



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:37 PM UTC

PDB ID : 1QHA / pdb_00001qha
Title : HUMAN HEXOKINASE TYPE I COMPLEXED WITH ATP ANALOGUE
AMP-PNP
Authors : Rosano, C.; Sabini, E.; Deriu, D.; Magnani, M.; Bolognesi, M.
Deposited on : 1999-05-11
Resolution : 2.25 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

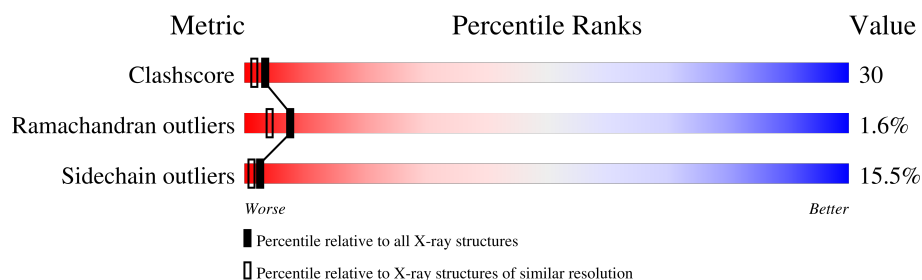
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	917	
1	B	917	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	G6P	A	919	X	-	X	-
3	G6P	A	921	X	-	-	-
3	G6P	B	1916	X	-	-	-
3	G6P	B	1918	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14737 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.

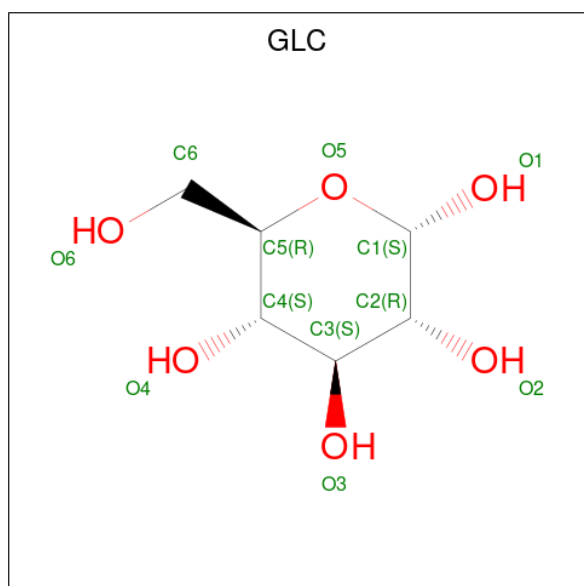
- Molecule 1 is a protein called PROTEIN (HEXOKINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	67	0	0
			7065	4428	1246	1338	53			
1	B	899	Total	C	N	O	S	62	0	0
			7032	4407	1241	1331	53			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	776	LEU	MET	conflict	UNP P19367
B	776	LEU	MET	conflict	UNP P19367

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



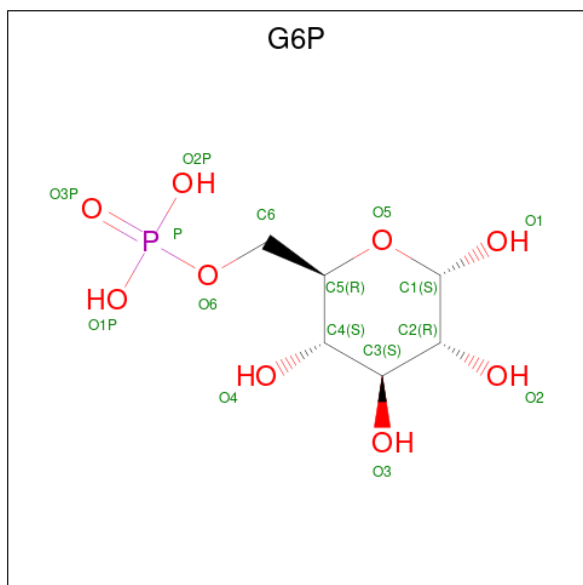
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

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

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: $C_6H_{13}O_9P$).

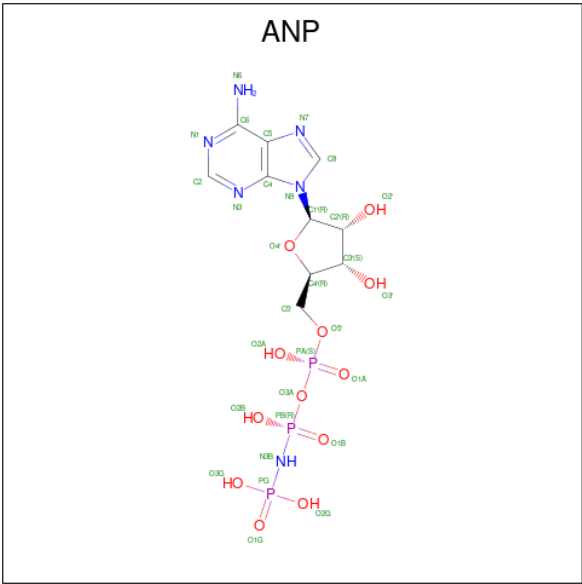


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	B	3	Total	Mg	0	0
			3	3		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

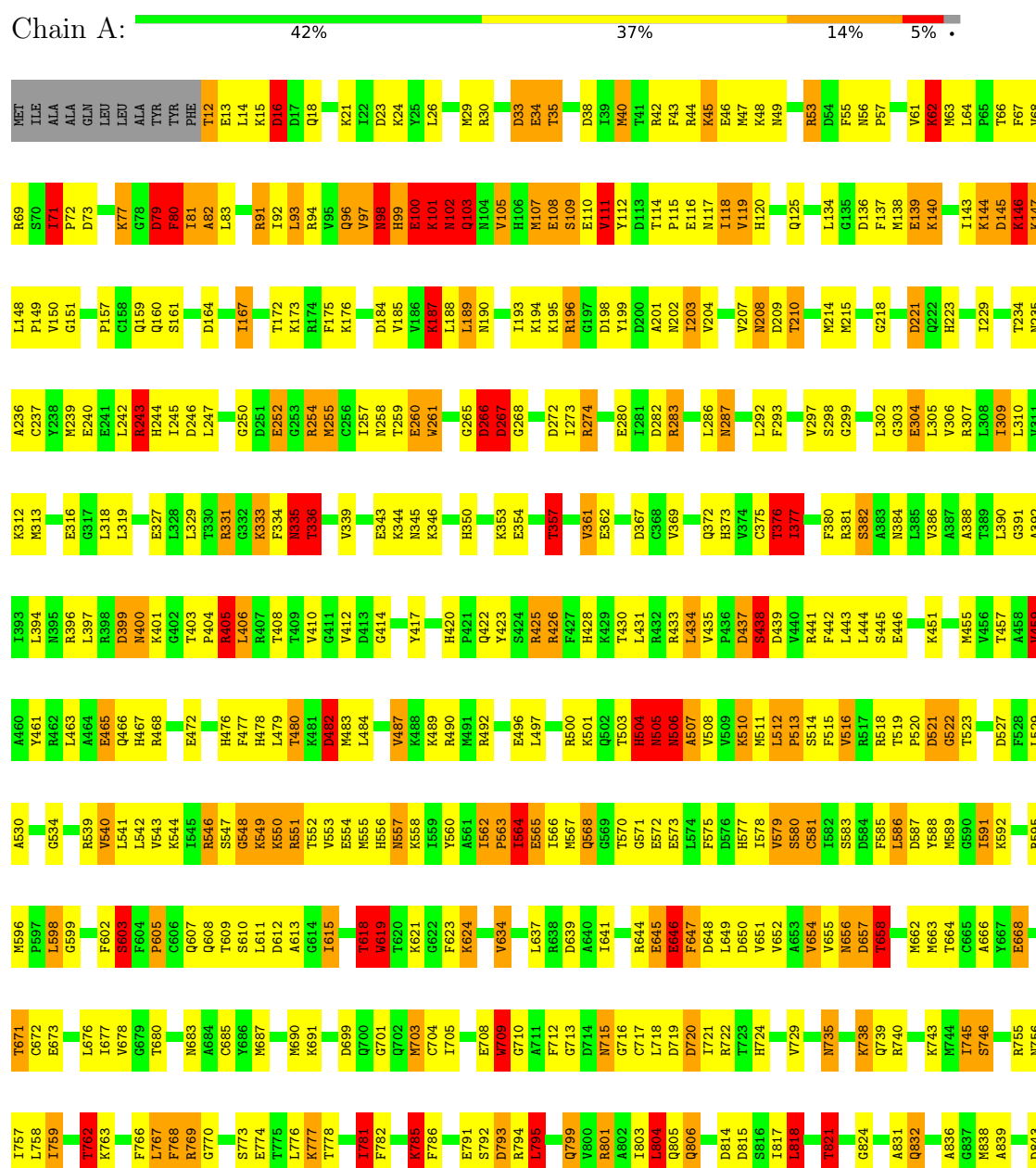


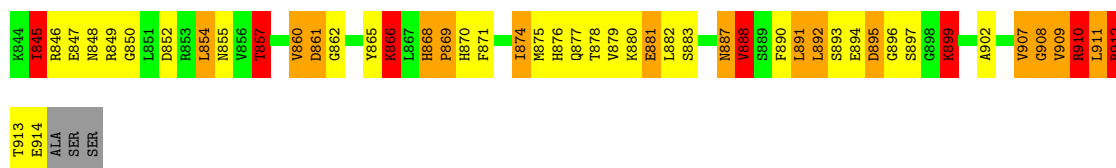
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

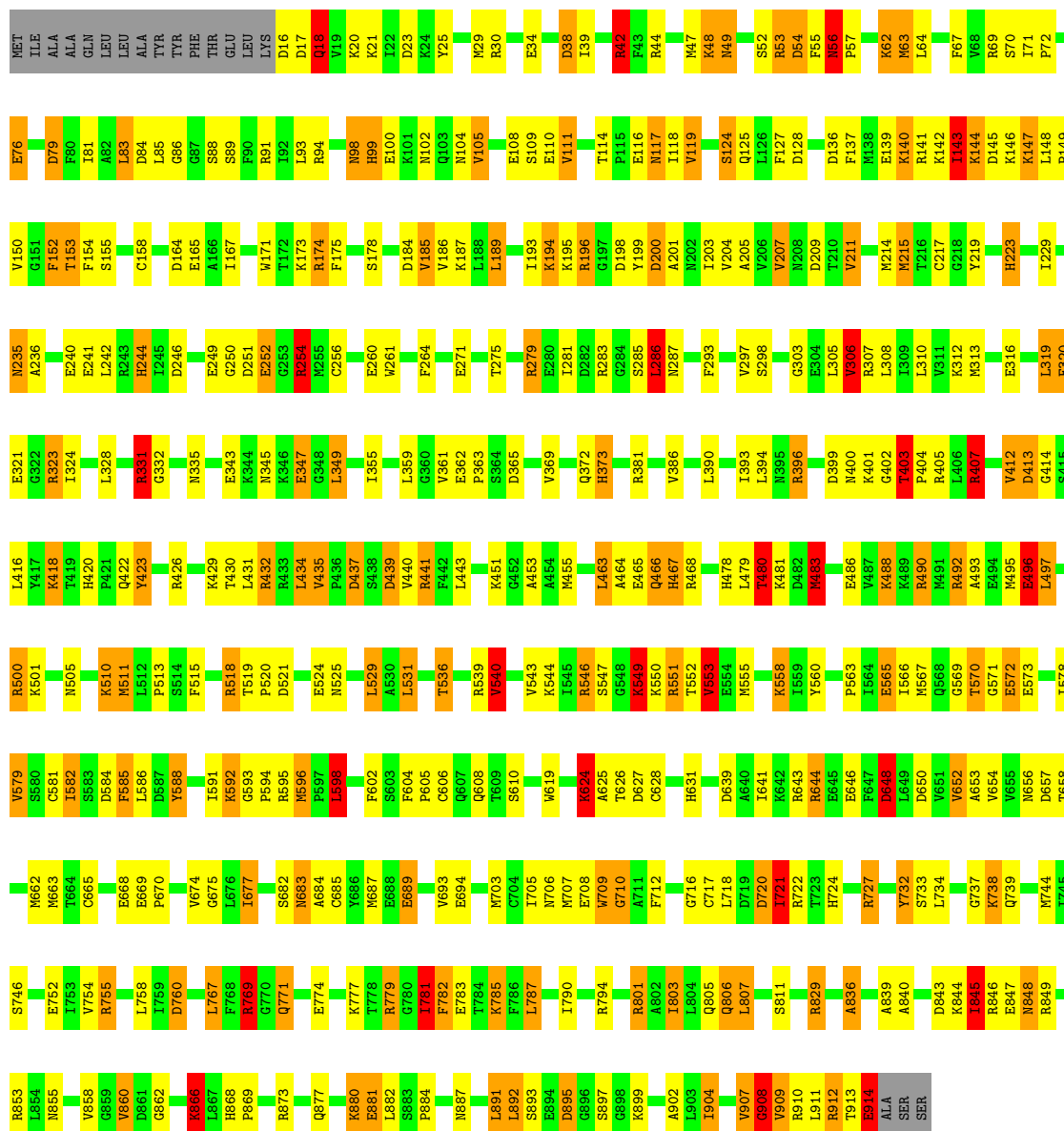
• Molecule 1: PROTEIN (HEXOKINASE)





● Molecule 1: PROTEIN (HEXOKINASE)

Chain B: 53% 30% 13%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.59Å 176.17Å 86.76Å 90.00° 90.53° 90.00°	Depositor
Resolution (Å)	12.00 – 2.25	Depositor
% Data completeness (in resolution range)	85.0 (12.00-2.25)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14737	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: ANP, GLC, G6P, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.95	9/7170 (0.1%)	2.13	263/9647 (2.7%)
1	B	1.00	7/7134 (0.1%)	2.17	258/9594 (2.7%)
All	All	0.97	16/14304 (0.1%)	2.15	521/19241 (2.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	28
1	B	0	16
All	All	0	44

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	HIS	C-N	24.40	1.68	1.33
1	B	914	GLU	CB-CG	-20.77	0.90	1.52
1	A	144	LYS	CG-CD	-20.23	0.91	1.52
1	A	99	HIS	C-N	-19.14	1.06	1.33
1	A	147	LYS	CG-CD	18.91	2.09	1.52
1	B	62	LYS	CG-CD	-15.35	1.06	1.52
1	B	18	GLN	CD-OE1	14.58	1.51	1.23
1	B	102	ASN	CA-CB	14.08	1.83	1.54
1	A	103	GLN	C-N	14.00	1.51	1.33
1	B	99	HIS	CA-CB	12.34	1.74	1.53
1	A	101	LYS	C-N	-8.17	1.22	1.33
1	A	912	ARG	CD-NE	8.07	1.57	1.46
1	A	100	GLU	C-N	-8.07	1.22	1.33
1	B	100	GLU	CA-CB	7.28	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	GLU	CA-CB	7.17	1.65	1.53
1	A	720	ASP	CA-CB	5.76	1.62	1.53

All (521) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ASN	N-CA-CB	-39.16	38.70	111.53
1	B	100	GLU	CB-CA-C	-30.44	60.37	110.29
1	A	99	HIS	O-C-N	-30.21	87.71	122.15
1	B	829	ARG	CD-NE-CZ	25.00	159.40	124.40
1	A	144	LYS	CB-CG-CD	23.89	166.24	111.30
1	B	99	HIS	O-C-N	21.00	150.53	122.59
1	A	912	ARG	CG-CD-NE	19.63	155.18	112.00
1	B	895	ASP	CA-CB-CG	17.97	130.57	112.60
1	A	101	LYS	O-C-N	-17.36	99.50	122.59
1	A	720	ASP	CA-CB-CG	-15.64	96.95	112.60
1	A	912	ARG	CD-NE-CZ	15.57	146.19	124.40
1	B	914	GLU	CB-CG-CD	-14.20	88.47	112.60
1	B	79	ASP	CA-CB-CG	13.94	126.54	112.60
1	B	829	ARG	NE-CZ-NH2	-13.85	106.73	119.20
1	B	755	ARG	NE-CZ-NH1	-13.56	107.94	121.50
1	B	42	ARG	CD-NE-CZ	13.00	142.60	124.40
1	B	441	ARG	NE-CZ-NH1	-12.96	108.54	121.50
1	B	18	GLN	OE1-CD-NE2	-12.95	109.65	122.60
1	B	873	ARG	CD-NE-CZ	12.85	142.38	124.40
1	A	639	ASP	CA-CB-CG	12.54	125.14	112.60
1	A	103	GLN	O-C-N	-12.46	106.02	122.59
1	B	648	ASP	CA-CB-CG	-12.40	100.20	112.60
1	B	877	GLN	CA-CB-CG	12.21	138.51	114.10
1	A	99	HIS	CB-CA-C	-11.92	90.59	110.85
1	B	914	GLU	CA-CB-CG	11.91	137.91	114.10
1	B	18	GLN	CG-CD-OE1	-11.75	97.30	120.80
1	A	283	ARG	NE-CZ-NH2	-11.61	108.76	119.20
1	A	102	ASN	N-CA-CB	-11.50	91.06	110.49
1	B	62	LYS	CB-CG-CD	11.38	137.46	111.30
1	A	719	ASP	CA-C-N	11.29	135.84	120.38
1	A	719	ASP	C-N-CA	11.29	135.84	120.38
1	A	71	ILE	CA-CB-CG2	11.15	129.45	110.50
1	A	103	GLN	CA-C-N	11.01	141.75	121.06
1	A	103	GLN	C-N-CA	11.01	141.75	121.06
1	B	99	HIS	N-CA-CB	-10.97	91.95	110.49
1	B	801	ARG	CD-NE-CZ	10.92	139.69	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASN	CA-CB-CG	10.84	123.44	112.60
1	A	67	PHE	CA-CB-CG	-10.71	103.09	113.80
1	A	377	ILE	CA-CB-CG2	10.49	128.33	110.50
1	A	516	VAL	N-CA-CB	10.41	123.39	111.21
1	B	490	ARG	CD-NE-CZ	10.30	138.82	124.40
1	B	102	ASN	CA-CB-CG	-10.22	102.38	112.60
1	A	654	VAL	N-CA-CB	10.21	125.49	111.41
1	B	98	ASN	CA-CB-CG	10.18	122.78	112.60
1	B	648	ASP	N-CA-CB	10.13	127.14	110.63
1	A	845	ILE	N-CA-CB	10.12	124.31	110.54
1	A	147	LYS	CB-CG-CD	-10.03	88.23	111.30
1	B	287	ASN	CA-CB-CG	10.02	122.62	112.60
1	A	38	ASP	CA-CB-CG	9.94	122.54	112.60
1	B	99	HIS	CA-C-N	-9.81	107.50	121.72
1	B	99	HIS	C-N-CA	-9.81	107.50	121.72
1	B	200	ASP	N-CA-CB	9.77	127.78	111.08
1	A	506	ASN	CA-CB-CG	-9.74	102.86	112.60
1	A	307	ARG	CD-NE-CZ	9.65	137.91	124.40
1	A	482	ASP	CA-CB-CG	9.64	122.24	112.60
1	B	722	ARG	CD-NE-CZ	9.37	137.51	124.40
1	A	221	ASP	CA-CB-CG	9.33	121.93	112.60
1	B	546	ARG	CD-NE-CZ	9.32	137.45	124.40
1	A	246	ASP	CA-CB-CG	9.31	121.91	112.60
1	A	793	ASP	CA-CB-CG	9.20	121.80	112.60
1	B	86	GLY	O-C-N	-9.16	115.38	122.71
1	A	712	PHE	CA-CB-CG	9.08	122.88	113.80
1	A	549	LYS	N-CA-C	-9.07	101.74	113.17
1	A	657	ASP	CA-CB-CG	9.00	121.60	112.60
1	A	99	HIS	CA-C-N	8.99	138.71	121.54
1	A	99	HIS	C-N-CA	8.99	138.71	121.54
1	B	785	LYS	CA-CB-CG	8.86	131.83	114.10
1	B	399	ASP	CA-CB-CG	8.81	121.41	112.60
1	B	654	VAL	CA-C-O	8.77	129.91	120.53
1	B	727	ARG	CD-NE-CZ	-8.72	112.19	124.40
1	A	815	ASP	CA-CB-CG	8.70	121.30	112.60
1	B	755	ARG	NE-CZ-NH2	8.65	126.99	119.20
1	A	767	LEU	N-CA-CB	-8.63	97.51	111.24
1	A	335	ASN	CA-CB-CG	-8.61	103.99	112.60
1	B	437	ASP	CA-CB-CG	-8.61	103.99	112.60
1	B	511	MET	O-C-N	-8.61	112.53	122.86
1	A	297	VAL	N-CA-C	8.59	118.94	111.56
1	B	441	ARG	NE-CZ-NH2	8.50	126.85	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	LYS	CA-C-O	-8.47	113.11	122.01
1	A	283	ARG	CD-NE-CZ	8.46	136.25	124.40
1	A	266	ASP	CA-CB-CG	-8.40	104.19	112.60
1	A	101	LYS	CA-C-N	8.40	137.58	121.54
1	A	101	LYS	C-N-CA	8.40	137.58	121.54
1	B	846	ARG	CD-NE-CZ	8.38	136.13	124.40
1	B	567	MET	CA-CB-CG	8.34	130.77	114.10
1	A	267	ASP	CA-C-O	-8.29	112.67	120.95
1	B	303	GLY	CA-C-N	8.24	132.83	120.31
1	B	303	GLY	C-N-CA	8.24	132.83	120.31
1	B	297	VAL	CB-CA-C	-8.21	103.64	111.44
1	B	721	ILE	CA-CB-CG2	8.16	124.38	110.50
1	A	161	SER	N-CA-C	-8.13	103.15	113.72
1	B	207	VAL	O-C-N	-8.10	113.76	123.00
1	B	553	VAL	N-CA-CB	8.04	123.26	111.52
1	A	801	ARG	CD-NE-CZ	8.04	135.65	124.40
1	A	399	ASP	CB-CA-C	8.00	127.02	110.31
1	B	866	LYS	CA-CB-CG	7.98	130.06	114.10
1	B	244	HIS	CA-C-N	-7.93	113.87	122.59
1	B	244	HIS	C-N-CA	-7.93	113.87	122.59
1	B	279	ARG	NE-CZ-NH2	-7.90	112.09	119.20
1	A	71	ILE	N-CA-CB	-7.86	100.20	111.21
1	B	174	ARG	CD-NE-CZ	-7.86	113.40	124.40
1	B	254	ARG	CD-NE-CZ	7.81	135.34	124.40
1	A	304	GLU	CB-CG-CD	7.75	125.78	112.60
1	B	540	VAL	O-C-N	-7.73	114.91	123.26
1	B	16	ASP	CA-CB-CG	7.70	120.30	112.60
1	B	845	ILE	N-CA-CB	7.68	120.41	110.57
1	A	12	THR	N-CA-CB	-7.66	98.48	111.50
1	B	500	ARG	NE-CZ-NH1	-7.65	113.85	121.50
1	B	69	ARG	NE-CZ-NH2	7.60	126.04	119.20
1	A	329	LEU	CA-C-N	7.59	132.55	122.30
1	A	329	LEU	C-N-CA	7.59	132.55	122.30
1	A	335	ASN	OD1-CG-ND2	7.58	130.18	122.60
1	A	568	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	B	598	LEU	CA-CB-CG	7.51	142.57	116.30
1	B	418	LYS	CA-C-O	-7.48	112.49	120.42
1	B	30	ARG	NE-CZ-NH1	-7.47	114.03	121.50
1	A	377	ILE	O-C-N	-7.46	114.64	121.87
1	B	86	GLY	N-CA-C	7.43	121.53	113.58
1	B	55	PHE	N-CA-C	7.39	122.32	113.16
1	B	641	ILE	CB-CA-C	-7.38	102.59	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	ASP	CA-CB-CG	-7.37	105.23	112.60
1	A	146	LYS	N-CA-C	-7.30	101.14	110.19
1	B	323	ARG	CD-NE-CZ	-7.30	114.18	124.40
1	B	407	ARG	O-C-N	-7.29	114.67	123.27
1	B	716	GLY	O-C-N	-7.28	113.31	122.41
1	B	767	LEU	N-CA-CB	-7.26	99.05	111.69
1	A	377	ILE	CA-C-N	7.26	129.70	120.56
1	A	377	ILE	C-N-CA	7.26	129.70	120.56
1	A	459	VAL	CA-C-N	7.25	130.72	120.28
1	A	459	VAL	C-N-CA	7.25	130.72	120.28
1	B	515	PHE	CA-CB-CG	-7.24	106.56	113.80
1	B	860	VAL	CB-CA-C	-7.23	99.56	110.55
1	A	646	GLU	CA-C-O	-7.22	115.65	119.77
1	B	892	LEU	CA-C-N	-7.21	112.56	122.30
1	B	892	LEU	C-N-CA	-7.21	112.56	122.30
1	B	100	GLU	N-CA-CB	7.20	121.61	109.87
1	A	377	ILE	N-CA-CB	7.20	120.33	110.54
1	A	709	TRP	CA-CB-CG	7.17	127.22	113.60
1	B	55	PHE	CA-CB-CG	-7.17	106.63	113.80
1	B	746	SER	N-CA-C	7.16	120.97	110.59
1	B	223	HIS	N-CA-CB	7.12	122.30	110.92
1	B	551	ARG	CD-NE-CZ	7.08	134.32	124.40
1	B	581	CYS	CA-C-O	7.08	127.55	119.27
1	B	718	LEU	N-CA-C	-7.08	102.47	113.02
1	A	350	HIS	CA-CB-CG	-7.03	106.77	113.80
1	A	100	GLU	CA-C-N	-7.02	108.12	121.54
1	A	100	GLU	C-N-CA	-7.02	108.12	121.54
1	B	286	LEU	CA-C-O	-7.02	110.93	119.43
1	B	246	ASP	N-CA-CB	6.99	120.39	110.12
1	A	147	LYS	CG-CD-CE	6.97	127.32	111.30
1	B	712	PHE	CA-CB-CG	6.95	120.75	113.80
1	B	293	PHE	CA-C-N	6.94	129.58	120.28
1	B	293	PHE	C-N-CA	6.94	129.58	120.28
1	A	69	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	B	441	ARG	CD-NE-CZ	-6.93	114.69	124.40
1	B	298	SER	N-CA-C	6.92	119.90	110.55
1	A	461	TYR	CA-C-N	6.90	129.53	120.28
1	A	461	TYR	C-N-CA	6.90	129.53	120.28
1	A	316	GLU	CB-CG-CD	6.88	124.30	112.60
1	B	63	MET	CA-C-N	6.88	133.25	121.35
1	B	63	MET	C-N-CA	6.88	133.25	121.35
1	A	53	ARG	NE-CZ-NH2	-6.86	113.03	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	467	HIS	CA-CB-CG	6.83	120.63	113.80
1	B	627	ASP	CA-C-O	-6.83	113.15	121.28
1	A	860	VAL	CB-CA-C	-6.82	99.77	110.69
1	B	805	GLN	OE1-CD-NE2	6.82	129.42	122.60
1	A	18	GLN	CA-C-N	6.81	129.38	120.60
1	A	18	GLN	C-N-CA	6.81	129.38	120.60
1	A	12	THR	CA-C-N	6.81	133.21	123.14
1	A	12	THR	C-N-CA	6.81	133.21	123.14
1	A	564	ILE	N-CA-CB	6.79	122.43	111.23
1	B	781	ILE	CB-CA-C	6.76	122.64	112.16
1	B	99	HIS	CB-CA-C	6.75	123.85	110.42
1	B	782	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	255	MET	CA-C-O	6.74	128.56	120.28
1	A	399	ASP	CA-CB-CG	-6.71	105.89	112.60
1	A	756	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	A	35	THR	N-CA-CB	6.69	120.61	110.30
1	B	483	MET	CA-CB-CG	6.69	127.48	114.10
1	A	821	THR	N-CA-CB	6.67	119.92	110.12
1	B	64	LEU	N-CA-C	6.66	121.23	109.58
1	A	292	LEU	N-CA-C	6.65	118.53	111.28
1	A	98	ASN	CA-CB-CG	6.64	119.24	112.60
1	B	38	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	250	GLY	CA-C-O	-6.61	114.42	122.15
1	A	455	MET	CA-C-N	6.60	128.88	120.56
1	A	455	MET	C-N-CA	6.60	128.88	120.56
1	A	255	MET	N-CA-CB	6.60	121.90	110.81
1	A	16	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	832	GLN	OE1-CD-NE2	-6.58	116.03	122.60
1	A	66	THR	CA-CB-OG1	-6.57	99.75	109.60
1	A	866	LYS	N-CA-CB	6.56	119.59	110.07
1	B	760	ASP	CA-CB-CG	-6.56	106.04	112.60
1	B	881	GLU	CA-CB-CG	6.56	127.22	114.10
1	B	727	ARG	NE-CZ-NH1	6.55	128.06	121.50
1	A	762	THR	N-CA-CB	6.55	120.44	110.28
1	A	425	ARG	CD-NE-CZ	6.54	133.56	124.40
1	A	868	HIS	CA-C-N	6.51	126.75	119.32
1	A	868	HIS	C-N-CA	6.51	126.75	119.32
1	A	439	ASP	CA-CB-CG	-6.51	106.09	112.60
1	A	814	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	781	ILE	CA-CB-CG2	6.49	121.54	110.50
1	A	267	ASP	N-CA-CB	-6.47	99.44	109.34
1	B	558	LYS	N-CA-CB	6.47	121.68	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	LYS	CA-C-N	6.47	129.24	120.38
1	A	187	LYS	C-N-CA	6.47	129.24	120.38
1	A	897	SER	CA-C-N	6.46	127.10	120.00
1	A	897	SER	C-N-CA	6.46	127.10	120.00
1	A	763	LYS	CA-CB-CG	6.45	127.01	114.10
1	A	243	ARG	CD-NE-CZ	-6.45	115.37	124.40
1	A	196	ARG	CB-CA-C	6.43	123.05	111.03
1	A	899	LYS	N-CA-C	-6.42	104.20	111.07
1	B	492	ARG	N-CA-CB	6.39	120.07	110.22
1	B	891	LEU	CA-C-O	-6.39	113.46	120.30
1	A	203	ILE	CA-C-N	-6.38	114.11	122.16
1	A	203	ILE	C-N-CA	-6.38	114.11	122.16
1	B	845	ILE	CA-CB-CG2	6.37	121.33	110.50
1	B	70	SER	O-C-N	6.37	129.15	123.41
1	B	505	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	B	720	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	785	LYS	N-CA-CB	6.34	119.54	110.16
1	B	732	TYR	CA-C-O	6.33	126.97	119.56
1	B	657	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	209	ASP	N-CA-CB	6.28	120.02	110.28
1	A	361	VAL	N-CA-C	6.28	120.83	112.98
1	A	459	VAL	O-C-N	-6.28	115.36	121.83
1	B	677	ILE	O-C-N	-6.26	116.44	123.20
1	A	208	ASN	CA-C-O	-6.25	113.86	121.36
1	A	818	LEU	CB-CA-C	6.25	123.14	110.38
1	A	298	SER	N-CA-C	6.25	118.98	110.55
1	A	297	VAL	O-C-N	-6.23	116.43	121.98
1	B	63	MET	O-C-N	-6.21	114.84	122.55
1	B	544	LYS	CA-C-N	-6.21	114.48	123.06
1	B	544	LYS	C-N-CA	-6.21	114.48	123.06
1	A	838	MET	CA-C-O	-6.20	112.84	119.97
1	A	658	THR	CA-CB-CG2	6.20	121.04	110.50
1	B	235	ASN	CA-CB-CG	6.20	118.80	112.60
1	B	644	ARG	NE-CZ-NH1	-6.20	115.30	121.50
1	A	619	TRP	O-C-N	-6.19	115.34	122.89
1	A	484	LEU	CA-C-O	6.19	126.98	120.42
1	A	880	LYS	CA-C-O	-6.18	113.87	120.42
1	A	602	PHE	CA-CB-CG	6.18	119.98	113.80
1	B	440	VAL	CB-CA-C	-6.17	101.64	110.83
1	B	653	ALA	CA-C-O	-6.17	113.34	120.31
1	A	467	HIS	CA-CB-CG	6.16	119.96	113.80
1	B	403	THR	N-CA-CB	-6.16	97.69	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASN	CA-CB-CG	-6.16	106.44	112.60
1	B	829	ARG	NH1-CZ-NH2	6.15	127.30	119.30
1	B	86	GLY	CA-C-O	6.14	125.05	119.83
1	B	803	ILE	CB-CA-C	-6.11	104.14	111.97
1	B	785	LYS	N-CA-CB	-6.09	100.86	109.94
1	A	243	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	B	500	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A	274	ARG	CD-NE-CZ	-6.06	115.91	124.40
1	A	782	PHE	CA-C-N	6.06	131.11	120.87
1	A	782	PHE	C-N-CA	6.06	131.11	120.87
1	B	393	ILE	O-C-N	-6.05	115.89	121.94
1	A	785	LYS	CA-CB-CG	6.05	126.19	114.10
1	A	327	GLU	O-C-N	-6.04	115.85	122.07
1	A	504	HIS	CA-CB-CG	-6.04	107.76	113.80
1	A	12	THR	O-C-N	-6.03	113.36	123.00
1	A	80	PHE	CA-CB-CG	6.03	119.83	113.80
1	B	683	ASN	CA-CB-CG	6.02	118.62	112.60
1	A	618	THR	CA-C-O	-6.01	114.84	121.33
1	B	173	LYS	CB-CA-C	-6.01	109.06	117.23
1	B	644	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	A	568	GLN	CA-C-N	6.00	129.21	122.42
1	A	568	GLN	C-N-CA	6.00	129.21	122.42
1	A	852	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	795	LEU	N-CA-C	5.99	118.48	108.96
1	B	250	GLY	CA-C-O	-5.99	116.06	122.05
1	A	400	ASN	CA-CB-CG	5.98	118.58	112.60
1	A	259	THR	CA-C-O	-5.97	113.10	119.97
1	A	376	THR	N-CA-CB	5.97	118.89	110.12
1	A	405	ARG	CA-C-O	-5.96	114.46	121.44
1	A	304	GLU	CA-C-O	5.95	126.73	120.42
1	B	510	LYS	N-CA-C	5.95	120.15	113.01
1	A	705	ILE	N-CA-CB	-5.91	104.01	111.46
1	A	720	ASP	N-CA-C	5.90	118.47	111.33
1	B	249	GLU	CA-C-O	5.90	127.27	120.60
1	A	260	GLU	CB-CG-CD	5.89	122.62	112.60
1	B	733	SER	CA-CB-OG	5.89	122.88	111.10
1	A	563	PRO	CA-C-O	-5.87	114.05	120.92
1	B	402	GLY	CA-C-O	5.87	125.81	119.06
1	A	55	PHE	CA-C-O	-5.86	113.04	119.08
1	B	279	ARG	CG-CD-NE	-5.86	99.11	112.00
1	B	654	VAL	O-C-N	-5.86	116.25	123.10
1	A	647	PHE	CA-CB-CG	-5.83	107.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ASP	CA-C-O	-5.82	114.35	120.58
1	B	323	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	B	584	ASP	CA-C-O	5.82	126.59	120.42
1	A	260	GLU	OE1-CD-OE2	-5.82	108.94	122.90
1	B	652	VAL	N-CA-CB	-5.81	103.24	112.07
1	A	478	HIS	O-C-N	-5.80	115.88	123.02
1	A	591	ILE	CB-CA-C	-5.80	104.41	112.36
1	A	476	HIS	CA-CB-CG	-5.80	108.00	113.80
1	B	293	PHE	CA-CB-CG	5.80	119.60	113.80
1	A	510	LYS	N-CA-C	5.79	119.61	112.54
1	A	362	GLU	CA-C-O	5.79	124.94	120.48
1	A	729	VAL	CA-C-O	5.79	126.97	120.95
1	B	331	ARG	NE-CZ-NH1	-5.79	115.71	121.50
1	A	639	ASP	CB-CA-C	-5.77	101.82	110.88
1	B	572	GLU	CB-CA-C	5.77	122.15	110.38
1	A	357	THR	N-CA-CB	5.76	118.59	110.12
1	A	845	ILE	CA-CB-CG2	5.76	120.29	110.50
1	A	12	THR	CA-C-O	5.76	130.58	120.80
1	B	868	HIS	CA-C-N	5.75	125.37	119.56
1	B	868	HIS	C-N-CA	5.75	125.37	119.56
1	A	603	SER	CA-CB-OG	-5.73	99.63	111.10
1	A	367	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	902	ALA	CA-C-N	5.71	127.94	120.28
1	B	902	ALA	C-N-CA	5.71	127.94	120.28
1	A	801	ARG	NE-CZ-NH2	-5.71	114.06	119.20
1	A	425	ARG	CA-C-O	-5.70	114.83	120.82
1	A	12	THR	CA-CB-CG2	5.70	120.19	110.50
1	A	297	VAL	CB-CA-C	-5.70	106.03	111.44
1	B	604	PHE	CA-CB-CG	-5.70	108.10	113.80
1	B	631	HIS	CB-CA-C	-5.70	100.60	110.45
1	B	308	LEU	N-CA-CB	5.67	118.46	110.12
1	A	144	LYS	CG-CD-CE	5.67	124.34	111.30
1	B	124	SER	CB-CA-C	-5.67	102.23	110.96
1	A	701	GLY	N-CA-C	5.67	118.42	111.45
1	A	719	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	479	LEU	CA-C-N	5.64	129.27	120.75
1	A	479	LEU	C-N-CA	5.64	129.27	120.75
1	B	153	THR	CA-CB-OG1	-5.64	101.14	109.60
1	A	45	LYS	CA-C-O	5.63	126.44	119.79
1	B	480	THR	O-C-N	5.63	129.25	122.94
1	A	568	GLN	CA-CB-CG	5.62	125.34	114.10
1	A	881	GLU	N-CA-CB	5.62	119.71	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ASN	OD1-CG-ND2	5.61	128.21	122.60
1	B	207	VAL	N-CA-CB	-5.60	101.45	111.92
1	A	111	VAL	N-CA-CB	5.59	120.46	111.23
1	A	331	ARG	CD-NE-CZ	-5.59	116.57	124.40
1	A	79	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	892	LEU	CA-C-O	-5.59	114.38	120.81
1	B	912	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	894	GLU	CA-C-O	-5.58	112.39	119.31
1	B	200	ASP	CA-CB-CG	-5.58	107.02	112.60
1	A	426	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	293	PHE	N-CA-C	-5.58	105.28	111.36
1	A	62	LYS	N-CA-C	5.57	119.18	112.38
1	B	500	ARG	CD-NE-CZ	-5.57	116.60	124.40
1	B	435	VAL	CA-C-N	5.57	125.18	119.56
1	B	435	VAL	C-N-CA	5.57	125.18	119.56
1	B	769	ARG	CD-NE-CZ	-5.56	116.61	124.40
1	B	34	GLU	CB-CG-CD	5.54	122.03	112.60
1	B	492	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	A	580	SER	N-CA-CB	5.54	118.36	110.16
1	B	724	HIS	N-CA-CB	-5.54	101.69	109.94
1	B	56	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	B	229	ILE	CA-CB-CG1	5.53	119.81	110.40
1	A	40	MET	CA-C-N	5.53	128.15	120.29
1	A	40	MET	C-N-CA	5.53	128.15	120.29
1	A	48	LYS	N-CA-C	-5.53	105.15	111.07
1	A	331	ARG	NE-CZ-NH2	5.53	124.17	119.20
1	B	152	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	438	SER	CA-C-O	-5.52	114.86	120.71
1	A	35	THR	CA-CB-OG1	5.52	117.88	109.60
1	A	38	ASP	CA-C-N	5.52	127.51	120.56
1	A	38	ASP	C-N-CA	5.52	127.51	120.56
1	B	187	LYS	N-CA-C	-5.52	105.28	112.23
1	B	365	ASP	CB-CA-C	5.51	119.94	110.79
1	B	207	VAL	CA-CB-CG1	5.51	119.77	110.40
1	A	539	ARG	N-CA-C	5.50	118.52	109.72
1	B	755	ARG	CD-NE-CZ	-5.50	116.70	124.40
1	A	357	THR	CA-CB-OG1	5.50	117.84	109.60
1	B	53	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	B	650	ASP	CA-CB-CG	-5.49	107.11	112.60
1	B	738	LYS	CA-C-N	5.49	130.16	122.36
1	B	738	LYS	C-N-CA	5.49	130.16	122.36
1	B	488	LYS	CA-C-O	5.48	126.58	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	860	VAL	CA-CB-CG1	5.48	119.72	110.40
1	B	345	ASN	N-CA-C	5.47	116.92	111.07
1	A	657	ASP	CA-C-O	5.47	126.32	120.20
1	B	760	ASP	CB-CA-C	-5.46	102.23	110.92
1	A	677	ILE	O-C-N	-5.46	116.72	123.10
1	B	283	ARG	NH1-CZ-NH2	5.46	126.39	119.30
1	A	699	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	307	ARG	CD-NE-CZ	5.45	132.03	124.40
1	B	860	VAL	CA-C-O	-5.45	115.95	121.67
1	B	94	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	B	345	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	699	ASP	N-CA-C	-5.43	105.35	112.41
1	A	785	LYS	CA-C-O	-5.43	114.67	120.42
1	A	209	ASP	N-CA-C	-5.42	105.92	112.54
1	A	283	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	A	857	THR	CA-CB-OG1	5.42	117.73	109.60
1	B	264	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	540	VAL	O-C-N	-5.41	117.50	123.18
1	B	246	ASP	CA-CB-CG	5.41	118.00	112.60
1	A	376	THR	CA-CB-CG2	5.38	119.65	110.50
1	B	912	ARG	N-CA-C	-5.38	106.67	113.18
1	A	512	LEU	N-CA-C	5.35	116.39	109.65
1	B	464	ALA	O-C-N	-5.35	115.96	122.22
1	B	811	SER	N-CA-C	5.35	117.96	109.24
1	A	745	ILE	N-CA-C	5.35	120.46	109.34
1	B	437	ASP	CB-CG-OD2	-5.35	106.10	118.40
1	B	217	CYS	CB-CA-C	5.34	120.50	110.63
1	A	817	ILE	CB-CA-C	-5.33	104.86	112.22
1	A	210	THR	CA-C-N	5.32	127.98	120.42
1	A	210	THR	C-N-CA	5.32	127.98	120.42
1	A	64	LEU	N-CA-C	5.32	116.78	110.07
1	A	866	LYS	CA-C-O	-5.32	115.22	120.70
1	B	869	PRO	CB-CA-C	-5.32	103.92	111.68
1	A	677	ILE	CA-C-N	5.32	128.01	122.96
1	A	677	ILE	C-N-CA	5.32	128.01	122.96
1	B	171	TRP	CG-CD2-CE3	-5.32	128.59	133.90
1	B	610	SER	CA-C-N	5.31	127.40	120.28
1	B	610	SER	C-N-CA	5.31	127.40	120.28
1	B	306	VAL	CA-CB-CG2	5.31	119.42	110.40
1	B	285	SER	N-CA-C	5.30	117.37	110.53
1	B	606	CYS	CA-C-N	-5.29	115.38	122.42
1	B	606	CYS	C-N-CA	-5.29	115.38	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	654	VAL	N-CA-CB	5.29	118.13	111.46
1	B	85	LEU	CA-C-O	-5.29	115.14	121.11
1	A	794	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	49	ASN	OD1-CG-ND2	5.28	127.88	122.60
1	A	30	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	B	67	PHE	CA-CB-CG	-5.27	108.53	113.80
1	B	882	LEU	CA-C-N	-5.26	116.95	123.21
1	B	882	LEU	C-N-CA	-5.26	116.95	123.21
1	B	155	SER	N-CA-C	5.26	117.75	109.39
1	A	516	VAL	CA-CB-CG2	5.26	119.34	110.40
1	B	706	ASN	CA-C-O	-5.25	115.46	120.92
1	A	768	PHE	O-C-N	-5.25	116.28	122.58
1	B	256	CYS	CA-C-O	-5.25	115.28	121.16
1	B	579	VAL	CA-C-O	5.25	126.42	120.85
1	B	608	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	B	335	ASN	CA-CB-CG	-5.25	107.35	112.60
1	B	178	SER	CB-CA-C	-5.24	99.89	109.54
1	B	413	ASP	CA-CB-CG	-5.24	107.36	112.60
1	A	720	ASP	CB-CA-C	-5.24	101.77	110.68
1	A	336	THR	N-CA-CB	5.24	119.23	110.32
1	A	103	GLN	N-CA-C	5.23	121.94	110.80
1	B	319	LEU	CA-C-O	-5.23	114.99	121.06
1	A	581	CYS	CA-C-O	-5.23	114.19	120.10
1	B	373	HIS	N-CA-CB	5.22	117.89	110.16
1	A	100	GLU	CB-CA-C	5.22	120.81	110.42
1	B	335	ASN	N-CA-C	5.22	117.59	110.55
1	A	354	GLU	CA-CB-CG	5.21	124.53	114.10
1	B	480	THR	CA-C-O	-5.21	115.57	121.72
1	B	453	ALA	N-CA-C	-5.21	105.60	111.28
1	B	585	PHE	N-CA-C	5.21	116.96	111.28
1	B	54	ASP	CB-CA-C	5.21	118.98	110.96
1	B	211	VAL	N-CA-C	5.20	115.93	110.62
1	A	786	PHE	CA-CB-CG	-5.20	108.60	113.80
1	B	866	LYS	N-CA-CB	5.20	117.86	110.16
1	A	272	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	42	ARG	CA-C-O	-5.19	115.04	120.55
1	A	396	ARG	NH1-CZ-NH2	5.19	126.05	119.30
1	B	416	LEU	N-CA-C	-5.19	105.54	111.14
1	B	884	PRO	N-CA-C	5.19	120.67	113.98
1	A	720	ASP	CB-CG-OD1	-5.19	106.47	118.40
1	A	190	ASN	CB-CA-C	-5.18	101.86	110.68
1	B	105	VAL	CB-CA-C	-5.18	102.79	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	MET	CA-C-O	5.18	126.12	120.58
1	A	335	ASN	CB-CG-ND2	-5.18	108.63	116.40
1	B	125	GLN	CA-CB-CG	5.17	124.44	114.10
1	B	347	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	207	VAL	CA-C-N	5.17	130.90	122.07
1	A	207	VAL	C-N-CA	5.17	130.90	122.07
1	A	821	THR	CA-CB-CG2	5.16	119.28	110.50
1	B	412	VAL	CB-CA-C	-5.16	102.43	110.69
1	B	423	TYR	N-CA-C	5.16	117.31	111.02
1	A	272	ASP	CA-C-O	-5.16	113.70	119.79
1	A	821	THR	CA-CB-OG1	5.16	117.33	109.60
1	A	513	PRO	CA-C-O	-5.15	115.16	121.03
1	A	381	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	B	744	MET	N-CA-CB	-5.15	102.56	110.44
1	A	354	GLU	CA-C-N	5.15	127.05	120.56
1	A	354	GLU	C-N-CA	5.15	127.05	120.56
1	A	897	SER	N-CA-CB	-5.15	103.45	110.56
1	A	804	LEU	N-CA-CB	-5.15	102.34	110.06
1	A	861	ASP	CA-CB-CG	-5.14	107.45	112.60
1	A	546	ARG	CA-C-O	-5.14	115.15	120.70
1	B	426	ARG	CD-NE-CZ	-5.13	117.21	124.40
1	B	143	ILE	CA-C-O	5.13	124.64	119.97
1	A	639	ASP	N-CA-CB	5.13	117.44	110.01
1	A	250	GLY	N-CA-C	-5.12	104.76	111.37
1	A	266	ASP	CB-CA-C	5.12	120.61	110.42
1	B	588	TYR	CA-CB-CG	5.12	123.12	113.90
1	A	282	ASP	O-C-N	-5.12	116.70	122.12
1	B	335	ASN	N-CA-CB	-5.12	102.67	110.45
1	A	869	PRO	CB-CA-C	-5.11	103.75	112.64
1	B	205	ALA	CA-C-O	-5.11	115.27	120.89
1	B	907	VAL	CB-CA-C	5.10	119.07	112.24
1	A	33	ASP	CA-CB-CG	-5.09	107.51	112.60
1	B	100	GLU	CA-CB-CG	5.09	124.27	114.10
1	B	582	ILE	N-CA-C	-5.08	105.75	110.53
1	B	154	PHE	CA-C-O	-5.08	114.90	120.70
1	B	400	ASN	CA-CB-CG	5.08	117.68	112.60
1	B	801	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	B	39	ILE	CA-C-N	5.08	127.09	120.28
1	B	39	ILE	C-N-CA	5.08	127.09	120.28
1	B	331	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	A	109	SER	N-CA-C	5.07	116.01	108.86
1	A	869	PRO	N-CD-CG	-5.07	95.60	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ASP	O-C-N	-5.07	115.64	122.43
1	A	763	LYS	CB-CA-C	-5.06	102.24	110.85
1	B	204	VAL	N-CA-C	5.06	117.84	112.83
1	B	275	THR	CA-C-N	5.06	127.57	120.28
1	B	275	THR	C-N-CA	5.06	127.57	120.28
1	B	602	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	382	SER	CA-C-O	-5.05	115.51	120.82
1	B	194	LYS	N-CA-C	-5.05	105.78	111.28
1	B	610	SER	O-C-N	-5.05	117.59	122.99
1	A	309	ILE	CB-CG1-CD1	5.04	124.39	113.80
1	A	410	VAL	O-C-N	-5.04	116.32	122.97
1	A	805	GLN	CA-C-O	5.03	125.75	119.97
1	B	912	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	B	782	PHE	N-CA-C	5.03	116.80	109.71
1	A	605	PRO	CA-C-O	5.02	126.76	121.03
1	B	579	VAL	CA-C-N	5.02	127.71	120.38
1	B	579	VAL	C-N-CA	5.02	127.71	120.38
1	B	904	ILE	N-CA-C	-5.02	105.53	111.00
1	B	211	VAL	O-C-N	-5.02	117.00	121.87
1	B	689	GLU	CA-CB-CG	-5.01	104.08	114.10
1	A	656	ASN	CA-C-O	-5.01	115.34	121.05
1	A	145	ASP	CA-CB-CG	-5.00	107.60	112.60
1	B	496	GLU	CA-C-O	-5.00	114.22	119.97

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	GLU	Mainchain
1	A	101	LYS	Peptide,Mainchain
1	A	114	THR	Mainchain
1	A	237	CYS	Mainchain
1	A	243	ARG	Mainchain
1	A	258	ASN	Mainchain
1	A	267	ASP	Mainchain
1	A	333	LYS	Mainchain
1	A	336	THR	Mainchain
1	A	346	LYS	Mainchain
1	A	399	ASP	Mainchain
1	A	459	VAL	Mainchain
1	A	505	ASN	Mainchain
1	A	507	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	568	GLN	Mainchain
1	A	618	THR	Mainchain
1	A	634	VAL	Mainchain
1	A	646	GLU	Mainchain
1	A	68	VAL	Mainchain
1	A	738	LYS	Mainchain
1	A	745	ILE	Mainchain
1	A	746	SER	Mainchain
1	A	79	ASP	Mainchain
1	A	854	LEU	Mainchain
1	A	887	ASN	Mainchain
1	A	888	VAL	Mainchain
1	A	99	HIS	Mainchain
1	B	128	ASP	Mainchain
1	B	18	GLN	Sidechain
1	B	286	LEU	Mainchain
1	B	363	PRO	Mainchain
1	B	435	VAL	Mainchain
1	B	466	GLN	Mainchain
1	B	480	THR	Mainchain
1	B	540	VAL	Mainchain
1	B	553	VAL	Mainchain
1	B	710	GLY	Mainchain
1	B	737	GLY	Mainchain
1	B	738	LYS	Mainchain
1	B	807	LEU	Mainchain
1	B	836	ALA	Mainchain
1	B	860	VAL	Mainchain
1	B	908	GLY	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7065	0	7124	498	0
1	B	7032	0	7087	347	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	22	7	0
3	B	32	0	21	8	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	31	0	13	1	0
5	B	31	0	13	1	0
6	A	188	0	0	33	0
6	B	272	0	0	36	0
All	All	14737	0	14328	851	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (851) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ASN:O	1:A:507:ALA:N	1.57	1.31
1:A:521:ASP:HB3	6:A:1169:HOH:O	1.34	1.24
1:B:71:ILE:HA	1:B:215:MET:HE1	1.20	1.17
1:A:29:MET:HB2	1:A:377:ILE:HD11	1.27	1.17
1:A:214:MET:HE3	1:A:215:MET:HE3	1.26	1.15
1:B:441:ARG:HH11	1:B:441:ARG:HG3	1.13	1.11
1:A:62:LYS:CE	6:A:1057:HOH:O	1.89	1.11
1:A:646:GLU:HG2	1:A:647:PHE:HD1	1.16	1.11
1:A:656:ASN:ND2	1:A:658:THR:HB	1.67	1.09
1:A:513:PRO:HB3	1:A:703:MET:HE3	1.33	1.06
1:B:215:MET:HA	1:B:215:MET:HE2	1.28	1.05
1:A:62:LYS:HE3	6:A:1057:HOH:O	1.44	1.04
1:A:778:THR:HB	1:A:781:ILE:HD13	1.38	1.03
1:A:441:ARG:NH1	1:A:443:LEU:HD22	1.74	1.02
1:B:752:GLU:CD	1:B:755:ARG:HH12	1.67	1.01
1:B:769:ARG:CD	6:B:2251:HOH:O	2.08	1.01
1:A:303:GLY:N	1:A:336:THR:HG22	1.77	1.00
1:B:71:ILE:CA	1:B:215:MET:HE1	1.93	0.99
1:A:71:ILE:HG23	6:A:1102:HOH:O	1.61	0.98
1:A:189:LEU:HD13	1:A:203:ILE:HD11	1.43	0.98
1:B:586:LEU:HD22	1:B:596:MET:HE1	1.45	0.98
1:A:598:LEU:HD12	1:A:599:GLY:N	1.79	0.98
1:A:40:MET:HE2	1:A:391:GLY:HA3	1.46	0.98
1:A:735:ASN:H	1:A:735:ASN:HD22	1.01	0.97
1:B:908:GLY:O	1:B:910:ARG:N	1.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:THR:H	1:B:483:MET:HG3	1.30	0.97
1:A:313:MET:HE3	1:A:319:LEU:HD11	1.46	0.97
1:B:441:ARG:HG3	1:B:441:ARG:NH1	1.72	0.96
1:A:690:MET:HE1	1:A:703:MET:HE2	1.46	0.96
1:A:313:MET:CE	1:A:319:LEU:HD11	1.93	0.96
1:A:313:MET:HE3	1:A:319:LEU:CD1	1.95	0.96
1:B:465:GLU:OE1	1:B:468:ARG:NH2	1.97	0.96
1:B:441:ARG:HH11	1:B:441:ARG:CG	1.66	0.95
1:A:138:MET:HE2	1:A:143:ILE:HD13	1.46	0.95
1:A:895:ASP:CG	1:A:895:ASP:O	2.09	0.95
1:A:110:GLU:O	1:A:111:VAL:HG23	1.67	0.94
1:B:71:ILE:HA	1:B:215:MET:CE	1.98	0.94
1:A:138:MET:HE2	1:A:143:ILE:CD1	1.97	0.94
1:A:435:VAL:HG12	1:A:438:SER:HB2	1.50	0.94
1:B:563:PRO:HB2	1:B:565:GLU:HG3	1.49	0.94
1:B:752:GLU:OE2	1:B:755:ARG:NH1	2.00	0.93
1:A:832:GLN:HG3	1:A:874:ILE:HD11	1.49	0.93
1:B:480:THR:HG22	1:B:483:MET:HG2	1.48	0.93
1:A:644:ARG:HG2	1:A:646:GLU:HB3	1.48	0.93
1:B:578:ILE:HG23	6:B:2246:HOH:O	1.66	0.93
1:B:71:ILE:HG22	1:B:215:MET:CE	1.98	0.92
1:B:578:ILE:CG2	6:B:2246:HOH:O	2.16	0.92
1:A:658:THR:HG23	1:A:685:CYS:HB3	1.50	0.92
1:B:769:ARG:HD2	6:B:2251:HOH:O	1.69	0.92
1:A:646:GLU:HG2	1:A:647:PHE:CD1	2.05	0.92
1:B:907:VAL:O	1:B:908:GLY:O	1.88	0.92
1:A:671:THR:HB	1:A:857:THR:HG23	1.49	0.91
1:B:493:ALA:O	1:B:497:LEU:HD23	1.70	0.91
3:B:1918:G6P:H62	6:B:2227:HOH:O	1.70	0.91
1:B:595:ARG:NH1	1:B:648:ASP:HB3	1.83	0.91
1:A:62:LYS:HE2	6:A:1173:HOH:O	1.71	0.91
1:A:81:ILE:HG22	1:A:82:ALA:H	1.35	0.91
1:A:562:ILE:HD11	6:A:1152:HOH:O	1.70	0.91
1:B:480:THR:HG22	1:B:483:MET:CG	2.01	0.90
1:A:26:LEU:HD22	1:A:29:MET:HE3	1.51	0.90
1:A:303:GLY:H	1:A:336:THR:HG22	1.31	0.89
1:A:792:SER:OG	1:A:795:LEU:HD23	1.72	0.89
3:B:1916:G6P:H62	6:B:2027:HOH:O	1.69	0.89
1:A:245:ILE:HD13	1:A:257:ILE:HD11	1.54	0.89
1:B:71:ILE:HG22	1:B:215:MET:HE1	1.52	0.89
1:A:634:VAL:HG23	1:A:654:VAL:CG2	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ASN:C	1:A:507:ALA:N	2.27	0.89
3:A:919:G6P:H61	6:A:1033:HOH:O	1.72	0.89
1:B:72:PRO:HB3	1:B:455:MET:CE	2.03	0.89
1:A:656:ASN:HD22	1:A:658:THR:CG2	1.85	0.88
1:A:656:ASN:HD22	1:A:658:THR:HB	1.28	0.88
1:A:335:ASN:C	1:A:335:ASN:HD22	1.72	0.88
1:B:420:HIS:HD2	1:B:422:GLN:H	1.20	0.88
1:B:769:ARG:NH2	6:B:2165:HOH:O	2.07	0.87
1:B:496:GLU:OE2	1:B:844:LYS:HE2	1.74	0.87
1:A:895:ASP:OD1	6:A:1161:HOH:O	1.93	0.87
1:A:71:ILE:HA	1:A:215:MET:HE1	1.57	0.86
1:A:690:MET:HE2	1:A:703:MET:CB	2.05	0.86
1:A:71:ILE:HG12	1:A:215:MET:HE1	1.57	0.86
1:B:189:LEU:HD13	1:B:203:ILE:HD11	1.56	0.86
1:B:480:THR:HG23	1:B:483:MET:H	1.41	0.86
1:B:76:GLU:HG3	1:B:455:MET:HE1	1.55	0.86
1:A:527:ASP:OD1	1:A:544:LYS:HG2	1.75	0.85
1:B:110:GLU:OE1	1:B:141:ARG:NH2	2.08	0.85
1:B:845:ILE:HD12	1:B:849:ARG:CZ	2.06	0.85
1:A:71:ILE:CD1	1:A:218:GLY:HA3	2.07	0.85
1:A:81:ILE:O	1:A:82:ALA:HB2	1.74	0.85
1:A:759:ILE:HD11	1:A:776:LEU:HG	1.56	0.85
1:A:353:LYS:O	1:A:357:THR:HG23	1.75	0.84
1:A:287:ASN:HD22	1:A:287:ASN:H	1.21	0.84
1:B:111:VAL:HG12	6:B:2155:HOH:O	1.77	0.84
1:A:33:ASP:OD2	1:A:433:ARG:NE	2.09	0.84
1:A:214:MET:CE	1:A:215:MET:HE3	2.06	0.84
1:A:646:GLU:HG2	1:A:647:PHE:H	1.42	0.84
1:B:76:GLU:HG3	1:B:455:MET:CE	2.05	0.84
1:B:585:PHE:O	6:B:2249:HOH:O	1.96	0.84
1:B:401:LYS:NZ	1:B:403:THR:HG21	1.91	0.84
1:A:762:THR:HG22	1:A:767:LEU:HD12	1.59	0.84
1:A:735:ASN:HD22	1:A:735:ASN:N	1.73	0.83
1:A:562:ILE:HD13	1:A:562:ILE:H	1.43	0.83
1:B:313:MET:CE	1:B:319:LEU:HD11	2.08	0.83
1:A:97:VAL:HG13	1:A:105:VAL:HA	1.61	0.83
1:B:200:ASP:OD1	1:B:201:ALA:N	2.12	0.83
1:B:540:VAL:HG12	1:B:585:PHE:CD2	2.13	0.82
1:A:634:VAL:CG2	1:A:654:VAL:CG2	2.58	0.82
1:A:71:ILE:HG12	1:A:215:MET:CE	2.10	0.82
1:B:23:ASP:OD1	1:B:373:HIS:HE1	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ARG:O	1:A:912:ARG:N	2.13	0.81
1:B:624:LYS:HD3	6:B:2229:HOH:O	1.80	0.81
1:A:687:MET:HE1	1:A:704:CYS:HB2	1.62	0.81
1:A:845:ILE:HD13	1:A:854:LEU:HD22	1.60	0.81
1:A:143:ILE:HG22	1:A:146:LYS:HD2	1.60	0.81
1:B:71:ILE:CG2	1:B:215:MET:HE1	2.11	0.81
1:A:522:GLY:HA2	1:A:551:ARG:HH21	1.46	0.80
1:A:662:MET:HE1	1:A:687:MET:HE3	1.63	0.80
1:B:513:PRO:HB3	1:B:703:MET:HE1	1.64	0.80
1:B:252:GLU:HG3	6:B:2028:HOH:O	1.79	0.80
3:B:1918:G6P:C6	6:B:2227:HOH:O	2.27	0.80
1:A:874:ILE:HD12	1:A:874:ILE:O	1.82	0.80
1:B:143:ILE:HG22	1:B:146:LYS:HE3	1.64	0.79
1:B:17:ASP:OD1	1:B:20:LYS:N	2.15	0.79
1:B:76:GLU:CG	1:B:455:MET:HE1	2.11	0.79
1:A:608:GLN:HG2	1:A:613:ALA:O	1.82	0.79
1:A:468:ARG:NH1	1:A:472:GLU:OE2	2.14	0.79
1:A:656:ASN:HD22	1:A:658:THR:CB	1.95	0.79
1:B:451:LYS:O	1:B:455:MET:HG2	1.83	0.78
1:A:544:LYS:HD2	1:A:554:GLU:OE1	1.84	0.78
1:A:690:MET:HE2	1:A:703:MET:HB2	1.63	0.78
1:B:72:PRO:HB3	1:B:455:MET:HE3	1.66	0.78
1:B:855:ASN:HD22	1:B:887:ASN:HB3	1.49	0.78
1:A:71:ILE:HD12	1:A:218:GLY:HA3	1.65	0.77
1:B:513:PRO:HB3	1:B:703:MET:CE	2.15	0.77
1:B:866:LYS:HD3	1:B:892:LEU:HD11	1.67	0.77
1:A:79:ASP:HB2	1:A:96:GLN:HG2	1.67	0.77
3:A:921:G6P:H61	6:A:1145:HOH:O	1.85	0.76
1:A:713:GLY:HA3	1:A:718:LEU:HD12	1.68	0.76
1:A:558:LYS:HG2	1:A:560:TYR:CE1	2.19	0.76
1:A:735:ASN:H	1:A:735:ASN:ND2	1.82	0.76
1:B:479:LEU:HD23	1:B:483:MET:HE3	1.66	0.76
1:A:563:PRO:HG2	1:A:566:ILE:HD12	1.65	0.76
1:B:492:ARG:HA	1:B:495:MET:CE	2.15	0.76
1:A:656:ASN:HD22	1:A:658:THR:HG22	1.50	0.76
1:A:866:LYS:NZ	1:A:892:LEU:HD11	2.01	0.76
1:B:420:HIS:CD2	1:B:422:GLN:H	2.03	0.76
1:B:624:LYS:HE2	1:B:734:LEU:HD22	1.68	0.76
1:A:96:GLN:O	1:A:105:VAL:HA	1.86	0.75
1:B:403:THR:CG2	1:B:405:ARG:O	2.34	0.75
1:B:401:LYS:HZ3	1:B:403:THR:HG21	1.47	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:ARG:HA	1:B:495:MET:HE2	1.68	0.75
1:A:343:GLU:OE2	1:A:420:HIS:HE1	1.69	0.75
1:B:215:MET:HA	1:B:215:MET:CE	2.11	0.75
1:A:405:ARG:NH2	1:A:437:ASP:HA	2.02	0.75
1:A:441:ARG:HH12	1:A:443:LEU:HD22	1.49	0.75
1:B:513:PRO:CB	1:B:703:MET:CE	2.65	0.75
1:B:531:LEU:HG	6:B:2246:HOH:O	1.87	0.74
1:A:595:ARG:NH1	1:A:650:ASP:HB2	2.02	0.74
1:A:671:THR:HB	1:A:857:THR:CG2	2.17	0.74
1:A:97:VAL:HG13	1:A:105:VAL:CA	2.18	0.74
1:A:283:ARG:NE	6:A:1172:HOH:O	2.19	0.74
1:B:479:LEU:HA	1:B:483:MET:HE2	1.70	0.74
1:B:518:ARG:HH12	1:B:521:ASP:H	1.34	0.74
1:B:465:GLU:CD	1:B:468:ARG:HH21	1.96	0.74
1:B:390:LEU:C	1:B:390:LEU:HD13	2.13	0.73
1:A:547:SER:O	1:A:548:GLY:O	2.06	0.73
1:A:562:ILE:HG12	1:A:562:ILE:O	1.88	0.73
1:B:774:GLU:OE2	1:B:777:LYS:NZ	2.21	0.73
1:A:607:GLN:O	1:A:615:ILE:HG12	1.88	0.73
1:B:480:THR:CG2	1:B:483:MET:HG2	2.18	0.73
1:A:343:GLU:OE2	1:A:420:HIS:CE1	2.41	0.73
1:A:534:GLY:O	1:A:621:LYS:HE3	1.89	0.72
1:A:527:ASP:OD1	1:A:546:ARG:NH2	2.22	0.72
1:A:607:GLN:HB3	1:A:615:ILE:HG13	1.71	0.72
1:A:687:MET:HE1	1:A:704:CYS:CB	2.19	0.72
1:A:896:GLY:O	6:A:1112:HOH:O	2.07	0.72
1:B:313:MET:HE3	1:B:319:LEU:CD1	2.20	0.72
1:B:492:ARG:HD2	1:B:495:MET:HE1	1.70	0.72
1:A:634:VAL:CG2	1:A:654:VAL:HG23	2.18	0.72
1:A:759:ILE:CD1	1:A:776:LEU:HG	2.18	0.72
1:B:323:ARG:NH2	1:B:362:GLU:HB2	2.04	0.72
1:A:492:ARG:NH1	1:A:847:GLU:OE1	2.22	0.71
1:A:715:ASN:H	1:A:715:ASN:ND2	1.88	0.71
1:A:831:ALA:HB3	1:A:874:ILE:HG13	1.71	0.71
1:A:570:THR:HB	1:A:573:GLU:OE1	1.88	0.71
1:B:323:ARG:NH2	1:B:361:VAL:O	2.21	0.71
1:A:414:GLY:HA2	3:A:919:G6P:H62	1.72	0.71
1:A:799:GLN:HG3	1:A:799:GLN:O	1.89	0.71
1:B:844:LYS:O	1:B:848:ASN:ND2	2.23	0.71
1:A:646:GLU:CG	1:A:647:PHE:H	2.03	0.71
1:A:116:GLU:HG3	1:A:120:HIS:HD1	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ILE:HA	1:A:215:MET:CE	2.20	0.71
1:A:564:ILE:HG22	1:A:567:MET:HG3	1.73	0.71
1:A:71:ILE:CA	1:A:215:MET:HE1	2.20	0.71
1:B:137:PHE:O	1:B:141:ARG:NH1	2.23	0.71
1:A:62:LYS:CE	6:A:1173:HOH:O	2.35	0.70
1:A:874:ILE:HD12	1:A:874:ILE:C	2.16	0.70
1:A:23:ASP:OD1	1:A:373:HIS:HE1	1.75	0.70
1:A:658:THR:CG2	1:A:685:CYS:HB3	2.21	0.70
1:A:339:VAL:HG13	1:A:375:CYS:HB3	1.74	0.70
1:A:72:PRO:HD2	6:A:1102:HOH:O	1.90	0.70
1:A:514:SER:OG	1:A:704:CYS:HB3	1.92	0.70
1:A:505:ASN:O	1:A:507:ALA:CA	2.39	0.70
1:B:497:LEU:CD1	6:B:2226:HOH:O	2.40	0.70
1:B:531:LEU:HD22	1:B:598:LEU:HD11	1.74	0.70
1:A:215:MET:HE2	1:A:215:MET:HA	1.73	0.70
1:A:480:THR:HG22	1:A:483:MET:H	1.57	0.70
1:A:722:ARG:CZ	1:A:740:ARG:HD3	2.22	0.70
1:A:891:LEU:N	1:A:891:LEU:HD22	2.06	0.70
1:A:857:THR:OG1	1:A:891:LEU:HD21	1.91	0.69
1:A:134:LEU:O	1:A:138:MET:HG3	1.92	0.69
1:B:518:ARG:NH1	1:B:521:ASP:H	1.90	0.69
1:A:832:GLN:HG3	1:A:874:ILE:CD1	2.22	0.69
1:A:845:ILE:CD1	1:A:854:LEU:CD2	2.70	0.69
1:A:534:GLY:HA3	1:A:603:SER:HB2	1.75	0.69
1:B:513:PRO:CB	1:B:703:MET:HE3	2.23	0.69
1:A:845:ILE:HD12	1:A:854:LEU:HD21	1.75	0.69
1:B:769:ARG:O	1:B:771:GLN:NE2	2.26	0.69
1:A:56:ASN:N	1:A:57:PRO:CD	2.55	0.69
1:A:81:ILE:HG22	1:A:82:ALA:N	2.08	0.69
1:A:513:PRO:HB3	1:A:703:MET:CE	2.17	0.69
1:B:908:GLY:O	1:B:909:VAL:C	2.35	0.69
1:A:646:GLU:CG	1:A:647:PHE:N	2.56	0.68
1:A:715:ASN:H	1:A:715:ASN:HD22	1.38	0.68
1:B:656:ASN:ND2	1:B:658:THR:OG1	2.25	0.68
1:B:549:LYS:HG2	1:B:550:LYS:H	1.56	0.68
1:A:768:PHE:O	1:A:770:GLY:N	2.27	0.68
1:B:513:PRO:HA	1:B:703:MET:HE3	1.74	0.68
1:B:727:ARG:NE	6:B:2180:HOH:O	2.16	0.68
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.58	0.68
1:B:540:VAL:CG1	1:B:585:PHE:CD2	2.76	0.68
1:A:519:THR:OG1	1:A:520:PRO:CD	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:PHE:O	1:A:624:LYS:HG3	1.94	0.68
1:B:200:ASP:CG	1:B:201:ALA:H	2.00	0.68
1:B:235:ASN:HD21	1:B:260:GLU:H	1.41	0.68
1:A:245:ILE:CD1	1:A:257:ILE:HD11	2.24	0.68
1:A:673:GLU:OE1	1:A:849:ARG:NH1	2.27	0.68
1:B:219:TYR:HD2	1:B:455:MET:HE2	1.58	0.67
1:A:79:ASP:OD2	1:A:148:LEU:HD22	1.93	0.67
1:A:16:ASP:CG	6:A:1055:HOH:O	2.38	0.67
1:A:91:ARG:HG2	1:A:93:LEU:CD2	2.24	0.67
1:A:521:ASP:O	1:A:523:THR:N	2.27	0.67
1:A:562:ILE:HD13	1:A:562:ILE:N	2.10	0.67
3:A:919:G6P:C6	6:A:1033:HOH:O	2.38	0.67
1:B:513:PRO:CA	1:B:703:MET:HE3	2.25	0.67
1:B:71:ILE:CB	1:B:215:MET:HE1	2.24	0.67
1:A:283:ARG:CZ	6:A:1172:HOH:O	2.43	0.67
1:B:588:TYR:N	6:B:2249:HOH:O	2.28	0.67
1:B:83:LEU:HD12	1:B:152:PHE:CD1	2.30	0.66
1:A:500:ARG:HB2	1:A:503:THR:OG1	1.96	0.66
1:A:845:ILE:CD1	1:A:854:LEU:HD22	2.26	0.66
1:B:478:HIS:O	1:B:483:MET:HE2	1.95	0.66
1:A:143:ILE:C	1:A:143:ILE:HD12	2.21	0.66
1:B:907:VAL:C	1:B:908:GLY:O	2.37	0.66
1:A:400:ASN:OD1	6:A:1147:HOH:O	2.14	0.66
1:B:513:PRO:CB	1:B:703:MET:HE1	2.26	0.66
1:B:525:ASN:HD22	1:B:547:SER:H	1.41	0.66
1:B:794:ARG:HD2	6:B:2247:HOH:O	1.95	0.66
3:B:1918:G6P:H61	6:B:2196:HOH:O	1.96	0.66
1:A:773:SER:O	1:A:777:LYS:HG2	1.96	0.66
1:A:242:LEU:HD23	1:A:252:GLU:O	1.96	0.66
1:B:200:ASP:CG	1:B:201:ALA:N	2.51	0.66
1:A:303:GLY:H	1:A:336:THR:CG2	2.08	0.65
1:B:479:LEU:HD23	1:B:483:MET:CE	2.25	0.65
1:B:480:THR:OG1	1:B:481:LYS:N	2.27	0.65
1:A:56:ASN:N	1:A:57:PRO:HD3	2.12	0.65
1:A:189:LEU:CD1	1:A:203:ILE:HD11	2.22	0.65
1:A:405:ARG:CZ	1:A:437:ASP:HA	2.26	0.65
1:A:575:PHE:O	1:A:579:VAL:HG13	1.96	0.65
1:A:145:ASP:OD1	6:A:1008:HOH:O	2.15	0.65
1:A:507:ALA:HA	6:A:1186:HOH:O	1.97	0.65
1:B:586:LEU:C	6:B:2249:HOH:O	2.40	0.65
1:A:492:ARG:HD3	6:A:1081:HOH:O	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:LEU:HD13	1:A:506:ASN:OD1	1.97	0.64
1:A:81:ILE:O	1:A:82:ALA:CB	2.46	0.64
1:A:598:LEU:HD12	1:A:598:LEU:C	2.23	0.64
1:A:662:MET:CE	1:A:687:MET:HE3	2.28	0.64
1:B:76:GLU:HG3	1:B:455:MET:SD	2.37	0.64
1:A:62:LYS:NZ	6:A:1057:HOH:O	1.77	0.64
1:A:515:PHE:HE2	1:A:608:GLN:O	1.81	0.64
1:B:72:PRO:HB3	1:B:455:MET:HE2	1.79	0.64
1:A:562:ILE:HD12	6:A:1140:HOH:O	1.98	0.63
1:A:778:THR:HB	1:A:781:ILE:CD1	2.22	0.63
1:A:26:LEU:HD22	1:A:29:MET:CE	2.27	0.63
1:B:76:GLU:CD	1:B:76:GLU:H	2.05	0.63
1:B:114:THR:CG2	1:B:118:ILE:HG21	2.27	0.63
1:B:244:HIS:CD2	1:B:396:ARG:HH21	2.16	0.63
1:B:496:GLU:CD	1:B:844:LYS:HE2	2.22	0.63
1:B:483:MET:HB3	6:B:2176:HOH:O	1.98	0.63
1:A:658:THR:HG23	1:A:685:CYS:CB	2.27	0.63
1:B:727:ARG:NH2	6:B:2180:HOH:O	2.21	0.63
1:A:80:PHE:HB3	1:A:149:PRO:O	1.99	0.63
1:A:768:PHE:C	1:A:770:GLY:H	2.06	0.63
1:A:71:ILE:HD13	1:A:218:GLY:HA3	1.81	0.63
1:B:313:MET:CE	1:B:319:LEU:CD1	2.77	0.63
1:A:23:ASP:OD1	1:A:373:HIS:CE1	2.52	0.63
1:A:710:GLY:O	1:A:739:GLN:HA	1.98	0.62
1:A:795:LEU:CD1	1:A:799:GLN:HG2	2.29	0.62
1:B:219:TYR:CD2	1:B:455:MET:HE2	2.33	0.62
1:B:734:LEU:HD13	6:B:2229:HOH:O	1.98	0.62
3:B:1916:G6P:C6	6:B:2027:HOH:O	2.38	0.62
1:B:114:THR:HG22	1:B:118:ILE:HB	1.81	0.62
1:B:845:ILE:CD1	1:B:849:ARG:CZ	2.77	0.62
1:A:518:ARG:NH1	1:A:521:ASP:HB2	2.15	0.62
1:A:313:MET:HG2	1:A:318:LEU:HD12	1.80	0.62
1:B:480:THR:HG22	1:B:483:MET:HG3	1.80	0.62
1:B:479:LEU:CD2	1:B:483:MET:HE3	2.28	0.62
1:B:549:LYS:CG	1:B:550:LYS:H	2.12	0.62
1:A:16:ASP:CB	6:A:1055:HOH:O	2.48	0.62
1:A:287:ASN:HD22	1:A:287:ASN:N	1.90	0.62
1:A:595:ARG:HG3	1:A:648:ASP:OD2	1.99	0.61
1:A:724:HIS:HE1	6:A:1115:HOH:O	1.82	0.61
1:A:875:MET:HE3	1:A:876:HIS:CD2	2.36	0.61
1:B:25:TYR:OH	1:B:312:LYS:HG2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:VAL:HG23	1:A:654:VAL:HG21	1.81	0.61
1:A:715:ASN:HD22	1:A:715:ASN:N	1.97	0.61
1:B:214:MET:HE3	1:B:215:MET:HE3	1.81	0.61
1:B:480:THR:N	1:B:483:MET:HG3	2.10	0.61
1:B:110:GLU:CD	1:B:141:ARG:HH22	2.08	0.61
1:B:463:LEU:HD23	1:B:467:HIS:NE2	2.16	0.61
1:A:306:VAL:HG11	1:A:334:PHE:CE1	2.36	0.60
1:A:437:ASP:OD1	1:A:437:ASP:N	2.33	0.60
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.16	0.60
1:A:29:MET:CB	1:A:377:ILE:HD11	2.16	0.60
1:A:157:PRO:HB3	1:A:260:GLU:CD	2.26	0.60
1:B:518:ARG:NH1	1:B:521:ASP:N	2.49	0.60
1:A:16:ASP:HB3	6:A:1055:HOH:O	2.00	0.60
1:A:671:THR:CB	1:A:857:THR:HG23	2.27	0.60
1:B:84:ASP:HA	1:B:153:THR:HB	1.83	0.60
1:A:313:MET:HE1	1:A:319:LEU:HD11	1.84	0.60
1:B:492:ARG:HG2	1:B:840:ALA:HB1	1.83	0.60
1:B:595:ARG:HH12	1:B:648:ASP:HB3	1.67	0.60
1:A:690:MET:CE	1:A:703:MET:HE2	2.24	0.60
1:A:857:THR:OG1	1:A:891:LEU:CD2	2.50	0.60
1:A:899:LYS:O	1:A:902:ALA:HB3	2.02	0.60
1:B:570:THR:HG22	1:B:573:GLU:H	1.67	0.60
1:A:115:PRO:HD2	1:A:118:ILE:HG13	1.83	0.59
1:B:323:ARG:HH21	1:B:362:GLU:HB2	1.64	0.59
1:B:72:PRO:HD3	1:B:215:MET:CE	2.32	0.59
1:B:143:ILE:HG22	1:B:146:LYS:CE	2.32	0.59
1:B:862:GLY:O	1:B:866:LYS:HG2	2.03	0.59
1:A:541:LEU:HG	1:A:557:ASN:HB3	1.85	0.59
1:A:550:LYS:O	1:A:552:THR:HG23	2.02	0.59
1:A:687:MET:CE	1:A:704:CYS:SG	2.91	0.59
1:A:792:SER:HG	1:A:795:LEU:HD23	1.67	0.59
1:A:722:ARG:NH1	1:A:740:ARG:HD3	2.17	0.59
1:A:832:GLN:CG	1:A:874:ILE:HD11	2.26	0.59
1:B:480:THR:HG23	1:B:483:MET:N	2.16	0.59
1:A:570:THR:HG22	1:A:571:GLY:N	2.16	0.59
1:B:164:ASP:OD1	6:B:2145:HOH:O	2.17	0.59
1:A:420:HIS:HD2	1:A:423:TYR:H	1.50	0.58
1:A:634:VAL:HG21	1:A:654:VAL:HG23	1.85	0.58
1:B:390:LEU:HD13	1:B:390:LEU:O	2.02	0.58
1:A:662:MET:SD	1:A:687:MET:HE3	2.43	0.58
1:B:136:ASP:OD1	1:B:140:LYS:NZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:VAL:O	1:A:908:GLY:O	2.21	0.58
1:A:138:MET:HB3	1:A:143:ILE:CD1	2.34	0.58
1:A:767:LEU:HD13	1:A:768:PHE:CD2	2.39	0.58
1:B:323:ARG:NH2	1:B:362:GLU:O	2.36	0.58
1:B:429:LYS:NZ	5:B:1999:ANP:O1B	2.36	0.58
1:A:845:ILE:CD1	1:A:854:LEU:HD21	2.32	0.58
1:B:71:ILE:HG22	1:B:215:MET:HE3	1.83	0.58
1:B:313:MET:HE3	1:B:319:LEU:HD11	1.78	0.58
1:A:588:TYR:CE1	1:B:331:ARG:HB2	2.38	0.58
1:B:721:ILE:HD11	6:B:2176:HOH:O	2.04	0.58
1:A:77:LYS:HD3	1:A:98:ASN:OD1	2.03	0.58
1:A:243:ARG:NH1	1:A:243:ARG:HB3	2.18	0.58
1:A:503:THR:O	1:A:505:ASN:N	2.37	0.58
1:A:662:MET:HE1	1:A:687:MET:CE	2.34	0.58
1:B:518:ARG:HD2	1:B:519:THR:O	2.03	0.58
1:A:550:LYS:O	1:A:551:ARG:C	2.47	0.57
1:B:479:LEU:HD22	1:B:721:ILE:HD11	1.85	0.57
1:A:866:LYS:HZ3	1:A:892:LEU:HD11	1.68	0.57
1:B:570:THR:HG22	1:B:572:GLU:H	1.68	0.57
1:A:176:LYS:HD2	1:A:286:LEU:HD22	1.85	0.57
1:A:91:ARG:HG2	1:A:93:LEU:HD21	1.85	0.57
1:A:116:GLU:HG3	1:A:120:HIS:ND1	2.20	0.57
1:A:875:MET:O	1:A:879:VAL:HG23	2.04	0.57
1:B:845:ILE:HD11	1:B:849:ARG:NH1	2.20	0.57
1:A:619:TRP:CD1	1:A:624:LYS:HA	2.40	0.57
1:A:306:VAL:O	1:A:310:LEU:HG	2.04	0.57
1:B:836:ALA:O	1:B:839:ALA:HB3	2.05	0.57
1:B:910:ARG:HG2	1:B:911:LEU:HD23	1.86	0.57
1:A:414:GLY:CA	3:A:919:G6P:H62	2.35	0.56
1:B:481:LYS:HA	6:B:2224:HOH:O	2.06	0.56
1:B:578:ILE:HG21	6:B:2246:HOH:O	1.92	0.56
1:A:299:GLY:O	1:A:336:THR:HG21	2.06	0.56
1:A:313:MET:CE	1:A:319:LEU:CD1	2.68	0.56
1:A:335:ASN:C	1:A:335:ASN:ND2	2.51	0.56
1:A:529:LEU:HD11	1:A:586:LEU:HD21	1.86	0.56
1:B:98:ASN:OD1	1:B:104:ASN:ND2	2.39	0.56
1:B:570:THR:HB	1:B:573:GLU:HG3	1.88	0.56
1:A:431:LEU:HD22	1:A:442:PHE:HZ	1.70	0.56
1:A:510:LYS:O	1:A:511:MET:C	2.49	0.56
1:A:888:VAL:HG22	1:A:890:PHE:CE1	2.41	0.56
1:B:550:LYS:HG2	1:B:552:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:LEU:HD23	1:A:911:LEU:N	2.20	0.56
1:B:480:THR:O	1:B:483:MET:N	2.36	0.56
1:A:77:LYS:HB2	1:A:98:ASN:HA	1.87	0.56
1:B:88:SER:OG	3:B:1916:G6P:O2P	2.20	0.56
1:A:652:VAL:CG1	1:A:908:GLY:HA3	2.35	0.55
1:B:136:ASP:OD1	1:B:140:LYS:CE	2.54	0.55
1:B:563:PRO:HB2	1:B:565:GLU:CG	2.30	0.55
1:B:782:PHE:O	1:B:787:LEU:HD22	2.06	0.55
1:B:911:LEU:HD12	6:B:2253:HOH:O	2.05	0.55
1:A:603:SER:OG	1:A:657:ASP:CG	2.49	0.55
1:A:875:MET:CE	1:A:876:HIS:CD2	2.89	0.55
1:B:769:ARG:HD3	6:B:2251:HOH:O	1.90	0.55
1:A:138:MET:HE2	1:A:143:ILE:HD11	1.86	0.55
1:B:29:MET:HE2	1:B:381:ARG:CZ	2.36	0.55
1:B:143:ILE:CG2	1:B:146:LYS:HE3	2.33	0.55
1:B:644:ARG:HH11	1:B:644:ARG:HG3	1.72	0.55
1:A:93:LEU:HD13	1:A:109:SER:HB3	1.89	0.55
1:A:507:ALA:O	1:A:510:LYS:NZ	2.37	0.55
1:B:401:LYS:HZ2	1:B:403:THR:HG21	1.72	0.55
1:A:77:LYS:HD3	1:A:98:ASN:CG	2.32	0.55
1:A:266:ASP:C	1:A:267:ASP:O	2.47	0.55
1:A:138:MET:HB3	1:A:143:ILE:HD12	1.88	0.55
1:A:846:ARG:HG2	1:A:846:ARG:HH11	1.72	0.55
1:B:136:ASP:O	1:B:140:LYS:HE2	2.07	0.55
1:B:579:VAL:O	1:B:582:ILE:HB	2.06	0.55
1:A:40:MET:HG3	1:A:388:ALA:O	2.07	0.55
1:A:91:ARG:HG2	1:A:93:LEU:HD22	1.87	0.55
1:A:430:THR:HG22	1:A:434:LEU:HD22	1.89	0.55
1:B:403:THR:HG23	1:B:405:ARG:O	2.06	0.55
1:B:668:GLU:OE1	1:B:668:GLU:N	2.35	0.55
1:A:93:LEU:CD2	1:A:93:LEU:N	2.70	0.54
1:A:519:THR:OG1	1:A:520:PRO:HD3	2.07	0.54
1:B:734:LEU:HB3	6:B:2229:HOH:O	2.07	0.54
1:A:265:GLY:O	1:A:267:ASP:O	2.25	0.54
1:B:240:GLU:HG3	1:B:241:GLU:N	2.22	0.54
1:B:862:GLY:HA2	3:B:1918:G6P:H62	1.89	0.54
1:A:62:LYS:HZ3	1:A:157:PRO:HB2	1.73	0.54
1:A:490:ARG:NH1	1:A:717:CYS:O	2.40	0.54
1:A:564:ILE:CD1	1:A:564:ILE:C	2.80	0.54
1:A:910:ARG:O	1:A:911:LEU:C	2.50	0.54
1:B:732:TYR:O	1:B:779:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:ND2	1:A:236:ALA:H	2.05	0.54
1:A:521:ASP:CB	6:A:1169:HOH:O	2.14	0.54
1:A:265:GLY:O	1:A:266:ASP:C	2.49	0.54
1:A:405:ARG:NH2	6:A:1077:HOH:O	2.40	0.54
1:B:53:ARG:HG3	1:B:54:ASP:N	2.22	0.54
1:A:299:GLY:O	1:A:336:THR:CG2	2.56	0.54
1:A:562:ILE:HG13	1:A:567:MET:SD	2.48	0.54
1:A:644:ARG:O	1:A:645:GLU:C	2.51	0.54
1:A:34:GLU:H	1:A:34:GLU:CD	2.14	0.54
1:A:676:LEU:O	1:A:860:VAL:HA	2.09	0.54
1:A:857:THR:CB	1:A:891:LEU:HD21	2.38	0.54
1:B:235:ASN:HD21	1:B:260:GLU:N	2.06	0.54
1:B:570:THR:CG2	1:B:572:GLU:H	2.20	0.54
1:B:361:VAL:O	1:B:362:GLU:C	2.51	0.53
1:A:145:ASP:C	1:A:146:LYS:O	2.48	0.53
1:A:422:GLN:O	1:A:426:ARG:HG3	2.08	0.53
1:A:583:SER:OG	1:A:592:LYS:NZ	2.41	0.53
1:B:563:PRO:CB	1:B:565:GLU:HG3	2.31	0.53
1:A:506:ASN:C	1:A:506:ASN:ND2	2.63	0.53
1:A:61:VAL:O	1:A:63:MET:HG2	2.08	0.53
1:A:110:GLU:O	1:A:111:VAL:CG2	2.51	0.53
1:A:265:GLY:O	1:A:266:ASP:O	2.27	0.53
1:A:505:ASN:O	1:A:507:ALA:C	2.51	0.53
1:A:570:THR:CG2	1:A:571:GLY:N	2.71	0.53
1:B:592:LYS:NZ	1:B:646:GLU:OE2	2.37	0.53
1:B:639:ASP:O	1:B:643:ARG:HG3	2.08	0.53
1:A:83:LEU:HD21	1:A:134:LEU:HD13	1.90	0.53
1:A:767:LEU:HD23	1:A:818:LEU:HD12	1.89	0.53
1:B:553:VAL:HG21	1:B:899:LYS:HG3	1.90	0.53
1:B:595:ARG:HH11	1:B:648:ASP:HB3	1.67	0.53
1:B:72:PRO:HD3	1:B:215:MET:HE2	1.91	0.53
1:A:522:GLY:CA	1:A:551:ARG:HH21	2.18	0.53
1:B:114:THR:HG23	1:B:118:ILE:HG21	1.90	0.53
1:A:56:ASN:H	1:A:57:PRO:HD3	1.72	0.53
1:A:895:ASP:O	1:A:895:ASP:OD1	2.26	0.53
1:B:605:PRO:HB3	1:B:708:GLU:HG3	1.91	0.53
1:B:644:ARG:HG3	1:B:644:ARG:NH1	2.24	0.53
1:B:652:VAL:HG13	1:B:908:GLY:HA3	1.90	0.53
1:B:193:ILE:HD13	1:B:201:ALA:HB3	1.91	0.53
1:A:562:ILE:O	1:A:562:ILE:CG1	2.56	0.52
1:A:641:ILE:CD1	1:A:649:LEU:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:ARG:HA	1:B:495:MET:HE3	1.91	0.52
1:A:647:PHE:HD1	1:A:647:PHE:H	1.58	0.52
1:A:690:MET:CE	1:A:703:MET:HB2	2.38	0.52
1:A:759:ILE:CD1	1:A:776:LEU:CD2	2.88	0.52
1:B:591:ILE:HB	1:B:596:MET:HE2	1.91	0.52
1:A:480:THR:HG23	1:A:482:ASP:H	1.73	0.52
1:A:656:ASN:HD21	1:A:658:THR:HB	1.68	0.52
1:B:492:ARG:HD2	1:B:495:MET:CE	2.39	0.52
1:A:397:LEU:O	1:A:401:LYS:HG2	2.09	0.52
1:A:735:ASN:N	1:A:735:ASN:ND2	2.41	0.52
1:B:324:ILE:HG23	1:B:328:LEU:HD23	1.91	0.52
1:B:665:CYS:SG	1:B:893:SER:HB3	2.49	0.52
1:B:752:GLU:CD	1:B:755:ARG:NH1	2.47	0.52
1:A:656:ASN:ND2	1:A:658:THR:CG2	2.64	0.52
1:B:79:ASP:OD1	1:B:148:LEU:HD13	2.09	0.52
1:B:114:THR:CG2	1:B:118:ILE:CG2	2.87	0.52
1:B:529:LEU:HB3	1:B:598:LEU:HB2	1.92	0.52
1:A:83:LEU:HD23	1:A:92:ILE:HG12	1.92	0.51
1:A:189:LEU:HD13	1:A:203:ILE:CD1	2.29	0.51
1:B:480:THR:CG2	1:B:483:MET:CG	2.82	0.51
1:A:907:VAL:O	1:A:908:GLY:C	2.52	0.51
1:A:198:ASP:HB3	1:A:199:TYR:HD1	1.75	0.51
1:A:208:ASN:ND2	1:A:210:THR:H	2.08	0.51
1:A:403:THR:OG1	1:A:405:ARG:O	2.22	0.51
1:A:444:LEU:O	1:A:446:GLU:N	2.43	0.51
1:B:570:THR:HG22	1:B:572:GLU:N	2.24	0.51
1:A:119:VAL:HG13	1:A:175:PHE:HA	1.93	0.51
1:A:240:GLU:O	1:A:254:ARG:HB3	2.11	0.51
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.23	0.51
1:A:267:ASP:OD1	1:A:267:ASP:C	2.53	0.51
1:A:673:GLU:OE1	1:A:849:ARG:NH2	2.43	0.51
1:A:83:LEU:N	1:A:151:GLY:O	2.37	0.51
1:A:406:LEU:HD23	1:A:438:SER:OG	2.11	0.51
1:A:414:GLY:HA2	3:A:919:G6P:C6	2.39	0.51
1:A:564:ILE:C	1:A:564:ILE:HD12	2.36	0.51
1:B:56:ASN:N	1:B:57:PRO:CD	2.74	0.51
1:B:193:ILE:O	1:B:196:ARG:O	2.29	0.51
1:A:287:ASN:H	1:A:287:ASN:ND2	2.01	0.51
1:A:514:SER:HG	1:A:704:CYS:HB3	1.75	0.51
1:A:758:LEU:O	1:A:762:THR:CG2	2.59	0.50
1:A:793:ASP:OD1	1:A:870:HIS:NE2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:O	1:B:310:LEU:HG	2.11	0.50
1:B:312:LYS:HG3	1:B:316:GLU:OE2	2.12	0.50
1:A:831:ALA:CB	1:A:874:ILE:HG13	2.41	0.50
1:B:136:ASP:OD1	1:B:140:LYS:HE2	2.11	0.50
1:A:553:VAL:HG11	1:A:899:LYS:HG3	1.94	0.50
1:B:570:THR:O	1:B:571:GLY:C	2.54	0.50
1:A:855:ASN:OD1	1:A:887:ASN:HB3	2.11	0.50
1:B:93:LEU:HG	1:B:109:SER:CB	2.41	0.50
1:B:845:ILE:CD1	1:B:849:ARG:NH1	2.74	0.50
1:A:806:GLN:NE2	1:A:806:GLN:HA	2.27	0.50
1:B:235:ASN:ND2	1:B:236:ALA:H	2.10	0.50
1:B:806:GLN:O	1:B:806:GLN:HG3	2.01	0.50
1:B:76:GLU:CD	1:B:455:MET:HE1	2.37	0.50
1:B:591:ILE:O	1:B:596:MET:CE	2.59	0.50
1:A:198:ASP:CB	1:A:199:TYR:HD1	2.25	0.50
1:B:845:ILE:HD12	1:B:849:ARG:NH2	2.27	0.50
1:B:343:GLU:OE2	1:B:420:HIS:CE1	2.65	0.50
1:B:531:LEU:HD11	1:B:582:ILE:HD11	1.93	0.50
1:A:466:GLN:HG3	1:A:766:PHE:CD1	2.47	0.49
1:B:76:GLU:CG	1:B:455:MET:CE	2.79	0.49
1:B:413:ASP:OD1	1:B:414:GLY:N	2.43	0.49
1:A:875:MET:CE	1:A:876:HIS:HD2	2.25	0.49
1:B:355:ILE:HG23	6:B:2019:HOH:O	2.11	0.49
1:A:507:ALA:O	1:A:510:LYS:HE2	2.12	0.49
1:A:713:GLY:CA	1:A:718:LEU:HD12	2.40	0.49
1:A:896:GLY:N	6:A:1112:HOH:O	2.45	0.49
1:B:349:LEU:HD13	1:B:372:GLN:NE2	2.28	0.49
1:B:549:LYS:HG2	1:B:550:LYS:N	2.25	0.49
1:B:595:ARG:HH12	1:B:648:ASP:CB	2.23	0.49
1:A:71:ILE:CG1	1:A:215:MET:CE	2.87	0.49
1:A:79:ASP:O	1:A:149:PRO:HD2	2.13	0.49
1:A:400:ASN:HB2	6:A:1147:HOH:O	2.11	0.49
1:B:543:VAL:HG13	1:B:555:MET:HG2	1.94	0.49
1:A:519:THR:OG1	1:A:520:PRO:HD2	2.12	0.49
1:A:29:MET:HE1	1:A:309:ILE:CD1	2.43	0.49
1:A:609:THR:O	1:A:610:SER:HB3	2.13	0.49
1:A:380:PHE:CE2	1:A:426:ARG:HD3	2.48	0.49
1:A:618:THR:HG23	1:A:618:THR:O	2.13	0.49
1:B:127:PHE:CE1	1:B:185:VAL:HG23	2.48	0.49
1:A:97:VAL:CG1	1:A:105:VAL:CA	2.90	0.49
1:A:394:LEU:HD22	1:A:408:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:THR:HG22	1:B:434:LEU:HD22	1.95	0.49
1:B:593:GLY:N	1:B:594:PRO:HD2	2.27	0.49
1:A:29:MET:HE1	1:A:309:ILE:HD11	1.94	0.48
1:A:420:HIS:HD2	1:A:423:TYR:N	2.11	0.48
1:A:530:ALA:HA	1:A:598:LEU:CD1	2.43	0.48
1:A:767:LEU:CD1	1:A:768:PHE:CD2	2.96	0.48
1:A:71:ILE:CG1	1:A:215:MET:HE1	2.36	0.48
1:A:112:TYR:OH	1:A:137:PHE:HB2	2.13	0.48
1:A:857:THR:HB	1:A:891:LEU:HD21	1.96	0.48
1:B:271:GLU:OE1	1:B:279:ARG:NH2	2.33	0.48
1:B:769:ARG:CG	1:B:769:ARG:HH11	2.25	0.48
1:A:46:GLU:HA	1:A:49:ASN:HB2	1.96	0.48
1:A:79:ASP:OD2	1:A:148:LEU:CD2	2.61	0.48
1:A:792:SER:OG	1:A:795:LEU:CD2	2.53	0.48
1:A:29:MET:HB2	1:A:377:ILE:CD1	2.20	0.48
1:B:683:ASN:HA	1:B:709:TRP:CD1	2.49	0.48
1:A:138:MET:CB	1:A:143:ILE:HD11	2.44	0.48
1:A:261:TRP:CD1	1:A:261:TRP:C	2.91	0.48
1:A:492:ARG:HD2	1:A:492:ARG:O	2.13	0.48
1:A:895:ASP:C	6:A:1112:HOH:O	2.57	0.48
1:A:529:LEU:O	1:A:598:LEU:HA	2.14	0.48
1:A:652:VAL:HG11	1:A:908:GLY:HA3	1.96	0.48
1:A:720:ASP:HB3	1:A:721:ILE:HG23	1.95	0.48
1:A:758:LEU:O	1:A:762:THR:HG23	2.13	0.48
1:B:119:VAL:CG2	1:B:175:PHE:CZ	2.97	0.48
1:A:62:LYS:NZ	1:A:260:GLU:HG3	2.29	0.48
1:A:150:VAL:HB	1:A:203:ILE:HA	1.95	0.48
1:A:214:MET:HE2	1:A:214:MET:HB3	1.76	0.48
1:A:425:ARG:NH1	5:A:999:ANP:O1A	2.44	0.48
1:A:892:LEU:HD13	1:A:893:SER:N	2.29	0.48
1:A:570:THR:HG22	1:A:572:GLU:H	1.79	0.48
1:B:83:LEU:HD12	1:B:152:PHE:HD1	1.75	0.48
1:A:598:LEU:HD12	1:A:599:GLY:H	1.71	0.48
1:A:267:ASP:O	1:A:267:ASP:OD1	2.31	0.48
1:A:577:HIS:O	1:A:578:ILE:C	2.55	0.48
1:B:174:ARG:HH11	1:B:174:ARG:CG	2.18	0.48
1:A:846:ARG:HG2	1:A:846:ARG:NH1	2.29	0.47
1:A:910:ARG:HB3	1:A:911:LEU:H	1.55	0.47
1:B:571:GLY:HA2	1:B:628:CYS:SG	2.54	0.47
1:B:675:GLY:O	1:B:684:ALA:HA	2.14	0.47
1:A:803:ILE:HG22	1:A:804:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ASP:CG	1:A:544:LYS:HG2	2.38	0.47
1:A:663:MET:O	1:A:664:THR:C	2.57	0.47
1:A:235:ASN:HD21	1:A:260:GLU:N	2.12	0.47
1:A:680:THR:O	1:A:746:SER:HB3	2.12	0.47
1:A:759:ILE:HD13	1:A:776:LEU:CD2	2.44	0.47
1:B:38:ASP:OD1	1:B:42:ARG:HD2	2.14	0.47
1:B:412:VAL:HG12	1:B:413:ASP:N	2.30	0.47
1:A:266:ASP:O	1:A:267:ASP:C	2.58	0.47
1:A:563:PRO:CG	1:A:566:ILE:HD12	2.39	0.47
1:A:570:THR:CB	1:A:573:GLU:OE1	2.58	0.47
1:B:48:LYS:HE2	1:B:48:LYS:HB3	1.56	0.47
1:A:414:GLY:N	3:A:919:G6P:H62	2.29	0.47
1:B:145:ASP:C	1:B:147:LYS:H	2.23	0.47
1:B:148:LEU:HA	1:B:149:PRO:HD3	1.79	0.47
1:B:571:GLY:N	1:B:626:THR:O	2.39	0.47
1:A:77:LYS:CD	1:A:98:ASN:CG	2.88	0.47
1:A:187:LYS:HE2	1:A:187:LYS:HB3	1.60	0.47
1:A:417:TYR:OH	1:A:428:HIS:NE2	2.40	0.47
1:A:512:LEU:HA	1:A:513:PRO:HD3	1.69	0.47
1:A:652:VAL:HG12	1:A:652:VAL:O	2.13	0.47
1:A:690:MET:HE2	1:A:703:MET:HB3	1.94	0.47
1:B:53:ARG:CG	1:B:54:ASP:N	2.77	0.47
1:B:185:VAL:HG23	1:B:185:VAL:O	2.13	0.47
1:B:525:ASN:ND2	1:B:546:ARG:HA	2.30	0.47
1:A:107:MET:HE3	1:A:107:MET:HB2	1.57	0.47
1:A:619:TRP:HA	1:A:619:TRP:CE3	2.50	0.47
1:A:567:MET:HE1	1:A:623:PHE:CE1	2.50	0.47
1:B:241:GLU:OE2	1:B:254:ARG:HD2	2.14	0.47
1:B:343:GLU:OE2	1:B:420:HIS:HE1	1.98	0.47
1:A:214:MET:HE3	1:A:215:MET:CE	2.19	0.46
1:A:287:ASN:N	1:A:287:ASN:ND2	2.57	0.46
1:A:444:LEU:C	1:A:444:LEU:HD13	2.40	0.46
1:A:487:VAL:HG12	1:A:836:ALA:CB	2.45	0.46
1:A:529:LEU:C	1:A:598:LEU:HD13	2.40	0.46
1:A:570:THR:HB	1:A:573:GLU:CD	2.39	0.46
1:B:158:CYS:HA	1:B:167:ILE:O	2.15	0.46
1:B:488:LYS:HD2	1:B:839:ALA:HB1	1.97	0.46
1:A:372:GLN:O	1:A:376:THR:HG23	2.15	0.46
1:A:847:GLU:O	1:A:848:ASN:C	2.57	0.46
1:A:878:THR:O	1:A:882:LEU:HG	2.14	0.46
1:B:136:ASP:O	1:B:139:GLU:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLU:OE2	1:A:15:LYS:HE3	2.15	0.46
1:A:143:ILE:CD1	1:A:143:ILE:C	2.87	0.46
1:A:506:ASN:N	1:A:506:ASN:HD22	2.13	0.46
1:A:678:VAL:HB	1:A:865:TYR:HB2	1.98	0.46
1:B:196:ARG:O	1:B:196:ARG:HG3	2.15	0.46
1:B:693:VAL:HG11	1:B:703:MET:HE2	1.98	0.46
1:B:619:TRP:CD1	1:B:624:LYS:HA	2.50	0.46
1:B:662:MET:HE1	1:B:687:MET:SD	2.56	0.46
1:A:193:ILE:HD13	1:A:201:ALA:CB	2.46	0.46
1:A:605:PRO:HB3	1:A:708:GLU:HG3	1.97	0.46
1:A:861:ASP:OD1	1:A:862:GLY:N	2.44	0.46
1:A:868:HIS:HA	1:A:869:PRO:HD2	1.65	0.46
1:A:93:LEU:HD22	1:A:93:LEU:N	2.31	0.46
1:A:235:ASN:HD21	1:A:260:GLU:H	1.63	0.46
1:B:93:LEU:HG	1:B:109:SER:HB3	1.98	0.45
1:B:480:THR:O	1:B:481:LYS:C	2.58	0.45
1:B:93:LEU:HD12	1:B:93:LEU:N	2.31	0.45
1:B:855:ASN:ND2	1:B:887:ASN:HB3	2.25	0.45
1:A:266:ASP:O	1:A:267:ASP:O	2.35	0.45
1:A:313:MET:HE3	1:A:319:LEU:CG	2.47	0.45
1:A:687:MET:CE	1:A:704:CYS:CB	2.92	0.45
1:A:739:GLN:O	1:A:743:LYS:HG3	2.16	0.45
1:A:891:LEU:N	1:A:891:LEU:CD2	2.75	0.45
1:B:119:VAL:HG22	1:B:175:PHE:CG	2.51	0.45
1:A:82:ALA:HA	1:A:151:GLY:O	2.16	0.45
1:A:791:GLU:OE1	1:A:824:GLY:HA2	2.16	0.45
1:B:189:LEU:HD13	1:B:203:ILE:CD1	2.38	0.45
1:B:521:ASP:OD1	1:B:521:ASP:C	2.58	0.45
1:B:529:LEU:HD22	1:B:596:MET:SD	2.56	0.45
1:A:480:THR:CG2	1:A:482:ASP:H	2.28	0.45
1:A:507:ALA:O	1:A:510:LYS:CE	2.65	0.45
1:B:203:ILE:O	1:B:203:ILE:HG22	2.16	0.45
1:B:119:VAL:CG2	1:B:175:PHE:CE1	2.99	0.45
1:B:144:LYS:HE2	1:B:199:TYR:HB3	1.98	0.45
1:B:710:GLY:O	1:B:739:GLN:HA	2.16	0.45
1:B:848:ASN:N	1:B:848:ASN:HD22	2.15	0.45
1:A:492:ARG:NH2	1:A:496:GLU:OE2	2.39	0.45
1:A:818:LEU:HA	1:A:821:THR:HG23	1.99	0.45
1:A:45:LYS:HD2	1:A:45:LYS:O	2.17	0.45
1:A:683:ASN:HA	1:A:709:TRP:CD1	2.51	0.45
1:B:89:SER:N	6:B:2250:HOH:O	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:THR:HG22	1:B:118:ILE:CB	2.47	0.45
1:B:880:LYS:HE2	1:B:880:LYS:HB2	1.48	0.45
1:A:598:LEU:C	1:A:598:LEU:CD1	2.90	0.45
1:A:759:ILE:HD13	1:A:776:LEU:HD21	1.98	0.45
1:A:866:LYS:HZ1	1:A:892:LEU:HD11	1.77	0.44
1:A:80:PHE:CD1	1:A:80:PHE:N	2.85	0.44
1:B:486:GLU:O	1:B:490:ARG:HG3	2.18	0.44
1:B:652:VAL:O	1:B:652:VAL:CG1	2.66	0.44
1:A:519:THR:HA	1:A:663:MET:SD	2.57	0.44
1:B:463:LEU:HD23	1:B:467:HIS:CE1	2.51	0.44
1:B:592:LYS:HE3	1:B:592:LYS:HB2	1.42	0.44
1:B:769:ARG:NH1	1:B:769:ARG:HG3	2.32	0.44
1:A:540:VAL:HG12	1:A:585:PHE:CD2	2.52	0.44
1:B:20:LYS:HA	1:B:20:LYS:HD3	1.75	0.44
1:B:754:VAL:O	1:B:758:LEU:HG	2.17	0.44
1:A:477:PHE:CZ	1:A:757:ILE:HD11	2.53	0.44
1:A:563:PRO:O	1:A:565:GLU:N	2.50	0.44
1:A:908:GLY:O	1:A:909:VAL:C	2.59	0.44
1:A:72:PRO:CD	6:A:1102:HOH:O	2.58	0.44
1:A:229:ILE:O	1:A:234:THR:HA	2.17	0.44
1:A:542:LEU:HB3	1:A:556:HIS:HB2	1.99	0.44
1:A:598:LEU:CD1	1:A:599:GLY:N	2.66	0.44
1:A:839:ALA:HB1	1:A:883:SER:OG	2.18	0.44
1:B:244:HIS:HD2	1:B:396:ARG:HH21	1.65	0.44
1:A:514:SER:O	1:A:515:PHE:HB2	2.17	0.44
1:B:407:ARG:HG3	1:B:439:ASP:HB3	2.00	0.44
1:A:13:GLU:OE2	1:A:15:LYS:CE	2.65	0.44
1:A:221:ASP:OD1	1:A:223:HIS:HB2	2.17	0.44
1:A:562:ILE:N	1:A:562:ILE:CD1	2.79	0.44
1:A:595:ARG:CZ	1:A:650:ASP:HB2	2.46	0.44
1:A:596:MET:O	1:A:649:LEU:HB2	2.17	0.44
1:B:313:MET:HE1	1:B:319:LEU:HD11	1.96	0.44
1:B:518:ARG:NH1	1:B:524:GLU:OE2	2.50	0.44
1:B:539:ARG:NH2	6:B:2193:HOH:O	2.21	0.44
1:B:563:PRO:CB	1:B:565:GLU:CG	2.94	0.44
1:B:71:ILE:HA	1:B:215:MET:SD	2.58	0.44
1:B:432:ARG:HH11	1:B:432:ARG:HD2	1.67	0.44
1:A:656:ASN:ND2	1:A:658:THR:CB	2.55	0.43
1:A:80:PHE:HD2	1:A:149:PRO:HB2	1.83	0.43
1:A:204:VAL:CG2	1:A:457:THR:HG23	2.48	0.43
1:A:607:GLN:HB3	1:A:615:ILE:CG1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:ILE:C	1:A:874:ILE:CD1	2.86	0.43
1:B:119:VAL:HG22	1:B:175:PHE:CD1	2.53	0.43
1:B:211:VAL:O	1:B:215:MET:HG2	2.18	0.43
1:B:286:LEU:O	1:B:286:LEU:HG	2.18	0.43
1:B:591:ILE:O	1:B:596:MET:HE1	2.17	0.43
1:A:560:TYR:CD2	1:A:581:CYS:HB3	2.53	0.43
1:B:536:THR:OG1	3:B:1918:G6P:O3P	2.29	0.43
1:A:558:LYS:HD3	1:A:560:TYR:OH	2.19	0.43
1:A:587:ASP:OD1	1:A:592:LYS:HE2	2.19	0.43
1:B:390:LEU:HD11	1:B:394:LEU:HD11	1.98	0.43
1:A:62:LYS:HZ3	1:A:157:PRO:CB	2.29	0.43
1:A:160:GLN:NE2	6:A:1108:HOH:O	2.14	0.43
1:B:72:PRO:CB	1:B:455:MET:HE2	2.47	0.43
1:B:140:LYS:HB2	1:B:140:LYS:HE3	1.36	0.43
1:B:251:ASP:OD1	1:B:801:ARG:NH2	2.42	0.43
1:B:510:LYS:O	1:B:511:MET:C	2.59	0.43
1:B:529:LEU:O	1:B:598:LEU:HA	2.18	0.43
1:A:666:ALA:C	1:A:668:GLU:N	2.74	0.43
1:A:871:PHE:CD1	1:A:871:PHE:C	2.97	0.43
1:B:76:GLU:CD	1:B:455:MET:CE	2.92	0.43
1:B:529:LEU:CD2	1:B:596:MET:SD	3.07	0.43
1:B:549:LYS:CG	1:B:550:LYS:N	2.79	0.43
1:B:669:GLU:OE2	1:B:670:PRO:HD2	2.18	0.43
1:A:529:LEU:O	1:A:598:LEU:HD13	2.19	0.43
1:A:759:ILE:CD1	1:A:776:LEU:CG	2.94	0.43
1:A:774:GLU:OE2	1:A:777:LYS:HE2	2.18	0.43
1:A:195:LYS:O	1:A:195:LYS:HG2	2.19	0.43
1:A:412:VAL:HG11	1:A:417:TYR:CE2	2.54	0.43
1:A:715:ASN:HD22	1:A:716:GLY:N	2.17	0.43
1:B:139:GLU:OE1	1:B:139:GLU:CA	2.66	0.43
1:B:139:GLU:OE1	1:B:139:GLU:HA	2.18	0.43
1:B:685:CYS:HA	1:B:705:ILE:O	2.19	0.43
1:A:208:ASN:ND2	1:A:210:THR:OG1	2.49	0.43
1:A:243:ARG:HG3	1:A:244:HIS:CD2	2.54	0.43
1:B:390:LEU:C	1:B:390:LEU:CD1	2.88	0.43
1:A:167:ILE:HD13	1:A:184:ASP:HB2	2.01	0.42
1:A:795:LEU:HD11	1:A:799:GLN:HG2	2.01	0.42
1:A:849:ARG:O	1:A:850:GLY:C	2.62	0.42
1:B:569:GLY:O	1:B:625:ALA:HA	2.19	0.42
1:A:71:ILE:HD13	1:A:215:MET:HE2	2.00	0.42
1:A:194:LYS:HB3	1:A:194:LYS:HE2	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TYR:HE2	1:A:444:LEU:HD23	1.84	0.42
1:A:672:CYS:HA	1:A:857:THR:O	2.19	0.42
1:B:519:THR:HB	1:B:520:PRO:CD	2.50	0.42
1:B:44:ARG:HD2	1:B:47:MET:HE3	2.01	0.42
1:B:104:ASN:N	1:B:104:ASN:OD1	2.52	0.42
1:A:73:ASP:C	1:A:73:ASP:OD1	2.62	0.42
1:A:157:PRO:HB3	1:A:260:GLU:OE1	2.19	0.42
1:A:487:VAL:HG12	1:A:836:ALA:HB1	2.01	0.42
1:B:558:LYS:HB3	1:B:560:TYR:CE1	2.55	0.42
1:B:682:SER:O	1:B:683:ASN:HB2	2.19	0.42
1:B:721:ILE:HD12	1:B:721:ILE:HG21	1.75	0.42
1:A:589:MET:HA	1:A:589:MET:HE2	2.01	0.42
1:A:77:LYS:HA	1:A:97:VAL:O	2.19	0.42
1:A:94:ARG:N	1:A:108:GLU:O	2.50	0.42
1:A:518:ARG:NH1	1:A:519:THR:O	2.50	0.42
1:B:479:LEU:HA	1:B:483:MET:CE	2.45	0.42
1:B:595:ARG:NH1	1:B:648:ASP:CB	2.66	0.42
1:B:674:VAL:HG12	1:B:858:VAL:HG13	2.01	0.42
1:A:673:GLU:CD	1:A:849:ARG:HH22	2.27	0.42
1:B:81:ILE:HB	1:B:150:VAL:HG22	2.02	0.42
1:A:176:LYS:HE2	6:A:1176:HOH:O	2.18	0.42
1:A:598:LEU:HD12	1:A:599:GLY:C	2.44	0.42
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.87	0.42
1:A:139:GLU:O	1:A:140:LYS:C	2.60	0.42
1:A:172:THR:O	1:A:173:LYS:HB2	2.20	0.42
1:A:274:ARG:HH11	1:A:274:ARG:HD3	1.61	0.42
1:A:382:SER:O	1:A:386:VAL:HG22	2.20	0.42
1:B:407:ARG:HG3	1:B:439:ASP:CB	2.50	0.42
1:B:709:TRP:CD1	1:B:709:TRP:C	2.98	0.42
1:A:138:MET:HB3	1:A:143:ILE:HD11	2.01	0.41
1:A:193:ILE:HD13	1:A:201:ALA:HB3	2.02	0.41
1:A:515:PHE:HA	1:A:703:MET:SD	2.60	0.41
1:A:637:LEU:HD23	1:A:651:VAL:HG21	2.01	0.41
1:B:332:GLY:HA2	6:B:2183:HOH:O	2.19	0.41
1:B:495:MET:HG2	1:B:707:MET:HE3	2.02	0.41
1:A:465:GLU:OE1	1:A:468:ARG:NH2	2.35	0.41
1:A:715:ASN:HD22	1:A:716:GLY:H	1.68	0.41
1:B:769:ARG:CG	1:B:769:ARG:NH1	2.78	0.41
1:B:774:GLU:CD	1:B:777:LYS:NZ	2.78	0.41
1:B:53:ARG:HH11	1:B:53:ARG:HD2	1.64	0.41
1:B:677:ILE:O	1:B:682:SER:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:LEU:HD13	1:A:768:PHE:CG	2.55	0.41
1:B:76:GLU:HA	6:B:2200:HOH:O	2.19	0.41
1:B:441:ARG:NH1	1:B:441:ARG:CG	2.38	0.41
1:A:403:THR:HB	1:A:404:PRO:CD	2.50	0.41
1:B:17:ASP:OD1	1:B:20:LYS:HG2	2.20	0.41
1:B:663:MET:HG3	1:B:904:ILE:HD11	2.03	0.41
1:A:43:PHE:HD2	1:A:392:ALA:HB3	1.86	0.41
1:A:911:LEU:HD23	1:A:911:LEU:H	1.83	0.41
1:B:386:VAL:O	1:B:386:VAL:CG2	2.68	0.41
1:B:777:LYS:HB2	1:B:777:LYS:HE3	1.81	0.41
1:A:890:PHE:C	1:A:891:LEU:HD22	2.45	0.41
1:B:29:MET:HE2	1:B:381:ARG:NH2	2.36	0.41
1:B:518:ARG:CZ	1:B:521:ASP:CG	2.94	0.41
1:A:615:ILE:HG12	1:A:615:ILE:H	1.12	0.41
1:B:755:ARG:HH11	1:B:755:ARG:HD3	1.15	0.41
1:B:913:THR:O	1:B:914:GLU:C	2.63	0.41
1:A:44:ARG:HA	1:A:47:MET:HE3	2.03	0.41
1:A:91:ARG:HG3	1:A:92:ILE:N	2.36	0.41
1:A:164:ASP:HB3	1:A:204:VAL:O	2.20	0.41
1:A:280:GLU:OE2	1:B:558:LYS:NZ	2.35	0.41
1:A:431:LEU:HD22	1:A:442:PHE:CZ	2.54	0.41
1:A:521:ASP:O	1:A:523:THR:HG23	2.20	0.41
1:A:785:LYS:HB3	1:A:785:LYS:HE3	1.37	0.41
1:B:320:PHE:O	1:B:321:GLU:C	2.63	0.41
1:B:781:ILE:CD1	1:B:807:LEU:HD13	2.51	0.41
1:B:783:GLU:HG3	6:B:2164:HOH:O	2.21	0.41
1:A:384:ASN:HD22	1:A:384:ASN:HA	1.67	0.41
1:A:755:ARG:HD2	1:A:776:LEU:O	2.20	0.41
1:B:593:GLY:N	1:B:594:PRO:CD	2.84	0.41
1:B:774:GLU:HA	1:B:777:LYS:CE	2.51	0.41
1:B:49:ASN:HD22	1:B:49:ASN:HA	1.54	0.40
1:B:570:THR:HG23	1:B:572:GLU:OE1	2.20	0.40
1:B:215:MET:CE	1:B:215:MET:CA	2.91	0.40
1:B:403:THR:HA	1:B:404:PRO:HD3	1.87	0.40
1:B:420:HIS:CD2	1:B:423:TYR:H	2.40	0.40
1:A:441:ARG:HH11	1:A:443:LEU:HD22	1.74	0.40
1:A:690:MET:HE2	1:A:703:MET:CG	2.51	0.40
1:A:874:ILE:O	1:A:874:ILE:CD1	2.64	0.40
1:A:331:ARG:HH11	1:A:331:ARG:HD3	1.52	0.40
1:B:62:LYS:O	1:B:63:MET:C	2.64	0.40
1:B:195:LYS:O	1:B:195:LYS:CG	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:ARG:HH11	1:B:500:ARG:HD3	1.57	0.40
1:B:501:LYS:HE3	1:B:694:GLU:O	2.22	0.40
1:A:40:MET:HE1	1:A:434:LEU:HB3	2.02	0.40
1:A:81:ILE:CD1	1:A:138:MET:HE3	2.51	0.40
1:A:543:VAL:CG2	1:A:555:MET:HE3	2.51	0.40
1:B:313:MET:HE3	1:B:319:LEU:CG	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	899/917 (98%)	825 (92%)	51 (6%)	23 (3%)	4	2
1	B	891/917 (97%)	861 (97%)	24 (3%)	6 (1%)	18	17
All	All	1790/1834 (98%)	1686 (94%)	75 (4%)	29 (2%)	7	4

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	A	100	GLU
1	A	111	VAL
1	A	504	HIS
1	A	506	ASN
1	A	522	GLY
1	A	548	GLY
1	A	769	ARG
1	A	910	ARG
1	A	911	LEU
1	B	909	VAL
1	A	81	ILE

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Mol	Chain	Res	Type
1	A	101	LYS
1	A	103	GLN
1	A	551	ARG
1	A	564	ILE
1	A	908	GLY
1	B	549	LYS
1	B	908	GLY
1	A	98	ASN
1	A	102	ASN
1	A	445	SER
1	A	505	ASN
1	B	624	LYS
1	B	147	LYS
1	A	266	ASP
1	B	105	VAL
1	A	268	GLY
1	A	909	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	778/788 (99%)	641 (82%)	137 (18%)	2	0
1	B	774/788 (98%)	671 (87%)	103 (13%)	4	2
All	All	1552/1576 (98%)	1312 (84%)	240 (16%)	2	1

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	14	LEU
1	A	16	ASP
1	A	21	LYS
1	A	24	LYS
1	A	34	GLU

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Mol	Chain	Res	Type
1	A	35	THR
1	A	53	ARG
1	A	62	LYS
1	A	71	ILE
1	A	77	LYS
1	A	79	ASP
1	A	80	PHE
1	A	91	ARG
1	A	93	LEU
1	A	96	GLN
1	A	97	VAL
1	A	102	ASN
1	A	103	GLN
1	A	105	VAL
1	A	107	MET
1	A	108	GLU
1	A	117	ASN
1	A	118	ILE
1	A	119	VAL
1	A	125	GLN
1	A	136	ASP
1	A	139	GLU
1	A	140	LYS
1	A	144	LYS
1	A	146	LYS
1	A	147	LYS
1	A	159	GLN
1	A	167	ILE
1	A	185	VAL
1	A	187	LYS
1	A	188	LEU
1	A	189	LEU
1	A	196	ARG
1	A	243	ARG
1	A	247	LEU
1	A	252	GLU
1	A	254	ARG
1	A	255	MET
1	A	261	TRP
1	A	273	ILE
1	A	287	ASN
1	A	302	LEU

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Mol	Chain	Res	Type
1	A	304	GLU
1	A	305	LEU
1	A	312	LYS
1	A	333	LYS
1	A	335	ASN
1	A	336	THR
1	A	344	LYS
1	A	357	THR
1	A	361	VAL
1	A	369	VAL
1	A	376	THR
1	A	377	ILE
1	A	390	LEU
1	A	405	ARG
1	A	406	LEU
1	A	434	LEU
1	A	437	ASP
1	A	438	SER
1	A	451	LYS
1	A	459	VAL
1	A	463	LEU
1	A	465	GLU
1	A	480	THR
1	A	482	ASP
1	A	487	VAL
1	A	489	LYS
1	A	501	LYS
1	A	504	HIS
1	A	506	ASN
1	A	508	VAL
1	A	516	VAL
1	A	521	ASP
1	A	549	LYS
1	A	550	LYS
1	A	557	ASN
1	A	562	ILE
1	A	564	ILE
1	A	565	GLU
1	A	579	VAL
1	A	580	SER
1	A	586	LEU
1	A	591	ILE

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Mol	Chain	Res	Type
1	A	598	LEU
1	A	603	SER
1	A	615	ILE
1	A	619	TRP
1	A	624	LYS
1	A	645	GLU
1	A	646	GLU
1	A	655	VAL
1	A	658	THR
1	A	668	GLU
1	A	671	THR
1	A	691	LYS
1	A	703	MET
1	A	709	TRP
1	A	715	ASN
1	A	735	ASN
1	A	738	LYS
1	A	759	ILE
1	A	762	THR
1	A	769	ARG
1	A	777	LYS
1	A	781	ILE
1	A	785	LYS
1	A	795	LEU
1	A	799	GLN
1	A	801	ARG
1	A	804	LEU
1	A	806	GLN
1	A	818	LEU
1	A	821	THR
1	A	843	ASP
1	A	845	ILE
1	A	857	THR
1	A	866	LYS
1	A	874	ILE
1	A	877	GLN
1	A	881	GLU
1	A	888	VAL
1	A	891	LEU
1	A	892	LEU
1	A	895	ASP
1	A	899	LYS

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Mol	Chain	Res	Type
1	A	907	VAL
1	A	910	ARG
1	A	912	ARG
1	A	913	THR
1	A	914	GLU
1	B	18	GLN
1	B	21	LYS
1	B	42	ARG
1	B	48	LYS
1	B	52	SER
1	B	56	ASN
1	B	76	GLU
1	B	83	LEU
1	B	91	ARG
1	B	99	HIS
1	B	108	GLU
1	B	111	VAL
1	B	116	GLU
1	B	117	ASN
1	B	119	VAL
1	B	124	SER
1	B	140	LYS
1	B	142	LYS
1	B	143	ILE
1	B	144	LYS
1	B	165	GLU
1	B	185	VAL
1	B	186	VAL
1	B	189	LEU
1	B	194	LYS
1	B	196	ARG
1	B	198	ASP
1	B	207	VAL
1	B	215	MET
1	B	223	HIS
1	B	242	LEU
1	B	252	GLU
1	B	254	ARG
1	B	261	TRP
1	B	281	ILE
1	B	305	LEU
1	B	306	VAL

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Mol	Chain	Res	Type
1	B	320	PHE
1	B	331	ARG
1	B	347	GLU
1	B	349	LEU
1	B	359	LEU
1	B	369	VAL
1	B	396	ARG
1	B	403	THR
1	B	407	ARG
1	B	418	LYS
1	B	431	LEU
1	B	432	ARG
1	B	434	LEU
1	B	437	ASP
1	B	439	ASP
1	B	443	LEU
1	B	463	LEU
1	B	466	GLN
1	B	483	MET
1	B	496	GLU
1	B	497	LEU
1	B	518	ARG
1	B	529	LEU
1	B	531	LEU
1	B	536	THR
1	B	549	LYS
1	B	551	ARG
1	B	553	VAL
1	B	565	GLU
1	B	566	ILE
1	B	570	THR
1	B	592	LYS
1	B	596	MET
1	B	598	LEU
1	B	624	LYS
1	B	648	ASP
1	B	689	GLU
1	B	709	TRP
1	B	717	CYS
1	B	720	ASP
1	B	721	ILE
1	B	760	ASP

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Mol	Chain	Res	Type
1	B	767	LEU
1	B	769	ARG
1	B	771	GLN
1	B	779	ARG
1	B	781	ILE
1	B	785	LYS
1	B	787	LEU
1	B	790	ILE
1	B	803	ILE
1	B	806	GLN
1	B	829	ARG
1	B	843	ASP
1	B	845	ILE
1	B	847	GLU
1	B	848	ASN
1	B	853	ARG
1	B	866	LYS
1	B	880	LYS
1	B	881	GLU
1	B	891	LEU
1	B	895	ASP
1	B	897	SER
1	B	912	ARG
1	B	914	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	117	ASN
1	A	208	ASN
1	A	222	GLN
1	A	235	ASN
1	A	244	HIS
1	A	287	ASN
1	A	335	ASN
1	A	345	ASN
1	A	373	HIS
1	A	384	ASN
1	A	420	HIS
1	A	467	HIS
1	A	476	HIS

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Mol	Chain	Res	Type
1	A	502	GLN
1	A	556	HIS
1	A	631	HIS
1	A	656	ASN
1	A	702	GLN
1	A	715	ASN
1	A	735	ASN
1	A	806	GLN
1	A	810	ASN
1	B	49	ASN
1	B	56	ASN
1	B	104	ASN
1	B	129	HIS
1	B	208	ASN
1	B	235	ASN
1	B	244	HIS
1	B	345	ASN
1	B	351	ASN
1	B	372	GLN
1	B	373	HIS
1	B	384	ASN
1	B	420	HIS
1	B	525	ASN
1	B	656	ASN
1	B	756	ASN
1	B	771	GLN
1	B	805	GLN
1	B	855	ASN
1	B	887	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	G6P	A	921	-	16,16,16	0.99	0	23,24,24	2.14	5 (21%)
2	GLC	B	1917	-	12,12,12	1.13	1 (8%)	17,17,17	2.01	6 (35%)
2	GLC	A	918	-	12,12,12	0.84	1 (8%)	17,17,17	1.74	4 (23%)
2	GLC	B	1915	-	12,12,12	0.55	0	17,17,17	1.45	2 (11%)
3	G6P	B	1918	-	16,16,16	1.38	4 (25%)	23,24,24	2.65	9 (39%)
5	ANP	B	1999	4	33,33,33	1.50	4 (12%)	45,52,52	1.29	5 (11%)
3	G6P	B	1916	-	16,16,16	0.97	1 (6%)	23,24,24	2.09	9 (39%)
2	GLC	A	920	-	12,12,12	0.95	1 (8%)	17,17,17	2.00	4 (23%)
5	ANP	A	999	-	33,33,33	1.54	5 (15%)	45,52,52	1.38	8 (17%)
3	G6P	A	919	-	16,16,16	1.29	3 (18%)	23,24,24	2.52	11 (47%)

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
3	G6P	A	921	-	1/1/6/6	5/6/26/26	0/1/1/1
2	GLC	B	1917	-	-	0/2/22/22	0/1/1/1
3	G6P	B	1918	-	1/1/6/6	3/6/26/26	0/1/1/1
2	GLC	A	918	-	-	0/2/22/22	0/1/1/1
2	GLC	B	1915	-	-	0/2/22/22	0/1/1/1
5	ANP	B	1999	4	-	7/18/38/38	0/3/3/3
3	G6P	B	1916	-	1/1/6/6	2/6/26/26	0/1/1/1
2	GLC	A	920	-	-	0/2/22/22	0/1/1/1
5	ANP	A	999	-	-	6/18/38/38	0/3/3/3
3	G6P	A	919	-	1/1/6/6	4/6/26/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	ANP	C5-N7	-4.37	1.31	1.39
5	B	1999	ANP	C5-N7	-3.89	1.32	1.39
5	A	999	ANP	PG-O3G	-3.09	1.48	1.56
5	A	999	ANP	PG-O2G	-3.07	1.48	1.56
5	B	1999	ANP	PG-O3G	-3.04	1.48	1.56
5	B	1999	ANP	PG-O2G	-3.04	1.48	1.56
5	B	1999	ANP	PB-O2B	-3.00	1.48	1.56
5	A	999	ANP	PB-O2B	-2.88	1.49	1.56
3	B	1918	G6P	O2-C2	-2.58	1.36	1.43
3	A	919	G6P	P-O2P	-2.36	1.46	1.54
3	A	919	G6P	O5-C5	2.23	1.49	1.44
5	A	999	ANP	C2-N1	2.21	1.37	1.33
3	A	919	G6P	C3-C2	2.20	1.58	1.52
3	B	1918	G6P	C3-C2	2.19	1.58	1.52
3	B	1918	G6P	P-O1P	-2.19	1.46	1.54
3	B	1916	G6P	O6-C6	2.17	1.52	1.44
2	A	920	GLC	C4-C3	2.16	1.57	1.52
3	B	1918	G6P	O6-C6	2.04	1.52	1.44
2	B	1917	GLC	C4-C5	2.04	1.57	1.53
2	A	918	GLC	C4-C5	2.03	1.57	1.53

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1918	G6P	O5-C5-C6	-6.96	92.91	106.69
3	A	919	G6P	C6-C5-C4	5.36	123.32	112.07
3	B	1918	G6P	C6-C5-C4	5.05	122.68	112.07
3	A	921	G6P	O5-C5-C4	5.04	118.79	109.70
3	A	921	G6P	O5-C1-C2	4.91	118.93	110.30
3	A	921	G6P	C4-C3-C2	-4.40	103.10	110.83
3	A	919	G6P	C4-C3-C2	-4.31	103.26	110.83
3	B	1916	G6P	O5-C1-C2	4.26	117.78	110.30
2	A	918	GLC	O5-C5-C4	-4.17	102.18	109.70
3	A	919	G6P	O1P-P-O6	-4.11	95.95	106.67
3	B	1918	G6P	C4-C3-C2	-4.08	103.66	110.83
3	A	919	G6P	O5-C5-C6	-4.06	98.64	106.69
5	B	1999	ANP	C4-N9-C8	-4.00	101.53	105.74
3	B	1916	G6P	O3-C3-C4	3.87	119.50	110.38
2	A	920	GLC	O4-C4-C3	-3.78	101.46	110.38
3	B	1916	G6P	O5-C5-C6	-3.76	99.24	106.69
3	A	921	G6P	O1P-P-O6	-3.73	96.93	106.67
2	A	920	GLC	O5-C5-C4	-3.69	103.05	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1918	G6P	O1-C1-O5	-3.67	99.50	110.41
2	A	920	GLC	C3-C4-C5	-3.64	103.63	110.23
3	A	919	G6P	O4-C4-C5	3.55	118.07	109.32
2	B	1917	GLC	O5-C5-C4	-3.49	103.41	109.70
2	B	1915	GLC	O5-C5-C4	-3.37	103.63	109.70
5	A	999	ANP	C4-N9-C8	-3.33	102.24	105.74
2	B	1917	GLC	C3-C4-C5	-3.26	104.32	110.23
3	A	919	G6P	O5-C5-C4	-3.26	103.83	109.70
3	B	1918	G6P	O2-C2-C3	-3.13	102.99	110.38
3	B	1916	G6P	O4-C4-C3	-3.12	103.02	110.38
2	B	1915	GLC	O5-C1-C2	-3.05	104.94	110.30
2	B	1917	GLC	O1-C1-O5	-3.01	101.46	110.41
3	A	919	G6P	C1-O5-C5	-2.99	107.86	113.65
2	B	1917	GLC	O4-C4-C3	-2.89	103.55	110.38
2	A	918	GLC	C3-C4-C5	-2.85	105.06	110.23
3	B	1916	G6P	C4-C3-C2	-2.85	105.83	110.83
2	B	1917	GLC	O5-C5-C6	2.80	113.39	106.44
5	A	999	ANP	C4-N9-C1'	2.74	133.05	126.63
3	B	1918	G6P	O3-C3-C4	2.72	116.80	110.38
3	B	1918	G6P	O4-C4-C3	-2.68	104.05	110.38
3	B	1918	G6P	O5-C1-C2	-2.66	105.61	110.30
2	A	918	GLC	O4-C4-C3	-2.62	104.21	110.38
5	B	1999	ANP	N9-C8-N7	2.60	117.63	113.94
5	A	999	ANP	C6-C5-N7	-2.60	127.08	132.09
3	B	1916	G6P	O6-P-O3P	2.58	113.41	106.44
5	B	1999	ANP	O3A-PB-N3B	-2.55	99.50	106.59
3	A	921	G6P	O2P-P-O1P	2.50	117.16	107.80
5	A	999	ANP	O2A-PA-O3A	2.48	113.98	107.27
5	B	1999	ANP	O4'-C1'-N9	2.43	112.76	108.09
5	A	999	ANP	O3A-PB-N3B	-2.43	99.86	106.59
3	B	1916	G6P	O2-C2-C3	-2.41	104.69	110.38
3	B	1918	G6P	C3-C4-C5	-2.38	105.92	110.23
5	A	999	ANP	N9-C8-N7	2.37	117.30	113.94
2	A	920	GLC	C6-C5-C4	-2.35	107.25	113.02
2	A	918	GLC	O2-C2-C3	2.33	115.88	110.38
3	B	1916	G6P	O3-C3-C2	2.28	115.76	110.38
3	A	919	G6P	C1-C2-C3	-2.26	105.75	110.36
5	A	999	ANP	O3G-PG-O1G	-2.21	107.90	113.45
5	A	999	ANP	C4-C5-N7	2.17	113.06	110.58
2	B	1917	GLC	C6-C5-C4	-2.16	107.72	113.02
3	A	919	G6P	O2P-P-O6	2.14	112.24	106.67
3	B	1916	G6P	C6-C5-C4	2.10	116.47	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	919	G6P	O2-C2-C1	-2.05	104.51	109.25
3	A	919	G6P	O4-C4-C3	-2.00	105.66	110.38
5	B	1999	ANP	O2G-PG-O1G	-2.00	108.43	113.45

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	919	G6P	C1
3	A	921	G6P	C1
3	B	1916	G6P	C1
3	B	1918	G6P	C1

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	919	G6P	C4-C5-C6-O6
3	A	919	G6P	O5-C5-C6-O6
3	A	921	G6P	C4-C5-C6-O6
3	A	921	G6P	O5-C5-C6-O6
3	A	921	G6P	C6-O6-P-O1P
3	A	921	G6P	C6-O6-P-O2P
3	B	1916	G6P	C4-C5-C6-O6
3	B	1916	G6P	O5-C5-C6-O6
3	B	1918	G6P	C4-C5-C6-O6
3	B	1918	G6P	O5-C5-C6-O6
5	A	999	ANP	PB-N3B-PG-O1G
5	A	999	ANP	PG-N3B-PB-O1B
5	A	999	ANP	PG-N3B-PB-O3A
5	A	999	ANP	PA-O3A-PB-O1B
5	B	1999	ANP	PG-N3B-PB-O3A
5	B	1999	ANP	C5'-O5'-PA-O1A
5	B	1999	ANP	C5'-O5'-PA-O3A
5	B	1999	ANP	O4'-C4'-C5'-O5'
5	B	1999	ANP	C3'-C4'-C5'-O5'
5	A	999	ANP	PB-O3A-PA-O5'
5	B	1999	ANP	C5'-O5'-PA-O2A
3	A	919	G6P	C6-O6-P-O3P
3	A	921	G6P	C6-O6-P-O3P
3	B	1918	G6P	C6-O6-P-O2P
3	A	919	G6P	C5-C6-O6-P
5	B	1999	ANP	PB-O3A-PA-O2A
5	A	999	ANP	C3'-C4'-C5'-O5'

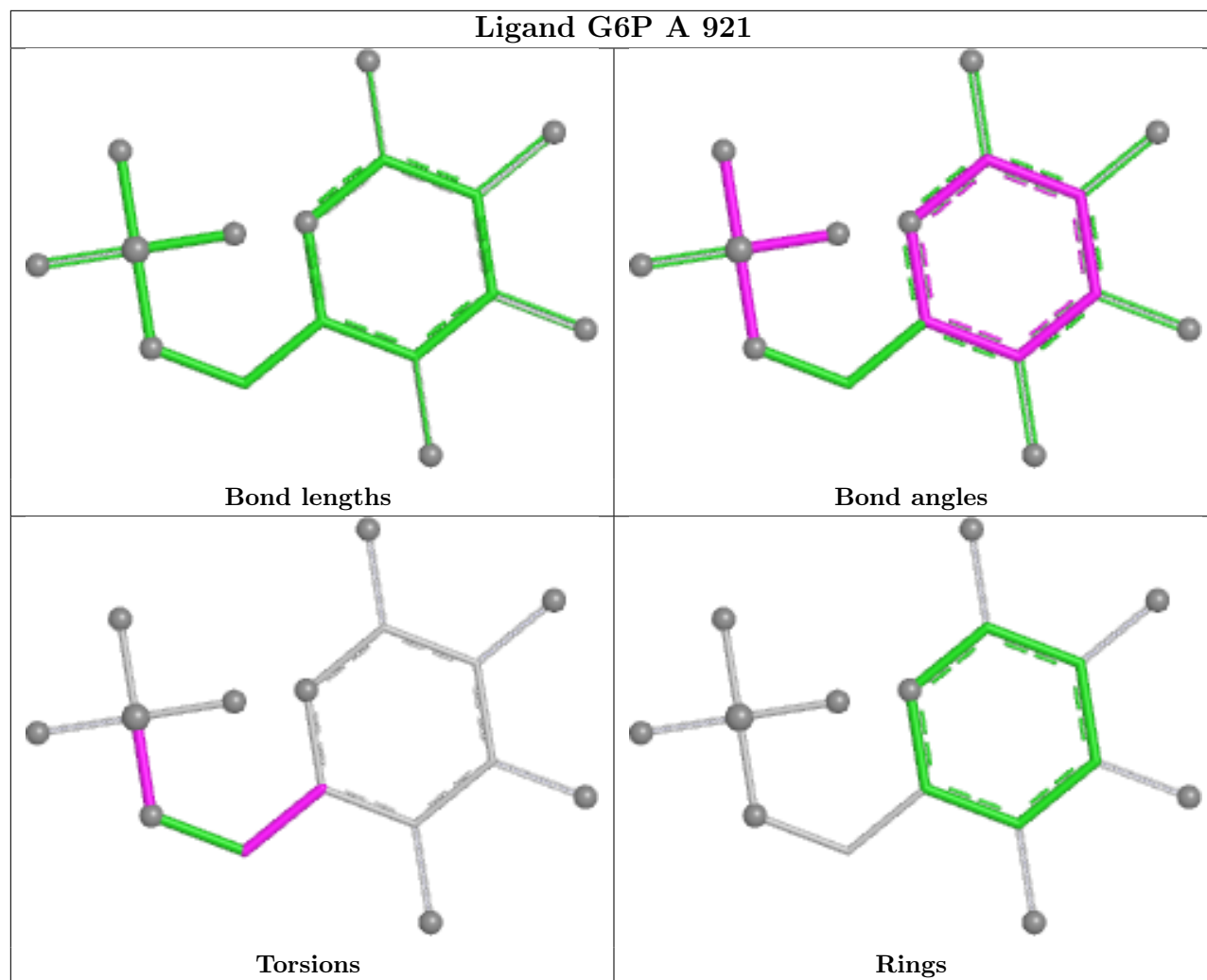
There are no ring outliers.

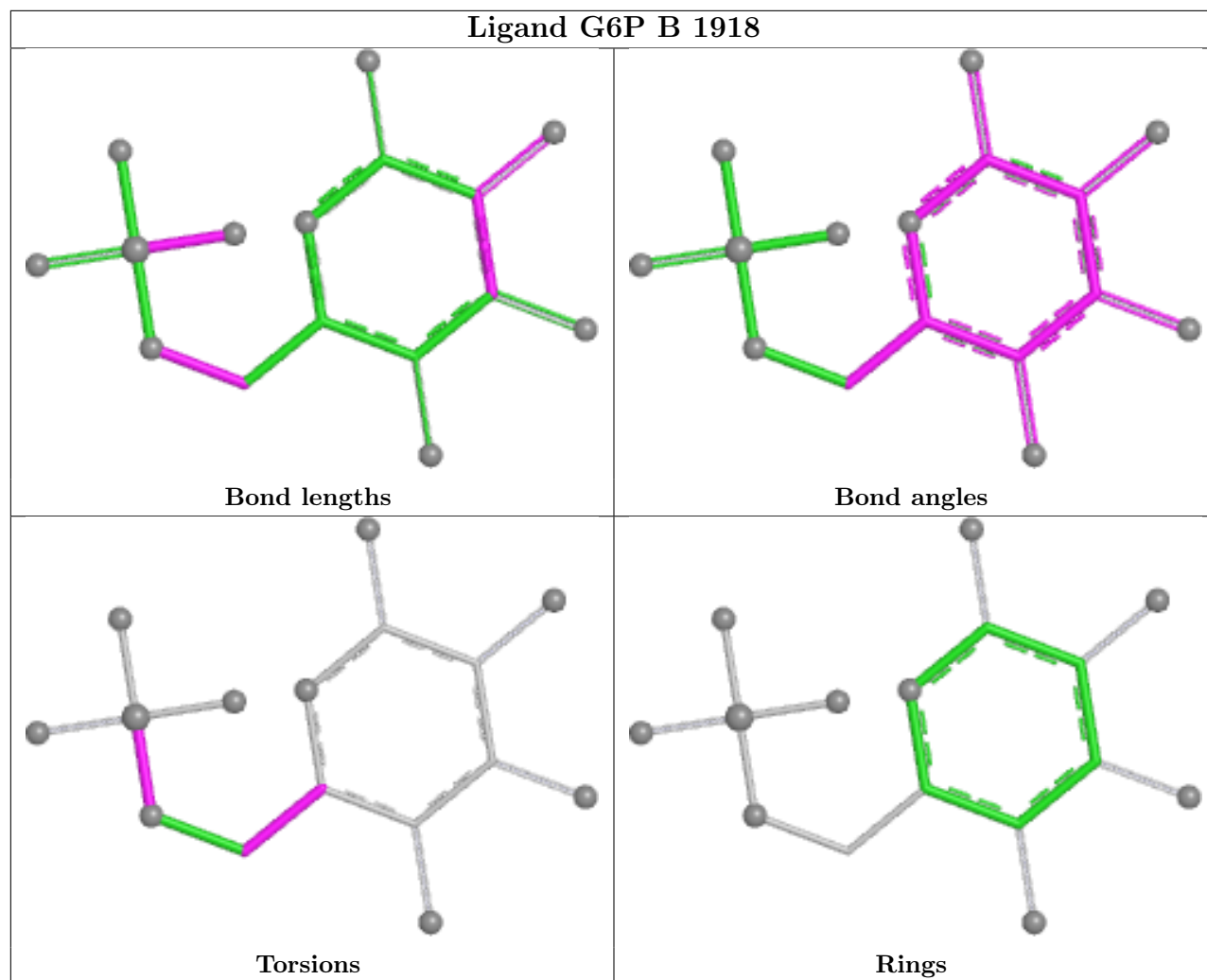
6 monomers are involved in 17 short contacts:

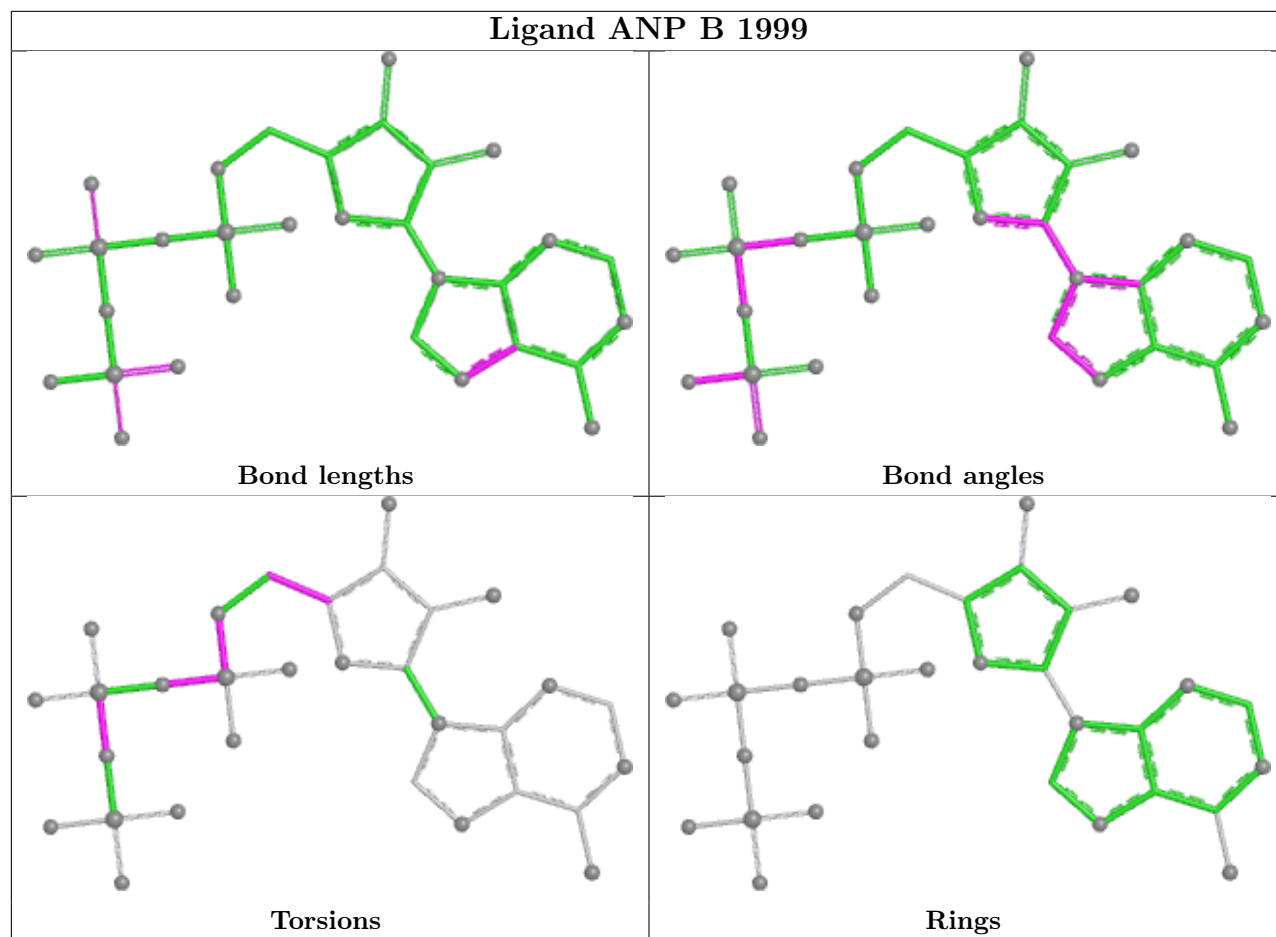
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	921	G6P	1	0
3	B	1918	G6P	5	0
5	B	1999	ANP	1	0
3	B	1916	G6P	3	0
5	A	999	ANP	1	0
3	A	919	G6P	6	0

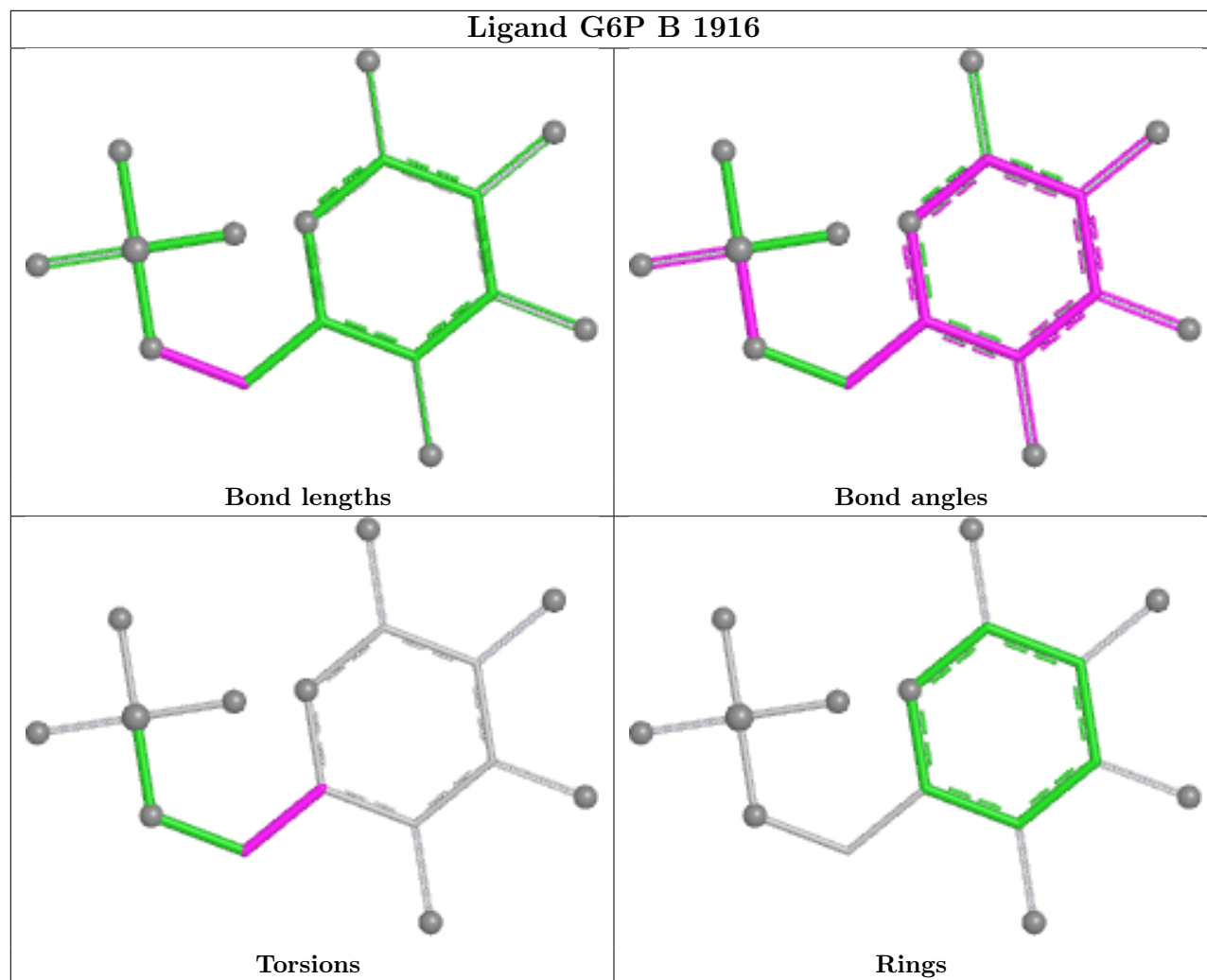
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

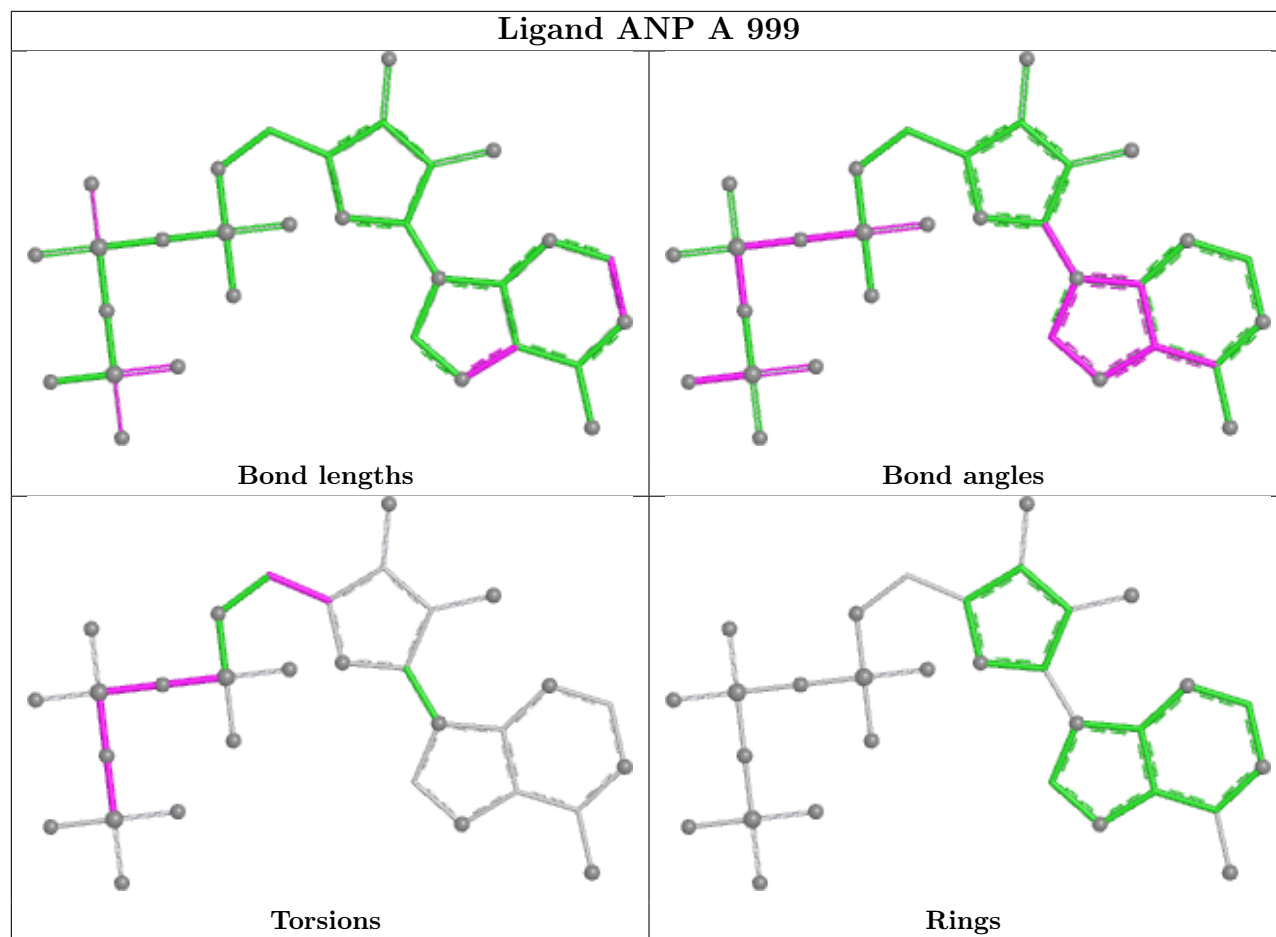
Ligand G6P A 921

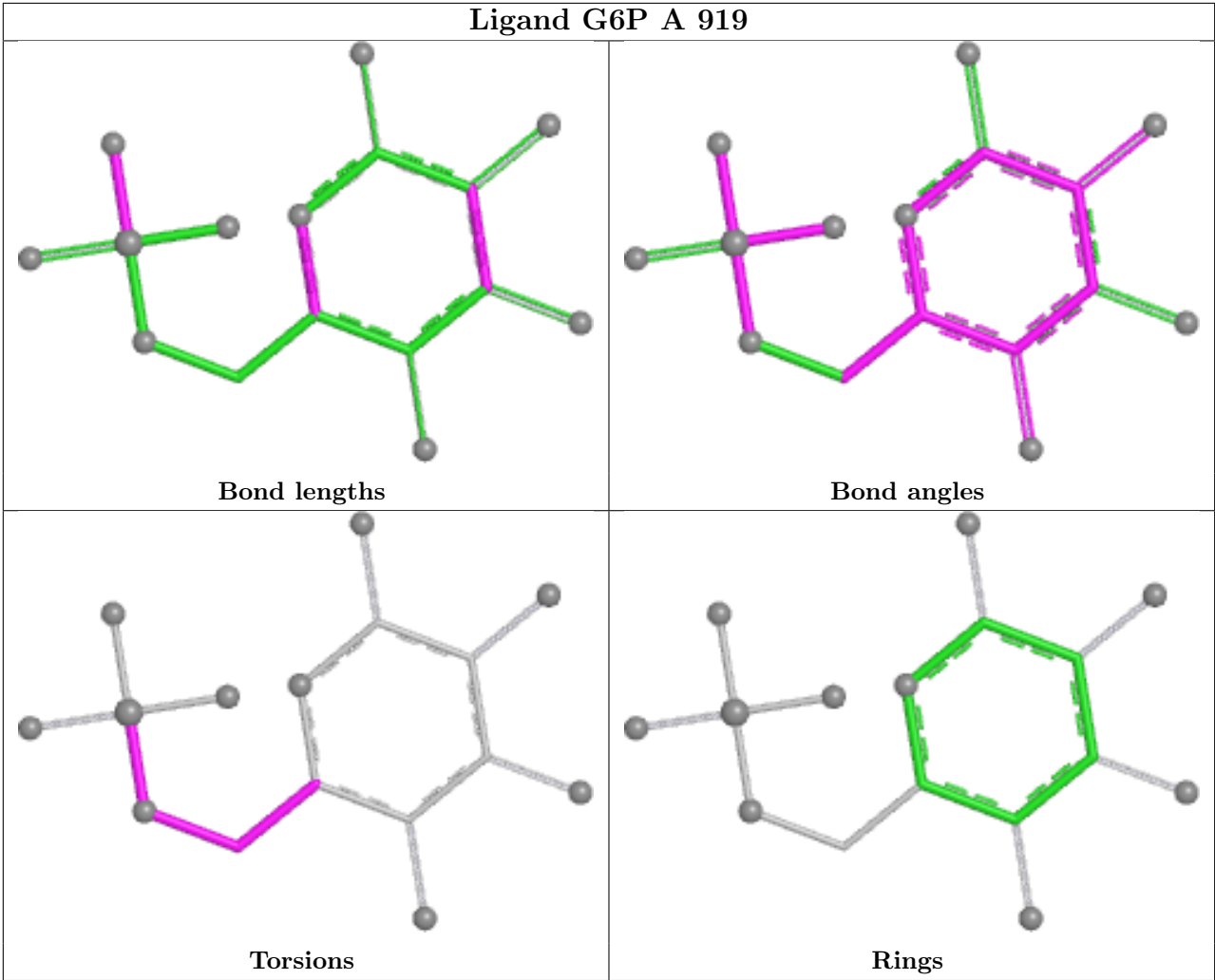












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	5
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	101:LYS	C	102:ASN	N	2.86

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	100:GLU	C	101:LYS	N	2.68
1	B	16:ASP	C	17:ASP	N	2.25
1	B	103:GLN	C	104:ASN	N	2.23
1	A	912:ARG	C	913:THR	N	2.03
1	B	99:HIS	C	100:GLU	N	1.68
1	A	99:HIS	C	100:GLU	N	1.06

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.