



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:01 am GMT

PDB ID : 1L6L
Title : Structures of Apolipoprotein A-II and a Lipid Surrogate Complex Provide Insights into Apolipoprotein-Lipid Interactions
Authors : Kumar, M.S.; Carson, M.; Hussain, M.M.; Murthy, H.M.K.
Deposited on : 2002-03-11
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

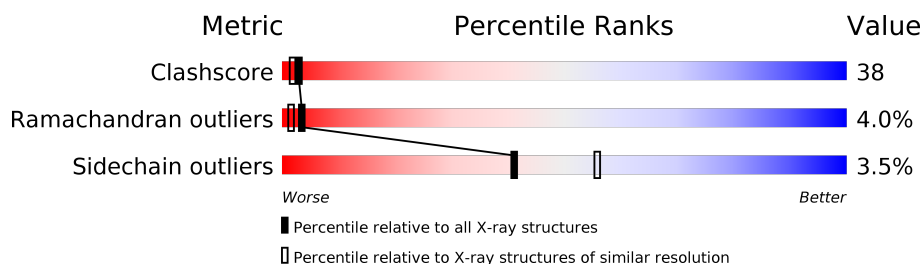
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)




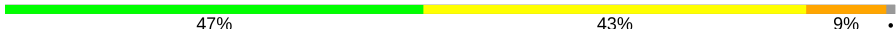

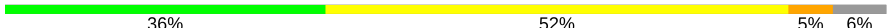



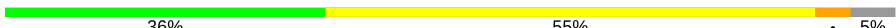












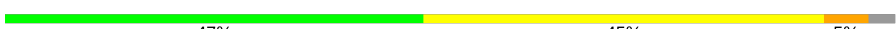

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	77	
1	2	77	
1	3	77	
1	4	77	
1	5	77	
1	6	77	
1	7	77	

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Mol	Chain	Length	Quality of chain
1	8	77	
1	A	77	
1	B	77	
1	C	77	
1	D	77	
1	E	77	
1	F	77	
1	G	77	
1	H	77	
1	I	77	
1	J	77	
1	K	77	
1	L	77	
1	M	77	
1	N	77	
1	P	77	
1	Q	77	
1	S	77	
1	T	77	
1	U	77	
1	V	77	
1	W	77	
1	X	77	
1	Y	77	
1	Z	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	3	1716	-	-	X	-
2	BOG	F	1619	-	-	X	-
2	BOG	G	1634	-	-	X	-
2	BOG	K	1610	-	-	X	-
2	BOG	K	1616	-	-	X	-
2	BOG	N	1624	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Apolipoprotein A-II.

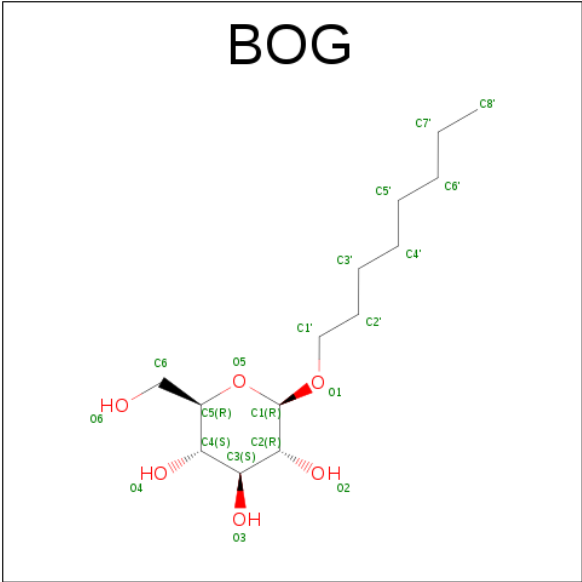
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	B	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	C	76	Total	C	N	O	S	0	0	0
			604	388	92	122	2			
1	D	74	Total	C	N	O	S	0	0	0
			590	380	90	118	2			
1	E	72	Total	C	N	O	S	0	0	0
			578	372	88	116	2			
1	F	75	Total	C	N	O	S	0	0	0
			595	383	91	119	2			
1	G	74	Total	C	N	O	S	0	0	0
			587	379	89	117	2			
1	H	74	Total	C	N	O	S	0	0	0
			587	379	89	117	2			
1	I	73	Total	C	N	O	S	0	0	0
			583	374	88	119	2			
1	J	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	K	74	Total	C	N	O	S	0	0	0
			590	380	90	118	2			
1	L	74	Total	C	N	O	S	0	0	0
			589	377	90	120	2			
1	M	76	Total	C	N	O	S	0	0	0
			604	388	92	122	2			
1	N	76	Total	C	N	O	S	0	0	0
			604	388	92	122	2			
1	P	73	Total	C	N	O	S	0	0	0
			582	376	88	116	2			
1	Q	73	Total	C	N	O	S	0	0	0
			576	370	88	116	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	T	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	U	76	Total	C	N	O	S	0	0	0
			604	388	92	122	2			
1	V	75	Total	C	N	O	S	0	0	0
			595	383	91	119	2			
1	W	73	Total	C	N	O	S	0	0	0
			587	377	89	119	2			
1	X	75	Total	C	N	O	S	0	0	0
			595	383	91	119	2			
1	Y	74	Total	C	N	O	S	0	0	0
			587	379	89	117	2			
1	Z	72	Total	C	N	O	S	0	0	0
			573	371	87	113	2			
1	1	73	Total	C	N	O	S	0	0	0
			583	374	88	119	2			
1	2	73	Total	C	N	O	S	0	0	0
			581	374	88	117	2			
1	3	73	Total	C	N	O	S	0	0	0
			585	377	89	117	2			
1	4	74	Total	C	N	O	S	0	0	0
			586	378	90	116	2			
1	5	75	Total	C	N	O	S	0	0	0
			597	384	91	120	2			
1	6	75	Total	C	N	O	S	0	0	0
			597	384	91	120	2			
1	7	70	Total	C	N	O	S	0	0	0
			559	362	84	111	2			
1	8	74	Total	C	N	O	S	0	0	0
			587	379	89	117	2			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			10	9	1		
2	B	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	I	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	J	1	Total	C	O	0	0
			20	14	6		
2	J	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	K	1	Total	C	O	0	0
			20	14	6		
2	D	1	Total	C	O	0	0
			20	14	6		
2	D	1	Total	C	O	0	0
			10	9	1		
2	C	1	Total	C	O	0	0
			20	14	6		
2	L	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	C	O	0	0
			20	14	6		
2	N	1	Total	C	O	0	0
			20	14	6		
2	N	1	Total	C	O	0	0
			20	14	6		
2	F	1	Total	C	O	0	0
			20	14	6		
2	M	1	Total	C	O	0	0
			20	14	6		
2	M	1	Total	C	O	0	0
			20	14	6		
2	N	1	Total	C	O	0	0
			20	14	6		
2	E	1	Total	C	O	0	0
			20	14	6		
2	N	1	Total	C	O	0	0
			20	14	6		
2	M	1	Total	C	O	0	0
			20	14	6		
2	H	1	Total	C	O	0	0
			20	14	6		
2	Q	1	Total	C	O	0	0
			20	14	6		
2	Q	1	Total	C	O	0	0
			20	14	6		
2	H	1	Total	C	O	0	0
			20	14	6		
2	Q	1	Total	C	O	0	0
			20	14	6		
2	H	1	Total	C	O	0	0
			20	14	6		
2	P	1	Total	C	O	0	0
			20	14	6		
2	G	1	Total	C	O	0	0
			20	14	6		
2	G	1	Total	C	O	0	0
			20	14	6		
2	T	1	Total	C	O	0	0
			20	14	6		
2	2	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	S	1	Total	C	O	0	0
			20	14	6		
2	1	1	Total	C	O	0	0
			20	14	6		
2	T	1	Total	C	O	0	0
			20	14	6		
2	1	1	Total	C	O	0	0
			20	14	6		
2	2	1	Total	C	O	0	0
			20	14	6		
2	1	1	Total	C	O	0	0
			20	14	6		
2	U	1	Total	C	O	0	0
			20	14	6		
2	3	1	Total	C	O	0	0
			20	14	6		
2	4	1	Total	C	O	0	0
			20	14	6		
2	U	1	Total	C	O	0	0
			20	14	6		
2	3	1	Total	C	O	0	0
			20	14	6		
2	6	1	Total	C	O	0	0
			20	14	6		
2	W	1	Total	C	O	0	0
			20	14	6		
2	5	1	Total	C	O	0	0
			20	14	6		
2	5	1	Total	C	O	0	0
			20	14	6		
2	5	1	Total	C	O	0	0
			20	14	6		
2	6	1	Total	C	O	0	0
			20	14	6		
2	W	1	Total	C	O	0	0
			20	14	6		
2	5	1	Total	C	O	0	0
			20	14	6		
2	X	1	Total	C	O	0	0
			20	14	6		
2	7	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	8	1	Total	C	O	0	0
			20	14	6		
2	8	1	Total	C	O	0	0
			20	14	6		
2	Z	1	Total	C	O	0	0
			20	14	6		
2	Y	1	Total	C	O	0	0
			20	14	6		
2	Z	1	Total	C	O	0	0
			20	14	6		
2	Z	1	Total	C	O	0	0
			20	14	6		
2	Y	1	Total	C	O	0	0
			20	14	6		
2	Y	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	19	Total	O	0	0
			19	19		
3	2	27	Total	O	0	0
			27	27		
3	3	31	Total	O	0	0
			31	31		
3	4	28	Total	O	0	0
			28	28		
3	5	21	Total	O	0	0
			21	21		
3	6	23	Total	O	0	0
			23	23		
3	7	42	Total	O	0	0
			42	42		
3	8	65	Total	O	0	0
			65	65		
3	A	36	Total	O	0	0
			36	36		
3	B	30	Total	O	0	0
			30	30		
3	C	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	19	Total O 19 19	0	0
3	E	46	Total O 46 46	0	0
3	F	26	Total O 26 26	0	0
3	G	70	Total O 70 70	0	0
3	H	20	Total O 20 20	0	0
3	I	38	Total O 38 38	0	0
3	J	32	Total O 32 32	0	0
3	K	32	Total O 32 32	0	0
3	L	26	Total O 26 26	0	0
3	M	31	Total O 31 31	0	0
3	N	56	Total O 56 56	0	0
3	P	34	Total O 34 34	0	0
3	Q	39	Total O 39 39	0	0
3	S	28	Total O 28 28	0	0
3	T	22	Total O 22 22	0	0
3	U	27	Total O 27 27	0	0
3	V	23	Total O 23 23	0	0
3	W	23	Total O 23 23	0	0
3	X	20	Total O 20 20	0	0
3	Y	38	Total O 38 38	0	0
3	Z	23	Total O 23 23	0	0

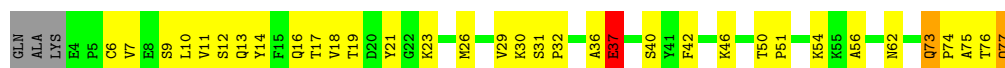
3 Residue-property plots [i](#)

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

Note EDS was not executed.

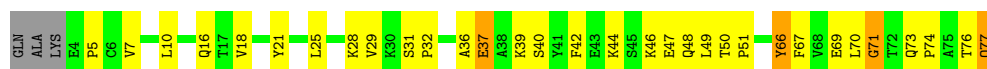
- Molecule 1: Apolipoprotein A-II

Chain A: 



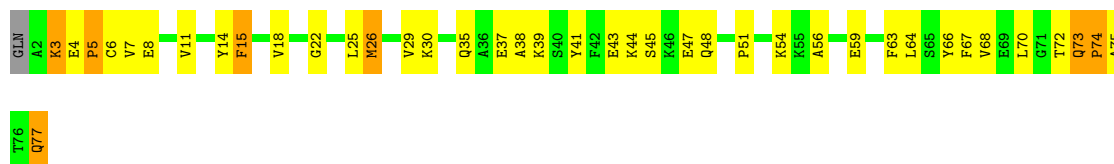
- Molecule 1: Apolipoprotein A-II

Chain B: 



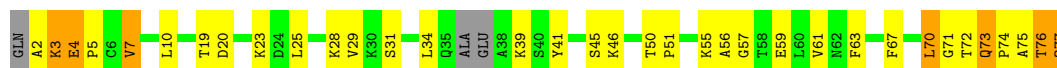
- Molecule 1: Apolipoprotein A-II

Chain C: 



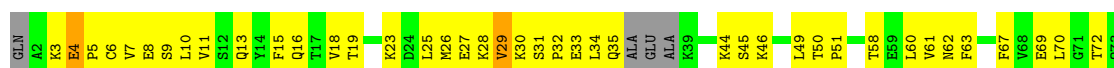
- Molecule 1: Apolipoprotein A-II

Chain D: 



- Molecule 1: Apolipoprotein A-II

Chain E: 





- Molecule 1: Apolipoprotein A-II

Chain F: 49% 42% 6% •



- Molecule 1: Apolipoprotein A-II

Chain G: 42% 53% • •



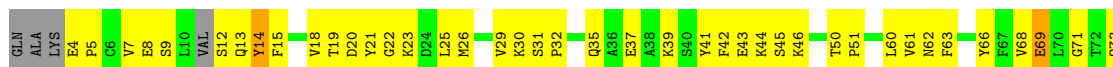
- Molecule 1: Apolipoprotein A-II

Chain H: 53% 36% 6% •



- Molecule 1: Apolipoprotein A-II

Chain I: 36% 55% • 5%



- Molecule 1: Apolipoprotein A-II

Chain J: 51% 38% 8% •



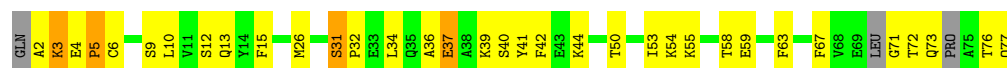
- Molecule 1: Apolipoprotein A-II

Chain K: 58% 31% 6% •



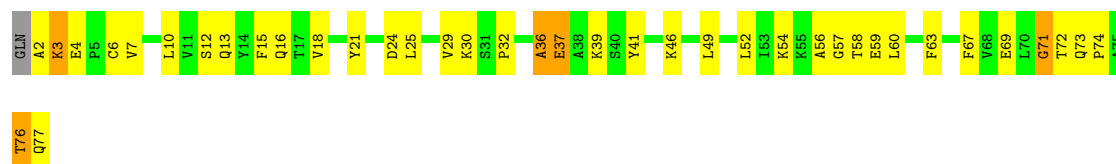
- Molecule 1: Apolipoprotein A-II

Chain L: 



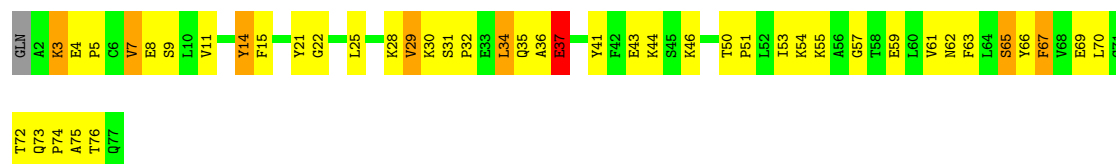
• Molecule 1: Apolipoprotein A-II

Chain M: 



• Molecule 1: Apolipoprotein A-II

Chain N: 



• Molecule 1: Apolipoprotein A-II

Chain P: 



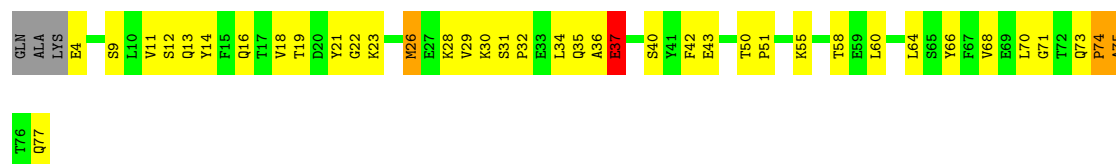
• Molecule 1: Apolipoprotein A-II

Chain Q: 



• Molecule 1: Apolipoprotein A-II

Chain S: 

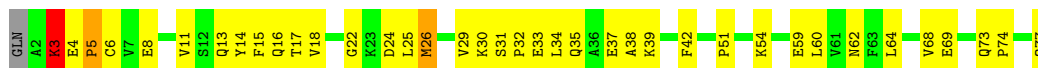


• Molecule 1: Apolipoprotein A-II

Chain T: 



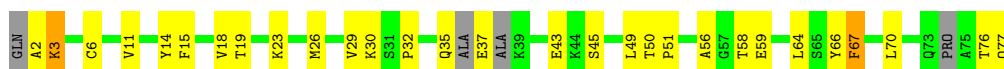
• Molecule 1: Apolipoprotein A-II



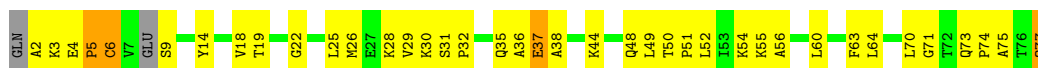
• Molecule 1: Apolipoprotein A-II



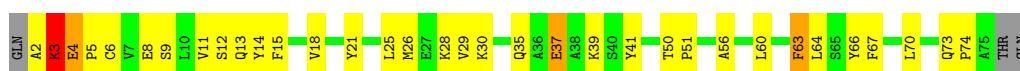
• Molecule 1: Apolipoprotein A-II



• Molecule 1: Apolipoprotein A-II



• Molecule 1: Apolipoprotein A-II



• Molecule 1: Apolipoprotein A-II



• Molecule 1: Apolipoprotein A-II



- Molecule 1: Apolipoprotein A-II

Chain 2:  60% 32% 5%



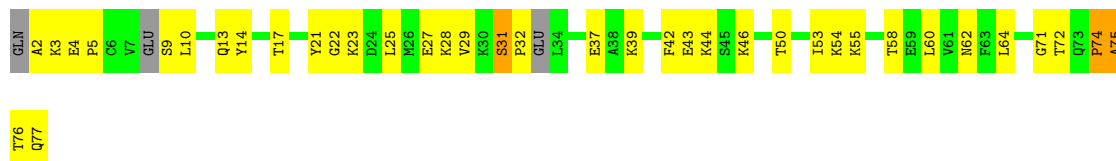
- Molecule 1: Apolipoprotein A-II

Chain 3:  52% 34% 9% 5%



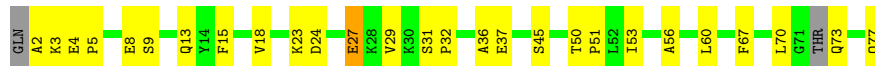
- Molecule 1: Apolipoprotein A-II

Chain 4:  47% 45%



- Molecule 1: Apolipoprotein A-II

Chain 5:  62% 34%



- Molecule 1: Apolipoprotein A-II

Chain 6:  61% 32%



- Molecule 1: Apolipoprotein A-II

Chain 7:  60% 30% 9%



- Molecule 1: Apolipoprotein A-II

Chain 8:  52% 35% 9%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	114.40Å 115.90Å 126.60Å 90.70° 96.20° 93.50°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	88.0 (8.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21106	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1	0.41	1/593 (0.2%)	0.49	0/797
1	2	0.41	1/591 (0.2%)	0.45	0/795
1	3	4.18	6/595 (1.0%)	0.53	0/799
1	4	0.42	1/595 (0.2%)	0.45	0/798
1	5	0.41	1/607 (0.2%)	0.49	0/815
1	6	0.41	1/607 (0.2%)	0.46	0/815
1	7	0.28	0/568	0.45	0/763
1	8	0.41	1/598 (0.2%)	0.46	0/806
1	A	0.40	1/601 (0.2%)	0.47	0/810
1	B	0.41	1/601 (0.2%)	0.48	0/810
1	C	0.40	1/615 (0.2%)	0.45	0/828
1	D	0.30	0/600	0.47	0/806
1	E	0.29	0/586	0.45	0/784
1	F	0.41	1/605 (0.2%)	0.51	0/813
1	G	0.41	1/598 (0.2%)	0.49	0/806
1	H	0.42	1/598 (0.2%)	0.47	0/806
1	I	0.41	1/593 (0.2%)	0.51	0/797
1	J	0.41	1/601 (0.2%)	0.45	0/810
1	K	4.11	6/600 (1.0%)	0.54	0/806
1	L	0.43	1/597 (0.2%)	0.45	0/799
1	M	0.42	1/615 (0.2%)	0.51	0/828
1	N	3.43	7/615 (1.1%)	0.63	2/828 (0.2%)
1	P	0.41	1/592 (0.2%)	0.47	0/796
1	Q	0.41	1/585 (0.2%)	0.49	0/787
1	S	0.41	1/601 (0.2%)	0.53	0/810
1	T	0.40	1/601 (0.2%)	0.47	0/810
1	U	0.41	1/615 (0.2%)	0.45	0/828
1	V	0.29	0/605	0.47	0/813
1	W	0.40	1/594 (0.2%)	0.44	0/793
1	X	0.41	1/605 (0.2%)	0.48	0/813
1	Y	0.40	1/598 (0.2%)	0.44	0/806
1	Z	0.42	1/583 (0.2%)	0.49	0/784

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.26	44/19158 (0.2%)	0.48	2/25759 (0.0%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	66	TYR	CD1-CE1	55.43	2.22	1.39
1	3	66	TYR	CD2-CE2	53.00	2.18	1.39
1	K	66	TYR	CD2-CE2	52.73	2.18	1.39
1	K	66	TYR	CD1-CE1	52.49	2.18	1.39
1	K	66	TYR	CE2-CZ	39.00	1.89	1.38
1	N	67	PHE	CD1-CE1	38.75	2.16	1.39
1	N	67	PHE	CD2-CE2	38.64	2.16	1.39
1	N	67	PHE	CE1-CZ	38.11	2.09	1.37
1	N	67	PHE	CE2-CZ	38.02	2.09	1.37
1	3	66	TYR	CE2-CZ	37.42	1.87	1.38
1	3	66	TYR	CE1-CZ	36.71	1.86	1.38
1	K	66	TYR	CE1-CZ	36.31	1.85	1.38
1	3	66	TYR	CG-CD2	29.24	1.77	1.39
1	K	66	TYR	CG-CD2	29.18	1.77	1.39
1	3	66	TYR	CG-CD1	29.15	1.77	1.39
1	K	66	TYR	CG-CD1	29.01	1.76	1.39
1	N	67	PHE	CG-CD1	25.02	1.76	1.38
1	N	67	PHE	CG-CD2	24.61	1.75	1.38
1	L	37	GLU	CD-OE2	7.18	1.33	1.25
1	4	37	GLU	CD-OE2	7.12	1.33	1.25
1	Q	37	GLU	CD-OE2	7.02	1.33	1.25
1	B	37	GLU	CD-OE2	6.99	1.33	1.25
1	H	37	GLU	CD-OE2	6.97	1.33	1.25
1	X	37	GLU	CD-OE2	6.95	1.33	1.25
1	6	37	GLU	CD-OE2	6.94	1.33	1.25
1	8	37	GLU	CD-OE2	6.94	1.33	1.25
1	Z	37	GLU	CD-OE2	6.94	1.33	1.25
1	2	37	GLU	CD-OE2	6.94	1.33	1.25
1	F	37	GLU	CD-OE2	6.92	1.33	1.25
1	U	37	GLU	CD-OE2	6.91	1.33	1.25
1	G	37	GLU	CD-OE2	6.91	1.33	1.25
1	I	37	GLU	CD-OE2	6.91	1.33	1.25
1	N	37	GLU	CD-OE2	6.91	1.33	1.25
1	J	37	GLU	CD-OE2	6.90	1.33	1.25
1	M	37	GLU	CD-OE2	6.88	1.33	1.25
1	P	37	GLU	CD-OE2	6.88	1.33	1.25
1	A	37	GLU	CD-OE2	6.86	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	37	GLU	CD-OE2	6.86	1.33	1.25
1	T	37	GLU	CD-OE2	6.86	1.33	1.25
1	Y	37	GLU	CD-OE2	6.86	1.33	1.25
1	1	37	GLU	CD-OE2	6.85	1.33	1.25
1	C	37	GLU	CD-OE2	6.84	1.33	1.25
1	5	37	GLU	CD-OE2	6.83	1.33	1.25
1	W	37	GLU	CD-OE2	6.79	1.33	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	67	PHE	CD1-CG-CD2	5.09	124.92	118.30
1	N	67	PHE	CB-CG-CD2	-5.05	117.27	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	583	0	576	27	9
1	2	581	0	579	22	0
1	3	585	0	587	93	0
1	4	586	0	590	41	0
1	5	597	0	596	27	0
1	6	597	0	596	34	2
1	7	559	0	558	33	0
1	8	587	0	589	69	2
1	A	590	0	586	51	0
1	B	590	0	586	45	0
1	C	604	0	604	60	0
1	D	590	0	590	45	0
1	E	578	0	579	72	9
1	F	595	0	597	39	0
1	G	587	0	589	67	0
1	H	587	0	589	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	583	0	576	51	0
1	J	590	0	586	59	0
1	K	590	0	591	75	0
1	L	589	0	584	46	0
1	M	604	0	604	56	0
1	N	604	0	604	111	0
1	P	582	0	583	35	0
1	Q	576	0	579	40	0
1	S	590	0	586	35	0
1	T	590	0	586	63	0
1	U	604	0	604	49	0
1	V	595	0	597	63	0
1	W	587	0	584	30	0
1	X	595	0	597	51	0
1	Y	587	0	589	51	0
1	Z	573	0	577	45	0
2	1	60	0	84	7	0
2	2	40	0	56	2	0
2	3	40	0	56	34	0
2	4	20	0	28	0	0
2	5	80	0	112	13	0
2	6	40	0	56	3	0
2	7	20	0	28	3	0
2	8	40	0	56	4	0
2	A	40	0	56	3	0
2	B	60	0	84	8	0
2	C	20	0	28	3	0
2	D	30	0	45	5	0
2	E	20	0	28	7	0
2	F	20	0	28	9	0
2	G	40	0	56	17	0
2	H	60	0	84	7	0
2	I	30	0	43	7	0
2	J	40	0	56	1	0
2	K	40	0	56	38	0
2	L	20	0	28	4	0
2	M	60	0	84	12	0
2	N	80	0	112	52	0
2	P	20	0	28	1	0
2	Q	60	0	84	11	0
2	S	20	0	28	1	0
2	T	40	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U	40	0	56	6	0
2	W	40	0	56	3	0
2	X	20	0	28	5	0
2	Y	60	0	84	6	0
2	Z	60	0	84	9	0
3	1	19	0	0	6	0
3	2	27	0	0	11	0
3	3	31	0	0	39	0
3	4	28	0	0	17	0
3	5	21	0	0	10	0
3	6	23	0	0	9	0
3	7	42	0	0	17	0
3	8	65	0	0	54	0
3	A	36	0	0	33	0
3	B	30	0	0	23	0
3	C	16	0	0	5	0
3	D	19	0	0	15	0
3	E	46	0	0	27	0
3	F	26	0	0	20	0
3	G	70	0	0	43	0
3	H	20	0	0	11	0
3	I	38	0	0	30	0
3	J	32	0	0	25	0
3	K	32	0	0	25	0
3	L	26	0	0	19	0
3	M	31	0	0	19	0
3	N	56	0	0	45	0
3	P	34	0	0	14	0
3	Q	39	0	0	20	0
3	S	28	0	0	20	0
3	T	22	0	0	12	0
3	U	27	0	0	21	0
3	V	23	0	0	12	0
3	W	23	0	0	15	0
3	X	20	0	0	23	0
3	Y	38	0	0	32	0
3	Z	23	0	0	29	0
All	All	21106	0	20586	1535	11

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (1535) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:66:TYR:CD2	1:3:66:TYR:CG	1.77	1.70
1:3:66:TYR:CG	1:3:66:TYR:CD1	1.77	1.68
1:K:66:TYR:CD1	1:K:66:TYR:CG	1.76	1.68
1:N:67:PHE:CG	1:N:67:PHE:CD2	1.75	1.68
1:K:66:TYR:CD2	1:K:66:TYR:CG	1.77	1.67
1:N:67:PHE:CG	1:N:67:PHE:CD1	1.76	1.64
1:K:66:TYR:CZ	1:K:66:TYR:CE1	1.85	1.64
1:3:66:TYR:CE1	1:3:66:TYR:CZ	1.86	1.63
1:3:66:TYR:CE2	1:3:66:TYR:CZ	1.87	1.62
1:K:66:TYR:CE2	1:K:66:TYR:CZ	1.89	1.60
1:H:2:ALA:HA	1:H:3:LYS:NZ	1.32	1.44
1:H:3:LYS:NZ	1:H:3:LYS:H	1.18	1.41
1:N:67:PHE:CE1	1:N:67:PHE:CZ	2.09	1.40
1:N:67:PHE:CE2	1:N:67:PHE:CZ	2.09	1.40
1:H:3:LYS:N	1:H:3:LYS:HZ2	0.93	1.36
1:N:67:PHE:CE1	1:N:67:PHE:CD1	2.16	1.33
1:H:3:LYS:N	1:H:3:LYS:NZ	1.72	1.33
1:2:76:THR:OG1	1:4:3:LYS:NZ	1.62	1.33
1:N:67:PHE:CD2	1:N:67:PHE:CE2	2.16	1.31
1:K:66:TYR:CE2	1:K:66:TYR:CD2	2.18	1.31
1:K:66:TYR:CD1	1:K:66:TYR:CE1	2.18	1.31
1:3:66:TYR:CD2	1:3:66:TYR:CE2	2.18	1.30
1:H:2:ALA:C	1:H:3:LYS:HZ2	1.34	1.30
1:K:54:LYS:HB3	3:K:249:HOH:O	1.30	1.29
1:Q:53:ILE:HG22	3:Q:1636:HOH:O	1.32	1.28
1:7:5:PRO:HB3	3:7:1737:HOH:O	1.32	1.28
1:E:62:ASN:HA	3:E:1660:HOH:O	1.28	1.28
1:3:66:TYR:CE1	1:3:66:TYR:CD1	2.22	1.26
1:Z:33:GLU:HG2	3:Z:1749:HOH:O	1.33	1.25
1:N:46:LYS:HD2	3:N:1657:HOH:O	1.29	1.25
1:T:77:GLN:HB3	1:V:3:LYS:NZ	1.47	1.25
1:H:2:ALA:CA	1:H:3:LYS:NZ	1.99	1.25
1:Q:9:SER:HA	3:Q:1643:HOH:O	1.36	1.24
1:4:77:GLN:O	1:6:3:LYS:HG2	1.35	1.23
1:N:4:GLU:HB2	3:N:1652:HOH:O	1.35	1.22
1:Y:74:PRO:HA	3:Y:1750:HOH:O	1.39	1.22
1:B:16:GLN:HB3	3:B:1610:HOH:O	1.39	1.19
1:6:66:TYR:HA	3:6:1743:HOH:O	1.38	1.19
1:5:5:PRO:HD2	3:5:712:HOH:O	1.37	1.19
1:I:71:GLY:HA2	3:I:1609:HOH:O	1.42	1.19
1:T:77:GLN:C	1:V:3:LYS:NZ	1.97	1.17
1:V:34:LEU:HD21	3:V:1034:HOH:O	1.43	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:44:LYS:HE2	3:P:1664:HOH:O	1.45	1.17
1:4:77:GLN:O	1:6:3:LYS:CG	1.93	1.16
1:H:2:ALA:CA	1:H:3:LYS:HZ3	1.57	1.15
1:8:39:LYS:HG3	3:8:1740:HOH:O	1.43	1.14
1:J:31:SER:HB3	3:J:1630:HOH:O	1.44	1.14
1:N:67:PHE:CD1	2:N:1624:BOG:H2'2	1.83	1.14
1:V:53:ILE:HD12	3:V:1332:HOH:O	1.48	1.14
1:3:66:TYR:CD1	2:3:1716:BOG:C4'	2.32	1.13
1:Y:26:MET:HA	3:Y:1742:HOH:O	1.46	1.13
1:2:24:ASP:HB3	3:2:1730:HOH:O	1.46	1.13
1:3:66:TYR:CE2	2:3:1716:BOG:C5'	2.32	1.13
3:P:1649:HOH:O	1:Q:2:ALA:HB2	1.45	1.13
1:T:77:GLN:CB	1:V:3:LYS:NZ	2.10	1.13
2:E:1623:BOG:H6'2	3:N:1649:HOH:O	1.47	1.13
1:N:67:PHE:CE1	2:N:1624:BOG:C2'	2.32	1.12
1:3:66:TYR:CE1	2:3:1716:BOG:C4'	2.33	1.12
1:G:51:PRO:HD3	3:G:1640:HOH:O	1.44	1.12
1:B:51:PRO:HG2	3:B:1632:HOH:O	1.49	1.12
1:8:33:GLU:HA	3:8:1760:HOH:O	1.48	1.12
1:Y:60:LEU:HB3	3:Y:1765:HOH:O	1.48	1.12
1:3:66:TYR:CD2	2:3:1716:BOG:C5'	2.33	1.11
1:C:8:GLU:HG2	3:K:238:HOH:O	1.49	1.11
1:K:66:TYR:CD1	2:K:1616:BOG:C4'	2.34	1.11
1:N:67:PHE:CD2	2:N:1624:BOG:C3'	2.34	1.11
1:3:30:LYS:HG2	3:3:1737:HOH:O	1.47	1.11
1:N:67:PHE:CE2	2:N:1624:BOG:C3'	2.32	1.11
1:K:66:TYR:CE1	2:K:1616:BOG:C5'	2.35	1.10
1:B:69:GLU:HB3	3:B:1630:HOH:O	1.50	1.10
1:8:28:LYS:HE2	3:8:1784:HOH:O	1.52	1.10
1:K:66:TYR:CD1	2:K:1616:BOG:C5'	2.34	1.10
1:K:66:TYR:CD2	2:K:1616:BOG:C5'	2.34	1.10
1:G:44:LYS:HD3	3:G:1645:HOH:O	1.50	1.10
1:L:39:LYS:HA	3:L:1632:HOH:O	1.51	1.10
1:N:67:PHE:CD2	2:N:1624:BOG:H3'1	1.86	1.10
1:K:66:TYR:CD2	2:K:1616:BOG:C4'	2.34	1.09
1:N:67:PHE:CD1	2:N:1624:BOG:C2'	2.34	1.09
1:N:73:GLN:HB3	3:N:1625:HOH:O	1.50	1.09
1:K:66:TYR:CE2	2:K:1616:BOG:C4'	2.35	1.09
1:K:66:TYR:CE1	2:K:1616:BOG:C4'	2.35	1.09
1:N:67:PHE:CE2	2:N:1624:BOG:H3'2	1.87	1.09
1:M:46:LYS:HD3	3:M:1649:HOH:O	1.51	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:43:GLU:HA	3:S:1705:HOH:O	1.50	1.09
1:K:66:TYR:CE2	2:K:1616:BOG:C5'	2.35	1.09
1:N:67:PHE:CZ	2:N:1624:BOG:C2'	2.36	1.08
1:3:66:TYR:CD2	2:3:1716:BOG:C4'	2.35	1.08
1:3:66:TYR:CZ	2:3:1716:BOG:C5'	2.36	1.08
1:8:30:LYS:HB2	3:8:1743:HOH:O	1.52	1.08
1:H:50:THR:HB	3:H:1648:HOH:O	1.51	1.08
1:N:67:PHE:CZ	2:N:1624:BOG:C3'	2.37	1.08
1:Q:7:VAL:HG23	3:Q:1631:HOH:O	1.53	1.07
1:3:66:TYR:CD2	2:3:1716:BOG:H5'2	1.89	1.07
1:U:39:LYS:HG2	3:U:1716:HOH:O	1.54	1.07
1:Y:8:GLU:HG3	3:Y:1755:HOH:O	1.53	1.07
1:3:66:TYR:CE1	2:3:1716:BOG:C5'	2.36	1.07
1:3:66:TYR:CD1	2:3:1716:BOG:C5'	2.37	1.07
1:K:75:ALA:HA	3:K:497:HOH:O	1.55	1.07
1:T:77:GLN:CB	1:V:3:LYS:HZ3	1.67	1.06
1:3:66:TYR:CE2	2:3:1716:BOG:C4'	2.39	1.06
1:K:54:LYS:HE3	3:K:429:HOH:O	1.55	1.06
1:N:67:PHE:CD1	2:N:1624:BOG:C3'	2.39	1.06
1:N:67:PHE:CE1	2:N:1624:BOG:C3'	2.39	1.06
1:T:77:GLN:NE2	1:V:3:LYS:HZ1	1.51	1.06
1:4:25:LEU:HB2	3:4:1725:HOH:O	1.53	1.05
1:K:66:TYR:CZ	2:K:1616:BOG:C5'	2.38	1.05
1:N:67:PHE:CE2	2:N:1624:BOG:C2'	2.39	1.05
1:3:66:TYR:CG	2:3:1716:BOG:C4'	2.39	1.05
1:3:66:TYR:CZ	2:3:1716:BOG:C4'	2.40	1.05
1:G:6:CYS:HB3	3:G:1687:HOH:O	1.54	1.05
1:3:66:TYR:CG	2:3:1716:BOG:H4'1	1.91	1.05
1:M:37:GLU:HG2	3:M:1648:HOH:O	1.56	1.05
1:K:66:TYR:CZ	2:K:1616:BOG:C4'	2.38	1.05
1:K:66:TYR:CD2	2:K:1616:BOG:H4'1	1.93	1.04
1:K:66:TYR:CG	2:K:1616:BOG:C4'	2.40	1.04
1:Y:74:PRO:HG3	3:Y:1735:HOH:O	1.56	1.04
1:3:66:TYR:CE1	2:3:1716:BOG:H4'2	1.93	1.04
1:D:10:LEU:HG	3:D:1632:HOH:O	1.56	1.04
1:3:66:TYR:CE2	2:3:1716:BOG:H5'1	1.92	1.03
1:K:66:TYR:CG	2:K:1616:BOG:C5'	2.40	1.03
1:N:7:VAL:HG11	3:N:1650:HOH:O	1.56	1.03
1:A:51:PRO:HB2	3:A:1622:HOH:O	1.59	1.03
1:3:3:LYS:HD3	1:3:3:LYS:H	0.89	1.03
1:N:67:PHE:CG	2:N:1624:BOG:C3'	2.42	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:66:TYR:CG	2:3:1716:BOG:C5'	2.42	1.03
1:Y:37:GLU:HA	3:Y:1768:HOH:O	1.54	1.03
1:L:55:LYS:HG2	3:L:1640:HOH:O	1.58	1.02
1:N:67:PHE:CD2	2:N:1624:BOG:C2'	2.41	1.02
1:S:66:TYR:HD1	3:S:1725:HOH:O	1.40	1.02
1:C:3:LYS:HD3	1:J:75:ALA:N	1.74	1.02
2:B:1606:BOG:H62	3:I:1628:HOH:O	1.59	1.02
1:1:41:TYR:HE2	3:1:1710:HOH:O	1.40	1.02
1:N:9:SER:HB3	3:N:1631:HOH:O	1.59	1.02
3:S:1731:HOH:O	1:T:70:LEU:HD13	1.55	1.01
1:T:77:GLN:HB3	1:V:3:LYS:HZ3	0.98	1.01
1:H:8:GLU:HB3	3:H:1650:HOH:O	1.58	1.01
1:T:77:GLN:C	1:V:3:LYS:HZ2	1.58	1.01
1:W:58:THR:HG23	3:W:641:HOH:O	1.60	1.01
1:7:42:PHE:HD1	3:7:1756:HOH:O	1.40	1.01
1:N:67:PHE:CG	2:N:1624:BOG:C2'	2.43	1.01
1:D:75:ALA:HB2	3:D:1617:HOH:O	1.60	1.01
2:E:1623:BOG:H5	3:E:1657:HOH:O	1.61	1.00
1:P:30:LYS:HD2	3:P:1644:HOH:O	1.58	1.00
1:3:3:LYS:HD3	1:3:3:LYS:N	1.73	1.00
1:K:66:TYR:CD2	2:K:1616:BOG:H5'1	1.94	1.00
1:F:61:VAL:HG23	3:F:581:HOH:O	1.59	1.00
1:Z:34:LEU:HD22	3:Z:1751:HOH:O	1.59	1.00
1:C:3:LYS:HD3	1:J:75:ALA:CA	1.92	0.99
1:A:54:LYS:HE3	3:A:1631:HOH:O	1.60	0.99
1:2:9:SER:HA	3:2:1719:HOH:O	1.62	0.99
1:7:14:TYR:HB2	3:7:1738:HOH:O	1.60	0.99
3:Z:1750:HOH:O	1:7:51:PRO:HB2	1.61	0.99
1:A:14:TYR:HB2	3:A:1618:HOH:O	1.60	0.99
1:3:34:LEU:HG	3:3:1733:HOH:O	1.62	0.98
1:K:66:TYR:CD1	2:K:1616:BOG:H5'2	1.97	0.98
1:G:3:LYS:HB3	1:N:74:PRO:HA	1.45	0.98
1:E:77:GLN:HE22	1:N:75:ALA:HB3	1.24	0.98
1:K:66:TYR:CD1	2:K:1616:BOG:H4'2	1.96	0.98
1:8:45:SER:HB3	3:8:1762:HOH:O	1.61	0.98
1:5:2:ALA:HB1	3:5:545:HOH:O	1.62	0.98
1:M:39:LYS:HG3	3:M:1629:HOH:O	1.63	0.98
1:J:44:LYS:HB2	3:J:1627:HOH:O	1.61	0.97
1:N:67:PHE:CZ	2:N:1624:BOG:H2'1	1.96	0.97
1:7:30:LYS:HG2	3:8:1769:HOH:O	1.62	0.97
1:Z:67:PHE:HE1	3:Z:1754:HOH:O	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1610:BOG:H6'2	3:K:1336:HOH:O	1.62	0.97
3:A:1612:HOH:O	1:B:10:LEU:HD13	1.63	0.97
1:N:5:PRO:HA	3:N:1637:HOH:O	1.66	0.96
1:M:24:ASP:HA	2:M:1620:BOG:H1'1	1.42	0.96
1:3:10:LEU:HG	3:3:1734:HOH:O	1.64	0.96
1:N:67:PHE:CE1	2:N:1624:BOG:H2'1	1.97	0.96
1:C:5:PRO:HA	1:J:76:THR:HA	1.46	0.96
3:W:271:HOH:O	1:6:60:LEU:HD11	1.64	0.96
1:T:77:GLN:NE2	1:V:3:LYS:NZ	2.15	0.95
1:N:67:PHE:CG	2:N:1624:BOG:H3'1	1.99	0.95
1:T:60:LEU:HB2	3:T:1396:HOH:O	1.66	0.95
1:G:44:LYS:HB2	3:G:1657:HOH:O	1.66	0.95
1:6:14:TYR:HE1	3:6:1737:HOH:O	1.48	0.95
1:H:60:LEU:HB2	3:H:1635:HOH:O	1.67	0.94
1:3:66:TYR:CZ	2:3:1716:BOG:H5'1	2.00	0.94
1:M:41:TYR:HA	3:M:1635:HOH:O	1.67	0.94
1:H:2:ALA:N	1:M:77:GLN:HA	1.80	0.94
1:M:54:LYS:HG3	2:M:1621:BOG:H2	1.50	0.94
2:K:1610:BOG:H4'1	3:K:1336:HOH:O	1.67	0.94
1:K:66:TYR:CG	2:K:1616:BOG:H5'1	2.02	0.93
1:N:3:LYS:HA	3:N:1662:HOH:O	1.68	0.93
2:Y:1730:BOG:H7'1	3:Z:1738:HOH:O	1.68	0.92
1:G:28:LYS:HD3	3:G:1673:HOH:O	1.69	0.92
1:E:75:ALA:HB2	1:M:76:THR:HB	1.51	0.92
1:3:24:ASP:HA	3:3:1718:HOH:O	1.70	0.92
1:K:66:TYR:CG	2:K:1616:BOG:H4'1	2.03	0.91
1:F:18:VAL:HG13	3:F:678:HOH:O	1.69	0.91
1:N:67:PHE:CZ	2:N:1624:BOG:H3'2	2.06	0.91
1:G:52:LEU:HD23	3:H:1639:HOH:O	1.71	0.91
1:T:77:GLN:O	1:V:3:LYS:CE	2.19	0.91
1:E:63:PHE:HZ	3:N:1629:HOH:O	1.54	0.90
1:A:46:LYS:HD3	3:A:1620:HOH:O	1.71	0.90
1:L:3:LYS:HD3	3:L:1617:HOH:O	1.70	0.90
1:8:32:PRO:HD2	3:8:1737:HOH:O	1.70	0.90
1:Y:70:LEU:CD1	3:Y:1735:HOH:O	2.20	0.90
1:N:65:SER:HB2	3:N:1651:HOH:O	1.71	0.90
1:3:3:LYS:CD	1:3:3:LYS:H	1.82	0.90
1:L:12:SER:HA	3:L:1618:HOH:O	1.70	0.90
1:4:39:LYS:HA	3:4:1742:HOH:O	1.70	0.90
1:F:18:VAL:HA	3:F:678:HOH:O	1.71	0.90
1:8:56:ALA:HB1	3:8:1770:HOH:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:34:LEU:HB2	3:Z:1751:HOH:O	1.73	0.89
1:1:64:LEU:HB3	3:1:1714:HOH:O	1.72	0.89
1:H:2:ALA:CA	1:H:3:LYS:HZ2	1.73	0.89
1:U:17:THR:HG23	3:U:1725:HOH:O	1.73	0.89
1:V:3:LYS:HD2	3:3:1725:HOH:O	1.72	0.89
1:E:34:LEU:HG	3:E:1648:HOH:O	1.72	0.89
1:3:39:LYS:HD2	3:3:1727:HOH:O	1.73	0.88
1:X:35:GLN:HG3	3:X:1738:HOH:O	1.71	0.88
1:X:54:LYS:HB2	3:X:1735:HOH:O	1.72	0.88
1:Z:12:SER:HB3	3:Z:1753:HOH:O	1.71	0.88
2:Q:1628:BOG:H2	3:Q:1654:HOH:O	1.73	0.88
1:8:39:LYS:HB2	3:8:1734:HOH:O	1.73	0.88
1:U:32:PRO:HG2	3:U:1734:HOH:O	1.72	0.87
1:T:77:GLN:HE21	1:V:3:LYS:HZ1	1.17	0.87
1:H:39:LYS:HG3	3:H:1645:HOH:O	1.73	0.87
3:V:734:HOH:O	2:3:1716:BOG:H2'2	1.75	0.87
1:N:67:PHE:CE1	2:N:1624:BOG:C4'	2.58	0.87
1:K:66:TYR:CE1	2:K:1616:BOG:H5'2	2.07	0.87
1:3:66:TYR:CE2	2:3:1716:BOG:C3'	2.58	0.87
2:T:1706:BOG:H61	1:1:44:LYS:HB3	1.57	0.86
1:Z:38:ALA:HB2	3:Z:1740:HOH:O	1.72	0.86
1:3:66:TYR:CD1	2:3:1716:BOG:H4'2	2.08	0.86
1:3:66:TYR:CG	2:3:1716:BOG:H5'2	2.10	0.86
1:4:43:GLU:HA	3:4:1733:HOH:O	1.75	0.86
1:K:15:PHE:HB2	3:K:1336:HOH:O	1.73	0.86
2:N:1624:BOG:C3'	2:N:1624:BOG:C2'	2.53	0.86
1:3:66:TYR:CD2	2:3:1716:BOG:H4'1	2.07	0.86
1:S:55:LYS:HA	3:S:1722:HOH:O	1.75	0.86
1:1:75:ALA:HB1	3:3:1721:HOH:O	1.74	0.86
1:E:77:GLN:NE2	1:N:75:ALA:HB3	1.88	0.86
1:T:77:GLN:O	1:V:3:LYS:HE2	1.74	0.86
1:Y:14:TYR:CD2	3:Y:1754:HOH:O	2.27	0.85
1:Y:70:LEU:HG	3:Y:1735:HOH:O	1.76	0.85
2:D:1612:BOG:H1	3:K:602:HOH:O	1.77	0.85
1:W:19:THR:HG21	3:W:409:HOH:O	1.74	0.85
1:8:60:LEU:HB2	3:8:1770:HOH:O	1.76	0.85
2:F:1619:BOG:C6	3:F:678:HOH:O	2.25	0.85
3:7:1741:HOH:O	1:8:70:LEU:HD11	1.76	0.85
3:S:1731:HOH:O	1:T:70:LEU:HD22	1.75	0.85
1:Z:27:GLU:HB2	3:Z:1747:HOH:O	1.75	0.85
1:2:41:TYR:HA	3:2:1716:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1619:BOG:H62	3:F:678:HOH:O	1.77	0.85
1:T:40:SER:HB2	3:T:1214:HOH:O	1.77	0.85
2:B:1606:BOG:H61	1:I:44:LYS:HB3	1.55	0.84
1:3:35:GLN:CB	3:3:1738:HOH:O	2.24	0.84
1:K:66:TYR:CE1	2:K:1616:BOG:H4'2	2.10	0.84
1:3:35:GLN:HA	3:3:1738:HOH:O	1.76	0.84
1:4:14:TYR:HD1	3:4:1717:HOH:O	1.60	0.84
1:D:61:VAL:HG11	3:D:1628:HOH:O	1.77	0.84
1:G:58:THR:HB	3:G:1686:HOH:O	1.75	0.84
1:V:62:ASN:HB2	3:V:1308:HOH:O	1.76	0.84
1:N:44:LYS:HB3	3:N:1660:HOH:O	1.77	0.84
1:Q:4:GLU:HB2	3:Q:1647:HOH:O	1.76	0.84
3:D:1630:HOH:O	2:K:1610:BOG:H6'1	1.77	0.84
1:T:17:THR:HG21	3:T:1111:HOH:O	1.78	0.84
1:U:35:GLN:HG3	3:U:1740:HOH:O	1.78	0.84
1:V:62:ASN:CB	3:V:1308:HOH:O	2.26	0.84
1:C:7:VAL:HG13	3:C:1616:HOH:O	1.76	0.83
1:N:67:PHE:CG	2:N:1624:BOG:H2'2	2.12	0.83
1:X:64:LEU:HD13	3:X:1744:HOH:O	1.78	0.83
1:K:66:TYR:CZ	2:K:1616:BOG:C3'	2.61	0.83
1:A:18:VAL:CG1	3:A:1626:HOH:O	2.25	0.83
1:G:43:GLU:HB3	3:G:1650:HOH:O	1.76	0.83
1:7:21:TYR:HB2	3:7:1766:HOH:O	1.78	0.83
1:E:58:THR:HB	3:E:1624:HOH:O	1.77	0.83
1:N:67:PHE:CE2	2:N:1624:BOG:C1'	2.62	0.83
1:I:20:ASP:HB3	3:I:1632:HOH:O	1.78	0.83
1:Y:28:LYS:HD3	3:Y:1766:HOH:O	1.78	0.83
1:3:30:LYS:HA	3:3:1737:HOH:O	1.78	0.83
1:A:56:ALA:HB1	3:B:1629:HOH:O	1.77	0.83
1:X:3:LYS:HE2	1:X:3:LYS:N	1.94	0.83
1:Y:13:GLN:HG2	3:Y:1743:HOH:O	1.78	0.82
1:8:50:THR:HG21	3:8:1729:HOH:O	1.78	0.82
3:A:1614:HOH:O	1:C:3:LYS:HE3	1.78	0.82
2:G:1634:BOG:C5	3:G:1698:HOH:O	2.28	0.82
1:4:77:GLN:O	1:6:3:LYS:HG3	1.79	0.82
1:G:18:VAL:HG23	3:Q:1652:HOH:O	1.79	0.82
3:A:1624:HOH:O	1:J:15:PHE:HD1	1.63	0.82
1:8:46:LYS:HD2	3:8:1766:HOH:O	1.80	0.82
1:4:3:LYS:HB2	3:4:1723:HOH:O	1.78	0.82
1:J:44:LYS:CB	3:J:1627:HOH:O	2.24	0.81
1:U:77:GLN:HA	3:U:1718:HOH:O	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:46:LYS:HD2	3:4:1733:HOH:O	1.80	0.81
1:Y:70:LEU:HD12	3:Y:1735:HOH:O	1.77	0.81
1:H:3:LYS:HZ1	1:H:3:LYS:H	1.24	0.81
1:8:36:ALA:HA	3:8:1764:HOH:O	1.81	0.81
1:K:66:TYR:CE2	2:K:1616:BOG:C6'	2.64	0.81
1:Z:14:TYR:CB	3:Z:1741:HOH:O	2.27	0.81
2:N:1622:BOG:C6	3:N:1656:HOH:O	2.28	0.81
1:S:66:TYR:CD1	3:S:1725:HOH:O	2.20	0.81
1:I:20:ASP:CB	3:I:1632:HOH:O	2.27	0.81
1:K:63:PHE:HB2	3:K:763:HOH:O	1.80	0.81
1:K:66:TYR:CZ	2:K:1616:BOG:C6'	2.62	0.81
1:N:67:PHE:CD2	2:N:1624:BOG:C1'	2.63	0.81
1:X:18:VAL:HG22	3:5:724:HOH:O	1.80	0.81
1:C:3:LYS:HD3	1:J:75:ALA:HA	1.63	0.80
1:V:30:LYS:HB3	3:V:1306:HOH:O	1.81	0.80
1:A:14:TYR:CB	3:A:1640:HOH:O	2.28	0.80
1:X:35:GLN:CB	3:X:1738:HOH:O	2.29	0.80
1:Y:18:VAL:HB	3:Y:1739:HOH:O	1.79	0.80
1:3:66:TYR:CD1	2:3:1716:BOG:C6'	2.64	0.80
1:1:76:THR:HB	1:1:77:GLN:OE1	1.80	0.80
1:G:62:ASN:HA	3:G:1663:HOH:O	1.80	0.80
3:G:1678:HOH:O	1:H:63:PHE:CE2	2.35	0.80
1:H:2:ALA:C	1:H:3:LYS:HD2	2.02	0.80
1:Q:7:VAL:CG2	3:Q:1631:HOH:O	2.21	0.80
1:N:67:PHE:CE2	2:N:1624:BOG:H1'2	2.17	0.80
1:3:66:TYR:CE1	2:3:1716:BOG:C6'	2.65	0.80
1:J:13:GLN:HG2	3:M:1645:HOH:O	1.80	0.80
1:Y:14:TYR:HD2	3:Y:1754:HOH:O	1.61	0.80
1:H:3:LYS:CE	1:H:3:LYS:N	2.44	0.80
1:N:5:PRO:CA	3:N:1637:HOH:O	2.24	0.80
1:G:47:GLU:HA	3:G:1640:HOH:O	1.80	0.79
1:T:70:LEU:HD11	3:2:1721:HOH:O	1.81	0.79
1:Y:70:LEU:CG	3:Y:1735:HOH:O	2.29	0.79
1:4:14:TYR:CD1	3:4:1717:HOH:O	2.35	0.79
2:N:1622:BOG:H62	3:N:1656:HOH:O	1.80	0.79
1:G:27:GLU:HB3	3:G:1697:HOH:O	1.82	0.79
1:P:59:GLU:HA	3:P:1639:HOH:O	1.83	0.79
3:W:762:HOH:O	2:6:1717:BOG:H8'2	1.82	0.79
1:K:66:TYR:CE2	2:K:1616:BOG:C3'	2.65	0.79
1:2:76:THR:HG21	3:2:1710:HOH:O	1.82	0.79
1:V:4:GLU:H	1:V:5:PRO:HD2	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:THR:HB	3:E:1625:HOH:O	1.82	0.79
1:T:77:GLN:O	1:V:3:LYS:NZ	2.15	0.79
1:Y:63:PHE:CE1	3:Y:1753:HOH:O	2.35	0.79
1:X:35:GLN:CG	3:X:1738:HOH:O	2.28	0.79
2:G:1634:BOG:H62	3:G:1698:HOH:O	1.82	0.78
1:N:34:LEU:HG	3:N:1654:HOH:O	1.83	0.78
1:N:9:SER:CB	3:N:1631:HOH:O	2.25	0.78
3:W:271:HOH:O	1:6:60:LEU:CD1	2.25	0.78
1:U:3:LYS:HZ1	1:U:5:PRO:HG3	1.46	0.78
1:X:70:LEU:HD21	3:Z:1746:HOH:O	1.82	0.78
1:X:9:SER:HB2	3:X:1730:HOH:O	1.83	0.78
1:B:49:LEU:HD11	3:I:1629:HOH:O	1.82	0.78
1:L:15:PHE:HB3	3:L:1618:HOH:O	1.83	0.78
1:6:14:TYR:CE1	3:6:1737:HOH:O	2.27	0.78
1:8:46:LYS:CD	3:8:1766:HOH:O	2.32	0.78
1:M:56:ALA:HB3	2:M:1621:BOG:H2'2	1.66	0.78
1:2:44:LYS:HB2	3:2:1716:HOH:O	1.84	0.78
1:E:26:MET:HA	3:E:1661:HOH:O	1.83	0.78
1:Q:6:CYS:SG	3:Q:1644:HOH:O	2.42	0.78
1:8:56:ALA:CB	3:8:1770:HOH:O	2.28	0.78
1:Q:5:PRO:HD2	3:Q:1631:HOH:O	1.84	0.78
1:G:65:SER:HA	3:G:1677:HOH:O	1.84	0.77
1:N:44:LYS:CB	3:N:1660:HOH:O	2.31	0.77
1:6:23:LYS:HD3	3:6:1739:HOH:O	1.84	0.77
1:P:28:LYS:HE3	3:P:1658:HOH:O	1.82	0.77
2:G:1633:BOG:H2'1	1:Q:64:LEU:HD13	1.65	0.77
1:B:69:GLU:CB	3:B:1630:HOH:O	2.20	0.77
1:E:46:LYS:HB2	3:E:1656:HOH:O	1.83	0.77
1:D:25:LEU:HB3	2:D:1612:BOG:H2'1	1.67	0.77
1:X:64:LEU:CD1	3:X:1744:HOH:O	2.32	0.77
1:8:38:ALA:HB2	3:8:1778:HOH:O	1.85	0.77
1:Y:5:PRO:C	3:Y:1736:HOH:O	2.23	0.77
3:5:1055:HOH:O	1:6:44:LYS:HD3	1.84	0.77
1:D:4:GLU:H	1:D:5:PRO:HD2	1.50	0.77
1:F:75:ALA:CB	3:F:142:HOH:O	2.32	0.76
1:7:53:ILE:HA	3:7:1742:HOH:O	1.84	0.76
1:A:77:GLN:NE2	1:C:3:LYS:NZ	2.33	0.76
3:A:1624:HOH:O	1:J:15:PHE:CD1	2.38	0.76
1:Z:27:GLU:CB	3:Z:1747:HOH:O	2.30	0.76
1:T:77:GLN:CA	1:V:3:LYS:NZ	2.47	0.76
1:A:23:LYS:HD3	3:A:1630:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:27:GLU:HA	3:P:1644:HOH:O	1.84	0.76
1:F:26:MET:SD	3:J:1616:HOH:O	2.43	0.76
1:G:35:GLN:CD	3:G:1646:HOH:O	2.23	0.76
1:C:5:PRO:HG2	1:D:3:LYS:HG3	1.68	0.76
1:I:22:GLY:HA3	3:I:1633:HOH:O	1.85	0.76
1:U:32:PRO:HB2	3:U:1731:HOH:O	1.86	0.76
1:G:34:LEU:HB2	3:G:1696:HOH:O	1.86	0.76
1:G:44:LYS:CD	3:G:1645:HOH:O	2.20	0.76
1:L:76:THR:HB	3:L:1629:HOH:O	1.86	0.76
1:N:67:PHE:CD2	2:N:1624:BOG:H1'2	2.20	0.76
2:M:1625:BOG:H7'1	1:N:67:PHE:CE1	2.21	0.76
1:Y:63:PHE:HE1	3:Y:1753:HOH:O	1.66	0.76
1:F:61:VAL:HG11	3:F:1459:HOH:O	1.84	0.76
1:J:16:GLN:HB3	3:J:1623:HOH:O	1.86	0.76
2:Y:1733:BOG:H5'1	1:8:63:PHE:HB3	1.66	0.75
1:A:7:VAL:HA	3:A:1638:HOH:O	1.85	0.75
1:K:26:MET:CA	3:K:602:HOH:O	2.35	0.75
1:T:77:GLN:HB3	1:V:3:LYS:HZ1	1.49	0.75
1:W:3:LYS:C	3:W:692:HOH:O	2.24	0.75
1:J:40:SER:HB2	3:J:1613:HOH:O	1.87	0.75
1:P:68:VAL:HG13	3:P:1637:HOH:O	1.86	0.75
1:T:4:GLU:HA	3:T:1100:HOH:O	1.86	0.75
1:W:19:THR:CG2	3:W:321:HOH:O	2.32	0.75
1:J:9:SER:HB2	3:J:1633:HOH:O	1.86	0.75
1:6:31:SER:H	1:6:32:PRO:HD2	1.52	0.75
1:S:4:GLU:HG3	3:S:1727:HOH:O	1.87	0.74
1:N:65:SER:CB	3:N:1651:HOH:O	2.30	0.74
1:X:63:PHE:HB3	3:X:1744:HOH:O	1.87	0.74
1:8:72:THR:HG23	3:8:1744:HOH:O	1.87	0.74
1:S:18:VAL:HG13	3:S:1719:HOH:O	1.87	0.74
1:Y:14:TYR:CE1	3:Y:1745:HOH:O	2.40	0.74
2:D:1612:BOG:H1'2	1:K:26:MET:SD	2.27	0.74
1:N:9:SER:CB	3:N:1646:HOH:O	2.35	0.74
3:F:1387:HOH:O	1:M:15:PHE:CZ	2.40	0.74
1:E:58:THR:CG2	3:E:1624:HOH:O	2.34	0.74
1:N:11:VAL:O	2:N:1618:BOG:H5'1	1.86	0.74
2:2:1708:BOG:H2	3:2:1734:HOH:O	1.88	0.74
1:F:18:VAL:HG13	2:F:1619:BOG:H62	1.70	0.74
1:P:2:ALA:N	1:P:3:LYS:HZ3	1.86	0.73
1:A:14:TYR:CD2	3:A:1618:HOH:O	2.40	0.73
1:D:73:GLN:HB3	1:D:74:PRO:HD3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:PHE:HA	2:N:1624:BOG:H7'2	1.68	0.73
1:7:60:LEU:HB2	3:7:1757:HOH:O	1.88	0.73
1:V:21:TYR:HH	1:4:21:TYR:HE1	1.36	0.73
1:D:75:ALA:CB	3:D:1617:HOH:O	2.27	0.73
1:E:63:PHE:CZ	3:N:1629:HOH:O	2.32	0.73
2:K:1610:BOG:H4	3:K:238:HOH:O	1.88	0.73
1:U:16:GLN:NE2	3:U:1722:HOH:O	2.21	0.73
1:E:19:THR:CB	3:E:1625:HOH:O	2.35	0.73
1:S:64:LEU:HB3	3:S:1730:HOH:O	1.87	0.73
1:E:34:LEU:CG	3:E:1648:HOH:O	2.32	0.73
1:D:61:VAL:HG21	3:D:1628:HOH:O	1.86	0.73
2:E:1623:BOG:H6'1	2:N:1624:BOG:H8'3	1.70	0.73
1:Y:56:ALA:HB3	3:Y:1746:HOH:O	1.88	0.73
1:Z:14:TYR:HB3	3:Z:1741:HOH:O	1.87	0.73
1:T:77:GLN:OXT	1:V:3:LYS:HD3	1.89	0.73
1:A:6:CYS:C	3:A:1638:HOH:O	2.27	0.72
1:X:22:GLY:CA	3:X:1737:HOH:O	2.36	0.72
1:X:35:GLN:C	3:X:1738:HOH:O	2.26	0.72
1:8:50:THR:HB	1:8:51:PRO:HD3	1.69	0.72
1:8:38:ALA:HB3	3:8:1741:HOH:O	1.88	0.72
1:Y:13:GLN:CD	3:Y:1743:HOH:O	2.26	0.72
2:3:1716:BOG:C5'	2:3:1716:BOG:C4'	2.67	0.72
1:I:9:SER:HB2	3:I:1636:HOH:O	1.87	0.72
1:F:20:ASP:HB3	3:F:1118:HOH:O	1.88	0.72
1:I:4:GLU:N	1:I:5:PRO:HD3	2.04	0.72
1:T:77:GLN:CD	1:V:3:LYS:NZ	2.43	0.72
1:N:9:SER:HB3	3:N:1646:HOH:O	1.88	0.72
1:E:61:VAL:HG11	3:E:1643:HOH:O	1.88	0.72
1:J:57:GLY:CA	3:J:1619:HOH:O	2.37	0.72
1:V:10:LEU:HG	3:V:345:HOH:O	1.89	0.72
1:8:50:THR:CG2	3:8:1729:HOH:O	2.37	0.72
1:U:3:LYS:NZ	1:U:5:PRO:HG3	2.05	0.71
1:J:33:GLU:HA	3:J:1622:HOH:O	1.89	0.71
1:Q:73:GLN:HB3	1:Q:74:PRO:HD3	1.71	0.71
1:3:66:TYR:CD1	2:3:1716:BOG:H6'1	2.25	0.71
2:I:1605:BOG:H4'1	3:I:1620:HOH:O	1.89	0.71
1:G:35:GLN:HB2	3:G:1646:HOH:O	1.90	0.71
1:W:43:GLU:CD	3:W:961:HOH:O	2.29	0.71
1:C:48:GLN:HB2	2:C:1614:BOG:H3'1	1.70	0.71
1:J:40:SER:CB	3:J:1613:HOH:O	2.39	0.71
1:T:18:VAL:HG13	2:T:1702:BOG:H3'1	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:66:TYR:CE1	2:3:1716:BOG:H6'2	2.25	0.71
1:3:66:TYR:CZ	2:3:1716:BOG:C3'	2.73	0.71
1:K:26:MET:HB2	3:K:602:HOH:O	1.90	0.71
1:X:77:GLN:O	1:Z:3:LYS:HA	1.90	0.71
1:3:35:GLN:CA	3:3:1738:HOH:O	2.30	0.71
1:Z:14:TYR:C	3:Z:1741:HOH:O	2.30	0.70
1:6:77:GLN:HB3	3:7:1758:HOH:O	1.88	0.70
1:8:39:LYS:N	3:8:1741:HOH:O	2.24	0.70
1:F:18:VAL:CA	3:F:678:HOH:O	2.35	0.70
1:G:21:TYR:HD2	3:G:1674:HOH:O	1.74	0.70
1:N:67:PHE:CE1	2:N:1624:BOG:H4'1	2.25	0.70
1:6:49:LEU:HD12	3:6:1728:HOH:O	1.91	0.70
1:8:34:LEU:HB2	3:8:1790:HOH:O	1.92	0.70
1:M:71:GLY:HA3	2:N:1624:BOG:H4	1.72	0.70
1:Q:3:LYS:HZ2	1:Q:3:LYS:HA	1.56	0.70
1:T:77:GLN:CA	1:V:3:LYS:HZ3	2.03	0.70
1:8:32:PRO:HB3	3:8:1733:HOH:O	1.92	0.70
2:K:1616:BOG:C5'	2:K:1616:BOG:C4'	2.68	0.70
1:M:57:GLY:HA3	2:M:1621:BOG:H62	1.71	0.70
1:A:18:VAL:HG13	3:A:1626:HOH:O	1.90	0.70
1:K:66:TYR:CZ	2:K:1616:BOG:H6'1	2.26	0.70
2:I:1601:BOG:C1'	3:I:1624:HOH:O	2.39	0.70
1:K:66:TYR:CE2	2:K:1616:BOG:H6'2	2.27	0.70
3:D:1617:HOH:O	1:M:7:VAL:HG13	1.92	0.70
1:A:77:GLN:HE22	1:C:3:LYS:NZ	1.90	0.70
1:A:77:GLN:HE22	1:C:3:LYS:HZ3	1.40	0.70
1:A:46:LYS:CD	3:A:1620:HOH:O	2.35	0.69
2:G:1634:BOG:C6	3:G:1698:HOH:O	2.40	0.69
1:F:50:THR:HB	1:F:51:PRO:HD3	1.74	0.69
1:B:51:PRO:CG	3:B:1632:HOH:O	2.20	0.69
1:L:3:LYS:CG	3:L:1617:HOH:O	2.38	0.69
1:X:35:GLN:HB3	3:X:1738:HOH:O	1.90	0.69
1:3:30:LYS:HE2	3:3:1723:HOH:O	1.91	0.69
1:8:36:ALA:C	3:8:1764:HOH:O	2.30	0.69
1:K:66:TYR:CZ	2:K:1616:BOG:H3'1	2.26	0.69
1:5:24:ASP:N	3:5:827:HOH:O	2.25	0.69
1:B:47:GLU:HA	3:B:1632:HOH:O	1.92	0.69
1:I:45:SER:HB3	3:I:1640:HOH:O	1.93	0.69
1:M:73:GLN:HB2	1:M:74:PRO:HD3	1.74	0.69
1:C:3:LYS:CD	1:J:75:ALA:CA	2.70	0.69
1:G:13:GLN:HB3	3:G:1658:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:67:PHE:CD1	2:N:1624:BOG:C4'	2.75	0.69
1:C:44:LYS:NZ	3:C:1620:HOH:O	2.25	0.69
1:N:69:GLU:CG	3:N:1639:HOH:O	2.42	0.69
1:B:49:LEU:CD1	3:I:1629:HOH:O	2.41	0.68
1:C:3:LYS:HZ3	1:J:74:PRO:HB2	1.57	0.68
1:K:66:TYR:CE2	2:K:1616:BOG:H3'2	2.27	0.68
1:3:25:LEU:CD1	3:3:1744:HOH:O	2.41	0.68
1:M:3:LYS:HE3	1:M:3:LYS:N	2.08	0.68
1:4:23:LYS:NZ	3:4:1719:HOH:O	2.26	0.68
1:X:56:ALA:HB3	3:X:1740:HOH:O	1.92	0.68
1:Z:64:LEU:HD12	3:Z:1754:HOH:O	1.93	0.68
1:C:75:ALA:HB3	1:E:7:VAL:HB	1.76	0.68
1:N:7:VAL:CG1	3:N:1652:HOH:O	2.41	0.68
1:V:77:GLN:HE22	1:X:5:PRO:HG3	1.58	0.68
1:X:50:THR:HB	1:X:51:PRO:HD3	1.75	0.68
1:8:36:ALA:CA	3:8:1764:HOH:O	2.38	0.68
1:B:18:VAL:HG13	2:B:1602:BOG:H3'1	1.76	0.68
1:H:3:LYS:HG2	1:M:74:PRO:HB3	1.74	0.68
1:7:11:VAL:HG11	2:7:1726:BOG:H6'1	1.75	0.68
3:K:763:HOH:O	1:L:63:PHE:CZ	2.47	0.68
1:G:18:VAL:HG22	3:G:1674:HOH:O	1.94	0.68
1:Y:13:GLN:CG	3:Y:1743:HOH:O	2.37	0.68
1:C:3:LYS:CD	1:J:75:ALA:HA	2.23	0.68
1:T:77:GLN:C	1:V:3:LYS:CE	2.60	0.67
1:M:2:ALA:C	1:M:3:LYS:HE3	2.14	0.67
1:Y:13:GLN:HG2	3:Y:1740:HOH:O	1.93	0.67
1:2:76:THR:CG2	3:2:1710:HOH:O	2.42	0.67
3:3:1723:HOH:O	1:4:28:LYS:HD2	1.93	0.67
1:Z:11:VAL:HA	3:Z:1739:HOH:O	1.93	0.67
1:B:42:PHE:HE2	3:B:1638:HOH:O	1.76	0.67
1:J:50:THR:HB	1:J:51:PRO:HD3	1.76	0.67
1:U:32:PRO:CB	3:U:1731:HOH:O	2.43	0.67
1:2:50:THR:HB	1:2:51:PRO:HD3	1.77	0.67
1:3:48:GLN:CD	3:3:1735:HOH:O	2.32	0.67
1:B:69:GLU:CG	3:B:1630:HOH:O	2.41	0.67
1:P:27:GLU:CB	3:P:1644:HOH:O	2.41	0.67
1:X:51:PRO:HA	3:X:1735:HOH:O	1.94	0.67
1:2:14:TYR:CZ	3:2:1733:HOH:O	2.48	0.67
1:D:61:VAL:CB	3:D:1628:HOH:O	2.41	0.67
1:B:47:GLU:CA	3:B:1632:HOH:O	2.43	0.67
1:L:50:THR:HG23	3:L:1630:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:50:THR:HB	1:V:51:PRO:HD3	1.77	0.66
1:N:32:PRO:HB3	3:N:1653:HOH:O	1.94	0.66
1:T:77:GLN:C	1:V:3:LYS:HZ3	1.83	0.66
1:J:45:SER:HB2	3:J:1638:HOH:O	1.95	0.66
1:Q:18:VAL:HG12	3:Q:1640:HOH:O	1.95	0.66
1:E:50:THR:HB	1:E:51:PRO:HD3	1.77	0.66
1:M:30:LYS:HA	3:M:1636:HOH:O	1.94	0.66
1:D:50:THR:HB	1:D:51:PRO:HD3	1.78	0.66
1:G:44:LYS:CE	3:G:1645:HOH:O	2.42	0.66
1:C:5:PRO:CA	1:J:76:THR:HA	2.25	0.66
1:M:3:LYS:HE2	3:M:1640:HOH:O	1.96	0.66
1:Z:5:PRO:HG2	1:Z:6:CYS:H	1.61	0.66
1:A:7:VAL:N	3:A:1638:HOH:O	2.29	0.66
2:B:1606:BOG:H1	1:I:41:TYR:HA	1.78	0.66
1:H:3:LYS:N	1:H:3:LYS:CD	2.59	0.65
2:H:1631:BOG:H4'2	1:P:52:LEU:HD22	1.77	0.65
1:3:66:TYR:CE2	2:3:1716:BOG:H3'2	2.29	0.65
2:K:1610:BOG:C6'	3:K:1336:HOH:O	2.29	0.65
1:X:56:ALA:CB	3:X:1740:HOH:O	2.43	0.65
1:3:66:TYR:CZ	2:3:1716:BOG:H3'1	2.31	0.65
1:G:28:LYS:CD	3:G:1673:HOH:O	2.33	0.65
1:W:59:GLU:HB2	3:W:641:HOH:O	1.97	0.65
1:8:4:GLU:H	1:8:5:PRO:HD2	1.61	0.65
1:A:31:SER:OG	1:A:32:PRO:HD3	1.97	0.65
1:4:42:PHE:HB2	3:4:1742:HOH:O	1.97	0.65
1:B:46:LYS:HA	3:B:1633:HOH:O	1.97	0.65
1:E:75:ALA:HB1	1:M:77:GLN:HB2	1.78	0.65
1:Q:46:LYS:HE3	3:Q:1653:HOH:O	1.95	0.65
1:U:35:GLN:CG	3:U:1740:HOH:O	2.39	0.65
1:B:50:THR:HB	1:B:51:PRO:HD3	1.79	0.65
1:W:50:THR:HB	1:W:51:PRO:HD3	1.79	0.65
1:Y:37:GLU:CA	3:Y:1768:HOH:O	2.25	0.65
1:8:17:THR:HA	3:8:1788:HOH:O	1.97	0.65
1:F:18:VAL:CG1	3:F:678:HOH:O	2.35	0.65
1:G:66:TYR:HD1	2:G:1634:BOG:H3'2	1.61	0.65
1:T:77:GLN:N	1:V:2:ALA:N	2.45	0.65
1:N:8:GLU:HB3	3:N:1642:HOH:O	1.96	0.64
1:A:14:TYR:CG	3:A:1618:HOH:O	2.50	0.64
1:N:50:THR:HB	1:N:51:PRO:HD3	1.79	0.64
1:2:31:SER:H	1:2:32:PRO:HD2	1.60	0.64
1:U:77:GLN:HB3	3:U:1718:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:38:ALA:HB2	3:8:1776:HOH:O	1.95	0.64
1:E:58:THR:HG22	3:E:1624:HOH:O	1.97	0.64
1:N:14:TYR:HB2	2:N:1618:BOG:H7'2	1.80	0.64
1:P:27:GLU:CA	3:P:1644:HOH:O	2.44	0.64
1:Y:64:LEU:HA	1:Y:67:PHE:HD1	1.63	0.64
1:B:76:THR:OG1	1:I:77:GLN:HG2	1.97	0.64
1:T:50:THR:HB	1:T:51:PRO:HD3	1.80	0.64
1:3:8:GLU:HA	1:3:11:VAL:HG22	1.77	0.64
1:3:21:TYR:CZ	3:3:1744:HOH:O	2.49	0.64
1:U:3:LYS:H	1:U:3:LYS:HD3	1.63	0.64
1:N:67:PHE:CD1	2:N:1624:BOG:H4'2	2.33	0.63
1:U:77:GLN:CB	3:U:1718:HOH:O	2.45	0.63
1:C:3:LYS:HD3	1:J:74:PRO:C	2.18	0.63
1:E:58:THR:CB	3:E:1624:HOH:O	2.38	0.63
1:I:68:VAL:HB	3:I:1622:HOH:O	1.97	0.63
1:B:5:PRO:HD2	3:B:1621:HOH:O	1.98	0.63
1:S:35:GLN:HG3	3:S:1713:HOH:O	1.98	0.63
1:3:35:GLN:HB3	3:3:1738:HOH:O	1.90	0.63
1:G:69:GLU:HB3	3:G:1698:HOH:O	1.99	0.63
1:P:67:PHE:HA	3:P:1633:HOH:O	1.97	0.63
1:8:46:LYS:NZ	3:8:1779:HOH:O	2.31	0.63
1:A:62:ASN:HB2	3:A:1617:HOH:O	1.98	0.63
1:C:8:GLU:HA	1:C:11:VAL:HG22	1.80	0.63
2:Z:1732:BOG:C2'	3:Z:1754:HOH:O	2.46	0.63
1:P:62:ASN:HB3	3:P:1666:HOH:O	1.99	0.63
1:L:39:LYS:CA	3:L:1632:HOH:O	2.25	0.63
2:6:1717:BOG:H4	3:6:1727:HOH:O	1.98	0.63
1:T:68:VAL:CG1	3:T:1305:HOH:O	2.46	0.63
1:W:19:THR:HG21	3:W:321:HOH:O	1.94	0.63
1:X:2:ALA:HB3	1:X:5:PRO:HB3	1.81	0.62
1:G:58:THR:CB	3:G:1686:HOH:O	2.38	0.62
1:A:7:VAL:CA	3:A:1638:HOH:O	2.46	0.62
3:B:1615:HOH:O	1:D:2:ALA:CB	2.46	0.62
3:7:1741:HOH:O	1:8:70:LEU:CD1	2.39	0.62
1:T:76:THR:O	1:T:77:GLN:O	2.17	0.62
1:U:42:PHE:HD1	3:U:1716:HOH:O	1.81	0.62
1:N:21:TYR:HD1	3:N:1647:HOH:O	1.82	0.62
1:X:19:THR:HG21	3:X:1739:HOH:O	1.98	0.62
1:V:52:LEU:HD23	3:V:826:HOH:O	2.00	0.62
1:B:77:GLN:H	1:I:75:ALA:HB1	1.64	0.62
1:E:15:PHE:HZ	2:N:1618:BOG:H6'1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:ALA:HA	1:H:3:LYS:HZ3	0.64	0.62
1:M:67:PHE:HA	2:N:1624:BOG:H3	1.81	0.62
3:E:1662:HOH:O	2:F:1619:BOG:H5'1	2.00	0.62
2:F:1619:BOG:H61	3:F:678:HOH:O	1.96	0.62
1:M:7:VAL:HG23	1:M:10:LEU:HD12	1.82	0.62
1:N:11:VAL:HB	2:N:1617:BOG:H5	1.81	0.62
1:5:56:ALA:HB3	2:5:1721:BOG:H4'2	1.82	0.62
2:A:1604:BOG:H5'2	3:A:1634:HOH:O	2.00	0.62
1:D:61:VAL:CG1	3:D:1628:HOH:O	2.42	0.62
1:I:50:THR:HB	1:I:51:PRO:HD3	1.80	0.62
2:D:1612:BOG:H1'1	1:K:29:VAL:HG21	1.81	0.62
1:N:3:LYS:HZ3	1:N:3:LYS:HB2	1.63	0.62
1:A:14:TYR:HB2	3:A:1640:HOH:O	1.96	0.62
1:A:36:ALA:HA	1:A:40:SER:HA	1.81	0.62
1:G:47:GLU:HB3	3:G:1667:HOH:O	2.00	0.62
1:N:44:LYS:C	3:N:1660:HOH:O	2.38	0.62
1:T:77:GLN:O	1:V:3:LYS:HB2	2.00	0.62
3:W:762:HOH:O	2:6:1717:BOG:C8'	2.45	0.61
1:A:73:GLN:HB3	1:A:74:PRO:HD3	1.81	0.61
2:I:1605:BOG:H2'1	3:I:1620:HOH:O	2.00	0.61
1:Q:54:LYS:HE3	3:Q:1636:HOH:O	1.99	0.61
1:4:75:ALA:HB1	1:4:77:GLN:HE22	1.64	0.61
1:3:77:GLN:HA	1:5:3:LYS:HZ2	1.63	0.61
1:J:31:SER:H	1:J:32:PRO:HD2	1.64	0.61
1:8:32:PRO:CD	3:8:1737:HOH:O	2.39	0.61
1:8:56:ALA:CA	3:8:1770:HOH:O	2.48	0.61
1:1:50:THR:HB	1:1:51:PRO:HD3	1.80	0.61
1:N:7:VAL:HG12	3:N:1652:HOH:O	1.99	0.61
1:Q:57:GLY:O	1:Q:61:VAL:HG12	2.00	0.61
1:S:34:LEU:HB2	3:S:1713:HOH:O	2.00	0.61
1:T:17:THR:CG2	3:T:1111:HOH:O	2.43	0.61
1:J:57:GLY:HA2	3:J:1619:HOH:O	1.98	0.60
1:K:34:LEU:H	1:K:34:LEU:HD23	1.66	0.60
1:S:31:SER:OG	1:S:32:PRO:HD3	2.01	0.60
1:1:62:ASN:HB3	2:1:1709:BOG:H1	1.84	0.60
1:E:69:GLU:CD	3:E:1639:HOH:O	2.38	0.60
1:6:50:THR:HB	1:6:51:PRO:HD3	1.82	0.60
1:E:26:MET:CA	3:E:1661:HOH:O	2.43	0.60
1:E:76:THR:N	1:M:77:GLN:HB3	2.16	0.60
1:E:44:LYS:HE3	3:E:1654:HOH:O	2.01	0.60
1:K:54:LYS:CE	3:K:89:HOH:O	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:77:GLN:CD	1:V:3:LYS:HZ2	2.04	0.60
1:K:54:LYS:NZ	3:K:89:HOH:O	2.28	0.60
1:3:48:GLN:NE2	3:3:1735:HOH:O	2.34	0.60
1:G:66:TYR:CD1	2:G:1634:BOG:H3'2	2.37	0.60
2:N:1622:BOG:H1'1	3:N:1626:HOH:O	1.99	0.60
1:3:25:LEU:CD2	3:3:1744:HOH:O	2.49	0.60
1:B:28:LYS:HE3	3:B:1620:HOH:O	2.01	0.60
1:G:2:ALA:C	1:G:3:LYS:HD3	2.21	0.60
1:W:59:GLU:N	3:W:641:HOH:O	2.35	0.60
1:1:64:LEU:CB	3:1:1714:HOH:O	2.40	0.60
1:7:14:TYR:CD2	3:7:1738:HOH:O	2.52	0.60
3:5:1055:HOH:O	1:6:44:LYS:CD	2.46	0.60
1:C:5:PRO:HG3	1:J:77:GLN:H	1.66	0.60
1:7:42:PHE:CD1	3:7:1756:HOH:O	2.28	0.59
1:7:49:LEU:HD12	1:7:52:LEU:HD12	1.84	0.59
2:G:1634:BOG:C6	3:G:1700:HOH:O	2.49	0.59
1:Z:34:LEU:CD2	3:Z:1751:HOH:O	2.31	0.59
1:4:42:PHE:CB	3:4:1742:HOH:O	2.48	0.59
1:7:60:LEU:CA	3:7:1757:HOH:O	2.49	0.59
1:G:3:LYS:HG3	1:N:72:THR:HG23	1.84	0.59
1:U:4:GLU:N	1:U:5:PRO:HD3	2.15	0.59
2:T:1706:BOG:H1	1:1:41:TYR:HA	1.83	0.59
1:A:77:GLN:HE22	1:J:74:PRO:HB2	1.66	0.59
1:V:77:GLN:OXT	1:X:3:LYS:NZ	2.35	0.59
1:I:20:ASP:HA	3:I:1632:HOH:O	2.01	0.59
2:Z:1731:BOG:H62	1:7:48:GLN:HG3	1.84	0.59
1:3:25:LEU:HD13	3:3:1744:HOH:O	2.03	0.59
1:D:4:GLU:N	1:D:5:PRO:HD2	2.17	0.59
1:H:35:GLN:HG2	1:H:36:ALA:H	1.68	0.59
1:T:73:GLN:N	1:T:74:PRO:HD2	2.16	0.59
1:3:26:MET:SD	2:3:1712:BOG:H1'2	2.42	0.59
2:W:1723:BOG:H8'3	1:6:63:PHE:HB3	1.84	0.59
1:8:28:LYS:CE	3:8:1784:HOH:O	2.27	0.59
1:P:27:GLU:HG2	3:P:1644:HOH:O	2.03	0.59
1:Y:8:GLU:CG	3:Y:1755:HOH:O	2.28	0.59
1:Z:67:PHE:CE1	3:Z:1754:HOH:O	2.33	0.59
1:8:58:THR:HA	3:8:1748:HOH:O	2.03	0.59
1:T:42:PHE:HB3	2:T:1706:BOG:H4	1.84	0.59
1:V:70:LEU:HD23	3:X:1729:HOH:O	2.02	0.59
1:3:17:THR:HB	3:3:1729:HOH:O	2.02	0.59
1:B:76:THR:HA	1:I:76:THR:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:GLU:HG3	1:G:60:LEU:H	1.68	0.59
1:1:60:LEU:HD21	1:2:59:GLU:HG2	1.84	0.58
1:F:74:PRO:HA	1:H:4:GLU:HB2	1.84	0.58
1:G:58:THR:N	3:G:1686:HOH:O	2.35	0.58
1:M:46:LYS:CD	3:M:1649:HOH:O	2.29	0.58
1:P:67:PHE:CD1	3:P:1633:HOH:O	2.51	0.58
1:B:16:GLN:HB2	3:B:1627:HOH:O	2.03	0.58
1:I:22:GLY:N	3:I:1620:HOH:O	2.36	0.58
1:J:57:GLY:HA3	3:J:1619:HOH:O	1.99	0.58
1:I:20:ASP:CA	3:I:1632:HOH:O	2.47	0.58
1:U:3:LYS:HZ1	1:U:5:PRO:CG	2.16	0.58
1:V:31:SER:N	1:V:32:PRO:HD2	2.17	0.58
1:5:31:SER:HB3	1:5:32:PRO:HD3	1.85	0.58
1:8:46:LYS:CE	3:8:1779:HOH:O	2.51	0.58
1:N:67:PHE:CD2	1:N:67:PHE:CB	2.78	0.58
1:U:39:LYS:CG	3:U:1716:HOH:O	2.28	0.58
1:U:39:LYS:HE2	3:U:1719:HOH:O	2.04	0.58
1:3:77:GLN:HA	1:5:3:LYS:NZ	2.18	0.58
1:H:2:ALA:C	1:H:3:LYS:CD	2.71	0.58
1:H:2:ALA:C	1:H:3:LYS:NZ	2.13	0.58
1:3:4:GLU:H	1:3:5:PRO:CD	2.17	0.58
1:7:15:PHE:HB3	3:7:1727:HOH:O	2.04	0.58
1:E:61:VAL:CG1	3:E:1643:HOH:O	2.47	0.58
1:3:30:LYS:CA	3:3:1737:HOH:O	2.45	0.58
3:B:1615:HOH:O	1:D:2:ALA:HB2	2.02	0.58
2:U:1710:BOG:H1'1	1:4:10:LEU:HB3	1.85	0.58
1:Z:35:GLN:HG2	1:Z:36:ALA:H	1.69	0.58
1:5:24:ASP:HA	2:5:1720:BOG:H3'1	1.86	0.58
1:6:21:TYR:HB2	3:6:1744:HOH:O	2.02	0.58
1:K:26:MET:HA	3:K:602:HOH:O	2.02	0.58
3:K:763:HOH:O	1:L:63:PHE:CE2	2.56	0.58
1:U:77:GLN:CA	3:U:1718:HOH:O	2.45	0.58
1:E:75:ALA:HB3	1:G:4:GLU:CB	2.34	0.58
2:K:1610:BOG:H1'1	1:L:10:LEU:HB3	1.86	0.58
1:T:74:PRO:HG2	3:T:1047:HOH:O	2.03	0.58
1:X:3:LYS:HE2	1:X:3:LYS:H	1.67	0.58
1:Z:34:LEU:CB	3:Z:1751:HOH:O	2.41	0.58
1:3:34:LEU:CD1	3:3:1733:HOH:O	2.52	0.57
1:E:16:GLN:HA	3:E:1625:HOH:O	2.04	0.57
1:E:70:LEU:HD21	1:N:70:LEU:HD12	1.86	0.57
1:Z:6:CYS:SG	1:Z:6:CYS:O	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:34:LEU:CB	3:8:1790:HOH:O	2.51	0.57
1:B:69:GLU:HA	1:B:73:GLN:HE21	1.69	0.57
1:I:45:SER:CB	3:I:1640:HOH:O	2.50	0.57
1:Z:54:LYS:HG3	3:Z:1734:HOH:O	2.04	0.57
1:3:4:GLU:H	1:3:5:PRO:HD2	1.67	0.57
1:K:26:MET:CB	3:K:602:HOH:O	2.48	0.57
1:L:5:PRO:HG2	1:L:6:CYS:H	1.68	0.57
1:B:66:TYR:CE1	1:B:70:LEU:HD11	2.39	0.57
1:J:13:GLN:CG	3:M:1645:HOH:O	2.46	0.57
1:Y:2:ALA:HB2	1:6:73:GLN:NE2	2.18	0.57
2:Z:1732:BOG:H2'2	3:Z:1754:HOH:O	2.04	0.57
1:F:73:GLN:HB2	1:F:74:PRO:HD3	1.86	0.57
2:I:1605:BOG:H8'2	3:I:1633:HOH:O	2.03	0.57
1:K:63:PHE:CB	3:K:763:HOH:O	2.46	0.57
1:C:54:LYS:NZ	3:C:1625:HOH:O	2.37	0.57
2:Q:1628:BOG:C2	3:Q:1654:HOH:O	2.40	0.57
2:G:1633:BOG:H4'1	1:Q:64:LEU:HA	1.86	0.57
1:U:51:PRO:HA	1:U:54:LYS:HB2	1.87	0.57
1:E:75:ALA:HB2	1:M:76:THR:CB	2.30	0.57
1:U:16:GLN:CD	3:U:1738:HOH:O	2.42	0.57
1:K:63:PHE:CE1	2:L:1615:BOG:H7'1	2.40	0.57
1:Q:33:GLU:HB2	1:Q:35:GLN:HE22	1.70	0.57
1:F:53:ILE:HG22	3:F:88:HOH:O	2.04	0.57
1:L:3:LYS:CD	3:L:1617:HOH:O	2.36	0.57
1:Q:17:THR:HA	3:Q:1639:HOH:O	2.04	0.57
1:B:42:PHE:HB3	2:B:1606:BOG:H4	1.87	0.56
1:H:68:VAL:CG2	3:H:1636:HOH:O	2.53	0.56
1:I:31:SER:HB2	3:I:1613:HOH:O	2.04	0.56
1:S:36:ALA:HA	1:S:40:SER:HA	1.87	0.56
1:T:40:SER:CB	3:T:1214:HOH:O	2.46	0.56
1:Z:3:LYS:HD2	1:Z:3:LYS:N	2.19	0.56
1:G:35:GLN:HG3	3:G:1696:HOH:O	2.05	0.56
1:M:13:GLN:HG2	3:M:1655:HOH:O	2.05	0.56
1:P:31:SER:H	1:P:32:PRO:HD2	1.69	0.56
1:W:64:LEU:HA	1:W:67:PHE:HB2	1.86	0.56
1:Y:14:TYR:CD1	3:Y:1745:HOH:O	2.58	0.56
1:8:45:SER:CB	3:8:1762:HOH:O	2.34	0.56
1:J:33:GLU:CA	3:J:1622:HOH:O	2.50	0.56
2:N:1622:BOG:H61	3:N:1656:HOH:O	1.97	0.56
1:T:77:GLN:CG	1:V:3:LYS:NZ	2.68	0.56
2:E:1623:BOG:H6'1	2:N:1624:BOG:C8'	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:77:GLN:CD	1:V:77:GLN:O	2.44	0.56
1:E:63:PHE:HD2	2:N:1624:BOG:H7'2	1.70	0.56
1:C:3:LYS:HB2	1:J:75:ALA:HA	1.87	0.56
1:G:35:GLN:HG2	3:G:1655:HOH:O	2.06	0.56
1:3:66:TYR:CD1	2:3:1716:BOG:H4'1	2.36	0.56
1:4:22:GLY:HA2	3:4:1725:HOH:O	2.05	0.56
1:N:31:SER:N	1:N:32:PRO:HD2	2.21	0.56
1:P:33:GLU:H	1:P:35:GLN:HE22	1.53	0.56
1:8:40:SER:CB	3:8:1746:HOH:O	2.53	0.56
1:8:73:GLN:N	1:8:74:PRO:HD2	2.20	0.56
1:T:63:PHE:HB3	2:1:1709:BOG:H4'2	1.88	0.55
1:I:60:LEU:HD21	1:J:59:GLU:HG2	1.88	0.55
1:S:37:GLU:HG3	2:S:1704:BOG:H1'1	1.86	0.55
1:W:32:PRO:HA	1:W:35:GLN:HB3	1.88	0.55
1:Z:31:SER:N	1:Z:32:PRO:HD2	2.21	0.55
1:F:13:GLN:NE2	3:F:1494:HOH:O	2.39	0.55
1:F:75:ALA:HB2	3:F:142:HOH:O	2.02	0.55
1:G:70:LEU:HD12	1:G:74:PRO:HG2	1.87	0.55
1:J:9:SER:CB	3:J:1633:HOH:O	2.50	0.55
1:C:73:GLN:HB3	1:C:74:PRO:HD3	1.87	0.55
1:N:31:SER:HB2	3:N:1671:HOH:O	2.05	0.55
1:5:45:SER:HB2	3:5:1055:HOH:O	2.05	0.55
1:U:24:ASP:CG	3:U:1735:HOH:O	2.45	0.55
1:M:59:GLU:HG3	3:M:1633:HOH:O	2.07	0.55
1:3:30:LYS:CE	3:3:1723:HOH:O	2.52	0.55
1:N:3:LYS:NZ	1:N:3:LYS:HB2	2.22	0.55
1:D:77:GLN:HE21	1:F:2:ALA:N	2.04	0.55
1:C:77:GLN:O	1:E:3:LYS:HG3	2.06	0.55
1:M:18:VAL:HA	1:M:21:TYR:CE2	2.40	0.55
2:F:1619:BOG:H6'1	1:N:21:TYR:HD2	1.72	0.55
1:E:18:VAL:HG12	2:F:1619:BOG:H8'1	1.89	0.55
1:K:8:GLU:HB2	1:L:6:CYS:SG	2.46	0.55
1:E:76:THR:O	1:P:3:LYS:HA	2.07	0.55
1:S:42:PHE:HZ	1:T:37:GLU:HA	1.72	0.55
1:W:30:LYS:HG2	1:X:28:LYS:HD2	1.87	0.55
1:1:4:GLU:N	1:1:5:PRO:HD2	2.22	0.55
1:8:28:LYS:NZ	3:8:1787:HOH:O	2.40	0.54
1:A:30:LYS:NZ	3:A:1627:HOH:O	2.41	0.54
1:N:9:SER:HB2	3:N:1646:HOH:O	2.02	0.54
1:W:77:GLN:O	1:Y:2:ALA:C	2.46	0.54
1:E:34:LEU:HD13	3:F:601:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:50:THR:OG1	1:7:51:PRO:HD3	2.08	0.54
1:E:46:LYS:CB	3:E:1656:HOH:O	2.49	0.54
1:X:74:PRO:HA	1:Z:3:LYS:O	2.07	0.54
1:Y:66:TYR:HD2	2:Y:1734:BOG:H3'2	1.72	0.54
1:A:75:ALA:O	1:A:76:THR:HG22	2.07	0.54
1:A:42:PHE:HZ	1:B:37:GLU:HA	1.73	0.54
1:H:2:ALA:HB3	1:M:77:GLN:N	2.22	0.54
1:N:73:GLN:HG2	1:N:74:PRO:HD2	1.88	0.54
1:V:7:VAL:O	1:V:11:VAL:HG13	2.08	0.54
1:X:22:GLY:HA2	3:X:1737:HOH:O	2.03	0.54
1:V:77:GLN:HE22	1:X:5:PRO:CG	2.20	0.54
1:E:28:LYS:HB2	1:N:29:VAL:HG23	1.89	0.54
1:4:71:GLY:N	3:4:1728:HOH:O	2.41	0.54
1:8:38:ALA:CB	3:8:1778:HOH:O	2.49	0.54
2:G:1634:BOG:H7'1	1:H:70:LEU:HD22	1.89	0.54
1:U:62:ASN:CB	2:U:1715:BOG:H1	2.37	0.54
1:F:30:LYS:HE3	3:F:548:HOH:O	2.07	0.54
1:H:50:THR:CB	3:H:1648:HOH:O	2.29	0.54
1:H:50:THR:CG2	3:H:1648:HOH:O	2.54	0.54
1:U:11:VAL:HA	1:U:14:TYR:CE1	2.43	0.54
1:V:53:ILE:CD1	3:V:1332:HOH:O	2.24	0.54
1:3:31:SER:H	1:3:32:PRO:HD2	1.72	0.54
1:J:71:GLY:N	3:J:1612:HOH:O	2.41	0.54
1:A:14:TYR:CB	3:A:1618:HOH:O	2.34	0.53
1:F:77:GLN:C	1:H:3:LYS:HZ1	2.12	0.53
1:N:29:VAL:HG13	1:N:30:LYS:HG3	1.91	0.53
1:N:73:GLN:CB	3:N:1625:HOH:O	2.30	0.53
1:S:28:LYS:HA	3:S:1706:HOH:O	2.07	0.53
1:V:34:LEU:CD2	3:V:1034:HOH:O	2.23	0.53
1:E:26:MET:HE3	3:E:1662:HOH:O	2.09	0.53
1:F:76:THR:HG22	1:F:77:GLN:H	1.73	0.53
1:N:69:GLU:CD	3:N:1639:HOH:O	2.46	0.53
1:A:14:TYR:HA	3:A:1640:HOH:O	2.07	0.53
1:D:4:GLU:O	1:D:7:VAL:HG12	2.07	0.53
1:L:76:THR:N	3:L:1629:HOH:O	2.41	0.53
1:T:21:TYR:HB3	2:T:1702:BOG:H3'2	1.91	0.53
2:X:1725:BOG:H6'2	2:5:1724:BOG:O2	2.07	0.53
1:B:49:LEU:HB2	3:B:1633:HOH:O	2.09	0.53
1:C:51:PRO:HA	1:C:54:LYS:HB2	1.90	0.53
1:K:55:LYS:NZ	1:K:55:LYS:HB3	2.23	0.53
1:L:59:GLU:HA	1:L:63:PHE:HD1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:22:GLY:N	3:X:1737:HOH:O	2.41	0.53
1:8:56:ALA:HA	3:8:1770:HOH:O	2.07	0.53
1:F:22:GLY:O	1:F:26:MET:HG2	2.09	0.53
1:N:67:PHE:CB	1:N:67:PHE:CD1	2.80	0.53
1:K:15:PHE:CB	3:K:1336:HOH:O	2.41	0.53
1:E:77:GLN:HG3	1:N:76:THR:O	2.09	0.53
1:4:17:THR:HB	3:4:1717:HOH:O	2.09	0.53
1:D:75:ALA:HB1	1:M:7:VAL:HG12	1.90	0.53
1:N:51:PRO:HB2	3:N:1638:HOH:O	2.07	0.53
1:S:77:GLN:HB2	1:U:5:PRO:HG2	1.88	0.53
1:4:3:LYS:CB	3:4:1723:HOH:O	2.47	0.53
1:5:60:LEU:HD11	1:6:59:GLU:HG2	1.91	0.53
1:H:34:LEU:O	1:H:39:LYS:HE2	2.09	0.53
1:I:22:GLY:CA	3:I:1620:HOH:O	2.55	0.53
1:Q:17:THR:HG21	2:Q:1628:BOG:H4'2	1.90	0.53
3:S:1731:HOH:O	1:T:70:LEU:CD1	2.32	0.53
1:W:58:THR:C	3:W:641:HOH:O	2.46	0.53
1:1:26:MET:HG2	1:1:30:LYS:HE3	1.91	0.53
1:8:72:THR:CG2	3:8:1744:HOH:O	2.51	0.53
1:D:70:LEU:HG	1:F:3:LYS:HB3	1.91	0.53
1:D:73:GLN:NE2	1:F:7:VAL:HB	2.24	0.53
1:G:73:GLN:HB2	1:G:74:PRO:HD3	1.91	0.53
1:P:3:LYS:NZ	1:P:3:LYS:H	2.07	0.53
1:P:3:LYS:NZ	1:P:3:LYS:N	2.56	0.53
1:A:37:GLU:HG3	2:A:1604:BOG:H1'1	1.91	0.52
1:X:5:PRO:HG2	1:X:6:CYS:H	1.73	0.52
1:I:46:LYS:HE2	3:I:1634:HOH:O	2.07	0.52
1:Q:2:ALA:CA	3:Q:1637:HOH:O	2.58	0.52
1:8:58:THR:HB	3:8:1793:HOH:O	2.08	0.52
1:E:29:VAL:HG21	3:N:1675:HOH:O	2.09	0.52
1:E:4:GLU:H	1:E:5:PRO:HD2	1.73	0.52
3:D:1620:HOH:O	1:K:7:VAL:HG11	2.09	0.52
1:7:3:LYS:NZ	1:7:3:LYS:HA	2.24	0.52
1:E:33:GLU:HB2	3:E:1648:HOH:O	2.10	0.52
1:E:32:PRO:HA	1:E:35:GLN:HB3	1.91	0.52
1:I:77:GLN:HA	1:K:2:ALA:N	2.24	0.52
1:S:60:LEU:HD11	1:T:59:GLU:HG2	1.92	0.52
1:G:51:PRO:CD	3:G:1640:HOH:O	2.25	0.52
1:I:26:MET:HG2	1:I:30:LYS:HE3	1.91	0.52
1:J:33:GLU:CB	3:J:1622:HOH:O	2.57	0.52
1:L:3:LYS:HG2	3:L:1617:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:3:LYS:NZ	1:U:5:PRO:CG	2.72	0.52
2:5:1724:BOG:H6'2	1:6:67:PHE:HD1	1.75	0.52
1:H:50:THR:HB	1:H:51:PRO:HD3	1.91	0.52
1:L:2:ALA:C	1:L:3:LYS:HE2	2.30	0.52
1:T:61:VAL:HG23	3:T:1396:HOH:O	2.09	0.52
1:3:61:VAL:HA	1:3:64:LEU:HD13	1.90	0.52
1:7:14:TYR:HD2	3:7:1738:HOH:O	1.87	0.52
1:8:40:SER:O	1:8:44:LYS:HG2	2.09	0.52
1:A:11:VAL:HA	1:A:14:TYR:CE1	2.45	0.52
1:U:64:LEU:O	1:U:68:VAL:HG23	2.09	0.52
1:V:64:LEU:O	1:V:68:VAL:HG23	2.10	0.52
1:4:72:THR:O	1:4:74:PRO:HD3	2.09	0.52
1:H:13:GLN:HG2	3:H:1646:HOH:O	2.10	0.52
1:2:58:THR:HG22	3:2:1726:HOH:O	2.09	0.51
1:5:53:ILE:O	2:5:1721:BOG:H6'1	2.10	0.51
1:V:25:LEU:O	1:V:29:VAL:HG23	2.09	0.51
1:5:70:LEU:HB2	2:5:1724:BOG:H4	1.92	0.51
1:6:35:GLN:HG2	1:6:36:ALA:H	1.74	0.51
2:G:1634:BOG:H5	3:G:1698:HOH:O	2.04	0.51
1:P:3:LYS:HZ2	1:P:3:LYS:H	1.58	0.51
1:S:58:THR:HG22	3:S:1722:HOH:O	2.10	0.51
1:V:19:THR:HG22	1:V:23:LYS:HE3	1.92	0.51
1:W:32:PRO:HA	1:W:35:GLN:CB	2.40	0.51
1:Y:50:THR:HB	1:Y:51:PRO:HD3	1.90	0.51
1:U:59:GLU:HA	2:U:1715:BOG:H1'2	1.93	0.51
1:H:45:SER:O	1:H:49:LEU:HG	2.10	0.51
1:L:53:ILE:HG13	1:L:54:LYS:HD2	1.92	0.51
1:N:53:ILE:HG12	2:N:1622:BOG:H5	1.93	0.51
2:H:1626:BOG:H6'1	1:P:11:VAL:HG11	1.92	0.51
1:Z:19:THR:O	1:Z:23:LYS:HG3	2.11	0.51
2:Y:1734:BOG:H7'1	1:Z:70:LEU:HD22	1.93	0.51
1:B:47:GLU:C	3:B:1632:HOH:O	2.48	0.51
1:A:77:GLN:C	1:C:3:LYS:HZ1	2.14	0.51
1:C:45:SER:HA	2:C:1614:BOG:H7'2	1.93	0.51
1:H:37:GLU:HG3	2:Q:1630:BOG:H2	1.92	0.51
2:E:1623:BOG:H8'1	1:N:67:PHE:HB2	1.93	0.51
1:U:14:TYR:O	1:U:18:VAL:HG23	2.11	0.51
1:U:33:GLU:N	3:U:1734:HOH:O	2.44	0.51
1:3:39:LYS:CD	3:3:1727:HOH:O	2.45	0.51
1:E:32:PRO:HA	1:E:35:GLN:CB	2.41	0.51
1:V:45:SER:HB2	1:3:48:GLN:HE22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:33:GLU:HB2	3:J:1622:HOH:O	2.10	0.51
1:S:73:GLN:O	1:U:6:CYS:HB2	2.10	0.51
1:5:8:GLU:HG3	1:6:6:CYS:O	2.11	0.51
1:C:77:GLN:OXT	1:C:77:GLN:NE2	2.43	0.51
1:B:76:THR:HA	1:I:75:ALA:HA	1.92	0.51
2:G:1634:BOG:H2'1	1:Q:67:PHE:HB3	1.92	0.51
1:3:47:GLU:HA	3:3:1720:HOH:O	2.10	0.51
1:4:25:LEU:O	1:4:29:VAL:HG23	2.11	0.51
1:8:44:LYS:HE3	1:8:44:LYS:HA	1.93	0.51
1:B:73:GLN:N	1:B:74:PRO:HD2	2.25	0.51
1:F:35:GLN:HB3	3:M:1635:HOH:O	2.08	0.51
1:I:14:TYR:O	1:I:18:VAL:HG23	2.11	0.51
1:A:18:VAL:HA	1:A:21:TYR:CE1	2.46	0.50
1:C:75:ALA:HB2	1:E:5:PRO:HG2	1.93	0.50
1:E:6:CYS:HB2	1:F:5:PRO:HB2	1.93	0.50
1:V:4:GLU:N	1:V:5:PRO:HD2	2.20	0.50
1:U:74:PRO:HA	1:W:2:ALA:N	2.26	0.50
1:X:22:GLY:O	1:X:26:MET:HG2	2.11	0.50
1:X:3:LYS:CE	1:X:3:LYS:N	2.72	0.50
1:Z:50:THR:HB	1:Z:51:PRO:HD3	1.92	0.50
1:8:39:LYS:CB	3:8:1734:HOH:O	2.46	0.50
1:L:72:THR:HG23	1:L:73:GLN:H	1.76	0.50
1:X:26:MET:O	1:X:30:LYS:HG3	2.12	0.50
1:4:60:LEU:O	1:4:64:LEU:HB2	2.11	0.50
1:D:75:ALA:CA	3:D:1617:HOH:O	2.56	0.50
1:I:12:SER:O	1:I:15:PHE:HB3	2.10	0.50
1:3:30:LYS:CB	3:3:1737:HOH:O	2.54	0.50
1:3:35:GLN:NE2	3:3:1730:HOH:O	2.30	0.50
1:3:50:THR:HG22	3:3:1743:HOH:O	2.12	0.50
1:W:11:VAL:HA	1:W:14:TYR:HD1	1.74	0.50
1:1:42:PHE:HB3	1:2:44:LYS:HZ2	1.76	0.50
1:I:22:GLY:HA2	3:I:1620:HOH:O	2.10	0.50
1:M:63:PHE:CE1	3:M:1633:HOH:O	2.55	0.50
1:T:25:LEU:O	1:T:29:VAL:HG23	2.11	0.50
1:U:34:LEU:HD22	3:U:1742:HOH:O	2.10	0.50
1:V:10:LEU:C	3:V:940:HOH:O	2.49	0.50
1:2:71:GLY:HA3	3:2:1728:HOH:O	2.11	0.50
1:8:46:LYS:HE2	3:8:1779:HOH:O	2.12	0.50
2:G:1634:BOG:H62	3:G:1700:HOH:O	2.07	0.50
1:I:13:GLN:NE2	3:I:1642:HOH:O	2.44	0.50
1:W:19:THR:HG23	3:W:321:HOH:O	2.03	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:14:TYR:CE2	3:Y:1754:HOH:O	2.60	0.50
1:8:34:LEU:O	3:8:1772:HOH:O	2.20	0.50
1:8:46:LYS:HD3	3:8:1766:HOH:O	2.06	0.50
2:B:1609:BOG:H3'2	1:I:63:PHE:CD2	2.47	0.50
1:G:35:GLN:CB	3:G:1646:HOH:O	2.52	0.50
1:G:14:TYR:HE2	2:Q:1627:BOG:H5	1.76	0.50
1:Z:64:LEU:HA	1:Z:67:PHE:HD1	1.77	0.50
1:3:30:LYS:CG	3:3:1737:HOH:O	2.23	0.50
1:4:31:SER:OG	1:4:32:PRO:HD3	2.12	0.50
1:D:10:LEU:N	3:D:1632:HOH:O	2.45	0.50
1:E:45:SER:O	1:E:49:LEU:HD23	2.11	0.50
2:M:1625:BOG:H2'2	2:M:1625:BOG:O5	2.09	0.50
1:T:77:GLN:CA	1:V:3:LYS:HZ2	2.16	0.50
1:L:31:SER:OG	1:L:32:PRO:HD3	2.12	0.49
1:U:62:ASN:HB3	2:U:1715:BOG:H1	1.93	0.49
1:3:29:VAL:HG21	2:3:1712:BOG:H1'1	1.94	0.49
1:4:55:LYS:HB3	1:4:55:LYS:NZ	2.28	0.49
1:E:33:GLU:HG2	3:N:1653:HOH:O	2.12	0.49
1:Q:2:ALA:N	3:Q:1637:HOH:O	2.44	0.49
1:W:45:SER:O	1:W:49:LEU:HD23	2.12	0.49
1:W:70:LEU:HD22	2:X:1725:BOG:H6'1	1.95	0.49
1:3:55:LYS:HB3	1:3:55:LYS:NZ	2.27	0.49
1:8:17:THR:HG21	2:8:1728:BOG:H4'2	1.92	0.49
1:G:47:GLU:CA	3:G:1640:HOH:O	2.48	0.49
1:M:30:LYS:CA	3:M:1636:HOH:O	2.57	0.49
1:N:73:GLN:CA	3:N:1625:HOH:O	2.59	0.49
1:S:11:VAL:HA	1:S:14:TYR:CE1	2.46	0.49
2:Z:1729:BOG:H8'1	1:8:17:THR:HG22	1.95	0.49
1:8:30:LYS:C	3:8:1767:HOH:O	2.51	0.49
1:F:75:ALA:HB1	3:F:142:HOH:O	2.07	0.49
1:J:52:LEU:HD23	2:J:1607:BOG:H62	1.94	0.49
1:N:69:GLU:HG3	3:N:1639:HOH:O	2.09	0.49
1:P:7:VAL:O	1:P:11:VAL:HG23	2.12	0.49
1:Q:3:LYS:NZ	1:Q:3:LYS:HA	2.26	0.49
1:6:60:LEU:HD23	1:6:60:LEU:H	1.76	0.49
1:I:39:LYS:O	1:I:43:GLU:HG3	2.12	0.49
1:L:4:GLU:N	1:L:5:PRO:HD3	2.28	0.49
1:N:63:PHE:HE2	2:N:1624:BOG:H5'1	1.77	0.49
1:T:64:LEU:O	1:T:68:VAL:HG23	2.12	0.49
1:4:14:TYR:HA	3:4:1717:HOH:O	2.11	0.49
1:5:9:SER:O	1:5:13:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:763:HOH:O	1:L:63:PHE:HZ	1.90	0.49
1:Q:2:ALA:HA	3:Q:1637:HOH:O	2.12	0.49
1:X:77:GLN:C	1:Z:3:LYS:HA	2.33	0.49
1:A:18:VAL:HG11	3:A:1626:HOH:O	2.02	0.49
1:D:3:LYS:H	1:K:3:LYS:HE3	1.78	0.49
1:D:63:PHE:O	1:D:67:PHE:HB2	2.13	0.49
1:G:55:LYS:NZ	1:G:55:LYS:HB3	2.27	0.49
1:K:4:GLU:H	1:K:5:PRO:HD2	1.77	0.49
1:L:59:GLU:HA	1:L:63:PHE:CD1	2.47	0.49
1:A:13:GLN:NE2	3:A:1608:HOH:O	2.23	0.49
1:B:37:GLU:HB2	3:B:1612:HOH:O	2.12	0.49
1:E:60:LEU:HD21	1:F:59:GLU:HG2	1.95	0.49
2:G:1634:BOG:H4'1	1:Q:67:PHE:CD2	2.47	0.49
1:1:31:SER:N	1:1:32:PRO:HD2	2.28	0.49
1:8:35:GLN:CD	3:8:1739:HOH:O	2.50	0.49
1:C:72:THR:HG23	1:E:9:SER:OG	2.13	0.49
1:E:26:MET:O	1:E:29:VAL:HG12	2.13	0.49
1:M:58:THR:HG22	3:M:1656:HOH:O	2.12	0.49
1:V:69:GLU:O	1:X:5:PRO:HA	2.12	0.49
1:Y:14:TYR:HE2	2:8:1727:BOG:H5	1.78	0.48
1:B:47:GLU:O	3:B:1632:HOH:O	2.20	0.48
1:N:57:GLY:O	1:N:61:VAL:HB	2.13	0.48
1:S:4:GLU:HA	3:S:1714:HOH:O	2.13	0.48
1:Y:26:MET:HG2	1:Y:30:LYS:HE3	1.94	0.48
1:3:33:GLU:HB2	3:3:1733:HOH:O	2.11	0.48
1:B:25:LEU:O	1:B:29:VAL:HG23	2.13	0.48
1:E:76:THR:H	1:M:77:GLN:HB3	1.77	0.48
2:Z:1732:BOG:H2'1	3:Z:1754:HOH:O	2.11	0.48
1:8:18:VAL:HG23	2:8:1728:BOG:H1'1	1.94	0.48
2:G:1633:BOG:H8'1	2:P:1632:BOG:H5'1	1.95	0.48
1:I:21:TYR:C	3:I:1620:HOH:O	2.51	0.48
2:W:1723:BOG:H7'2	2:5:1724:BOG:H8'3	1.94	0.48
1:E:72:THR:HG22	1:G:4:GLU:HG2	1.95	0.48
1:J:68:VAL:O	3:J:1612:HOH:O	2.20	0.48
1:M:60:LEU:HD11	1:N:59:GLU:HG2	1.96	0.48
1:T:36:ALA:HA	1:T:39:LYS:HB2	1.93	0.48
1:Z:27:GLU:CD	3:Z:1747:HOH:O	2.50	0.48
1:C:8:GLU:HA	3:C:1616:HOH:O	2.12	0.48
1:K:26:MET:N	3:K:602:HOH:O	2.46	0.48
1:X:30:LYS:HG2	1:2:19:THR:HG21	1.94	0.48
1:4:4:GLU:N	1:4:5:PRO:CD	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:LYS:CE	3:F:548:HOH:O	2.60	0.48
1:K:8:GLU:HA	1:K:11:VAL:HG22	1.95	0.48
1:K:31:SER:H	1:K:32:PRO:HD2	1.78	0.48
3:S:1731:HOH:O	1:T:70:LEU:CD2	2.46	0.48
1:2:63:PHE:CD1	2:2:1708:BOG:H2'2	2.49	0.48
1:4:46:LYS:NZ	3:4:1731:HOH:O	2.45	0.48
1:C:4:GLU:O	1:J:75:ALA:HB1	2.14	0.48
1:1:22:GLY:HA3	2:1:1705:BOG:H6'1	1.96	0.48
1:4:50:THR:O	1:4:54:LYS:HD3	2.14	0.48
1:4:53:ILE:HG13	1:4:54:LYS:HD2	1.96	0.48
1:B:21:TYR:HB3	2:B:1602:BOG:H3'2	1.96	0.48
1:B:77:GLN:N	1:I:75:ALA:HB1	2.29	0.48
1:1:35:GLN:NE2	3:1:1717:HOH:O	2.47	0.48
1:1:63:PHE:HA	2:1:1709:BOG:H3'2	1.96	0.48
1:3:59:GLU:HA	3:3:1736:HOH:O	2.13	0.48
1:5:50:THR:HB	1:5:51:PRO:HD3	1.96	0.48
1:E:34:LEU:N	3:E:1648:HOH:O	2.47	0.48
2:G:1634:BOG:H8'1	1:H:67:PHE:HA	1.96	0.48
1:G:47:GLU:C	3:G:1640:HOH:O	2.52	0.48
1:I:31:SER:CB	3:I:1613:HOH:O	2.60	0.48
1:I:61:VAL:HG21	3:I:1626:HOH:O	2.13	0.48
1:Q:37:GLU:HB3	3:Q:1656:HOH:O	2.13	0.48
1:T:66:TYR:CE1	1:T:70:LEU:HD21	2.49	0.48
1:3:25:LEU:HD22	3:3:1744:HOH:O	2.14	0.48
2:5:1724:BOG:H5	1:6:67:PHE:CE2	2.48	0.48
1:G:63:PHE:CD2	2:G:1633:BOG:H3'1	2.49	0.48
1:P:6:CYS:SG	3:Q:1644:HOH:O	2.60	0.48
1:C:43:GLU:O	1:C:47:GLU:HG3	2.14	0.47
1:E:30:LYS:HG2	1:F:28:LYS:HD2	1.96	0.47
1:I:77:GLN:C	1:K:2:ALA:N	2.68	0.47
1:M:74:PRO:HB2	2:M:1625:BOG:H4	1.96	0.47
1:X:2:ALA:C	1:X:3:LYS:HE2	2.34	0.47
1:Z:54:LYS:HA	3:Z:1734:HOH:O	2.12	0.47
1:8:70:LEU:HD23	1:8:70:LEU:H	1.78	0.47
1:E:29:VAL:HG21	1:N:28:LYS:HE2	1.94	0.47
1:E:8:GLU:HA	1:E:11:VAL:HG12	1.96	0.47
1:G:18:VAL:O	1:G:21:TYR:HB3	2.14	0.47
1:I:4:GLU:N	1:I:5:PRO:CD	2.76	0.47
1:1:41:TYR:CE2	3:1:1710:HOH:O	2.31	0.47
1:U:8:GLU:HA	1:U:11:VAL:HG22	1.96	0.47
1:1:25:LEU:O	1:1:29:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PRO:HG3	1:J:77:GLN:N	2.29	0.47
1:E:4:GLU:N	1:E:5:PRO:HD2	2.30	0.47
1:N:54:LYS:HG3	2:N:1622:BOG:H6'1	1.97	0.47
1:N:54:LYS:HD2	2:N:1622:BOG:H3'2	1.96	0.47
1:W:70:LEU:CD2	2:X:1725:BOG:H6'1	2.44	0.47
1:Y:28:LYS:CE	3:Y:1766:HOH:O	2.62	0.47
1:5:29:VAL:O	1:5:32:PRO:HD2	2.15	0.47
3:E:1661:HOH:O	1:N:25:LEU:HD13	2.13	0.47
1:Y:37:GLU:C	3:Y:1768:HOH:O	2.48	0.47
3:3:1746:HOH:O	1:4:2:ALA:HB2	2.15	0.47
1:E:75:ALA:HB3	1:G:4:GLU:HB2	1.97	0.47
1:G:26:MET:HG2	1:G:30:LYS:HE3	1.95	0.47
1:G:5:PRO:HB3	3:N:1677:HOH:O	2.13	0.47
1:I:12:SER:N	3:I:1624:HOH:O	2.48	0.47
1:I:25:LEU:O	1:I:29:VAL:HG23	2.14	0.47
1:J:36:ALA:HB1	1:J:39:LYS:HG2	1.97	0.47
1:H:2:ALA:HB3	1:M:76:THR:C	2.34	0.47
1:V:63:PHE:HA	1:V:66:TYR:CE2	2.50	0.47
1:D:3:LYS:HE2	1:D:3:LYS:HB2	1.57	0.47
1:E:34:LEU:CB	3:E:1648:HOH:O	2.59	0.47
1:K:54:LYS:HE2	3:K:89:HOH:O	2.11	0.47
1:Q:73:GLN:HG3	3:Q:1632:HOH:O	2.14	0.47
1:F:31:SER:N	1:F:32:PRO:HD2	2.30	0.47
1:G:9:SER:O	1:G:13:GLN:HG3	2.14	0.47
2:A:1603:BOG:H1	1:J:4:GLU:HG2	1.96	0.47
1:K:66:TYR:CB	1:K:66:TYR:CD1	2.82	0.47
1:T:66:TYR:OH	2:1:1709:BOG:H8'3	2.15	0.47
1:D:72:THR:HG23	1:D:76:THR:HA	1.95	0.47
2:E:1623:BOG:H61	3:E:1650:HOH:O	2.14	0.47
2:F:1619:BOG:H6'1	1:N:21:TYR:CD2	2.49	0.47
1:I:9:SER:CB	3:I:1636:HOH:O	2.53	0.47
1:P:2:ALA:N	1:P:3:LYS:NZ	2.61	0.47
1:8:55:LYS:O	1:8:59:GLU:HG2	2.15	0.47
1:T:77:GLN:CD	1:V:3:LYS:HZ1	2.07	0.47
1:B:36:ALA:HA	1:B:39:LYS:HB2	1.97	0.47
1:H:19:THR:O	1:H:23:LYS:HG3	2.14	0.47
1:L:15:PHE:CB	3:L:1618:HOH:O	2.54	0.47
1:L:67:PHE:HB2	2:L:1615:BOG:H62	1.96	0.47
3:J:1640:HOH:O	1:M:25:LEU:CD1	2.62	0.47
1:P:12:SER:O	1:P:16:GLN:HG3	2.15	0.47
1:U:22:GLY:O	1:U:26:MET:SD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:70:LEU:HB3	3:3:1747:HOH:O	2.14	0.46
1:C:64:LEU:O	1:C:68:VAL:HG23	2.15	0.46
1:E:75:ALA:HB1	1:M:77:GLN:CB	2.44	0.46
2:I:1601:BOG:H5'2	1:J:10:LEU:HB3	1.98	0.46
1:P:50:THR:OG1	1:P:51:PRO:HD3	2.15	0.46
1:B:31:SER:N	1:B:32:PRO:HD2	2.30	0.46
2:H:1626:BOG:H1'2	1:P:11:VAL:HG22	1.96	0.46
1:M:67:PHE:CA	2:N:1624:BOG:H3	2.46	0.46
1:S:18:VAL:HA	1:S:21:TYR:CE1	2.51	0.46
1:W:26:MET:O	1:W:29:VAL:HG12	2.15	0.46
1:Y:12:SER:HB2	1:Z:14:TYR:OH	2.15	0.46
1:Y:25:LEU:O	1:Y:29:VAL:HG23	2.15	0.46
1:2:36:ALA:HB1	1:2:39:LYS:HG2	1.98	0.46
1:C:3:LYS:HB2	1:C:4:GLU:H	1.62	0.46
1:E:25:LEU:HD22	1:N:29:VAL:HG11	1.97	0.46
2:G:1633:BOG:H2'1	1:Q:64:LEU:CD1	2.42	0.46
1:K:19:THR:HG22	1:K:23:LYS:HE3	1.97	0.46
1:K:4:GLU:H	1:K:5:PRO:CD	2.27	0.46
1:L:55:LYS:NZ	1:L:55:LYS:HB3	2.30	0.46
1:Y:28:LYS:CD	3:Y:1766:HOH:O	2.51	0.46
1:8:28:LYS:HE3	3:8:1769:HOH:O	2.15	0.46
1:I:31:SER:N	1:I:32:PRO:HD2	2.30	0.46
1:W:6:CYS:O	1:W:6:CYS:SG	2.74	0.46
1:B:5:PRO:HD2	3:B:1636:HOH:O	2.16	0.46
1:W:35:GLN:CD	3:W:190:HOH:O	2.54	0.46
1:X:31:SER:N	1:X:32:PRO:HD2	2.30	0.46
1:D:34:LEU:HB2	1:D:39:LYS:NZ	2.31	0.46
1:E:31:SER:OG	1:E:32:PRO:HD3	2.15	0.46
1:E:77:GLN:O	1:G:3:LYS:HE2	2.15	0.46
1:N:15:PHE:HA	2:N:1618:BOG:H1'1	1.98	0.46
1:T:44:LYS:O	1:T:48:GLN:HG3	2.16	0.46
1:T:77:GLN:CB	1:V:3:LYS:HZ2	2.14	0.46
1:Y:35:GLN:HA	1:Y:39:LYS:CD	2.46	0.46
1:Z:4:GLU:N	1:Z:5:PRO:HD3	2.30	0.46
1:G:14:TYR:HD1	3:G:1636:HOH:O	1.99	0.46
1:N:35:GLN:HB3	1:N:37:GLU:OE1	2.15	0.46
1:N:43:GLU:HA	3:N:1657:HOH:O	2.15	0.46
1:T:31:SER:N	1:T:32:PRO:HD2	2.31	0.46
1:C:25:LEU:O	1:C:29:VAL:HG23	2.16	0.46
1:L:50:THR:CG2	3:L:1630:HOH:O	2.59	0.46
1:S:70:LEU:O	1:T:70:LEU:HD22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:35:GLN:HG2	3:3:1738:HOH:O	2.16	0.46
2:B:1609:BOG:H3	1:I:62:ASN:HB3	1.98	0.46
1:D:61:VAL:CG2	3:D:1628:HOH:O	2.49	0.46
1:I:12:SER:N	3:I:1638:HOH:O	2.48	0.46
1:Z:15:PHE:N	3:Z:1741:HOH:O	2.49	0.46
1:5:45:SER:CB	3:5:1055:HOH:O	2.63	0.45
1:C:35:GLN:HG2	1:C:39:LYS:NZ	2.31	0.45
1:A:74:PRO:CB	1:J:74:PRO:HB3	2.46	0.45
1:J:9:SER:C	3:J:1633:HOH:O	2.54	0.45
1:1:14:TYR:O	1:1:18:VAL:HG23	2.15	0.45
1:A:17:THR:HB	3:A:1616:HOH:O	2.17	0.45
1:B:39:LYS:HG2	3:B:1628:HOH:O	2.15	0.45
1:E:72:THR:O	1:G:4:GLU:HB3	2.17	0.45
2:H:1629:BOG:H61	1:P:25:LEU:HB3	1.99	0.45
1:U:73:GLN:HB2	1:U:74:PRO:HD3	1.97	0.45
1:D:73:GLN:HB2	1:F:4:GLU:HG2	1.97	0.45
1:C:3:LYS:NZ	1:J:74:PRO:HB2	2.27	0.45
1:N:53:ILE:N	1:N:53:ILE:HD12	2.31	0.45
1:Y:6:CYS:CB	3:Y:1736:HOH:O	2.64	0.45
1:C:48:GLN:HB3	2:C:1614:BOG:H5'1	1.98	0.45
1:N:54:LYS:O	2:N:1622:BOG:H7'2	2.17	0.45
1:P:8:GLU:HB3	1:Q:10:LEU:HD11	1.97	0.45
1:S:9:SER:O	1:S:13:GLN:HG3	2.17	0.45
1:Z:73:GLN:N	1:Z:74:PRO:HD2	2.31	0.45
1:A:17:THR:HG21	3:A:1616:HOH:O	2.16	0.45
1:C:22:GLY:O	1:C:26:MET:SD	2.74	0.45
1:F:25:LEU:O	1:F:29:VAL:HG23	2.16	0.45
2:K:1610:BOG:H1'1	1:L:10:LEU:HD22	1.98	0.45
1:P:9:SER:O	1:P:13:GLN:HG3	2.17	0.45
1:V:70:LEU:HG	1:X:2:ALA:HB1	1.97	0.45
2:Z:1729:BOG:H5	1:7:22:GLY:HA2	1.98	0.45
1:Z:31:SER:O	1:Z:35:GLN:HB2	2.16	0.45
1:G:3:LYS:HB2	1:G:3:LYS:HE2	1.83	0.45
1:Q:18:VAL:CG2	2:Q:1628:BOG:H1'1	2.46	0.45
1:Y:18:VAL:O	1:Y:21:TYR:HB3	2.17	0.45
2:1:1707:BOG:H62	1:2:52:LEU:HD23	1.98	0.45
1:8:60:LEU:CB	3:8:1770:HOH:O	2.47	0.45
1:J:55:LYS:NZ	1:J:55:LYS:HB3	2.32	0.45
1:M:24:ASP:O	2:M:1620:BOG:H61	2.16	0.45
1:Y:35:GLN:HA	1:Y:39:LYS:HD3	1.99	0.45
1:4:76:THR:C	1:6:3:LYS:HZ2	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:O	1:B:48:GLN:HG3	2.16	0.45
1:F:61:VAL:CG2	3:F:581:HOH:O	2.39	0.45
1:H:2:ALA:HA	1:H:3:LYS:CE	2.36	0.45
1:I:73:GLN:HA	1:I:74:PRO:HD3	1.72	0.45
1:M:32:PRO:HA	1:M:36:ALA:HB3	1.99	0.45
1:M:72:THR:H	2:M:1625:BOG:H62	1.82	0.45
1:U:3:LYS:H	1:U:3:LYS:CD	2.29	0.45
1:X:4:GLU:N	1:X:5:PRO:CD	2.80	0.45
1:3:50:THR:CG2	3:3:1743:HOH:O	2.64	0.45
1:H:73:GLN:HB2	1:H:74:PRO:HD3	1.99	0.45
1:K:15:PHE:HE1	2:K:1610:BOG:HO2	1.64	0.45
1:6:53:ILE:HD12	1:6:53:ILE:N	2.32	0.44
1:C:11:VAL:HA	1:C:14:TYR:CE1	2.53	0.44
1:Z:64:LEU:CD1	3:Z:1754:HOH:O	2.60	0.44
1:D:3:LYS:N	1:D:3:LYS:HE2	2.32	0.44
1:I:32:PRO:HA	1:I:35:GLN:O	2.17	0.44
1:X:35:GLN:O	3:X:1738:HOH:O	2.21	0.44
1:A:10:LEU:HD23	3:A:1608:HOH:O	2.17	0.44
1:A:17:THR:CB	3:A:1616:HOH:O	2.65	0.44
1:D:56:ALA:HA	1:D:59:GLU:HB2	1.99	0.44
1:J:73:GLN:HA	1:J:74:PRO:HD3	1.83	0.44
1:T:74:PRO:HA	1:V:2:ALA:HB2	2.00	0.44
1:1:12:SER:O	1:1:15:PHE:HB3	2.18	0.44
1:8:3:LYS:HB2	1:8:3:LYS:HZ2	1.83	0.44
1:B:40:SER:O	1:B:44:LYS:HG3	2.18	0.44
1:C:73:GLN:CB	1:C:74:PRO:HD3	2.46	0.44
1:I:22:GLY:HA3	2:I:1605:BOG:H6'1	1.99	0.44
1:J:77:GLN:O	1:J:77:GLN:HG3	2.18	0.44
1:S:22:GLY:O	1:S:26:MET:SD	2.75	0.44
1:Y:67:PHE:HD2	2:Y:1734:BOG:H5'2	1.82	0.44
1:1:25:LEU:HB2	2:1:1705:BOG:H1'1	1.99	0.44
1:4:77:GLN:N	1:6:3:LYS:HZ2	2.16	0.44
1:7:3:LYS:HZ1	1:7:3:LYS:HA	1.83	0.44
1:A:75:ALA:HB2	1:C:6:CYS:O	2.17	0.44
1:F:26:MET:O	1:F:30:LYS:HG3	2.17	0.44
1:I:42:PHE:HB3	1:J:44:LYS:HZ2	1.83	0.44
1:J:75:ALA:O	1:J:76:THR:HB	2.18	0.44
1:C:41:TYR:HB3	1:L:42:PHE:HD2	1.83	0.44
3:S:1731:HOH:O	1:T:70:LEU:CG	2.59	0.44
1:U:26:MET:O	1:U:30:LYS:HG3	2.17	0.44
1:V:3:LYS:HE3	1:3:3:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:23:LYS:HB3	1:5:23:LYS:NZ	2.32	0.44
1:D:3:LYS:O	1:D:4:GLU:HB2	2.18	0.44
1:D:57:GLY:O	1:D:61:VAL:HB	2.18	0.44
1:L:37:GLU:HA	1:L:40:SER:OG	2.18	0.44
1:L:76:THR:CB	3:L:1629:HOH:O	2.56	0.44
1:3:66:TYR:CD2	1:3:66:TYR:CB	2.84	0.44
1:A:19:THR:O	1:A:23:LYS:HG3	2.17	0.44
1:C:8:GLU:HG2	2:K:1610:BOG:H4	2.00	0.44
1:D:19:THR:HG22	1:D:23:LYS:HE3	2.00	0.44
2:H:1626:BOG:H3	3:H:1643:HOH:O	2.17	0.44
1:Q:18:VAL:HG23	2:Q:1628:BOG:H1'1	2.00	0.44
2:X:1725:BOG:H61	1:5:73:GLN:NE2	2.33	0.44
1:3:25:LEU:O	1:3:29:VAL:HG23	2.18	0.44
1:6:32:PRO:HA	1:6:35:GLN:HE21	1.83	0.44
1:7:73:GLN:HB2	1:7:74:PRO:HD3	1.99	0.44
1:D:4:GLU:HA	3:D:1620:HOH:O	2.17	0.44
1:W:66:TYR:O	2:5:1724:BOG:H5'2	2.18	0.44
1:4:9:SER:O	1:4:13:GLN:HG3	2.18	0.44
2:5:1724:BOG:H5	1:6:67:PHE:CZ	2.53	0.44
1:D:45:SER:HB2	1:K:48:GLN:HE22	1.82	0.44
1:G:25:LEU:O	1:G:29:VAL:HG23	2.18	0.44
1:G:35:GLN:NE2	3:G:1646:HOH:O	2.45	0.44
1:G:50:THR:N	1:G:51:PRO:HD2	2.33	0.44
1:T:40:SER:O	1:T:44:LYS:HG3	2.17	0.44
1:U:3:LYS:HB2	1:U:3:LYS:HE2	1.61	0.44
1:Y:9:SER:O	1:Y:13:GLN:HG3	2.18	0.44
1:Y:4:GLU:HG2	1:Y:4:GLU:O	2.18	0.44
1:2:55:LYS:HB3	1:2:55:LYS:NZ	2.33	0.43
1:3:66:TYR:CD1	1:3:66:TYR:CB	2.83	0.43
1:5:27:GLU:HB3	2:5:1720:BOG:H1'2	1.99	0.43
1:L:3:LYS:N	1:L:3:LYS:HE2	2.33	0.43
1:2:76:THR:HG1	1:4:3:LYS:HZ2	1.62	0.43
1:6:50:THR:HG21	3:6:1736:HOH:O	2.18	0.43
1:S:12:SER:O	1:S:16:GLN:HG3	2.18	0.43
1:W:14:TYR:O	1:W:18:VAL:HG23	2.19	0.43
2:X:1725:BOG:O3	3:X:1733:HOH:O	2.21	0.43
1:Y:73:GLN:N	1:Y:74:PRO:HD2	2.33	0.43
1:Z:64:LEU:HA	1:Z:67:PHE:CD1	2.53	0.43
1:G:30:LYS:HE2	1:H:28:LYS:HD2	2.00	0.43
1:I:19:THR:O	1:I:23:LYS:HG3	2.16	0.43
1:I:69:GLU:N	3:I:1622:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:4:GLU:HG3	3:N:1650:HOH:O	2.18	0.43
1:N:73:GLN:HA	1:N:74:PRO:HD3	1.86	0.43
1:2:25:LEU:O	1:2:29:VAL:HG23	2.18	0.43
1:E:76:THR:HG22	1:E:77:GLN:N	2.33	0.43
2:M:1625:BOG:H7'1	1:N:67:PHE:HE1	1.76	0.43
1:M:54:LYS:HD2	1:M:54:LYS:N	2.34	0.43
1:N:35:GLN:HG2	1:N:36:ALA:H	1.83	0.43
1:U:62:ASN:HB2	2:U:1715:BOG:H1	1.99	0.43
1:U:25:LEU:O	1:U:29:VAL:HG23	2.18	0.43
1:X:25:LEU:O	1:X:29:VAL:HG23	2.17	0.43
2:Z:1731:BOG:H2'2	1:7:52:LEU:HD11	2.00	0.43
1:4:10:LEU:HD23	1:4:13:GLN:NE2	2.34	0.43
1:5:3:LYS:HZ2	1:5:3:LYS:HB2	1.83	0.43
1:A:74:PRO:HB3	1:J:74:PRO:HB3	2.01	0.43
2:F:1619:BOG:H7'2	1:N:22:GLY:HA2	1.98	0.43
1:Q:43:GLU:O	1:Q:47:GLU:HG3	2.18	0.43
1:V:70:LEU:CD2	3:X:1729:HOH:O	2.63	0.43
1:Z:49:LEU:O	1:Z:52:LEU:HG	2.18	0.43
1:1:19:THR:O	1:1:23:LYS:HG3	2.18	0.43
1:6:77:GLN:HE22	1:7:5:PRO:HA	1.84	0.43
1:L:59:GLU:O	2:L:1615:BOG:H2	2.19	0.43
1:Q:55:LYS:HB3	1:Q:55:LYS:NZ	2.34	0.43
1:S:19:THR:O	1:S:23:LYS:HG3	2.18	0.43
1:U:60:LEU:O	1:U:64:LEU:HD13	2.18	0.43
1:B:67:PHE:CE2	1:B:71:GLY:HA3	2.53	0.43
1:C:66:TYR:HB3	3:C:1622:HOH:O	2.17	0.43
1:D:74:PRO:HD2	1:D:77:GLN:NE2	2.33	0.43
1:G:44:LYS:CE	3:G:1657:HOH:O	2.66	0.43
1:J:8:GLU:HB3	3:J:1640:HOH:O	2.17	0.43
1:M:41:TYR:CA	3:M:1635:HOH:O	2.46	0.43
1:N:22:GLY:C	3:N:1664:HOH:O	2.57	0.43
1:U:69:GLU:HB3	1:U:73:GLN:HE21	1.84	0.43
1:Q:41:TYR:CD1	2:Q:1630:BOG:H3	2.54	0.43
1:Q:51:PRO:O	1:Q:55:LYS:HB2	2.18	0.43
1:S:29:VAL:O	1:S:32:PRO:HD2	2.19	0.43
1:5:4:GLU:N	1:5:5:PRO:HD3	2.34	0.43
1:G:28:LYS:NZ	3:G:1689:HOH:O	2.52	0.43
1:L:55:LYS:O	1:L:58:THR:HG22	2.18	0.43
1:Z:7:VAL:HG23	2:7:1726:BOG:H2'1	2.00	0.43
1:B:69:GLU:HG2	3:B:1630:HOH:O	2.14	0.43
3:A:1614:HOH:O	1:C:3:LYS:CE	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:HA	1:C:67:PHE:HD1	1.83	0.43
1:K:76:THR:HG22	1:K:77:GLN:N	2.33	0.43
1:Z:7:VAL:O	1:Z:11:VAL:HG23	2.19	0.43
1:6:18:VAL:HA	1:6:21:TYR:CE1	2.54	0.42
1:8:70:LEU:HA	1:8:73:GLN:HG3	2.00	0.42
1:A:9:SER:O	1:A:13:GLN:HG3	2.19	0.42
1:D:3:LYS:CE	1:D:3:LYS:N	2.82	0.42
1:J:65:SER:HB2	3:J:1637:HOH:O	2.19	0.42
1:L:42:PHE:HB3	3:L:1632:HOH:O	2.19	0.42
1:M:59:GLU:CG	3:M:1633:HOH:O	2.64	0.42
1:P:3:LYS:N	1:P:3:LYS:HZ3	2.16	0.42
1:X:54:LYS:CB	3:X:1735:HOH:O	2.48	0.42
1:Y:11:VAL:HA	1:Y:14:TYR:CE1	2.54	0.42
2:Y:1730:BOG:C7'	3:Z:1738:HOH:O	2.45	0.42
1:7:12:SER:O	1:7:16:GLN:HG3	2.19	0.42
1:7:15:PHE:HD1	3:7:1727:HOH:O	2.02	0.42
1:P:33:GLU:N	1:P:35:GLN:HE22	2.15	0.42
1:P:68:VAL:HA	3:P:1637:HOH:O	2.17	0.42
1:T:68:VAL:HG11	3:T:1305:HOH:O	2.17	0.42
2:Z:1729:BOG:H61	1:7:25:LEU:HB3	2.00	0.42
1:4:27:GLU:HG2	3:4:1739:HOH:O	2.18	0.42
1:5:23:LYS:HB3	3:5:827:HOH:O	2.19	0.42
1:C:56:ALA:HA	1:C:59:GLU:HB3	2.01	0.42
1:K:20:ASP:HA	1:K:23:LYS:HD2	1.99	0.42
2:T:1706:BOG:H1'2	1:1:41:TYR:HA	2.01	0.42
1:5:67:PHE:HA	2:5:1724:BOG:O4	2.18	0.42
1:7:25:LEU:O	1:7:29:VAL:HG23	2.19	0.42
1:E:75:ALA:HB3	1:G:4:GLU:HB3	2.00	0.42
1:G:44:LYS:HE3	3:G:1657:HOH:O	2.19	0.42
1:M:71:GLY:HA3	2:N:1624:BOG:C4	2.43	0.42
1:X:49:LEU:O	1:X:52:LEU:HG	2.20	0.42
1:5:27:GLU:CB	2:5:1720:BOG:H1'2	2.50	0.42
1:8:37:GLU:O	3:8:1778:HOH:O	2.21	0.42
1:C:15:PHE:HD2	1:C:15:PHE:HA	1.69	0.42
1:Q:50:THR:CG2	1:Q:51:PRO:HD3	2.48	0.42
1:V:20:ASP:HA	1:V:23:LYS:HD2	2.01	0.42
1:Z:49:LEU:HG	2:Z:1731:BOG:H1	2.01	0.42
1:G:11:VAL:HA	1:G:14:TYR:CE1	2.54	0.42
2:H:1629:BOG:H8'1	1:Q:17:THR:HG22	2.01	0.42
1:M:54:LYS:HA	2:M:1621:BOG:H2'1	2.02	0.42
1:S:43:GLU:CA	3:S:1705:HOH:O	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:73:GLN:N	1:X:74:PRO:HD2	2.34	0.42
1:Y:3:LYS:HG3	1:Y:3:LYS:H	1.52	0.42
1:G:56:ALA:HB1	1:G:60:LEU:HB2	2.02	0.42
1:1:33:GLU:HB3	3:1:1718:HOH:O	2.20	0.42
1:7:60:LEU:N	3:7:1757:HOH:O	2.52	0.42
1:H:31:SER:OG	1:H:32:PRO:HD3	2.20	0.42
1:Q:4:GLU:N	1:Q:5:PRO:CD	2.83	0.42
1:U:13:GLN:NE2	3:U:1717:HOH:O	2.51	0.42
1:3:25:LEU:HD11	3:3:1744:HOH:O	2.16	0.42
1:A:14:TYR:CA	3:A:1640:HOH:O	2.60	0.42
1:J:60:LEU:O	1:J:64:LEU:HD13	2.19	0.42
1:L:59:GLU:O	1:L:63:PHE:HB2	2.20	0.42
1:F:25:LEU:HD13	1:M:29:VAL:HG11	2.02	0.42
1:S:73:GLN:HB2	1:S:74:PRO:HD3	2.01	0.42
1:V:63:PHE:HB3	3:V:730:HOH:O	2.19	0.42
1:X:44:LYS:O	1:X:48:GLN:HG3	2.20	0.42
1:2:60:LEU:O	1:2:64:LEU:HD13	2.20	0.42
1:3:35:GLN:CG	3:3:1738:HOH:O	2.61	0.42
1:A:50:THR:N	1:A:51:PRO:HD2	2.35	0.42
2:D:1612:BOG:H5	3:K:602:HOH:O	2.18	0.42
1:F:60:LEU:O	1:F:64:LEU:HD13	2.19	0.42
1:H:4:GLU:HA	1:H:5:PRO:HD2	1.86	0.42
1:I:7:VAL:HG13	1:I:8:GLU:HG3	2.01	0.42
1:L:9:SER:O	1:L:13:GLN:HG3	2.20	0.42
1:N:53:ILE:HA	3:N:1676:HOH:O	2.20	0.42
1:S:50:THR:N	1:S:51:PRO:HD2	2.34	0.42
1:Y:6:CYS:HB2	3:Y:1736:HOH:O	2.20	0.42
1:4:58:THR:O	1:4:62:ASN:HB2	2.20	0.41
1:A:12:SER:O	1:A:16:GLN:HG3	2.19	0.41
1:D:3:LYS:HE2	1:K:3:LYS:HE2	1.08	0.41
3:M:1639:HOH:O	1:N:44:LYS:HD3	2.20	0.41
1:S:26:MET:O	1:S:30:LYS:HG3	2.21	0.41
1:S:74:PRO:O	1:S:75:ALA:HB2	2.20	0.41
1:D:46:LYS:HD3	3:D:1622:HOH:O	2.19	0.41
1:D:55:LYS:O	1:D:59:GLU:HG3	2.20	0.41
1:D:41:TYR:HD1	1:L:41:TYR:HH	1.68	0.41
3:J:1640:HOH:O	1:M:25:LEU:HD13	2.20	0.41
1:M:32:PRO:O	1:M:37:GLU:HB2	2.20	0.41
1:Y:15:PHE:O	1:Y:18:VAL:HG12	2.20	0.41
1:7:60:LEU:HA	3:7:1757:HOH:O	2.19	0.41
1:B:69:GLU:HA	1:B:73:GLN:NE2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:TYR:O	1:C:18:VAL:HG23	2.19	0.41
1:C:63:PHE:CD2	2:L:1615:BOG:H3'1	2.55	0.41
1:H:23:LYS:O	1:H:27:GLU:HG3	2.21	0.41
1:J:4:GLU:N	1:J:5:PRO:CD	2.83	0.41
1:L:76:THR:CA	3:L:1629:HOH:O	2.68	0.41
1:P:11:VAL:HA	1:P:14:TYR:CE1	2.56	0.41
1:X:60:LEU:O	1:X:64:LEU:HD13	2.20	0.41
1:A:29:VAL:O	1:A:32:PRO:HD2	2.20	0.41
1:A:77:GLN:NE2	1:C:3:LYS:HZ1	2.12	0.41
1:G:7:VAL:HA	1:G:10:LEU:HD12	2.02	0.41
1:J:33:GLU:HG3	1:J:34:LEU:N	2.36	0.41
1:K:4:GLU:N	1:K:5:PRO:CD	2.84	0.41
1:K:66:TYR:CB	1:K:66:TYR:CD2	2.83	0.41
1:L:26:MET:HG2	3:L:1641:HOH:O	2.19	0.41
1:X:56:ALA:HB1	3:X:1740:HOH:O	2.17	0.41
1:3:29:VAL:HG11	2:3:1712:BOG:H2'2	2.01	0.41
1:A:7:VAL:O	1:A:11:VAL:HG23	2.20	0.41
1:B:77:GLN:NE2	1:B:77:GLN:O	2.54	0.41
1:C:66:TYR:O	1:C:70:LEU:HD13	2.20	0.41
2:E:1623:BOG:H8'2	2:N:1624:BOG:H6'2	2.03	0.41
1:L:72:THR:HG23	1:L:73:GLN:N	2.35	0.41
2:H:1629:BOG:H5	1:P:22:GLY:HA2	2.02	0.41
1:U:31:SER:N	1:U:32:PRO:HD2	2.34	0.41
1:V:77:GLN:OE1	1:X:5:PRO:HD2	2.20	0.41
1:1:26:MET:O	1:1:30:LYS:HG3	2.21	0.41
1:3:56:ALA:HB1	1:3:60:LEU:HD12	2.02	0.41
1:8:41:TYR:O	3:8:1762:HOH:O	2.22	0.41
1:C:59:GLU:O	1:C:63:PHE:HB2	2.21	0.41
1:G:55:LYS:O	1:G:55:LYS:HD2	2.21	0.41
1:K:42:PHE:HA	1:L:44:LYS:NZ	2.36	0.41
1:S:21:TYR:OH	3:S:1719:HOH:O	2.22	0.41
1:U:38:ALA:HB2	3:U:1736:HOH:O	2.21	0.41
1:3:4:GLU:N	1:3:5:PRO:CD	2.82	0.41
1:M:12:SER:O	1:M:16:GLN:HG3	2.21	0.41
1:Q:2:ALA:O	1:Q:3:LYS:HB2	2.20	0.41
1:S:68:VAL:HG22	3:S:1715:HOH:O	2.19	0.41
1:6:35:GLN:HB3	1:6:37:GLU:OE1	2.21	0.41
1:7:34:LEU:HD23	1:7:34:LEU:N	2.36	0.41
1:F:5:PRO:HG2	1:F:6:CYS:H	1.85	0.41
1:H:31:SER:O	1:H:35:GLN:HB2	2.21	0.41
1:M:56:ALA:HA	1:M:59:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:67:PHE:CD2	1:N:67:PHE:N	2.89	0.41
3:G:1674:HOH:O	2:Q:1628:BOG:H1'2	2.21	0.41
1:T:61:VAL:N	3:T:1396:HOH:O	2.54	0.41
1:Z:23:LYS:O	1:Z:27:GLU:HG3	2.20	0.41
1:Z:25:LEU:O	1:Z:29:VAL:HG23	2.20	0.41
1:5:24:ASP:HB3	3:5:827:HOH:O	2.21	0.41
1:8:50:THR:HG23	3:8:1747:HOH:O	2.21	0.41
1:L:31:SER:H	1:L:32:PRO:CD	2.34	0.41
1:M:13:GLN:HA	1:M:16:GLN:HE21	1.86	0.41
1:S:74:PRO:HA	1:U:4:GLU:O	2.20	0.41
1:W:15:PHE:HZ	2:W:1718:BOG:H6'2	1.86	0.41
1:W:19:THR:O	1:W:23:LYS:HG3	2.21	0.41
3:Z:1750:HOH:O	1:7:52:LEU:N	2.54	0.41
1:8:39:LYS:CG	3:8:1740:HOH:O	2.28	0.41
1:8:45:SER:N	3:8:1762:HOH:O	2.52	0.41
1:D:28:LYS:HA	1:D:31:SER:OG	2.21	0.41
1:T:18:VAL:HG23	3:T:1013:HOH:O	2.20	0.41
1:X:2:ALA:CA	1:X:3:LYS:HE2	2.51	0.41
1:X:51:PRO:O	1:X:55:LYS:HB2	2.21	0.41
1:5:15:PHE:O	1:5:18:VAL:HG12	2.21	0.41
1:W:76:THR:O	1:7:3:LYS:HG3	2.20	0.41
1:8:43:GLU:HB3	3:8:1786:HOH:O	2.21	0.41
1:F:2:ALA:N	1:F:3:LYS:HZ3	2.19	0.41
1:H:61:VAL:HG23	3:H:1635:HOH:O	2.21	0.41
1:J:7:VAL:HG13	1:J:8:GLU:N	2.35	0.41
1:K:2:ALA:N	1:K:3:LYS:HZ3	2.19	0.41
1:V:57:GLY:O	1:V:61:VAL:HB	2.21	0.41
1:Z:55:LYS:O	1:Z:58:THR:HG22	2.21	0.41
1:1:39:LYS:O	1:1:43:GLU:HG3	2.20	0.40
1:6:21:TYR:CB	3:6:1744:HOH:O	2.66	0.40
1:D:20:ASP:HA	1:D:23:LYS:HD2	2.03	0.40
1:D:25:LEU:O	1:D:29:VAL:HG23	2.20	0.40
1:J:52:LEU:CD1	3:J:1625:HOH:O	2.69	0.40
1:L:71:GLY:C	3:L:1625:HOH:O	2.59	0.40
1:7:11:VAL:HG22	2:7:1726:BOG:H1'2	2.03	0.40
1:C:26:MET:O	1:C:30:LYS:HG3	2.21	0.40
1:C:38:ALA:HA	1:C:41:TYR:CZ	2.56	0.40
1:F:49:LEU:O	1:F:52:LEU:HG	2.21	0.40
1:H:25:LEU:O	1:H:29:VAL:HG23	2.21	0.40
2:M:1621:BOG:H5'1	1:N:55:LYS:HG3	2.04	0.40
2:U:1710:BOG:H2	1:3:8:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:GLU:HA	1:C:11:VAL:CG2	2.51	0.40
1:E:26:MET:N	3:E:1661:HOH:O	2.52	0.40
1:N:62:ASN:ND2	3:N:1641:HOH:O	2.55	0.40
1:3:42:PHE:HA	1:4:44:LYS:NZ	2.36	0.40
1:8:14:TYR:CE2	2:8:1728:BOG:H2'1	2.57	0.40
1:E:10:LEU:HA	1:E:13:GLN:HE21	1.87	0.40
1:H:48:GLN:HE22	2:Q:1630:BOG:H7'1	1.86	0.40
1:I:25:LEU:HB2	2:I:1605:BOG:H1'1	2.03	0.40
1:B:77:GLN:CD	1:B:77:GLN:O	2.59	0.40
1:E:23:LYS:O	1:E:27:GLU:HG3	2.22	0.40
1:E:75:ALA:C	1:G:4:GLU:HB2	2.42	0.40
1:K:50:THR:N	1:K:51:PRO:HD2	2.36	0.40
1:M:39:LYS:CG	3:M:1629:HOH:O	2.44	0.40
1:M:49:LEU:O	1:M:52:LEU:HG	2.22	0.40
1:Q:14:TYR:CE2	2:Q:1628:BOG:H2'1	2.56	0.40
1:V:4:GLU:H	1:V:5:PRO:CD	2.27	0.40
1:W:56:ALA:HA	1:W:59:GLU:HB3	2.02	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LYS:CE	1:1:73:GLN:CD[1_455]	0.76	1.44
1:E:28:LYS:CE	1:1:73:GLN:OE1[1_455]	1.14	1.06
1:E:28:LYS:NZ	1:1:73:GLN:CG[1_455]	1.17	1.03
1:E:28:LYS:NZ	1:1:73:GLN:CB[1_455]	1.18	1.02
1:E:28:LYS:CE	1:1:73:GLN:CG[1_455]	1.26	0.94
1:E:28:LYS:NZ	1:1:73:GLN:CD[1_455]	1.69	0.51
1:E:28:LYS:CD	1:1:73:GLN:OE1[1_455]	1.71	0.49
1:E:28:LYS:CE	1:1:73:GLN:NE2[1_455]	2.08	0.12
1:6:16:GLN:NE2	1:8:43:GLU:OE2[1_556]	2.08	0.12
1:E:28:LYS:CG	1:1:73:GLN:OE1[1_455]	2.11	0.09
1:6:16:GLN:OE1	1:8:43:GLU:OE2[1_556]	2.16	0.04

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	1	69/77 (90%)	63 (91%)	5 (7%)	1 (1%)	13	13
1	2	69/77 (90%)	57 (83%)	9 (13%)	3 (4%)	3	1
1	3	69/77 (90%)	55 (80%)	11 (16%)	3 (4%)	3	1
1	4	68/77 (88%)	59 (87%)	6 (9%)	3 (4%)	3	1
1	5	71/77 (92%)	55 (78%)	14 (20%)	2 (3%)	6	4
1	6	72/77 (94%)	59 (82%)	8 (11%)	5 (7%)	1	0
1	7	64/77 (83%)	58 (91%)	4 (6%)	2 (3%)	5	3
1	8	72/77 (94%)	63 (88%)	6 (8%)	3 (4%)	3	1
1	A	72/77 (94%)	62 (86%)	8 (11%)	2 (3%)	6	4
1	B	72/77 (94%)	64 (89%)	6 (8%)	2 (3%)	6	4
1	C	74/77 (96%)	63 (85%)	8 (11%)	3 (4%)	3	1
1	D	70/77 (91%)	61 (87%)	3 (4%)	6 (9%)	1	0
1	E	66/77 (86%)	60 (91%)	3 (4%)	3 (4%)	3	1
1	F	71/77 (92%)	58 (82%)	8 (11%)	5 (7%)	1	0
1	G	72/77 (94%)	66 (92%)	6 (8%)	0	100	100
1	H	72/77 (94%)	62 (86%)	7 (10%)	3 (4%)	3	1
1	I	69/77 (90%)	59 (86%)	8 (12%)	2 (3%)	5	3
1	J	72/77 (94%)	59 (82%)	7 (10%)	6 (8%)	1	0
1	K	70/77 (91%)	58 (83%)	9 (13%)	3 (4%)	3	1
1	L	68/77 (88%)	54 (79%)	10 (15%)	4 (6%)	2	1
1	M	74/77 (96%)	54 (73%)	16 (22%)	4 (5%)	2	1
1	N	74/77 (96%)	59 (80%)	11 (15%)	4 (5%)	2	1
1	P	69/77 (90%)	61 (88%)	6 (9%)	2 (3%)	5	3
1	Q	69/77 (90%)	63 (91%)	6 (9%)	0	100	100
1	S	72/77 (94%)	61 (85%)	8 (11%)	3 (4%)	3	1
1	T	72/77 (94%)	67 (93%)	3 (4%)	2 (3%)	6	4
1	U	74/77 (96%)	65 (88%)	7 (10%)	2 (3%)	6	4
1	V	71/77 (92%)	60 (84%)	7 (10%)	4 (6%)	2	1
1	W	66/77 (86%)	56 (85%)	10 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	X	71/77 (92%)	56 (79%)	9 (13%)	6 (8%)	1	0
1	Y	72/77 (94%)	69 (96%)	2 (3%)	1 (1%)	13	13
1	Z	68/77 (88%)	59 (87%)	7 (10%)	2 (3%)	5	3
All	All	2254/2464 (92%)	1925 (85%)	238 (11%)	91 (4%)	3	1

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	C	73	GLN
1	D	4	GLU
1	E	4	GLU
1	E	76	THR
1	I	74	PRO
1	J	7	VAL
1	J	31	SER
1	J	74	PRO
1	K	4	GLU
1	L	5	PRO
1	L	31	SER
1	N	7	VAL
1	N	65	SER
1	N	66	TYR
1	S	75	ALA
1	U	5	PRO
1	V	4	GLU
1	X	5	PRO
1	Y	3	LYS
1	Z	5	PRO
1	2	31	SER
1	3	4	GLU
1	4	31	SER
1	A	37	GLU
1	C	74	PRO
1	D	7	VAL
1	D	70	LEU
1	D	73	GLN
1	D	76	THR
1	F	37	GLU
1	J	36	ALA
1	J	76	THR

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Mol	Chain	Res	Type
1	L	34	LEU
1	L	36	ALA
1	M	36	ALA
1	P	36	ALA
1	S	37	GLU
1	S	71	GLY
1	T	7	VAL
1	V	7	VAL
1	V	34	LEU
1	V	70	LEU
1	X	71	GLY
1	X	75	ALA
1	2	36	ALA
1	6	5	PRO
1	6	7	VAL
1	6	31	SER
1	7	3	LYS
1	8	38	ALA
1	A	73	GLN
1	F	5	PRO
1	F	38	ALA
1	F	71	GLY
1	H	4	GLU
1	I	69	GLU
1	M	6	CYS
1	U	3	LYS
1	X	37	GLU
1	X	38	ALA
1	1	71	GLY
1	2	5	PRO
1	3	31	SER
1	4	75	ALA
1	5	27	GLU
1	7	71	GLY
1	8	4	GLU
1	F	75	ALA
1	H	5	PRO
1	M	69	GLU
1	Z	4	GLU
1	6	3	LYS
1	6	13	GLN
1	8	60	LEU

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Mol	Chain	Res	Type
1	C	5	PRO
1	E	29	VAL
1	X	36	ALA
1	3	6	CYS
1	5	36	ALA
1	B	71	GLY
1	K	31	SER
1	T	71	GLY
1	M	71	GLY
1	N	29	VAL
1	D	71	GLY
1	4	74	PRO
1	H	7	VAL
1	J	71	GLY
1	K	71	GLY
1	P	31	SER

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	1	66/69 (96%)	63 (96%)	3 (4%)	32	44
1	2	66/69 (96%)	64 (97%)	2 (3%)	46	63
1	3	67/69 (97%)	63 (94%)	4 (6%)	22	30
1	4	66/69 (96%)	66 (100%)	0	100	100
1	5	67/69 (97%)	66 (98%)	1 (2%)	70	83
1	6	67/69 (97%)	65 (97%)	2 (3%)	46	63
1	7	64/69 (93%)	63 (98%)	1 (2%)	68	82
1	8	66/69 (96%)	63 (96%)	3 (4%)	32	44
1	A	67/69 (97%)	65 (97%)	2 (3%)	46	63
1	B	67/69 (97%)	65 (97%)	2 (3%)	46	63
1	C	68/69 (99%)	64 (94%)	4 (6%)	23	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	67/69 (97%)	65 (97%)	2 (3%)	46	63
1	E	66/69 (96%)	64 (97%)	2 (3%)	46	63
1	F	67/69 (97%)	63 (94%)	4 (6%)	22	30
1	G	66/69 (96%)	64 (97%)	2 (3%)	46	63
1	H	66/69 (96%)	64 (97%)	2 (3%)	46	63
1	I	66/69 (96%)	64 (97%)	2 (3%)	46	63
1	J	67/69 (97%)	67 (100%)	0	100	100
1	K	67/69 (97%)	64 (96%)	3 (4%)	32	44
1	L	66/69 (96%)	64 (97%)	2 (3%)	46	63
1	M	68/69 (99%)	65 (96%)	3 (4%)	33	45
1	N	68/69 (99%)	63 (93%)	5 (7%)	16	20
1	P	66/69 (96%)	66 (100%)	0	100	100
1	Q	65/69 (94%)	62 (95%)	3 (5%)	31	42
1	S	67/69 (97%)	65 (97%)	2 (3%)	46	63
1	T	67/69 (97%)	65 (97%)	2 (3%)	46	63
1	U	68/69 (99%)	65 (96%)	3 (4%)	33	45
1	V	67/69 (97%)	65 (97%)	2 (3%)	46	63
1	W	67/69 (97%)	65 (97%)	2 (3%)	46	63
1	X	67/69 (97%)	64 (96%)	3 (4%)	32	44
1	Y	66/69 (96%)	62 (94%)	4 (6%)	22	29
1	Z	65/69 (94%)	62 (95%)	3 (5%)	31	42
All	All	2130/2208 (96%)	2055 (96%)	75 (4%)	41	56

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	77	GLN
1	B	66	TYR
1	B	77	GLN
1	C	3	LYS
1	C	15	PHE
1	C	26	MET
1	C	77	GLN
1	D	3	LYS

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Mol	Chain	Res	Type
1	D	77	GLN
1	E	67	PHE
1	E	77	GLN
1	F	3	LYS
1	F	34	LEU
1	F	67	PHE
1	F	76	THR
1	G	41	TYR
1	G	55	LYS
1	H	3	LYS
1	H	34	LEU
1	I	14	TYR
1	I	66	TYR
1	K	3	LYS
1	K	55	LYS
1	K	73	GLN
1	L	3	LYS
1	L	77	GLN
1	M	3	LYS
1	M	4	GLU
1	M	76	THR
1	N	3	LYS
1	N	14	TYR
1	N	34	LEU
1	N	37	GLU
1	N	41	TYR
1	Q	33	GLU
1	Q	37	GLU
1	Q	54	LYS
1	S	26	MET
1	S	74	PRO
1	T	66	TYR
1	T	77	GLN
1	U	3	LYS
1	U	15	PHE
1	U	26	MET
1	V	3	LYS
1	V	77	GLN
1	W	3	LYS
1	W	67	PHE
1	X	6	CYS
1	X	14	TYR

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Mol	Chain	Res	Type
1	X	77	GLN
1	Y	3	LYS
1	Y	4	GLU
1	Y	41	TYR
1	Y	63	PHE
1	Z	3	LYS
1	Z	34	LEU
1	Z	59	GLU
1	1	14	TYR
1	1	66	TYR
1	1	77	GLN
1	2	66	TYR
1	2	77	GLN
1	3	3	LYS
1	3	5	PRO
1	3	34	LEU
1	3	55	LYS
1	5	77	GLN
1	6	37	GLU
1	6	41	TYR
1	7	3	LYS
1	8	3	LYS
1	8	44	LYS
1	8	73	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	B	73	GLN
1	B	77	GLN
1	D	13	GLN
1	D	35	GLN
1	D	73	GLN
1	E	13	GLN
1	E	77	GLN
1	F	35	GLN
1	G	13	GLN
1	G	73	GLN
1	H	13	GLN
1	H	35	GLN
1	I	13	GLN

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Mol	Chain	Res	Type
1	K	48	GLN
1	K	73	GLN
1	M	16	GLN
1	P	13	GLN
1	P	35	GLN
1	Q	35	GLN
1	Q	73	GLN
1	S	73	GLN
1	T	73	GLN
1	T	77	GLN
1	U	73	GLN
1	V	35	GLN
1	V	77	GLN
1	X	73	GLN
1	Z	13	GLN
1	1	13	GLN
1	2	13	GLN
1	3	48	GLN
1	4	13	GLN
1	4	35	GLN
1	4	77	GLN
1	5	73	GLN
1	6	35	GLN
1	6	73	GLN
1	7	13	GLN
1	7	73	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

64 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	BOG	1	1705	-	20,20,20	0.83	1 (5%)	25,25,25	0.64	0
2	BOG	1	1707	-	20,20,20	0.83	1 (5%)	25,25,25	0.65	0
2	BOG	1	1709	-	20,20,20	0.82	1 (5%)	25,25,25	0.66	0
2	BOG	2	1703	-	20,20,20	0.82	1 (5%)	25,25,25	0.64	0
2	BOG	2	1708	-	20,20,20	0.82	1 (5%)	25,25,25	0.65	0
2	BOG	3	1712	-	20,20,20	0.82	1 (5%)	25,25,25	0.63	0
2	BOG	3	1716	-	20,20,20	4.61	2 (10%)	25,25,25	1.06	2 (8%)
2	BOG	4	1714	-	20,20,20	0.84	1 (5%)	25,25,25	0.64	0
2	BOG	5	1719	-	20,20,20	0.82	1 (5%)	25,25,25	0.66	0
2	BOG	5	1720	-	20,20,20	0.81	1 (5%)	25,25,25	0.65	0
2	BOG	5	1721	-	20,20,20	0.85	1 (5%)	25,25,25	0.63	0
2	BOG	5	1724	-	20,20,20	0.80	1 (5%)	25,25,25	0.64	0
2	BOG	6	1717	-	20,20,20	0.83	1 (5%)	25,25,25	0.64	0
2	BOG	6	1722	-	20,20,20	0.82	1 (5%)	25,25,25	0.65	0
2	BOG	7	1726	-	20,20,20	0.82	1 (5%)	25,25,25	0.64	0
2	BOG	8	1727	-	20,20,20	0.82	1 (5%)	25,25,25	0.65	0
2	BOG	8	1728	-	20,20,20	0.82	1 (5%)	25,25,25	0.68	0
2	BOG	A	1603	-	20,20,20	0.81	1 (5%)	25,25,25	0.66	0
2	BOG	A	1604	-	20,20,20	0.82	1 (5%)	25,25,25	0.63	0
2	BOG	B	1602	-	20,20,20	0.82	1 (5%)	25,25,25	0.65	0
2	BOG	B	1606	-	20,20,20	0.81	1 (5%)	25,25,25	0.66	0
2	BOG	B	1609	-	20,20,20	0.81	1 (5%)	25,25,25	0.67	0
2	BOG	C	1614	-	20,20,20	0.78	1 (5%)	25,25,25	0.66	0
2	BOG	D	1612	-	20,20,20	0.78	1 (5%)	25,25,25	0.68	0
2	BOG	D	1613	-	9,9,20	0.17	0	8,8,25	0.57	0
2	BOG	E	1623	-	20,20,20	0.84	1 (5%)	25,25,25	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BOG	F	1619	-	20,20,20	0.79	1 (5%)	25,25,25	0.64	0
2	BOG	G	1633	-	20,20,20	0.82	1 (5%)	25,25,25	0.66	0
2	BOG	G	1634	-	20,20,20	0.81	1 (5%)	25,25,25	0.64	0
2	BOG	H	1626	-	20,20,20	0.82	1 (5%)	25,25,25	0.64	0
2	BOG	H	1629	-	20,20,20	0.81	1 (5%)	25,25,25	0.63	0
2	BOG	H	1631	-	20,20,20	0.81	1 (5%)	25,25,25	0.63	0
2	BOG	I	1601	-	8,8,20	0.17	0	6,6,25	0.52	0
2	BOG	I	1605	-	20,20,20	0.83	1 (5%)	25,25,25	0.65	0
2	BOG	J	1607	-	20,20,20	0.83	1 (5%)	25,25,25	0.64	0
2	BOG	J	1608	-	20,20,20	0.83	1 (5%)	25,25,25	0.65	0
2	BOG	K	1610	-	20,20,20	0.81	1 (5%)	25,25,25	0.66	0
2	BOG	K	1616	-	20,20,20	4.68	2 (10%)	25,25,25	1.13	2 (8%)
2	BOG	L	1615	-	20,20,20	0.82	1 (5%)	25,25,25	0.67	0
2	BOG	M	1620	-	20,20,20	0.80	1 (5%)	25,25,25	0.70	0
2	BOG	M	1621	-	20,20,20	0.90	1 (5%)	25,25,25	0.65	0
2	BOG	M	1625	-	20,20,20	0.86	2 (10%)	25,25,25	0.67	0
2	BOG	N	1617	-	20,20,20	0.82	1 (5%)	25,25,25	0.66	0
2	BOG	N	1618	-	20,20,20	0.90	1 (5%)	25,25,25	0.66	0
2	BOG	N	1622	-	20,20,20	0.84	1 (5%)	25,25,25	0.64	0
2	BOG	N	1624	-	20,20,20	4.11	2 (10%)	25,25,25	1.19	2 (8%)
2	BOG	P	1632	-	20,20,20	0.82	1 (5%)	25,25,25	0.65	0
2	BOG	Q	1627	-	20,20,20	0.82	1 (5%)	25,25,25	0.65	0
2	BOG	Q	1628	-	20,20,20	0.82	1 (5%)	25,25,25	0.69	0
2	BOG	Q	1630	-	20,20,20	0.81	1 (5%)	25,25,25	0.64	0
2	BOG	S	1704	-	20,20,20	0.81	1 (5%)	25,25,25	0.64	0
2	BOG	T	1702	-	20,20,20	0.83	1 (5%)	25,25,25	0.64	0
2	BOG	T	1706	-	20,20,20	0.81	1 (5%)	25,25,25	0.67	0
2	BOG	U	1710	-	20,20,20	0.81	1 (5%)	25,25,25	0.65	0
2	BOG	U	1715	-	20,20,20	0.80	1 (5%)	25,25,25	0.67	0
2	BOG	W	1718	-	20,20,20	0.84	1 (5%)	25,25,25	0.64	0
2	BOG	W	1723	-	20,20,20	0.82	1 (5%)	25,25,25	0.65	0
2	BOG	X	1725	-	20,20,20	0.84	1 (5%)	25,25,25	0.64	0
2	BOG	Y	1730	-	20,20,20	0.81	1 (5%)	25,25,25	0.65	0
2	BOG	Y	1733	-	20,20,20	0.80	1 (5%)	25,25,25	0.65	0
2	BOG	Y	1734	-	20,20,20	0.81	1 (5%)	25,25,25	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BOG	Z	1729	-	20,20,20	0.81	1 (5%)	25,25,25	0.63	0
2	BOG	Z	1731	-	20,20,20	0.82	1 (5%)	25,25,25	0.63	0
2	BOG	Z	1732	-	20,20,20	0.82	1 (5%)	25,25,25	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	1	1705	-	-	0/11/31/31	0/1/1/1
2	BOG	1	1707	-	-	0/11/31/31	0/1/1/1
2	BOG	1	1709	-	-	0/11/31/31	0/1/1/1
2	BOG	2	1703	-	-	0/11/31/31	0/1/1/1
2	BOG	2	1708	-	-	0/11/31/31	0/1/1/1
2	BOG	3	1712	-	-	0/11/31/31	0/1/1/1
2	BOG	3	1716	-	-	0/11/31/31	0/1/1/1
2	BOG	4	1714	-	-	0/11/31/31	0/1/1/1
2	BOG	5	1719	-	-	0/11/31/31	0/1/1/1
2	BOG	5	1720	-	-	0/11/31/31	0/1/1/1
2	BOG	5	1721	-	-	0/11/31/31	0/1/1/1
2	BOG	5	1724	-	-	0/11/31/31	0/1/1/1
2	BOG	6	1717	-	-	0/11/31/31	0/1/1/1
2	BOG	6	1722	-	-	0/11/31/31	0/1/1/1
2	BOG	7	1726	-	-	0/11/31/31	0/1/1/1
2	BOG	8	1727	-	-	0/11/31/31	0/1/1/1
2	BOG	8	1728	-	-	0/11/31/31	0/1/1/1
2	BOG	A	1603	-	-	0/11/31/31	0/1/1/1
2	BOG	A	1604	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1602	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1606	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1609	-	-	0/11/31/31	0/1/1/1
2	BOG	C	1614	-	-	0/11/31/31	0/1/1/1
2	BOG	D	1612	-	-	0/11/31/31	0/1/1/1
2	BOG	D	1613	-	-	0/7/7/31	0/0/0/1
2	BOG	E	1623	-	-	0/11/31/31	0/1/1/1
2	BOG	F	1619	-	-	0/11/31/31	0/1/1/1
2	BOG	G	1633	-	-	0/11/31/31	0/1/1/1
2	BOG	G	1634	-	-	0/11/31/31	0/1/1/1
2	BOG	H	1626	-	-	0/11/31/31	0/1/1/1
2	BOG	H	1629	-	-	0/11/31/31	0/1/1/1
2	BOG	H	1631	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	I	1601	-	-	0/5/5/31	0/0/0/1
2	BOG	I	1605	-	-	0/11/31/31	0/1/1/1
2	BOG	J	1607	-	-	0/11/31/31	0/1/1/1
2	BOG	J	1608	-	-	0/11/31/31	0/1/1/1
2	BOG	K	1610	-	-	0/11/31/31	0/1/1/1
2	BOG	K	1616	-	-	0/11/31/31	0/1/1/1
2	BOG	L	1615	-	-	0/11/31/31	0/1/1/1
2	BOG	M	1620	-	-	0/11/31/31	0/1/1/1
2	BOG	M	1621	-	-	0/11/31/31	0/1/1/1
2	BOG	M	1625	-	-	0/11/31/31	0/1/1/1
2	BOG	N	1617	-	-	0/11/31/31	0/1/1/1
2	BOG	N	1618	-	-	0/11/31/31	0/1/1/1
2	BOG	N	1622	-	-	0/11/31/31	0/1/1/1
2	BOG	N	1624	-	-	0/11/31/31	0/1/1/1
2	BOG	P	1632	-	-	0/11/31/31	0/1/1/1
2	BOG	Q	1627	-	-	0/11/31/31	0/1/1/1
2	BOG	Q	1628	-	-	0/11/31/31	0/1/1/1
2	BOG	Q	1630	-	-	0/11/31/31	0/1/1/1
2	BOG	S	1704	-	-	0/11/31/31	0/1/1/1
2	BOG	T	1702	-	-	0/11/31/31	0/1/1/1
2	BOG	T	1706	-	-	0/11/31/31	0/1/1/1
2	BOG	U	1710	-	-	0/11/31/31	0/1/1/1
2	BOG	U	1715	-	-	0/11/31/31	0/1/1/1
2	BOG	W	1718	-	-	0/11/31/31	0/1/1/1
2	BOG	W	1723	-	-	0/11/31/31	0/1/1/1
2	BOG	X	1725	-	-	0/11/31/31	0/1/1/1
2	BOG	Y	1730	-	-	0/11/31/31	0/1/1/1
2	BOG	Y	1733	-	-	0/11/31/31	0/1/1/1
2	BOG	Y	1734	-	-	0/11/31/31	0/1/1/1
2	BOG	Z	1729	-	-	0/11/31/31	0/1/1/1
2	BOG	Z	1731	-	-	0/11/31/31	0/1/1/1
2	BOG	Z	1732	-	-	0/11/31/31	0/1/1/1

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1625	BOG	O1-C1	2.01	1.43	1.40
2	L	1615	BOG	O5-C1	2.27	1.47	1.41
2	D	1612	BOG	O5-C1	2.30	1.47	1.41
2	3	1716	BOG	O5-C1	2.34	1.47	1.41
2	C	1614	BOG	O5-C1	2.34	1.47	1.41
2	U	1715	BOG	O5-C1	2.34	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1633	BOG	O5-C1	2.35	1.47	1.41
2	B	1606	BOG	O5-C1	2.35	1.47	1.41
2	N	1617	BOG	O5-C1	2.36	1.47	1.41
2	T	1706	BOG	O5-C1	2.36	1.47	1.41
2	3	1712	BOG	O5-C1	2.36	1.47	1.41
2	G	1634	BOG	O5-C1	2.36	1.47	1.41
2	2	1708	BOG	O5-C1	2.37	1.47	1.41
2	B	1609	BOG	O5-C1	2.37	1.47	1.41
2	A	1603	BOG	O5-C1	2.37	1.47	1.41
2	M	1625	BOG	O5-C1	2.37	1.47	1.41
2	Y	1733	BOG	O5-C1	2.38	1.47	1.41
2	H	1631	BOG	O5-C1	2.38	1.47	1.41
2	Q	1630	BOG	O5-C1	2.38	1.47	1.41
2	5	1720	BOG	O5-C1	2.38	1.47	1.41
2	1	1709	BOG	O5-C1	2.38	1.47	1.41
2	W	1723	BOG	O5-C1	2.39	1.47	1.41
2	F	1619	BOG	O5-C1	2.39	1.47	1.41
2	2	1703	BOG	O5-C1	2.39	1.47	1.41
2	U	1710	BOG	O5-C1	2.40	1.47	1.41
2	5	1724	BOG	O5-C1	2.40	1.47	1.41
2	H	1626	BOG	O5-C1	2.40	1.47	1.41
2	S	1704	BOG	O5-C1	2.40	1.47	1.41
2	Y	1730	BOG	O5-C1	2.40	1.47	1.41
2	Z	1729	BOG	O5-C1	2.40	1.47	1.41
2	K	1610	BOG	O5-C1	2.40	1.47	1.41
2	4	1714	BOG	O5-C1	2.41	1.47	1.41
2	7	1726	BOG	O5-C1	2.41	1.47	1.41
2	Q	1627	BOG	O5-C1	2.41	1.47	1.41
2	H	1629	BOG	O5-C1	2.41	1.47	1.41
2	M	1620	BOG	O5-C1	2.41	1.47	1.41
2	Y	1734	BOG	O5-C1	2.41	1.47	1.41
2	B	1602	BOG	O5-C1	2.41	1.47	1.41
2	N	1624	BOG	O5-C1	2.41	1.47	1.41
2	A	1604	BOG	O5-C1	2.42	1.47	1.41
2	Z	1732	BOG	O5-C1	2.42	1.47	1.41
2	W	1718	BOG	O5-C1	2.42	1.47	1.41
2	P	1632	BOG	O5-C1	2.43	1.47	1.41
2	5	1719	BOG	O5-C1	2.43	1.47	1.41
2	J	1608	BOG	O5-C1	2.43	1.47	1.41
2	1	1707	BOG	O5-C1	2.44	1.47	1.41
2	I	1605	BOG	O5-C1	2.44	1.47	1.41
2	1	1705	BOG	O5-C1	2.44	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1616	BOG	O5-C1	2.44	1.47	1.41
2	8	1727	BOG	O5-C1	2.44	1.47	1.41
2	6	1722	BOG	O5-C1	2.44	1.47	1.41
2	E	1623	BOG	O5-C1	2.44	1.47	1.41
2	T	1702	BOG	O5-C1	2.44	1.47	1.41
2	Z	1731	BOG	O5-C1	2.45	1.47	1.41
2	5	1721	BOG	O5-C1	2.45	1.47	1.41
2	6	1717	BOG	O5-C1	2.46	1.47	1.41
2	N	1622	BOG	O5-C1	2.46	1.47	1.41
2	J	1607	BOG	O5-C1	2.46	1.47	1.41
2	8	1728	BOG	O5-C1	2.47	1.48	1.41
2	Q	1628	BOG	O5-C1	2.50	1.48	1.41
2	N	1618	BOG	O5-C1	2.51	1.48	1.41
2	X	1725	BOG	O5-C1	2.51	1.48	1.41
2	M	1621	BOG	O5-C1	2.59	1.48	1.41
2	N	1624	BOG	C3'-C2'	17.93	2.53	1.51
2	3	1716	BOG	C5'-C4'	20.25	2.67	1.51
2	K	1616	BOG	C5'-C4'	20.53	2.68	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	1716	BOG	C6'-C5'-C4'	2.89	129.36	114.45
2	3	1716	BOG	C5'-C4'-C3'	3.21	131.01	114.45
2	K	1616	BOG	C6'-C5'-C4'	3.35	131.74	114.45
2	N	1624	BOG	C4'-C3'-C2'	3.35	131.74	114.45
2	K	1616	BOG	C5'-C4'-C3'	3.36	131.79	114.45
2	N	1624	BOG	C3'-C2'-C1'	3.68	130.03	113.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

58 monomers are involved in 281 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	1705	BOG	2	0
2	1	1707	BOG	1	0
2	1	1709	BOG	4	0
2	2	1708	BOG	2	0
2	3	1712	BOG	3	0
2	3	1716	BOG	31	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5	1720	BOG	3	0
2	5	1721	BOG	2	0
2	5	1724	BOG	8	0
2	6	1717	BOG	3	0
2	7	1726	BOG	3	0
2	8	1727	BOG	1	0
2	8	1728	BOG	3	0
2	A	1603	BOG	1	0
2	A	1604	BOG	2	0
2	B	1602	BOG	2	0
2	B	1606	BOG	4	0
2	B	1609	BOG	2	0
2	C	1614	BOG	3	0
2	D	1612	BOG	5	0
2	E	1623	BOG	7	0
2	F	1619	BOG	9	0
2	G	1633	BOG	5	0
2	G	1634	BOG	12	0
2	H	1626	BOG	3	0
2	H	1629	BOG	3	0
2	H	1631	BOG	1	0
2	I	1601	BOG	2	0
2	I	1605	BOG	5	0
2	J	1607	BOG	1	0
2	K	1610	BOG	9	0
2	K	1616	BOG	29	0
2	L	1615	BOG	4	0
2	M	1620	BOG	2	0
2	M	1621	BOG	5	0
2	M	1625	BOG	5	0
2	N	1617	BOG	1	0
2	N	1618	BOG	4	0
2	N	1622	BOG	8	0
2	N	1624	BOG	39	0
2	P	1632	BOG	1	0
2	Q	1627	BOG	1	0
2	Q	1628	BOG	7	0
2	Q	1630	BOG	3	0
2	S	1704	BOG	1	0
2	T	1702	BOG	2	0
2	T	1706	BOG	4	0
2	U	1710	BOG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	U	1715	BOG	4	0
2	W	1718	BOG	1	0
2	W	1723	BOG	2	0
2	X	1725	BOG	5	0
2	Y	1730	BOG	2	0
2	Y	1733	BOG	1	0
2	Y	1734	BOG	3	0
2	Z	1729	BOG	3	0
2	Z	1731	BOG	3	0
2	Z	1732	BOG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.