4
1	A	118	LYS	5.4
1	O	221	ASP	5.4
1	P	189	VAL	5.3
1	P	101	MET	5.3
1	A	150	LEU	5.3
1	G	94	PHE	5.3
1	P	185	ASP	5.3
1	P	129	GLN	5.3
1	A	133	LYS	5.3
1	O	56	SER	5.3
1	G	339	PRO	5.3
1	N	444	ALA	5.3
1	L	158	GLU	5.3
1	A	228	PRO	5.2
1	P	228	PRO	5.2
1	O	133	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	N	103	ARG	5.2
1	N	183	ASP	5.2
1	P	153	GLN	5.2
1	G	82	LEU	5.2
1	O	231	ARG	5.2
1	M	104	GLY	5.2
1	N	117	ASP	5.2
1	P	161	LEU	5.2
1	O	441	PHE	5.2
1	P	160	THR	5.2
1	P	199	PHE	5.2
1	O	75	GLY	5.1
1	O	369	LEU	5.1
1	A	124	PHE	5.1
1	N	150	LEU	5.1
1	G	153	GLN	5.1
1	O	136	ARG	5.1
1	O	165	VAL	5.1
1	N	247	ASN	5.1
1	O	55	GLY	5.1
1	O	455	HIS	5.1
1	A	135	VAL	5.1
1	G	185	ASP	5.0
1	P	14	PRO	5.0
1	O	201	VAL	5.0
1	N	118	LYS	5.0
1	N	182	CYS	5.0
1	N	131	LEU	5.0
1	N	166	THR	5.0
1	O	13	ASP	5.0
1	G	115	PHE	5.0
1	M	185	ASP	5.0
1	O	450	ASP	5.0
1	N	185	ASP	5.0
1	O	474	ASP	5.0
1	M	156	GLU	5.0
1	P	442	PHE	5.0
1	O	111	THR	4.9
1	O	34	VAL	4.9
1	G	12	PHE	4.9
1	M	140	TYR	4.9
1	O	159	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	197	LEU	4.9
1	O	224	LYS	4.9
1	H	157	ASP	4.9
1	P	391	THR	4.9
1	G	226	LEU	4.9
1	O	14	PRO	4.9
1	P	111	THR	4.9
1	M	107	CYS	4.8
1	N	105	ALA	4.8
1	M	12	PHE	4.8
1	N	154	SER	4.8
1	O	93	GLN	4.8
1	P	198	GLN	4.8
1	O	96	GLY	4.8
1	A	171	ILE	4.8
1	N	136	ARG	4.8
1	G	116	ALA	4.8
1	O	181	GLY	4.8
1	P	43	SER	4.8
1	E	115	PHE	4.8
1	P	73	GLU	4.8
1	P	106	THR	4.8
1	P	103	ARG	4.8
1	P	37	LEU	4.8
1	G	133	LYS	4.8
1	M	95	VAL	4.8
1	A	152	VAL	4.7
1	O	470	VAL	4.7
1	P	16	ALA	4.7
1	H	293	ILE	4.7
1	O	8	THR	4.7
1	A	158	GLU	4.7
1	O	371	HIS	4.7
1	H	12	PHE	4.7
1	I	134	VAL	4.7
1	P	165	VAL	4.7
1	O	114	ALA	4.7
1	O	41	ILE	4.7
1	P	75	GLY	4.7
1	O	107	CYS	4.7
1	N	153	GLN	4.6
1	O	443	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	P	443	ASP	4.6
1	G	161	LEU	4.6
1	E	14	PRO	4.6
1	O	183	ASP	4.6
1	O	423	THR	4.6
1	G	109	VAL	4.6
1	I	135	VAL	4.6
1	N	483	HIS	4.6
1	O	458	ALA	4.6
1	O	495	LEU	4.6
1	O	287	VAL	4.6
1	O	142	TYR	4.6
1	O	115	PHE	4.6
1	M	96	GLY	4.6
1	O	484	LYS	4.6
1	A	155	HIS	4.6
1	M	136	ARG	4.6
1	F	228	PRO	4.6
1	G	107	CYS	4.6
1	O	198	GLN	4.6
1	E	136	ARG	4.6
1	N	94	PHE	4.6
1	O	204	GLY	4.6
1	P	133	LYS	4.6
1	N	168	SER	4.5
1	G	447	LEU	4.5
1	O	126	ILE	4.5
1	A	102	GLU	4.5
1	E	12	PHE	4.5
1	O	110	THR	4.5
1	G	74	LEU	4.5
1	C	293	ILE	4.5
1	A	120	THR	4.5
1	N	170	THR	4.5
1	A	98	ASP	4.5
1	H	181	GLY	4.5
1	O	372	ILE	4.5
1	P	475	TYR	4.5
1	N	225	ALA	4.5
1	E	155	HIS	4.5
1	P	136	ARG	4.5
1	F	326	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	52	PHE	4.5
1	L	97	GLY	4.5
1	O	104	GLY	4.5
1	P	454	GLU	4.5
1	P	168	SER	4.5
1	A	137	PRO	4.5
1	N	113	PRO	4.5
1	P	137	PRO	4.5
1	O	160	THR	4.5
1	G	152	VAL	4.5
1	O	189	VAL	4.5
1	H	129	GLN	4.4
1	E	261	ALA	4.4
1	N	230	GLY	4.4
1	N	163	CYS	4.4
1	O	152	VAL	4.4
1	O	457	VAL	4.4
1	P	497	VAL	4.4
1	M	4	ALA	4.4
1	O	468	GLY	4.4
1	P	97	GLY	4.4
1	P	487	GLY	4.4
1	E	140	TYR	4.4
1	P	304	TYR	4.4
1	M	129	GLN	4.4
1	M	132	SER	4.4
1	C	326	CYS	4.4
1	E	135	VAL	4.4
1	G	165	VAL	4.4
1	M	134	VAL	4.4
1	P	227	GLY	4.4
1	P	109	VAL	4.4
1	G	163	CYS	4.4
1	P	471	GLN	4.4
1	C	261	ALA	4.4
1	M	121	LYS	4.4
1	N	1	SER	4.4
1	G	140	TYR	4.4
1	O	3	LEU	4.4
1	N	14	PRO	4.4
1	G	184	VAL	4.4
1	N	8	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	P	99	ALA	4.3
1	G	171	ILE	4.3
1	G	154	SER	4.3
1	L	12	PHE	4.3
1	O	404	ARG	4.3
1	P	102	GLU	4.3
1	O	190	SER	4.3
1	G	102	GLU	4.3
1	O	483	HIS	4.3
1	N	228	PRO	4.3
1	O	9	LEU	4.3
1	A	93	GLN	4.3
1	G	120	THR	4.3
1	N	151	GLN	4.3
1	M	116	ALA	4.3
1	A	111	THR	4.3
1	P	110	THR	4.3
1	E	132	SER	4.3
1	F	47	VAL	4.3
1	N	157	ASP	4.3
1	O	446	LYS	4.3
1	G	141	ILE	4.3
1	O	99	ALA	4.3
1	P	452	GLY	4.3
1	P	307	ARG	4.3
1	O	179	LEU	4.2
1	N	106	THR	4.2
1	N	107	CYS	4.2
1	N	372	ILE	4.2
1	A	115	PHE	4.2
1	F	115	PHE	4.2
1	P	394	LYS	4.2
1	M	106	THR	4.2
1	O	101	MET	4.2
1	A	293	ILE	4.2
1	P	17	ASN	4.2
1	O	339	PRO	4.2
1	O	122	ASP	4.2
1	C	409	VAL	4.2
1	E	137	PRO	4.2
1	N	199	PHE	4.2
1	N	69	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	O	351	LEU	4.2
1	P	425	LEU	4.2
1	L	134	VAL	4.2
1	N	465	LYS	4.2
1	P	441	PHE	4.2
1	E	158	GLU	4.2
1	O	197	LEU	4.2
1	A	134	VAL	4.2
1	M	133	LYS	4.2
1	K	293	ILE	4.2
1	O	94	PHE	4.2
1	O	164	THR	4.2
1	P	130	ASN	4.2
1	H	159	GLN	4.2
1	M	113	PRO	4.2
1	P	34	VAL	4.1
1	O	473	GLY	4.1
1	O	486	LYS	4.1
1	A	114	ALA	4.1
1	E	292	VAL	4.1
1	P	488	TYR	4.1
1	M	130	ASN	4.1
1	H	185	ASP	4.1
1	N	58	GLU	4.1
1	P	120	THR	4.1
1	E	133	LYS	4.1
1	O	373	PRO	4.1
1	O	168	SER	4.1
1	O	102	GLU	4.1
1	G	223	ARG	4.1
1	G	97	GLY	4.1
1	O	112	ASP	4.1
1	P	138	GLY	4.1
1	P	157	ASP	4.1
1	E	295	ALA	4.1
1	G	134	VAL	4.1
1	G	292	VAL	4.1
1	H	108	TYR	4.1
1	O	451	GLU	4.1
1	P	466	SER	4.1
1	O	118	LYS	4.1
1	N	114	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	95	VAL	4.1
1	H	160	THR	4.1
1	G	249	ASP	4.0
1	I	185	ASP	4.0
1	O	121	LYS	4.0
1	N	194	ARG	4.0
1	O	76	VAL	4.0
1	E	168	SER	4.0
1	A	156	GLU	4.0
1	C	294	CYS	4.0
1	P	428	CYS	4.0
1	J	295	ALA	4.0
1	O	116	ALA	4.0
1	P	31	THR	4.0
1	C	259	MET	4.0
1	H	114	ALA	4.0
1	H	292	VAL	4.0
1	N	164	THR	4.0
1	A	168	SER	4.0
1	A	55	GLY	4.0
1	F	227	GLY	4.0
1	O	338	TYR	4.0
1	A	226	LEU	4.0
1	G	70	ALA	4.0
1	O	424	ARG	4.0
1	G	293	ILE	4.0
1	P	141	ILE	4.0
1	P	58	GLU	4.0
1	N	34	VAL	4.0
1	N	246	GLN	4.0
1	P	170	THR	4.0
1	N	327	VAL	4.0
1	O	498	GLU	4.0
1	A	113	PRO	4.0
1	M	98	ASP	4.0
1	O	469	TYR	4.0
1	N	102	GLU	3.9
1	O	5	HIS	3.9
1	P	93	GLN	3.9
1	G	224	LYS	3.9
1	F	24	ILE	3.9
1	P	162	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	449	HIS	3.9
1	G	114	ALA	3.9
1	P	72	ALA	3.9
1	H	104	GLY	3.9
1	M	158	GLU	3.9
1	O	32	GLN	3.9
1	O	399	LEU	3.9
1	H	188	ALA	3.9
1	N	72	ALA	3.9
1	C	327	VAL	3.9
1	E	152	VAL	3.9
1	C	258	ILE	3.9
1	O	59	TYR	3.9
1	N	217	GLU	3.9
1	G	188	ALA	3.9
1	M	139	ASN	3.9
1	C	260	VAL	3.9
1	M	433	ILE	3.9
1	I	114	ALA	3.9
1	F	409	VAL	3.9
1	N	245	VAL	3.9
1	P	371	HIS	3.9
1	G	98	ASP	3.9
1	A	224	LYS	3.9
1	G	119	GLY	3.9
1	O	158	GLU	3.9
1	O	228	PRO	3.9
1	H	133	LYS	3.8
1	A	103	ARG	3.8
1	O	35	GLU	3.8
1	O	223	ARG	3.8
1	F	191	ALA	3.8
1	M	15	VAL	3.8
1	N	93	GLN	3.8
1	E	104	GLY	3.8
1	A	99	ALA	3.8
1	M	99	ALA	3.8
1	O	377	ASP	3.8
1	A	97	GLY	3.8
1	G	132	SER	3.8
1	G	182	CYS	3.8
1	H	132	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	292	VAL	3.8
1	K	292	VAL	3.8
1	N	446	LYS	3.8
1	P	372	ILE	3.8
1	A	21	ALA	3.8
1	H	94	PHE	3.8
1	I	183	ASP	3.8
1	P	164	THR	3.8
1	P	231	ARG	3.8
1	O	381	CYS	3.8
1	N	293	ILE	3.8
1	F	112	ASP	3.8
1	M	3	LEU	3.8
1	P	94	PHE	3.8
1	H	119	GLY	3.8
1	H	123	LYS	3.8
1	F	449	HIS	3.8
1	E	324	ALA	3.8
1	G	105	ALA	3.8
1	N	338	TYR	3.8
1	P	224	LYS	3.8
1	H	95	VAL	3.8
1	E	326	CYS	3.7
1	F	226	LEU	3.7
1	O	425	LEU	3.7
1	P	142	TYR	3.7
1	M	103	ARG	3.7
1	N	162	GLU	3.7
1	F	293	ILE	3.7
1	M	105	ALA	3.7
1	D	135	VAL	3.7
1	O	205	VAL	3.7
1	D	293	ILE	3.7
1	E	293	ILE	3.7
1	A	229	LYS	3.7
1	P	15	VAL	3.7
1	G	197	LEU	3.7
1	O	401	ASN	3.7
1	P	495	LEU	3.7
1	F	381	CYS	3.7
1	O	227	GLY	3.7
1	O	403	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	N	98	ASP	3.7
1	G	444	ALA	3.7
1	N	143	ILE	3.7
1	I	115	PHE	3.7
1	O	150	LEU	3.7
1	N	231	ARG	3.7
1	N	445	ASP	3.7
1	O	232	ASP	3.7
1	A	446	LYS	3.7
1	N	224	LYS	3.7
1	G	135	VAL	3.7
1	H	116	ALA	3.7
1	O	70	ALA	3.7
1	G	202	GLU	3.7
1	M	131	LEU	3.7
1	O	73	GLU	3.7
1	O	226	LEU	3.7
1	H	134	VAL	3.6
1	I	177	VAL	3.6
1	J	292	VAL	3.6
1	N	110	THR	3.6
1	O	219	VAL	3.6
1	A	24	ILE	3.6
1	P	80	ILE	3.6
1	N	129	GLN	3.6
1	E	381	CYS	3.6
1	M	117	ASP	3.6
1	N	173	ASP	3.6
1	N	10	SER	3.6
1	M	17	ASN	3.6
1	O	459	ALA	3.6
1	M	11	ILE	3.6
1	N	148	LEU	3.6
1	A	160	THR	3.6
1	C	328	MET	3.6
1	O	161	LEU	3.6
1	B	326	CYS	3.6
1	N	254	GLU	3.6
1	F	118	LYS	3.6
1	G	31	THR	3.6
1	N	125	TYR	3.6
1	G	55	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	O	15	VAL	3.6
1	G	99	ALA	3.6
1	P	39	GLY	3.6
1	F	236	ILE	3.6
1	L	183	ASP	3.6
1	G	50	MET	3.6
1	O	138	GLY	3.5
1	P	468	GLY	3.5
1	F	109	VAL	3.5
1	L	159	GLN	3.5
1	P	182	CYS	3.5
1	G	121	LYS	3.5
1	P	33	SER	3.5
1	G	112	ASP	3.5
1	M	155	HIS	3.5
1	O	40	LEU	3.5
1	F	12	PHE	3.5
1	H	156	GLU	3.5
1	I	181	GLY	3.5
1	M	166	THR	3.5
1	A	183	ASP	3.5
1	E	345	TYR	3.5
1	F	177	VAL	3.5
1	F	410	ALA	3.5
1	G	190	SER	3.5
1	H	295	ALA	3.5
1	M	128	TYR	3.5
1	M	157	ASP	3.5
1	P	195	VAL	3.5
1	A	337	LYS	3.5
1	E	120	THR	3.5
1	A	109	VAL	3.5
1	F	384	ALA	3.5
1	H	102	GLU	3.5
1	N	188	ALA	3.5
1	H	155	HIS	3.5
1	O	431	LEU	3.5
1	L	160	THR	3.5
1	O	185	ASP	3.5
1	P	13	ASP	3.5
1	P	156	GLU	3.5
1	O	17	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	97	GLY	3.5
1	I	326	CYS	3.5
1	A	161	LEU	3.5
1	G	159	GLN	3.5
1	G	193	ASP	3.5
1	O	58	GLU	3.5
1	O	253	GLU	3.5
1	N	215	SER	3.5
1	C	384	ALA	3.5
1	N	219	VAL	3.5
1	P	140	TYR	3.5
1	L	157	ASP	3.4
1	N	294	CYS	3.4
1	O	106	THR	3.4
1	F	14	PRO	3.4
1	F	478	VAL	3.4
1	G	173	ASP	3.4
1	H	183	ASP	3.4
1	O	482	ASP	3.4
1	P	152	VAL	3.4
1	A	23	ILE	3.4
1	F	46	SER	3.4
1	M	496	LEU	3.4
1	O	170	THR	3.4
1	D	294	CYS	3.4
1	O	52	PHE	3.4
1	O	117	ASP	3.4
1	H	39	GLY	3.4
1	M	184	VAL	3.4
1	P	461	VAL	3.4
1	G	58	GLU	3.4
1	G	106	THR	3.4
1	N	250	SER	3.4
1	P	8	THR	3.4
1	L	449	HIS	3.4
1	O	340	ASN	3.4
1	C	381	CYS	3.4
1	F	221	ASP	3.4
1	L	182	CYS	3.4
1	P	55	GLY	3.4
1	A	58	GLU	3.4
1	G	34	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	156	GLU	3.4
1	G	327	VAL	3.4
1	H	470	VAL	3.4
1	N	424	ARG	3.4
1	G	151	GLN	3.4
1	G	252	ILE	3.4
1	H	106	THR	3.4
1	M	94	PHE	3.4
1	N	441	PHE	3.4
1	L	451	GLU	3.4
1	N	121	LYS	3.4
1	K	295	ALA	3.4
1	G	294	CYS	3.4
1	N	152	VAL	3.4
1	A	46	SER	3.4
1	E	434	THR	3.4
1	O	360	TYR	3.4
1	O	239	ILE	3.4
1	A	447	LEU	3.4
1	P	112	ASP	3.4
1	P	373	PRO	3.4
1	O	72	ALA	3.4
1	A	184	VAL	3.4
1	M	165	VAL	3.4
1	M	122	ASP	3.4
1	O	465	LYS	3.4
1	O	63	THR	3.4
1	G	24	ILE	3.4
1	N	11	ILE	3.4
1	D	319	ALA	3.3
1	N	191	ALA	3.3
1	M	112	ASP	3.3
1	F	398	VAL	3.3
1	N	184	VAL	3.3
1	G	237	CYS	3.3
1	N	120	THR	3.3
1	F	23	ILE	3.3
1	H	128	TYR	3.3
1	J	293	ILE	3.3
1	M	448	GLY	3.3
1	A	209	PHE	3.3
1	M	137	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	229	LYS	3.3
1	P	139	ASN	3.3
1	O	57	HIS	3.3
1	E	100	VAL	3.3
1	N	134	VAL	3.3
1	O	7	LEU	3.3
1	G	136	ARG	3.3
1	H	154	SER	3.3
1	A	100	VAL	3.3
1	O	222	VAL	3.3
1	K	433	ILE	3.3
1	O	27	ILE	3.3
1	N	59	TYR	3.3
1	A	182	CYS	3.3
1	A	20	ALA	3.3
1	M	5	HIS	3.3
1	A	189	VAL	3.3
1	A	385	VAL	3.3
1	C	478	VAL	3.3
1	O	245	VAL	3.3
1	P	421	VAL	3.3
1	P	249	ASP	3.3
1	F	258	ILE	3.3
1	H	186	LEU	3.3
1	O	335	LYS	3.3
1	A	12	PHE	3.3
1	G	243	GLN	3.3
1	E	176	GLY	3.3
1	O	92	GLY	3.3
1	P	123	LYS	3.3
1	A	149	ILE	3.3
1	M	1	SER	3.3
1	M	159	GLN	3.3
1	P	10	SER	3.3
1	H	101	MET	3.3
1	N	442	PHE	3.3
1	O	393	ALA	3.3
1	P	116	ALA	3.3
1	A	104	GLY	3.3
1	N	227	GLY	3.3
1	C	185	ASP	3.3
1	G	17	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	98	ASP	3.3
1	O	374	MET	3.2
1	C	295	ALA	3.2
1	D	176	GLY	3.2
1	G	216	ALA	3.2
1	I	12	PHE	3.2
1	I	295	ALA	3.2
1	M	498	GLU	3.2
1	P	4	ALA	3.2
1	E	183	ASP	3.2
1	F	185	ASP	3.2
1	O	172	SER	3.2
1	A	80	ILE	3.2
1	A	258	ILE	3.2
1	D	24	ILE	3.2
1	F	408	LEU	3.2
1	O	162	GLU	3.2
1	M	97	GLY	3.2
1	M	183	ASP	3.2
1	F	295	ALA	3.2
1	O	199	PHE	3.2
1	A	231	ARG	3.2
1	H	326	CYS	3.2
1	O	184	VAL	3.2
1	P	242	HIS	3.2
1	G	433	ILE	3.2
1	C	319	ALA	3.2
1	M	102	GLU	3.2
1	O	466	SER	3.2
1	C	292	VAL	3.2
1	N	135	VAL	3.2
1	P	342	VAL	3.2
1	J	294	CYS	3.2
1	P	28	GLY	3.2
1	P	226	LEU	3.2
1	A	132	SER	3.2
1	E	10	SER	3.2
1	M	168	SER	3.2
1	A	130	ASN	3.2
1	C	385	VAL	3.2
1	D	316	VAL	3.2
1	J	260	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	96	GLY	3.2
1	G	103	ARG	3.2
1	N	27	ILE	3.2
1	I	324	ALA	3.2
1	M	242	HIS	3.2
1	L	118	LYS	3.2
1	O	243	GLN	3.2
1	P	38	LYS	3.2
1	P	243	GLN	3.2
1	A	136	ARG	3.2
1	O	149	ILE	3.1
1	F	319	ALA	3.1
1	M	163	CYS	3.1
1	H	122	ASP	3.1
1	H	162	GLU	3.1
1	C	304	TYR	3.1
1	O	43	SER	3.1
1	M	138	GLY	3.1
1	O	97	GLY	3.1
1	N	177	VAL	3.1
1	P	148	LEU	3.1
1	H	384	ALA	3.1
1	P	167	ASN	3.1
1	C	237	CYS	3.1
1	H	294	CYS	3.1
1	D	380	VAL	3.1
1	O	485	VAL	3.1
1	P	485	VAL	3.1
1	G	186	LEU	3.1
1	F	406	ALA	3.1
1	G	225	ALA	3.1
1	N	17	ASN	3.1
1	P	250	SER	3.1
1	A	291	PRO	3.1
1	H	96	GLY	3.1
1	A	163	CYS	3.1
1	G	219	VAL	3.1
1	N	122	ASP	3.1
1	A	148	LEU	3.1
1	K	21	ALA	3.1
1	H	158	GLU	3.1
1	C	12	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	469	TYR	3.1
1	O	103	ARG	3.1
1	E	285	CYS	3.1
1	G	229	LYS	3.1
1	L	47	VAL	3.1
1	N	371	HIS	3.1
1	A	81	ALA	3.1
1	I	261	ALA	3.1
1	P	9	LEU	3.1
1	C	492	THR	3.1
1	P	61	GLN	3.1
1	P	35	GLU	3.1
1	E	380	VAL	3.1
1	C	48	ALA	3.1
1	F	433	ILE	3.1
1	P	105	ALA	3.1
1	O	467	LYS	3.1
1	P	486	LYS	3.1
1	C	176	GLY	3.0
1	A	444	ALA	3.0
1	C	296	THR	3.0
1	D	158	GLU	3.0
1	H	182	CYS	3.0
1	J	326	CYS	3.0
1	L	295	ALA	3.0
1	P	339	PRO	3.0
1	D	433	ILE	3.0
1	P	64	ILE	3.0
1	M	124	PHE	3.0
1	F	158	GLU	3.0
1	H	135	VAL	3.0
1	L	409	VAL	3.0
1	N	443	ASP	3.0
1	C	324	ALA	3.0
1	E	21	ALA	3.0
1	H	261	ALA	3.0
1	I	431	LEU	3.0
1	M	9	LEU	3.0
1	P	369	LEU	3.0
1	C	23	ILE	3.0
1	M	293	ILE	3.0
1	G	194	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	231	ARG	3.0
1	H	98	ASP	3.0
1	N	452	GLY	3.0
1	O	173	ASP	3.0
1	A	165	VAL	3.0
1	G	201	VAL	3.0
1	C	210	ALA	3.0
1	C	408	LEU	3.0
1	N	242	HIS	3.0
1	G	199	PHE	3.0
1	H	445	ASP	3.0
1	M	119	GLY	3.0
1	C	437	VAL	3.0
1	E	259	MET	3.0
1	H	34	VAL	3.0
1	M	497	VAL	3.0
1	N	222	VAL	3.0
1	N	396	MET	3.0
1	N	451	GLU	3.0
1	N	329	LEU	3.0
1	L	418	ILE	3.0
1	O	248	ILE	3.0
1	G	183	ASP	3.0
1	P	439	SER	3.0
1	H	163	CYS	3.0
1	A	125	TYR	3.0
1	F	291	PRO	3.0
1	A	434	THR	3.0
1	G	478	VAL	3.0
1	D	384	ALA	3.0
1	E	114	ALA	3.0
1	O	376	ALA	3.0
1	H	11	ILE	3.0
1	P	337	LYS	3.0
1	P	474	ASP	3.0
1	D	159	GLN	3.0
1	G	214	ARG	3.0
1	O	66	ASN	3.0
1	D	137	PRO	2.9
1	E	177	VAL	2.9
1	O	123	LYS	2.9
1	O	347	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	236	ILE	2.9
1	E	97	GLY	2.9
1	O	230	GLY	2.9
1	A	194	ARG	2.9
1	O	174	ARG	2.9
1	A	62	THR	2.9
1	C	84	THR	2.9
1	D	396	MET	2.9
1	L	324	ALA	2.9
1	N	15	VAL	2.9
1	N	109	VAL	2.9
1	P	201	VAL	2.9
1	O	11	ILE	2.9
1	N	156	GLU	2.9
1	A	69	GLN	2.9
1	F	21	ALA	2.9
1	G	128	TYR	2.9
1	G	129	GLN	2.9
1	P	166	THR	2.9
1	M	125	TYR	2.9
1	D	326	CYS	2.9
1	D	437	VAL	2.9
1	I	133	LYS	2.9
1	F	80	ILE	2.9
1	N	89	ILE	2.9
1	H	217	GLU	2.9
1	E	157	ASP	2.9
1	F	223	ARG	2.9
1	E	106	THR	2.9
1	P	298	MET	2.9
1	A	188	ALA	2.9
1	D	409	VAL	2.9
1	G	15	VAL	2.9
1	J	81	ALA	2.9
1	N	181	GLY	2.9
1	P	401	ASN	2.9
1	M	7	LEU	2.9
1	P	7	LEU	2.9
1	G	233	ILE	2.9
1	O	171	ILE	2.9
1	H	137	PRO	2.9
1	P	180	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	101	MET	2.9
1	M	410	ALA	2.9
1	G	69	GLN	2.9
1	G	218	GLN	2.9
1	P	69	GLN	2.9
1	P	203	GLN	2.9
1	J	258	ILE	2.9
1	N	180	PRO	2.9
1	E	160	THR	2.9
1	F	20	ALA	2.9
1	F	79	ALA	2.9
1	K	261	ALA	2.9
1	M	295	ALA	2.9
1	O	36	ALA	2.9
1	P	179	LEU	2.8
1	F	479	ILE	2.8
1	M	147	ILE	2.8
1	O	269	ILE	2.8
1	A	107	CYS	2.8
1	E	296	THR	2.8
1	G	170	THR	2.8
1	K	176	GLY	2.8
1	A	223	ARG	2.8
1	I	319	ALA	2.8
1	N	116	ALA	2.8
1	A	409	VAL	2.8
1	C	479	ILE	2.8
1	G	139	ASN	2.8
1	J	433	ILE	2.8
1	L	433	ILE	2.8
1	N	171	ILE	2.8
1	P	233	ILE	2.8
1	F	181	GLY	2.8
1	G	56	SER	2.8
1	P	194	ARG	2.8
1	G	326	CYS	2.8
1	K	434	THR	2.8
1	F	48	ALA	2.8
1	M	16	ALA	2.8
1	N	186	LEU	2.8
1	D	236	ILE	2.8
1	H	113	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	198	GLN	2.8
1	N	218	GLN	2.8
1	N	252	ILE	2.8
1	G	162	GLU	2.8
1	P	92	GLY	2.8
1	A	191	ALA	2.8
1	F	188	ALA	2.8
1	L	326	CYS	2.8
1	F	292	VAL	2.8
1	G	100	VAL	2.8
1	L	292	VAL	2.8
1	P	76	VAL	2.8
1	A	187	PRO	2.8
1	N	128	TYR	2.8
1	E	154	SER	2.8
1	C	433	ILE	2.8
1	H	64	ILE	2.8
1	F	296	THR	2.8
1	G	123	LYS	2.8
1	M	111	THR	2.8
1	B	158	GLU	2.8
1	B	295	ALA	2.8
1	H	136	ARG	2.8
1	H	139	ASN	2.8
1	O	454	GLU	2.8
1	A	294	CYS	2.8
1	B	409	VAL	2.8
1	F	327	VAL	2.8
1	I	327	VAL	2.8
1	M	292	VAL	2.8
1	M	360	TYR	2.8
1	N	229	LYS	2.8
1	G	258	ILE	2.8
1	O	233	ILE	2.8
1	P	462	GLU	2.8
1	A	129	GLN	2.8
1	B	259	MET	2.8
1	N	101	MET	2.8
1	A	292	VAL	2.8
1	E	138	GLY	2.8
1	E	182	CYS	2.8
1	F	25	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	291	PRO	2.8
1	J	409	VAL	2.8
1	L	177	VAL	2.8
1	N	137	PRO	2.8
1	O	215	SER	2.8
1	I	294	CYS	2.8
1	P	59	TYR	2.8
1	E	24	ILE	2.8
1	A	112	ASP	2.7
1	E	319	ALA	2.7
1	O	249	ASP	2.7
1	N	330	SER	2.7
1	C	398[A]	VAL	2.7
1	E	385	VAL	2.7
1	I	118	LYS	2.7
1	G	160	THR	2.7
1	N	64	ILE	2.7
1	N	167	ASN	2.7
1	O	193	ASP	2.7
1	B	324	ALA	2.7
1	I	259	MET	2.7
1	K	259	MET	2.7
1	L	261	ALA	2.7
1	P	104	GLY	2.7
1	A	327	VAL	2.7
1	O	153	GLN	2.7
1	G	131	LEU	2.7
1	N	130	ASN	2.7
1	A	141	ILE	2.7
1	M	338	TYR	2.7
1	N	235	ILE	2.7
1	O	304	TYR	2.7
1	F	209	PHE	2.7
1	J	12	PHE	2.7
1	P	463	PHE	2.7
1	F	132	SER	2.7
1	J	48	ALA	2.7
1	P	484	LYS	2.7
1	L	137	PRO	2.7
1	M	14	PRO	2.7
1	D	260	VAL	2.7
1	G	65	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	117	ASP	2.7
1	D	434	THR	2.7
1	M	394	LYS	2.7
1	N	204	GLY	2.7
1	L	383	SER	2.7
1	F	114	ALA	2.7
1	I	21	ALA	2.7
1	L	116	ALA	2.7
1	P	36	ALA	2.7
1	C	158	GLU	2.7
1	G	245	VAL	2.7
1	H	184	VAL	2.7
1	A	431	LEU	2.7
1	D	296	THR	2.7
1	B	24	ILE	2.7
1	E	433	ILE	2.7
1	F	230	GLY	2.7
1	M	471	GLN	2.7
1	P	336	GLY	2.7
1	L	156	GLU	2.7
1	E	379	ALA	2.7
1	L	21	ALA	2.7
1	G	117	ASP	2.7
1	N	85	LYS	2.7
1	A	197	LEU	2.7
1	F	385	VAL	2.7
1	F	431	LEU	2.7
1	M	437	VAL	2.7
1	M	164	THR	2.7
1	N	198	GLN	2.7
1	O	42	GLN	2.7
1	E	23	ILE	2.7
1	K	236	ILE	2.7
1	P	18	TYR	2.7
1	C	291	PRO	2.7
1	H	99	ALA	2.7
1	K	209	PHE	2.7
1	N	81	ALA	2.7
1	B	327	VAL	2.6
1	D	329	LEU	2.6
1	F	447	LEU	2.6
1	F	477	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	265	LEU	2.6
1	K	177	VAL	2.6
1	L	100	VAL	2.6
1	P	440	VAL	2.6
1	F	176	GLY	2.6
1	P	230	GLY	2.6
1	A	121	LYS	2.6
1	G	149	ILE	2.6
1	M	372	ILE	2.6
1	A	22	ARG	2.6
1	A	304	TYR	2.6
1	P	459	ALA	2.6
1	A	38	LYS	2.6
1	C	434	THR	2.6
1	D	26	THR	2.6
1	G	179	LEU	2.6
1	H	161	LEU	2.6
1	L	447	LEU	2.6
1	M	34	VAL	2.6
1	N	62	THR	2.6
1	O	1	SER	2.6
1	O	10	SER	2.6
1	A	214	ARG	2.6
1	C	183	ASP	2.6
1	N	175	ARG	2.6
1	P	183	ASP	2.6
1	E	102	GLU	2.6
1	P	149	ILE	2.6
1	P	217	GLU	2.6
1	A	79	ALA	2.6
1	A	116	ALA	2.6
1	D	324	ALA	2.6
1	G	81	ALA	2.6
1	N	4	ALA	2.6
1	E	289	GLY	2.6
1	N	403	GLY	2.6
1	A	195	VAL	2.6
1	C	46	SER	2.6
1	G	320	VAL	2.6
1	N	192	LYS	2.6
1	H	259	MET	2.6
1	M	334	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	N	52	PHE	2.6
1	P	209	PHE	2.6
1	A	181	GLY	2.6
1	H	164	THR	2.6
1	H	296	THR	2.6
1	E	260	VAL	2.6
1	M	123	LYS	2.6
1	A	169	HIS	2.6
1	J	24	ILE	2.6
1	O	141	ILE	2.6
1	A	324	ALA	2.6
1	F	94	PHE	2.6
1	F	212	PHE	2.6
1	G	158	GLU	2.6
1	J	328	MET	2.6
1	L	20	ALA	2.6
1	P	254	GLU	2.6
1	A	445	ASP	2.6
1	E	123	LYS	2.6
1	F	133	LYS	2.6
1	G	110	THR	2.6
1	D	134	VAL	2.6
1	F	100	VAL	2.6
1	I	437	VAL	2.6
1	H	103	ARG	2.6
1	N	149	ILE	2.6
1	A	326	CYS	2.6
1	H	121	LYS	2.6
1	A	227	GLY	2.6
1	E	130	ASN	2.6
1	I	13	ASP	2.6
1	F	129	GLN	2.6
1	I	176	GLY	2.6
1	O	344	GLN	2.6
1	G	63	THR	2.6
1	C	388	VAL	2.6
1	G	437	VAL	2.6
1	M	431	LEU	2.6
1	N	165	VAL	2.6
1	G	196	ASP	2.5
1	N	220	GLY	2.5
1	A	199	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	326	CYS	2.5
1	G	217	GLU	2.5
1	O	250	SER	2.5
1	A	60	HIS	2.5
1	C	238	LYS	2.5
1	D	447	LEU	2.5
1	F	131	LEU	2.5
1	F	437	VAL	2.5
1	H	260	VAL	2.5
1	L	408	LEU	2.5
1	E	151	GLN	2.5
1	G	122	ASP	2.5
1	P	29	PRO	2.5
1	A	220	GLY	2.5
1	A	436	GLY	2.5
1	C	24	ILE	2.5
1	P	366	ILE	2.5
1	C	209	PHE	2.5
1	D	209	PHE	2.5
1	P	467	LYS	2.5
1	I	296	THR	2.5
1	A	157	ASP	2.5
1	C	265	LEU	2.5
1	F	82	LEU	2.5
1	I	398[A]	VAL	2.5
1	O	82	LEU	2.5
1	P	66	ASN	2.5
1	A	217	GLU	2.5
1	C	236	ILE	2.5
1	D	379	ALA	2.5
1	F	383	SER	2.5
1	I	24	ILE	2.5
1	I	328	MET	2.5
1	K	258	ILE	2.5
1	P	71	ALA	2.5
1	P	225	ALA	2.5
1	G	338	TYR	2.5
1	O	333	THR	2.5
1	O	492	THR	2.5
1	P	163	CYS	2.5
1	H	220	GLY	2.5
1	P	197	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	80	ILE	2.5
1	I	81	ALA	2.5
1	M	10	SER	2.5
1	M	171	ILE	2.5
1	N	479	ILE	2.5
1	E	159	GLN	2.5
1	M	93	GLN	2.5
1	N	253	GLU	2.5
1	F	434	THR	2.5
1	H	26	THR	2.5
1	N	142	TYR	2.5
1	O	91	THR	2.5
1	O	345	TYR	2.5
1	A	138	GLY	2.5
1	G	181	GLY	2.5
1	G	220	GLY	2.5
1	M	473	GLY	2.5
1	O	461	VAL	2.5
1	L	154	SER	2.5
1	F	198	GLN	2.5
1	H	451	GLU	2.5
1	C	410	ALA	2.5
1	J	444	ALA	2.5
1	L	444	ALA	2.5
1	P	57	HIS	2.5
1	I	418	ILE	2.5
1	A	117	ASP	2.5
1	G	157	ASP	2.5
1	A	432	ASN	2.5
1	I	103	ARG	2.5
1	P	174	ARG	2.5
1	O	28	GLY	2.5
1	D	435	GLN	2.5
1	H	153	GLN	2.5
1	H	398[A]	VAL	2.5
1	I	260	VAL	2.5
1	L	382	SER	2.5
1	P	326	CYS	2.5
1	D	295	ALA	2.5
1	I	384	ALA	2.5
1	I	410	ALA	2.5
1	O	225	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	139	ASN	2.5
1	C	103	ARG	2.5
1	N	248	ILE	2.5
1	B	434	THR	2.4
1	N	73	GLU	2.4
1	P	202	GLU	2.4
1	M	151	GLN	2.4
1	P	151	GLN	2.4
1	E	337	LYS	2.4
1	F	224	LYS	2.4
1	G	38	LYS	2.4
1	P	121	LYS	2.4
1	M	172	SER	2.4
1	E	409	VAL	2.4
1	E	497	VAL	2.4
1	F	117	ASP	2.4
1	M	169	HIS	2.4
1	O	109	VAL	2.4
1	O	343	VAL	2.4
1	O	497	VAL	2.4
1	J	410	ALA	2.4
1	J	259	MET	2.4
1	A	202	GLU	2.4
1	B	479	ILE	2.4
1	D	23	ILE	2.4
1	J	236	ILE	2.4
1	N	233	ILE	2.4
1	P	341	GLU	2.4
1	M	8	THR	2.4
1	J	449	HIS	2.4
1	P	450	ASP	2.4
1	H	131	LEU	2.4
1	I	292	VAL	2.4
1	O	186	LEU	2.4
1	P	299	LEU	2.4
1	C	20	ALA	2.4
1	G	101	MET	2.4
1	A	153	GLN	2.4
1	F	42	GLN	2.4
1	M	153	GLN	2.4
1	N	80	ILE	2.4
1	L	120	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	262	ARG	2.4
1	J	291	PRO	2.4
1	K	291	PRO	2.4
1	F	183	ASP	2.4
1	G	169	HIS	2.4
1	N	169	HIS	2.4
1	P	30	SER	2.4
1	H	140	TYR	2.4
1	A	123	LYS	2.4
1	C	177	VAL	2.4
1	I	316	VAL	2.4
1	L	477	VAL	2.4
1	O	437	VAL	2.4
1	O	440	VAL	2.4
1	E	20	ALA	2.4
1	H	105	ALA	2.4
1	K	210	ALA	2.4
1	P	328	MET	2.4
1	H	282	ILE	2.4
1	M	181	GLY	2.4
1	N	296	THR	2.4
1	A	185	ASP	2.4
1	C	228	PRO	2.4
1	H	14	PRO	2.4
1	M	35	GLU	2.4
1	O	378	GLU	2.4
1	K	294	CYS	2.4
1	P	476	CYS	2.4
1	O	203	GLN	2.4
1	E	81	ALA	2.4
1	H	216	ALA	2.4
1	E	396	MET	2.4
1	H	263	GLY	2.4
1	O	71	ALA	2.4
1	P	424	ARG	2.4
1	A	170	THR	2.4
1	F	445	ASP	2.4
1	G	41	ILE	2.4
1	G	84	THR	2.4
1	H	120	THR	2.4
1	H	434	THR	2.4
1	I	434	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	252	ILE	2.4
1	N	291	PRO	2.4
1	B	294	CYS	2.4
1	A	179	LEU	2.4
1	A	351	LEU	2.4
1	E	281	LEU	2.4
1	P	493	ARG	2.4
1	A	260	VAL	2.4
1	C	263	GLY	2.4
1	E	436	GLY	2.4
1	I	409	VAL	2.4
1	F	157	ASP	2.4
1	G	377	ASP	2.4
1	I	48	ALA	2.4
1	P	377	ASP	2.4
1	G	130	ASN	2.4
1	B	209	PHE	2.4
1	D	12	PHE	2.4
1	H	337	LYS	2.3
1	N	337	LYS	2.3
1	F	13	ASP	2.3
1	P	389	TYR	2.3
1	I	436	GLY	2.3
1	E	410	ALA	2.3
1	G	47	VAL	2.3
1	M	328	MET	2.3
1	N	243	GLN	2.3
1	O	303	THR	2.3
1	L	132	SER	2.3
1	P	1	SER	2.3
1	N	158	GLU	2.3
1	A	174	ARG	2.3
1	B	133	LYS	2.3
1	O	493	ARG	2.3
1	H	112	ASP	2.3
1	H	117	ASP	2.3
1	K	263	GLY	2.3
1	L	92	GLY	2.3
1	O	323	GLY	2.3
1	P	331	GLY	2.3
1	C	329	LEU	2.3
1	E	150	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	431	LEU	2.3
1	L	140	TYR	2.3
1	N	304	TYR	2.3
1	A	48	ALA	2.3
1	E	210	ALA	2.3
1	N	32	GLN	2.3
1	N	240	GLU	2.3
1	E	382	SER	2.3
1	F	22	ARG	2.3
1	G	14	PRO	2.3
1	H	111	THR	2.3
1	M	449	HIS	2.3
1	A	236	ILE	2.3
1	C	282	ILE	2.3
1	F	494	ILE	2.3
1	L	293	ILE	2.3
1	C	83	ASP	2.3
1	G	200	GLY	2.3
1	L	146	GLY	2.3
1	A	35	GLU	2.3
1	C	42	GLN	2.3
1	L	130	ASN	2.3
1	H	330	SER	2.3
1	J	261	ALA	2.3
1	J	483[A]	HIS	2.3
1	O	380	VAL	2.3
1	O	237	CYS	2.3
1	E	239	ILE	2.3
1	N	433	ILE	2.3
1	C	198	GLN	2.3
1	N	35[A]	GLU	2.3
1	G	448	GLY	2.3
1	H	446	LYS	2.3
1	N	138	GLY	2.3
1	P	220	GLY	2.3
1	P	465	LYS	2.3
1	G	49	ARG	2.3
1	A	225	ALA	2.3
1	B	261	ALA	2.3
1	E	383	SER	2.3
1	D	34	VAL	2.3
1	E	384	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	291	PRO	2.3
1	E	397	VAL	2.3
1	F	328	MET	2.3
1	I	298	MET	2.3
1	B	183	ASP	2.3
1	E	162	GLU	2.3
1	G	35	GLU	2.3
1	P	173	ASP	2.3
1	N	326	CYS	2.3
1	D	479	ILE	2.3
1	E	282	ILE	2.3
1	I	293	ILE	2.3
1	N	24	ILE	2.3
1	G	442	PHE	2.3
1	N	209	PHE	2.3
1	M	154	SER	2.3
1	B	156	GLU	2.3
1	F	379	ALA	2.3
1	P	186	LEU	2.3
1	A	388	VAL	2.3
1	B	15	VAL	2.3
1	C	380	VAL	2.3
1	C	396	MET	2.3
1	G	26	THR	2.3
1	H	385	VAL	2.3
1	L	113	PRO	2.3
1	L	135	VAL	2.3
1	N	31	THR	2.3
1	N	368	LYS	2.3
1	I	159	GLN	2.3
1	L	436	GLY	2.3
1	L	448	GLY	2.3
1	P	126	ILE	2.3
1	G	441	PHE	2.3
1	L	124	PHE	2.3
1	O	375	SER	2.3
1	P	98	ASP	2.3
1	G	42	GLN	2.3
1	H	410	ALA	2.3
1	A	140	TYR	2.2
1	A	259	MET	2.2
1	F	412	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	136	ARG	2.2
1	P	26	THR	2.3
1	J	207	MET	2.2
1	N	477	VAL	2.2
1	L	178	ASN	2.2
1	N	119	GLY	2.2
1	A	147	ILE	2.2
1	D	418	ILE	2.2
1	O	254	GLU	2.2
1	C	212	PHE	2.2
1	E	294	CYS	2.2
1	A	159	GLN	2.2
1	P	83	ASP	2.2
1	D	136	ARG	2.2
1	F	216	ALA	2.2
1	J	296	THR	2.2
1	L	319	ALA	2.2
1	M	261	ALA	2.2
1	N	7	LEU	2.2
1	O	379	ALA	2.2
1	A	380	VAL	2.2
1	B	260	VAL	2.2
1	G	409	VAL	2.2
1	G	412	TYR	2.2
1	K	260	VAL	2.2
1	N	269	ILE	2.2
1	L	325	ASP	2.2
1	N	13	ASP	2.2
1	O	69	GLN	2.2
1	P	42	GLN	2.2
1	F	168	SER	2.2
1	F	382	SER	2.2
1	I	209	PHE	2.2
1	N	362	PHE	2.2
1	I	158	GLU	2.2
1	L	381	CYS	2.2
1	L	417	PRO	2.2
1	F	311	ALA	2.2
1	H	406	ALA	2.2
1	D	259	MET	2.2
1	D	328	MET	2.2
1	E	134	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	177	VAL	2.2
1	L	152	VAL	2.2
1	O	259	MET	2.2
1	O	316	VAL	2.2
1	A	13	ASP	2.2
1	F	404	ARG	2.2
1	O	242	HIS	2.2
1	C	239	ILE	2.2
1	D	330	SER	2.2
1	E	418	ILE	2.2
1	G	215	SER	2.2
1	P	27	ILE	2.2
1	N	202	GLU	2.2
1	O	306	PRO	2.2
1	D	261	ALA	2.2
1	E	492	THR	2.2
1	I	311	ALA	2.2
1	L	84	THR	2.2
1	L	406	ALA	2.2
1	P	204	GLY	2.2
1	J	408	LEU	2.2
1	L	25	CYS	2.2
1	P	82	LEU	2.2
1	E	328	MET	2.2
1	A	398	VAL	2.2
1	D	398	VAL	2.2
1	I	313	VAL	2.2
1	K	47	VAL	2.2
1	L	136	ARG	2.2
1	E	236	ILE	2.2
1	E	258	ILE	2.2
1	F	213	ILE	2.2
1	P	89	ILE	2.2
1	J	209	PHE	2.2
1	E	181	GLY	2.2
1	G	104	GLY	2.2
1	J	176	GLY	2.2
1	D	49	ARG	2.2
1	E	22	ARG	2.2
1	A	173	ASP	2.2
1	H	328	MET	2.2
1	K	328	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	396	MET	2.2
1	A	34	VAL	2.2
1	D	327	VAL	2.2
1	F	397	VAL	2.2
1	L	437	VAL	2.2
1	O	342	VAL	2.2
1	O	358	ASN	2.2
1	I	236	ILE	2.2
1	A	119	GLY	2.2
1	A	323	GLY	2.2
1	I	14	PRO	2.2
1	O	209	PHE	2.2
1	E	121	LYS	2.2
1	G	335	LYS	2.2
1	M	110	THR	2.2
1	P	232	ASP	2.2
1	H	444	ALA	2.2
1	I	317	ALA	2.2
1	L	99	ALA	2.2
1	P	295	ALA	2.2
1	E	101	MET	2.2
1	B	47	VAL	2.2
1	C	132	SER	2.2
1	J	327	VAL	2.2
1	L	385	VAL	2.2
1	N	267	VAL	2.2
1	N	461	VAL	2.2
1	O	33	SER	2.2
1	O	276	VAL	2.2
1	K	51	ASN	2.2
1	C	89	ILE	2.1
1	L	78	ILE	2.1
1	L	435	GLN	2.1
1	N	484	LYS	2.1
1	H	414	PRO	2.1
1	G	209	PHE	2.1
1	D	81	ALA	2.1
1	H	72	ALA	2.1
1	M	216	ALA	2.1
1	A	101	MET	2.1
1	K	207	MET	2.1
1	N	299	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	383	SER	2.1
1	C	397	VAL	2.1
1	E	320	VAL	2.1
1	I	95	VAL	2.1
1	G	93	GLN	2.1
1	A	235	ILE	2.1
1	E	257	GLY	2.1
1	I	433	ILE	2.1
1	K	479	ILE	2.1
1	L	23	ILE	2.1
1	N	381	CYS	2.1
1	O	420	CYS	2.1
1	P	176	GLY	2.1
1	L	228	PRO	2.1
1	L	291	PRO	2.1
1	O	29	PRO	2.1
1	J	434	THR	2.1
1	O	60	HIS	2.1
1	E	105	ALA	2.1
1	G	395	ALA	2.1
1	M	451	GLU	2.1
1	N	123	LYS	2.1
1	O	217	GLU	2.1
1	P	192	LYS	2.1
1	E	207	MET	2.1
1	E	408	LEU	2.1
1	F	211	SER	2.1
1	B	320	VAL	2.1
1	D	320	VAL	2.1
1	I	385	VAL	2.1
1	E	263	GLY	2.1
1	L	445	ASP	2.1
1	M	436	GLY	2.1
1	C	451[A]	GLU	2.1
1	F	38	LYS	2.1
1	F	111	THR	2.1
1	G	337	LYS	2.1
1	O	463	PHE	2.1
1	P	62	THR	2.1
1	C	435	GLN	2.1
1	G	203	GLN	2.1
1	J	379	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	435	GLN	2.1
1	P	159	GLN	2.1
1	C	211	SER	2.1
1	D	408	LEU	2.1
1	E	495	LEU	2.1
1	M	150	LEU	2.1
1	M	259	MET	2.1
1	E	264	ASP	2.1
1	A	257	GLY	2.1
1	C	477	VAL	2.1
1	G	380	VAL	2.1
1	O	289	GLY	2.1
1	M	162	GLU	2.1
1	N	38	LYS	2.1
1	N	367	LYS	2.1
1	G	142	TYR	2.1
1	D	483[A]	HIS	2.1
1	E	103	ARG	2.1
1	M	194	ARG	2.1
1	O	280	ILE	2.1
1	P	143	ILE	2.1
1	G	66	ASN	2.1
1	D	387	SER	2.1
1	K	211	SER	2.1
1	K	326	CYS	2.1
1	L	209	PHE	2.1
1	N	190	SER	2.1
1	O	301	SER	2.1
1	N	196	ASP	2.1
1	D	299	LEU	2.1
1	E	161	LEU	2.1
1	E	265	LEU	2.1
1	G	329	LEU	2.1
1	I	320	VAL	2.1
1	C	417	PRO	2.1
1	A	412	TYR	2.1
1	C	51	ASN	2.1
1	O	286	ASN	2.1
1	H	23	ILE	2.1
1	D	492	THR	2.1
1	A	319	ALA	2.1
1	C	395	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	70	ALA	2.1
1	F	98	ASP	2.1
1	F	261	ALA	2.1
1	G	443	ASP	2.1
1	I	79	ALA	2.1
1	N	145	ASP	2.1
1	O	277	ALA	2.1
1	P	393	ALA	2.1
1	C	420	CYS	2.1
1	C	257	GLY	2.1
1	C	431	LEU	2.1
1	H	431	LEU	2.1
1	M	179	LEU	2.1
1	N	259	MET	2.1
1	O	281	LEU	2.1
1	A	47	VAL	2.1
1	H	409	VAL	2.1
1	P	67	VAL	2.1
1	G	113	PRO	2.1
1	B	433	ILE	2.1
1	C	412	TYR	2.1
1	G	125	TYR	2.1
1	F	387	SER	2.1
1	H	433	ILE	2.1
1	L	434	THR	2.1
1	M	475	TYR	2.1
1	P	91	THR	2.1
1	J	324	ALA	2.1
1	M	92	GLY	2.0
1	E	449	HIS	2.0
1	E	477	VAL	2.0
1	F	134	VAL	2.0
1	K	437	VAL	2.0
1	M	276	VAL	2.0
1	A	154	SER	2.0
1	E	269	ILE	2.0
1	F	304	TYR	2.0
1	G	27	ILE	2.0
1	H	8	THR	2.0
1	H	171	ILE	2.0
1	K	262	ARG	2.0
1	M	248	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	68	ARG	2.0
1	P	345	TYR	2.0
1	G	362	PHE	2.0
1	K	212	PHE	2.0
1	F	207	MET	2.0
1	E	82	LEU	2.0
1	G	73	GLU	2.0
1	G	241	ASN	2.0
1	N	9	LEU	2.0
1	O	462	GLU	2.0
1	P	253	GLU	2.0
1	B	137	PRO	2.0
1	G	325	ASP	2.0
1	J	25	CYS	2.0
1	M	109	VAL	2.0
1	O	83	ASP	2.0
1	G	314	SER	2.0
1	N	223	ARG	2.0
1	O	348	ARG	2.0
1	A	492	THR	2.0
1	C	69	GLN	2.0
1	K	472	THR	2.0
1	B	446	LYS	2.0
1	E	208	ILE	2.0
1	G	269	ILE	2.0
1	L	258	ILE	2.0
1	B	498	GLU	2.0
1	C	323	GLY	2.0
1	F	55	GLY	2.0
1	G	254	GLU	2.0
1	G	319	ALA	2.0
1	A	442	PHE	2.0
1	F	259	MET	2.0
1	M	483	HIS	2.0
1	P	60	HIS	2.0
1	G	425	LEU	2.0
1	M	161	LEU	2.0
1	A	419	VAL	2.0
1	G	274	VAL	2.0
1	H	276	VAL	2.0
1	K	478	VAL	2.0
1	M	337	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	O	30	SER	2.0
1	B	296	THR	2.0
1	L	110	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	N	500	1/1	0.63	28.88	88,88,88,88	0
2	MG	P	500	1/1	0.73	12.84	94,94,94,94	0
7	GOL	O	499	6/6	0.64	11.21	74,75,75,75	0
3	K	G	501	1/1	0.35	11.04	137,137,137,137	0
3	K	A	504	1/1	0.58	10.05	106,106,106,106	0
2	MG	G	500	1/1	0.56	9.85	81,81,81,81	0
7	GOL	I	501	6/6	0.41	9.43	85,85,85,85	0
2	MG	H	502	1/1	0.50	8.19	61,61,61,61	0
3	K	N	499	1/1	0.20	7.30	107,107,107,107	0
2	MG	A	502	1/1	0.35	7.11	58,58,58,58	0
7	GOL	J	499	6/6	0.35	6.60	69,71,71,72	0
3	K	P	504	1/1	0.52	6.41	98,98,98,98	0
4	OXL	P	510	6/6	0.38	5.97	85,85,85,86	0
4	OXL	F	510	6/6	0.45	5.55	83,83,83,83	0
2	MG	G	502	1/1	0.31	4.96	66,66,66,66	0
3	K	G	504	1/1	0.42	4.21	82,82,82,82	0
2	MG	F	500	1/1	0.41	4.19	67,67,67,67	0
3	K	M	504	1/1	0.27	4.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	M	500	1/1	0.34	3.96	69,69,69,69	0
3	K	B	499	1/1	0.20	3.90	60,60,60,60	0
3	K	N	504	1/1	0.45	3.82	84,84,84,84	0
2	MG	F	502	1/1	0.34	3.51	60,60,60,60	0
2	MG	N	502	1/1	0.40	2.96	76,76,76,76	0
2	MG	M	502	1/1	0.31	2.87	60,60,60,60	0
7	GOL	I	499	6/6	0.28	2.84	91,91,91,92	0
4	OXL	A	510	6/6	0.32	2.65	63,65,66,66	0
7	GOL	E	499	6/6	0.33	2.57	78,79,80,80	0
4	OXL	N	510	6/6	0.37	2.56	77,79,80,80	0
2	MG	A	500	1/1	0.35	2.53	77,77,77,77	0
3	K	F	504	1/1	0.32	2.50	69,69,69,69	0
4	OXL	M	510	6/6	0.32	2.39	64,66,67,67	0
2	MG	B	502	1/1	0.30	2.34	28,28,28,28	0
2	MG	C	500	1/1	0.38	2.32	45,45,45,45	0
2	MG	K	500	1/1	0.30	2.26	29,29,29,29	0
2	MG	I	500	1/1	0.33	2.09	36,36,36,36	0
3	K	O	501	1/1	0.30	2.02	30,30,30,30	0
4	OXL	G	510	6/6	0.31	1.95	71,74,75,75	0
2	MG	J	502	1/1	0.27	1.91	26,26,26,26	0
2	MG	I	502	1/1	0.32	1.68	30,30,30,30	0
4	OXL	J	510	6/6	0.31	1.66	30,31,32,33	0
6	ATP	K	1001	31/31	0.29	1.63	28,31,37,38	0
4	OXL	H	510	6/6	0.32	1.60	54,54,55,55	0
3	K	M	499	1/1	0.18	1.59	106,106,106,106	0
2	MG	L	502	1/1	0.28	1.56	37,37,37,37	0
5	FDP	B	700	20/20	0.22	1.54	37,40,45,46	0
6	ATP	J	1001	31/31	0.24	1.51	26,34,36,36	0
3	K	C	504	1/1	0.33	1.50	56,56,56,56	0
2	MG	H	500	1/1	0.30	1.44	63,63,63,63	0
2	MG	L	500	1/1	0.27	1.43	46,46,46,46	0
4	OXL	C	510	6/6	0.36	1.41	39,40,41,41	0
5	FDP	I	700	20/20	0.21	1.40	29,32,34,35	0
4	OXL	I	510	6/6	0.30	1.35	32,33,34,35	0
6	ATP	B	1001	31/31	0.25	1.28	31,35,39,40	0
2	MG	J	500	1/1	0.29	1.27	27,27,27,27	0
3	K	E	504	1/1	0.25	1.26	48,48,48,48	0
6	ATP	P	1001	31/31	0.30	1.20	132,134,134,134	0
3	K	L	504	1/1	0.25	1.17	52,52,52,52	0
2	MG	P	502	1/1	0.23	1.16	64,64,64,64	0
4	OXL	L	510	6/6	0.26	1.00	37,38,38,39	0
6	ATP	H	1001	31/31	0.23	1.00	62,69,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	K	J	504	1/1	0.25	0.97	35,35,35,35	0
4	OXL	E	510	6/6	0.31	0.88	48,49,49,50	0
4	OXL	D	510	6/6	0.27	0.83	37,38,39,39	0
2	MG	E	502	1/1	0.31	0.80	48,48,48,48	0
2	MG	B	500	1/1	0.25	0.72	35,35,35,35	0
3	K	K	504	1/1	0.27	0.69	29,29,29,29	0
4	OXL	K	510	6/6	0.28	0.64	25,27,28,28	0
3	K	D	504	1/1	0.25	0.60	33,33,33,33	0
6	ATP	E	1001	31/31	0.20	0.59	52,58,63,63	0
6	ATP	G	1001	31/31	0.27	0.59	77,97,101,101	0
5	FDP	D	700	20/20	0.18	0.57	32,40,43,45	0
4	OXL	B	510	6/6	0.25	0.55	30,32,33,33	0
6	ATP	I	1001	31/31	0.21	0.54	36,37,39,40	0
6	ATP	D	1001	31/31	0.22	0.53	35,42,44,44	0
2	MG	E	500	1/1	0.24	0.42	55,55,55,55	0
5	FDP	E	700	20/20	0.17	0.41	38,41,46,47	0
3	K	H	504	1/1	0.20	0.41	59,59,59,59	0
2	MG	C	502	1/1	0.31	0.31	38,38,38,38	0
2	MG	D	502	1/1	0.24	0.24	34,34,34,34	0
6	ATP	C	1001	31/31	0.22	0.12	43,52,54,54	0
6	ATP	F	1001	31/31	0.21	-0.02	64,73,76,76	0
5	FDP	M	700	20/20	0.16	-0.04	55,59,62,64	0
3	K	B	504	1/1	0.20	-0.12	38,38,38,38	0
5	FDP	K	700	20/20	0.16	-0.14	36,38,42,43	0
6	ATP	N	1001	31/31	0.21	-0.15	83,94,95,95	0
5	FDP	J	700	20/20	0.15	-0.19	25,32,34,35	0
3	K	E	501	1/1	0.14	-0.32	75,75,75,75	0
2	MG	K	502	1/1	0.25	-0.34	28,28,28,28	0
5	FDP	F	700	20/20	0.16	-0.37	48,53,55,56	0
6	ATP	A	1001	31/31	0.20	-0.40	70,85,87,87	0
5	FDP	H	700	20/20	0.15	-0.41	54,57,59,60	0
6	ATP	L	1001	31/31	0.16	-0.42	44,55,59,59	0
2	MG	D	500	1/1	0.24	-0.53	37,37,37,37	0
6	ATP	M	1001	31/31	0.15	-0.53	66,73,76,76	0
5	FDP	L	700	20/20	0.14	-0.54	37,41,43,43	0
5	FDP	C	700	20/20	0.15	-0.54	36,45,48,50	0
5	FDP	G	700	20/20	0.14	-0.58	69,74,75,75	0
3	K	L	499	1/1	0.13	-0.58	47,47,47,47	0
3	K	D	499	1/1	0.12	-0.68	53,53,53,53	0
7	GOL	G	499	6/6	0.18	-0.69	97,97,97,97	0
5	FDP	P	700	20/20	0.16	-0.78	110,115,119,119	0
3	K	I	504	1/1	0.17	-0.81	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	FDP	A	700	20/20	0.13	-0.88	53,58,61,64	0
5	FDP	N	700	20/20	0.13	-0.88	76,78,81,82	0
5	FDP	O	700	20/20	0.16	-1.16	118,119,121,121	0
3	K	H	499	1/1	0.12	-1.46	76,76,76,76	0
3	K	P	499	1/1	0.14	-1.51	119,119,119,119	0
3	K	J	501	1/1	0.08	-2.09	50,50,50,50	0
3	K	A	499	1/1	0.07	-2.65	60,60,60,60	0
3	K	K	499	1/1	0.08	-3.18	52,52,52,52	0
3	K	O	500	1/1	0.07	-3.36	122,122,122,122	0
3	K	C	499	1/1	0.09	-3.77	68,68,68,68	0
3	K	F	499	1/1	0.11	-3.89	85,85,85,85	0
3	K	I	503	1/1	0.09	-4.57	47,47,47,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.