



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:24 AM UTC

PDB ID : 3OPY / pdb_00003opy
Title : Crystal structure of Pichia pastoris phosphofructokinase in the T-state
Authors : Strater, N.; Marek, S.; Kuettner, E.B.; Kloos, M.; Keim, A.; Bruser, A.; Kirchberger, J.; Schoneberg, T.
Deposited on : 2010-09-02
Resolution : 3.05 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

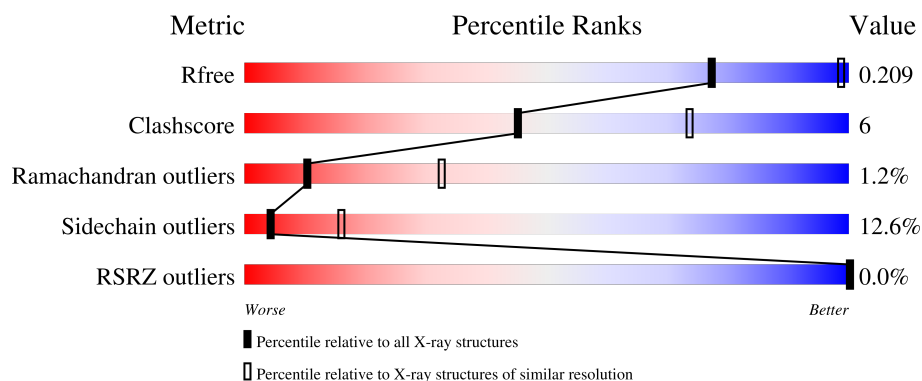
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	989	 71% 21% • 5%
1	C	989	 71% 20% • 5%
1	E	989	 71% 20% • 5%
1	G	989	 71% 20% • 5%
2	B	941	 72% 18% • 6%

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Mol	Chain	Length	Quality of chain
2	D	941	
2	F	941	
2	H	941	
3	I	351	
3	J	351	
3	K	351	
3	L	351	

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
4	SO4	C	991	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65025 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 6-phosphofructo-1-kinase alpha-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	C	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	E	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			
1	G	936	Total	C	N	O	S	0	0	0
			7008	4410	1200	1373	25			

- Molecule 2 is a protein called 6-phosphofructo-1-kinase beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	D	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	F	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			
2	H	884	Total	C	N	O	S	0	0	0
			6546	4093	1165	1254	34			

- Molecule 3 is a protein called 6-phosphofructo-1-kinase gamma-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	J	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	K	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			
3	L	323	Total	C	N	O	S	0	0	0
			2590	1650	439	492	9			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

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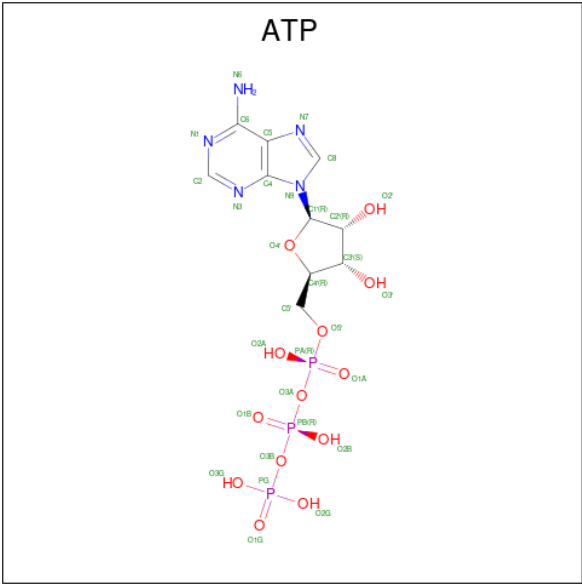
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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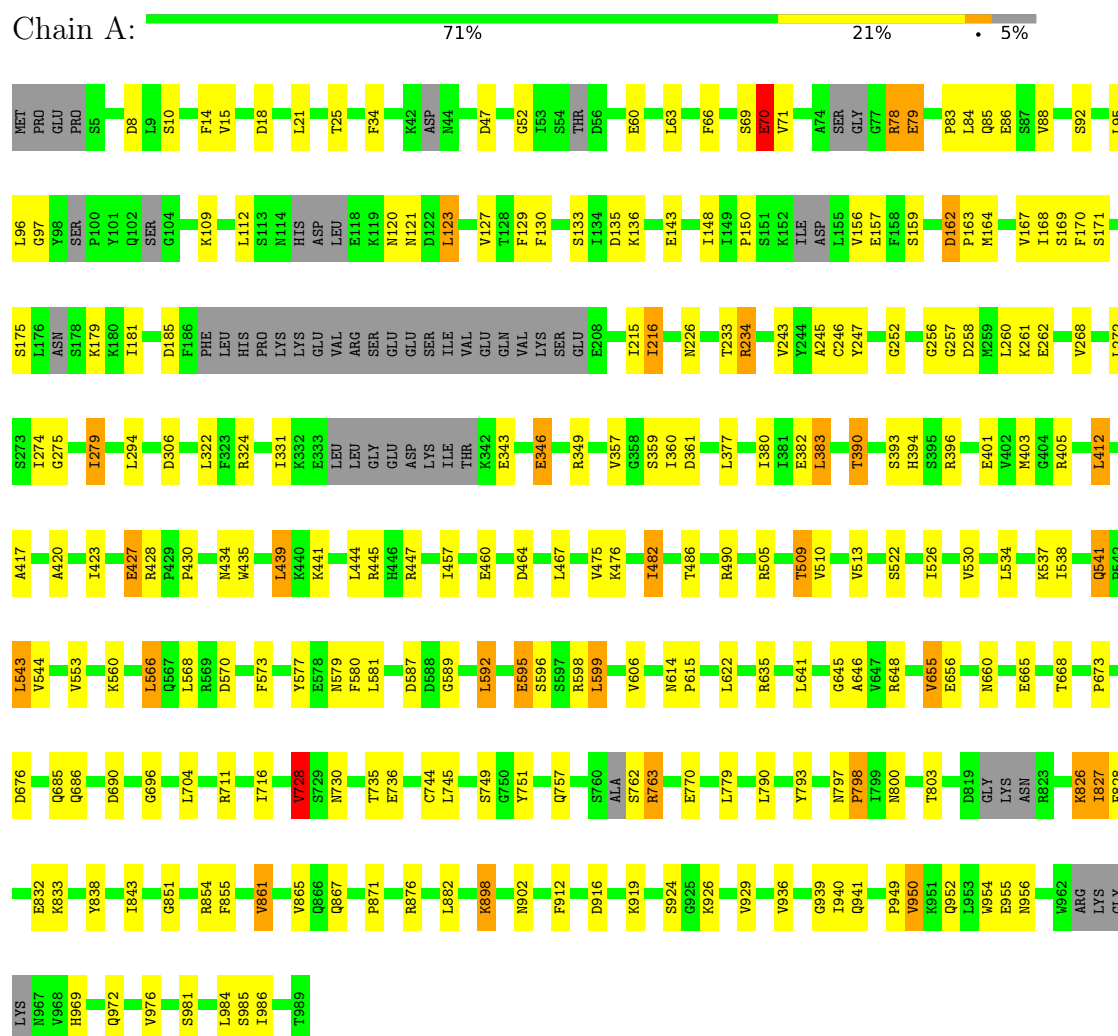
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

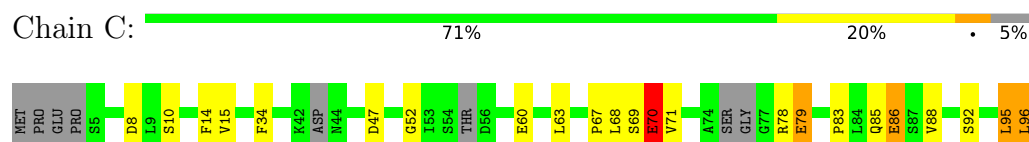
3 Residue-property plots [i](#)

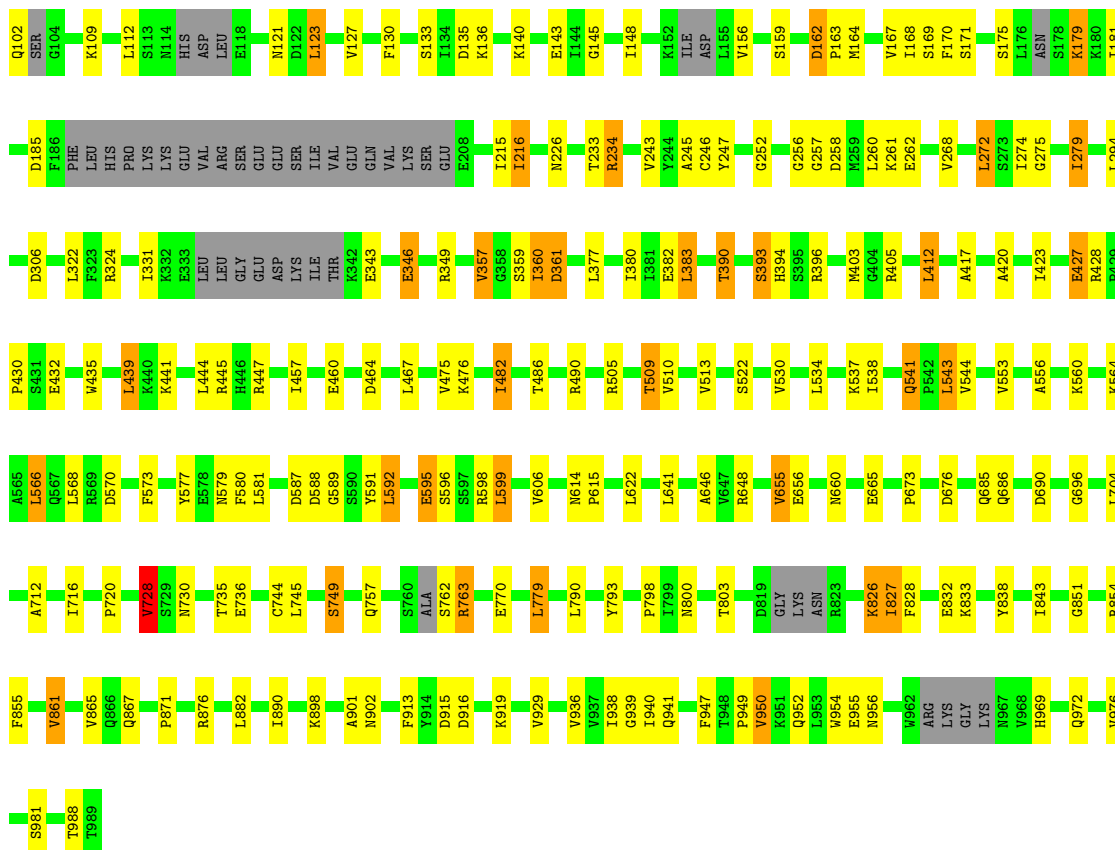
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

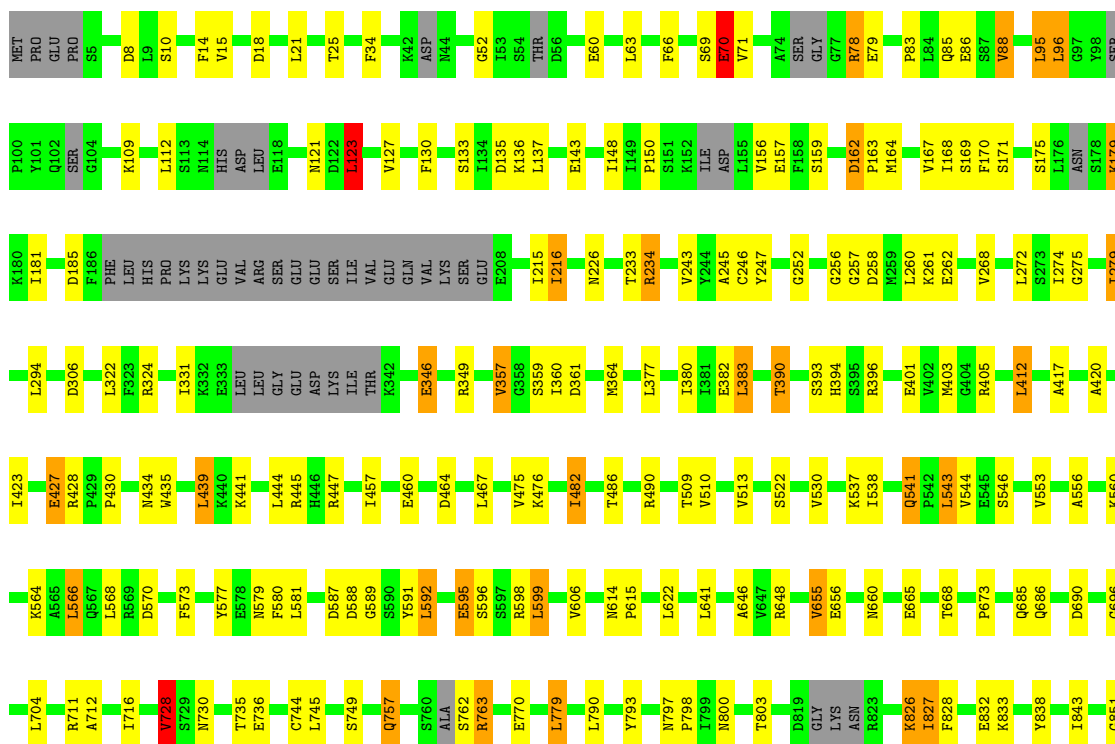


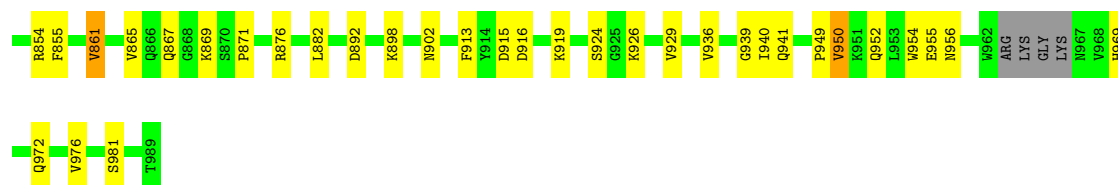
- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit





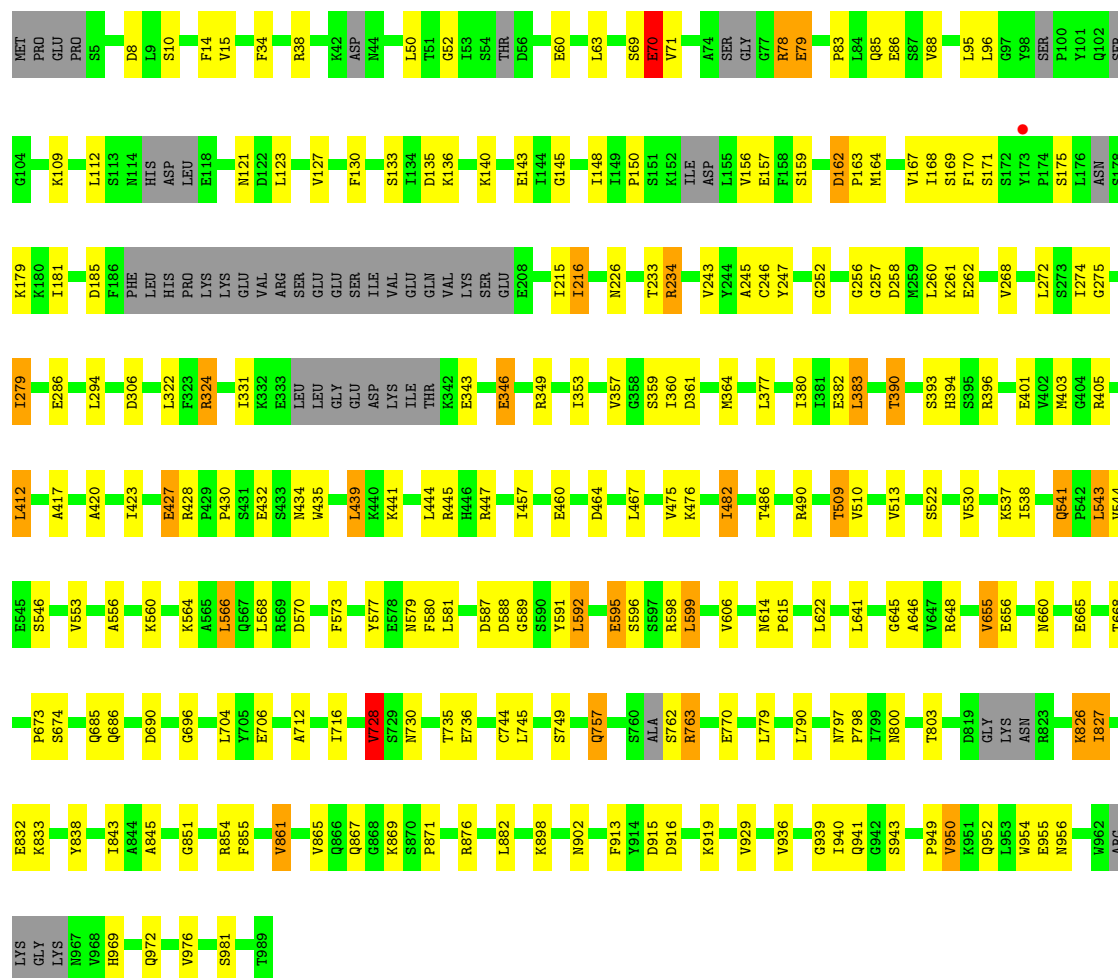
- Molecule 1: 6-phosphofructo-1-kinase alpha-subunit





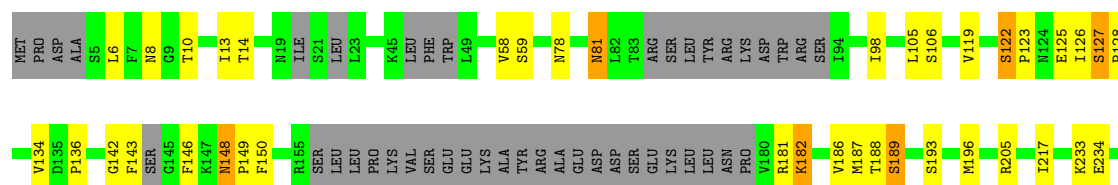
• Molecule 1: 6-phosphofructo-1-kinase alpha-subunit

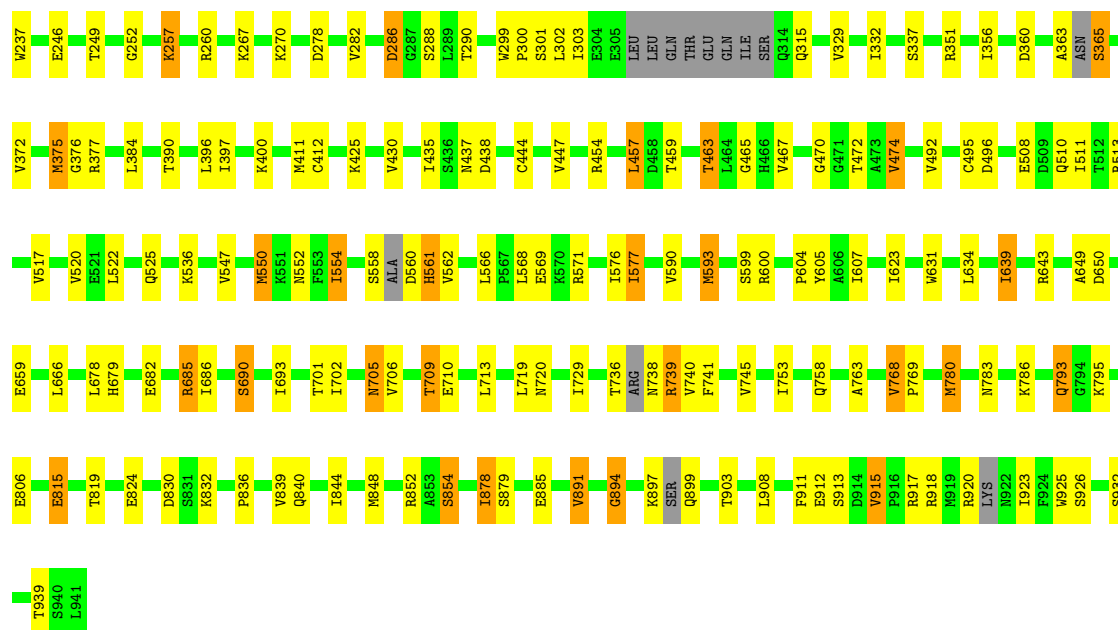
Chain G: 71% 20% 5%



• Molecule 2: 6-phosphofructo-1-kinase beta-subunit

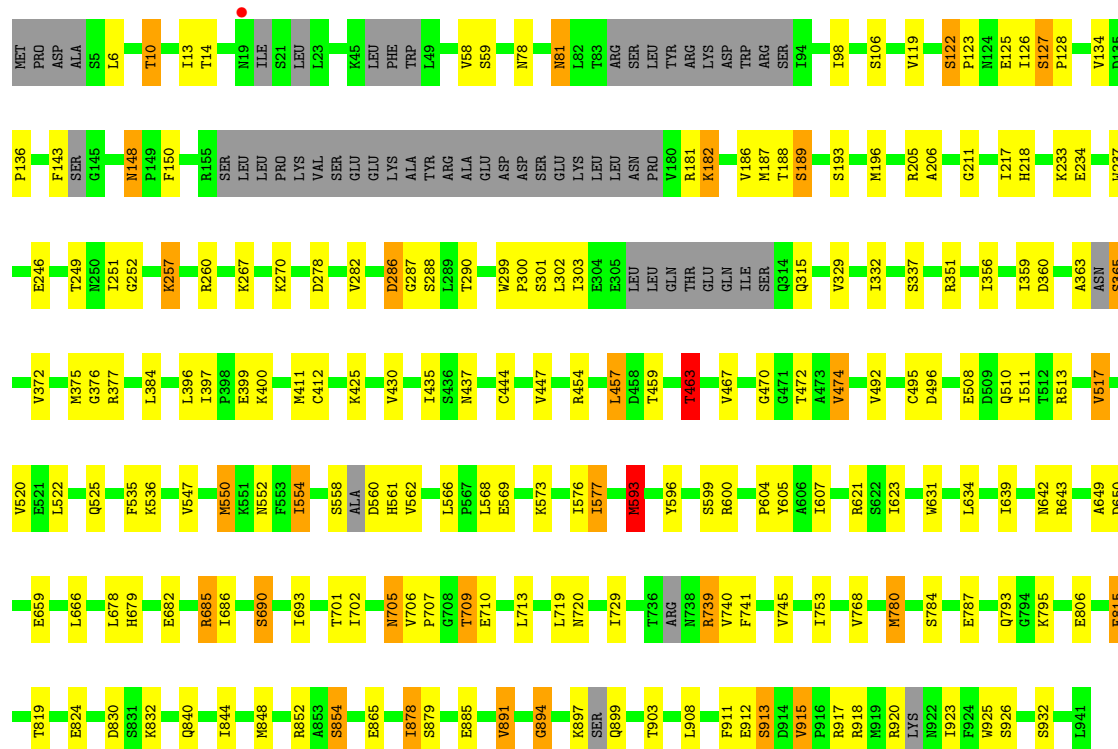
Chain B: 72% 18% 6%





- Molecule 2: 6-phosphofructo-1-kinase beta-subunit

Chain D: 73% 18% 6%



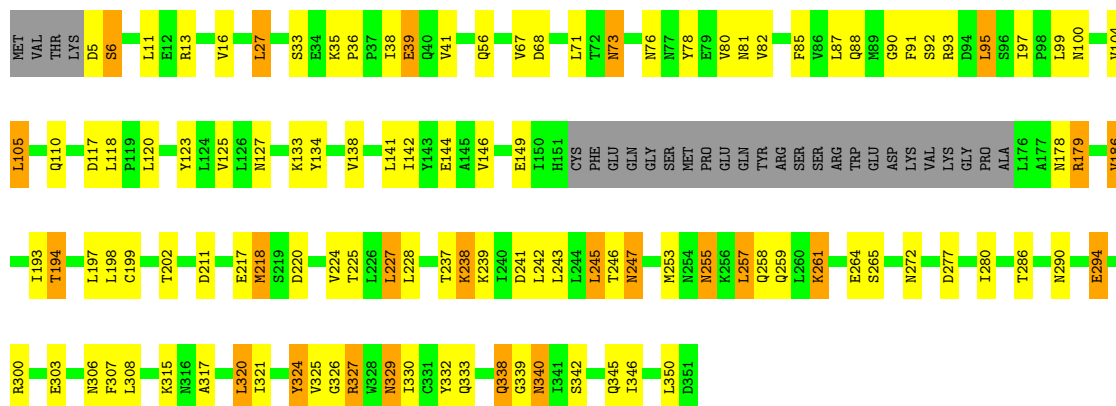
- Molecule 2: 6-phosphofructo-1-kinase beta-subunit

Chain F: 73% 18% 6%



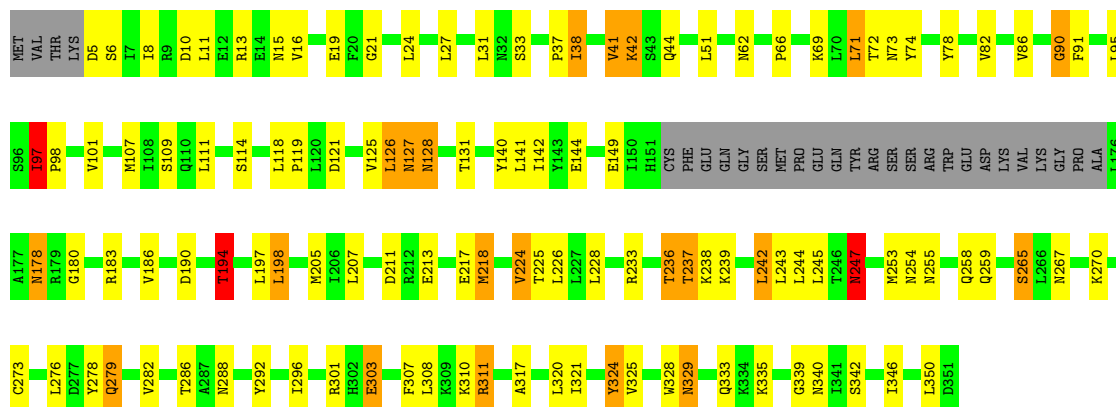
• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain I: 60% 26% 7% 8%



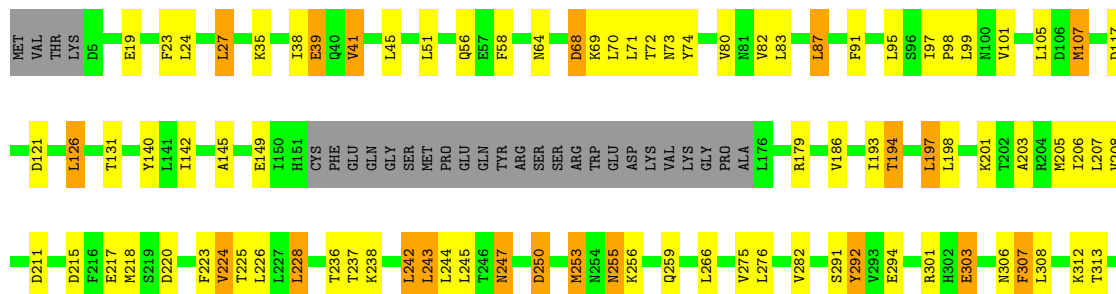
• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

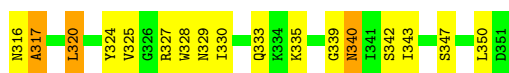
Chain J: 58% 27% 6% 8%



• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

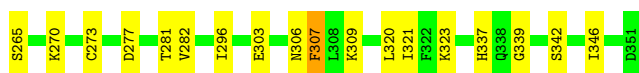
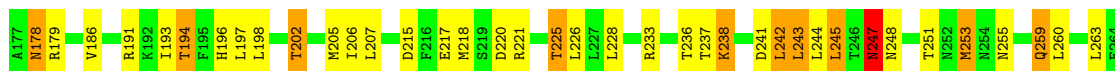
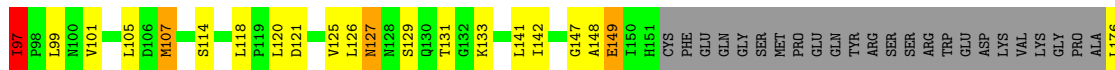
Chain K: 62% 24% 7% 8%





• Molecule 3: 6-phosphofructo-1-kinase gamma-subunit

Chain L: 60% 26% 5% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	161.66Å 188.30Å 231.56Å 90.00° 92.85° 90.00°	Depositor
Resolution (Å)	29.80 – 3.05 29.80 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.80-3.05) 84.0 (29.80-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.06Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.200 , 0.232 0.216 , 0.209	Depositor DCC
R_{free} test set	5145 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	65025	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, SO4

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	0.86	0/7125	1.45	49/9664 (0.5%)
1	C	0.86	0/7125	1.44	54/9664 (0.6%)
1	E	0.81	0/7125	1.44	47/9664 (0.5%)
1	G	0.83	0/7125	1.44	46/9664 (0.5%)
2	B	0.88	0/6651	1.45	43/9002 (0.5%)
2	D	0.89	1/6651 (0.0%)	1.46	44/9002 (0.5%)
2	F	0.83	0/6651	1.45	33/9002 (0.4%)
2	H	0.84	0/6651	1.44	33/9002 (0.4%)
3	I	1.02	5/2640 (0.2%)	1.62	36/3578 (1.0%)
3	J	0.97	1/2640 (0.0%)	1.57	37/3578 (1.0%)
3	K	0.90	0/2640	1.53	25/3578 (0.7%)
3	L	0.92	3/2640 (0.1%)	1.51	26/3578 (0.7%)
All	All	0.87	10/65664 (0.0%)	1.46	473/88976 (0.5%)

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	E	0	1
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	218	MET	SD-CE	-6.57	1.63	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	218	MET	SD-CE	-5.72	1.65	1.79
2	D	593	MET	SD-CE	-5.55	1.65	1.79
3	I	261	LYS	CA-C	5.49	1.60	1.52
3	L	97	ILE	CA-CB	5.27	1.56	1.54
3	L	296	ILE	CA-C	5.21	1.58	1.52
3	L	306	ASN	CG-OD1	5.14	1.33	1.23
3	I	73	ASN	CG-OD1	5.08	1.33	1.23
3	I	338	GLN	CA-C	-5.03	1.47	1.52
3	I	338	GLN	CD-OE1	5.01	1.33	1.23

All (473) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	67	VAL	CA-C-N	10.74	135.04	120.54
3	I	67	VAL	C-N-CA	10.74	135.04	120.54
3	L	194	THR	CB-CA-C	9.55	125.00	111.82
3	J	127	ASN	N-CA-C	9.45	121.18	111.07
1	A	394	HIS	N-CA-C	9.07	121.17	111.28
1	C	394	HIS	N-CA-C	9.03	121.12	111.28
1	E	394	HIS	N-CA-C	9.00	121.09	111.28
1	G	394	HIS	N-CA-C	8.96	121.04	111.28
3	L	127	ASN	N-CA-C	8.62	121.62	111.71
1	E	88	VAL	N-CA-C	8.57	119.14	110.23
3	I	280	ILE	N-CA-C	-8.56	104.86	111.62
2	D	148	ASN	CA-CB-CG	8.47	121.07	112.60
2	B	148	ASN	CA-CB-CG	8.43	121.03	112.60
3	I	6	SER	CA-C-N	8.35	131.08	120.56
3	I	6	SER	C-N-CA	8.35	131.08	120.56
1	C	86	GLU	N-CA-C	-8.26	101.22	113.61
2	F	337	SER	N-CA-C	8.23	120.33	111.36
2	H	148	ASN	CA-CB-CG	8.23	120.83	112.60
2	F	148	ASN	CA-CB-CG	8.16	120.76	112.60
1	E	86	GLU	N-CA-C	-8.11	101.44	113.61
1	A	86	GLU	N-CA-C	-8.03	101.57	113.61
3	K	91	PHE	CA-CB-CG	7.99	121.79	113.80
2	B	377	ARG	N-CA-C	7.97	120.05	111.36
2	D	377	ARG	N-CA-C	7.94	120.01	111.36
1	G	86	GLU	N-CA-C	-7.88	101.80	113.61
1	C	179	LYS	CA-C-N	7.78	131.33	120.29
1	C	179	LYS	C-N-CA	7.78	131.33	120.29
3	J	325	VAL	N-CA-C	7.56	122.36	112.76
3	J	324	TYR	CA-C-N	7.54	133.90	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	324	TYR	C-N-CA	7.54	133.90	121.54
2	D	182	LYS	N-CA-C	7.50	120.86	110.35
2	B	182	LYS	N-CA-C	7.48	120.82	110.35
1	G	85	GLN	CA-C-N	7.46	133.93	122.29
1	G	85	GLN	C-N-CA	7.46	133.93	122.29
3	K	58	PHE	CA-CB-CG	7.35	121.15	113.80
2	D	337	SER	N-CA-C	7.28	120.64	111.69
2	H	182	LYS	N-CA-C	7.22	120.45	110.35
2	B	332	ILE	CA-C-N	7.19	129.92	120.28
2	B	332	ILE	C-N-CA	7.19	129.92	120.28
2	B	649	ALA	N-CA-C	-7.16	99.61	110.14
2	B	337	SER	N-CA-C	7.16	120.49	111.69
2	F	125	GLU	CA-C-N	7.15	134.57	121.70
2	F	125	GLU	C-N-CA	7.15	134.57	121.70
2	F	182	LYS	N-CA-C	7.13	120.34	110.35
1	A	360	ILE	CA-C-N	7.12	130.16	120.54
1	A	360	ILE	C-N-CA	7.12	130.16	120.54
1	E	85	GLN	CA-C-N	7.12	133.39	122.29
1	E	85	GLN	C-N-CA	7.12	133.39	122.29
2	B	125	GLU	CA-C-N	7.10	134.49	121.70
2	B	125	GLU	C-N-CA	7.10	134.49	121.70
1	G	360	ILE	CA-C-N	7.10	130.12	120.54
1	G	360	ILE	C-N-CA	7.10	130.12	120.54
1	E	360	ILE	CA-C-N	7.04	130.04	120.54
1	E	360	ILE	C-N-CA	7.04	130.04	120.54
3	I	315	LYS	CA-C-N	7.04	129.71	120.28
3	I	315	LYS	C-N-CA	7.04	129.71	120.28
2	H	337	SER	N-CA-C	7.02	120.32	111.69
1	C	85	GLN	CA-C-N	7.00	133.20	122.29
1	C	85	GLN	C-N-CA	7.00	133.20	122.29
2	H	125	GLU	CA-C-N	6.99	134.27	121.70
2	H	125	GLU	C-N-CA	6.99	134.27	121.70
2	D	125	GLU	CA-C-N	6.98	134.26	121.70
2	D	125	GLU	C-N-CA	6.98	134.26	121.70
2	F	377	ARG	N-CA-C	6.97	118.96	111.36
2	D	332	ILE	CA-C-N	6.94	129.58	120.28
2	D	332	ILE	C-N-CA	6.94	129.58	120.28
2	D	649	ALA	N-CA-C	-6.93	99.95	110.14
3	K	194	THR	CB-CA-C	6.92	121.06	111.51
2	B	830	ASP	CA-CB-CG	6.83	119.43	112.60
1	C	360	ILE	CA-C-N	6.81	129.73	120.54
1	C	360	ILE	C-N-CA	6.81	129.73	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	830	ASP	CA-CB-CG	6.78	119.38	112.60
2	H	377	ARG	N-CA-C	6.78	118.75	111.36
2	F	649	ALA	N-CA-C	-6.78	100.18	110.14
2	F	332	ILE	CA-C-N	6.76	129.34	120.28
2	F	332	ILE	C-N-CA	6.76	129.34	120.28
3	J	126	LEU	CA-C-N	6.76	129.22	120.44
3	J	126	LEU	C-N-CA	6.76	129.22	120.44
3	I	144	GLU	CA-C-N	6.68	129.56	120.54
3	I	144	GLU	C-N-CA	6.68	129.56	120.54
2	H	649	ALA	N-CA-C	-6.68	100.32	110.14
2	H	332	ILE	CA-C-N	6.67	129.22	120.28
2	H	332	ILE	C-N-CA	6.67	129.22	120.28
3	I	36	PRO	N-CA-C	6.67	118.84	110.70
2	D	710	GLU	N-CA-C	-6.66	105.06	113.72
1	E	902	ASN	CA-CB-CG	6.66	119.26	112.60
2	F	710	GLU	N-CA-C	-6.65	105.08	113.72
1	G	673	PRO	CA-C-N	6.61	129.43	120.38
1	G	673	PRO	C-N-CA	6.61	129.43	120.38
2	B	710	GLU	N-CA-C	-6.58	105.17	113.72
1	C	969	HIS	N-CA-C	6.58	119.87	108.76
3	K	126	LEU	CA-C-N	6.55	134.04	121.54
3	K	126	LEU	C-N-CA	6.55	134.04	121.54
2	B	536	LYS	CA-C-N	6.52	129.31	120.44
2	B	536	LYS	C-N-CA	6.52	129.31	120.44
3	I	100	ASN	CA-C-N	6.51	129.00	120.60
3	I	100	ASN	C-N-CA	6.51	129.00	120.60
3	I	300	ARG	CA-C-N	6.51	128.91	120.44
3	I	300	ARG	C-N-CA	6.51	128.91	120.44
1	G	981	SER	N-CA-C	-6.51	102.14	110.53
1	E	673	PRO	CA-C-N	6.50	129.28	120.38
1	E	673	PRO	C-N-CA	6.50	129.28	120.38
3	I	33	SER	N-CA-C	6.50	118.69	110.24
2	H	536	LYS	CA-C-N	6.49	129.27	120.44
2	H	536	LYS	C-N-CA	6.49	129.27	120.44
1	C	673	PRO	CA-C-N	6.48	129.26	120.38
1	C	673	PRO	C-N-CA	6.48	129.26	120.38
3	L	126	LEU	CA-C-N	6.46	129.58	120.28
3	L	126	LEU	C-N-CA	6.46	129.58	120.28
1	A	85	GLN	CA-C-N	6.44	132.34	122.29
1	A	85	GLN	C-N-CA	6.44	132.34	122.29
3	K	193	ILE	CA-C-N	6.41	130.81	121.26
3	K	193	ILE	C-N-CA	6.41	130.81	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	536	LYS	CA-C-N	6.40	129.15	120.44
2	F	536	LYS	C-N-CA	6.40	129.15	120.44
1	E	969	HIS	N-CA-C	6.40	119.57	108.76
1	A	673	PRO	CA-C-N	6.39	129.13	120.38
1	A	673	PRO	C-N-CA	6.39	129.13	120.38
3	L	307	PHE	CA-C-N	6.37	128.72	120.44
3	L	307	PHE	C-N-CA	6.37	128.72	120.44
3	J	194	THR	CB-CA-C	6.34	120.24	111.23
2	D	360	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	434	ASN	N-CA-C	6.32	118.52	110.61
1	C	902	ASN	CA-CB-CG	6.30	118.90	112.60
2	B	360	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	969	HIS	N-CA-C	6.27	119.35	108.76
3	J	213	GLU	CB-CG-CD	6.26	123.23	112.60
2	D	830	ASP	CA-CB-CG	6.25	118.85	112.60
1	C	464	ASP	CA-CB-CG	6.22	118.82	112.60
2	H	710	GLU	N-CA-C	-6.21	105.65	113.72
3	J	288	ASN	CA-CB-CG	6.21	118.81	112.60
3	I	149	GLU	N-CA-C	-6.20	103.06	111.55
2	F	360	ASP	CA-CB-CG	6.16	118.76	112.60
2	D	536	LYS	CA-C-N	6.13	128.78	120.44
2	D	536	LYS	C-N-CA	6.13	128.78	120.44
3	K	247	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	950	VAL	N-CA-C	6.12	116.78	110.36
1	E	522	SER	CA-C-N	6.11	132.04	122.26
1	E	522	SER	C-N-CA	6.11	132.04	122.26
3	J	311	ARG	N-CA-C	6.11	120.81	113.23
2	H	830	ASP	CA-CB-CG	6.11	118.71	112.60
1	E	950	VAL	N-CA-C	6.10	116.77	110.36
3	I	5	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	902	ASN	CA-CB-CG	6.08	118.68	112.60
3	K	306	ASN	CA-CB-CG	6.08	118.68	112.60
3	L	129	SER	CA-C-N	6.08	130.42	120.63
3	L	129	SER	C-N-CA	6.08	130.42	120.63
3	I	194	THR	CB-CA-C	6.06	119.84	111.23
3	I	255	ASN	CA-C-N	6.04	128.29	120.44
3	I	255	ASN	C-N-CA	6.04	128.29	120.44
1	G	175	SER	N-CA-C	6.03	118.13	109.14
1	A	526	ILE	CB-CA-C	6.01	117.92	110.95
1	E	464	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	464	ASP	CA-CB-CG	5.97	118.57	112.60
1	G	736	GLU	N-CA-C	-5.96	106.17	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	969	HIS	N-CA-C	5.95	118.82	108.76
1	G	464	ASP	CA-CB-CG	5.95	118.55	112.60
2	H	360	ASP	CA-CB-CG	5.94	118.54	112.60
3	K	255	ASN	CA-C-N	5.93	129.72	120.82
3	K	255	ASN	C-N-CA	5.93	129.72	120.82
1	C	522	SER	CA-C-N	5.93	131.75	122.26
1	C	522	SER	C-N-CA	5.93	131.75	122.26
1	A	175	SER	N-CA-C	5.92	117.96	109.14
3	J	224	VAL	N-CA-CB	5.92	117.47	110.55
1	A	656	GLU	N-CA-C	5.91	119.16	110.30
2	F	457	LEU	N-CA-C	5.90	119.14	109.76
3	J	10	ASP	CA-CB-CG	5.88	118.48	112.60
2	B	81	ASN	CA-C-N	5.87	130.32	121.40
2	B	81	ASN	C-N-CA	5.87	130.32	121.40
2	D	913	SER	N-CA-C	5.87	118.32	109.23
1	E	441	LYS	CA-C-N	5.86	128.16	120.60
1	E	441	LYS	C-N-CA	5.86	128.16	120.60
3	I	306	ASN	CA-CB-CG	5.84	118.44	112.60
1	C	441	LYS	CA-C-N	5.83	128.12	120.60
1	C	441	LYS	C-N-CA	5.83	128.12	120.60
1	E	175	SER	N-CA-C	5.82	117.82	109.14
3	J	71	LEU	CA-C-N	5.82	129.55	120.82
3	J	71	LEU	C-N-CA	5.82	129.55	120.82
1	E	179	LYS	CA-C-N	5.82	128.55	120.29
1	E	179	LYS	C-N-CA	5.82	128.55	120.29
1	G	950	VAL	N-CA-C	5.82	116.47	110.36
1	A	522	SER	CA-C-N	5.80	131.54	122.26
1	A	522	SER	C-N-CA	5.80	131.54	122.26
2	H	457	LEU	N-CA-C	5.80	118.98	109.76
1	G	656	GLU	N-CA-C	5.77	118.96	110.30
2	B	554	ILE	N-CA-CB	5.77	118.38	110.54
3	J	97	ILE	N-CA-CB	5.75	114.12	110.50
2	B	913	SER	N-CA-C	5.75	118.15	109.23
2	D	702	ILE	CA-C-N	5.75	128.45	120.29
2	D	702	ILE	C-N-CA	5.75	128.45	120.29
2	B	702	ILE	CA-C-N	5.75	128.45	120.29
2	B	702	ILE	C-N-CA	5.75	128.45	120.29
3	J	15	ASN	CA-C-N	5.74	128.20	120.50
3	J	15	ASN	C-N-CA	5.74	128.20	120.50
3	J	149	GLU	N-CA-C	-5.74	103.42	110.65
1	A	589	GLY	N-CA-C	-5.73	107.27	115.64
2	D	457	LEU	N-CA-C	5.73	118.87	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	702	ILE	CA-C-N	5.73	128.43	120.29
2	H	702	ILE	C-N-CA	5.73	128.43	120.29
3	K	68	ASP	CA-CB-CG	5.72	118.32	112.60
3	I	227	LEU	CA-C-N	5.72	127.94	120.28
3	I	227	LEU	C-N-CA	5.72	127.94	120.28
2	H	181	ARG	CA-C-N	5.71	129.82	121.31
2	H	181	ARG	C-N-CA	5.71	129.82	121.31
1	C	656	GLU	N-CA-C	5.71	118.86	110.30
3	J	247	ASN	CA-CB-CG	5.70	118.30	112.60
3	I	127	ASN	N-CA-C	5.69	120.22	113.16
3	J	180	GLY	N-CA-C	5.69	123.95	112.34
1	C	534	LEU	CA-C-N	-5.69	113.94	122.24
1	C	534	LEU	C-N-CA	-5.69	113.94	122.24
1	G	522	SER	CA-C-N	5.69	131.36	122.26
1	G	522	SER	C-N-CA	5.69	131.36	122.26
3	I	91	PHE	CA-CB-CG	5.68	119.48	113.80
2	H	552	ASN	CA-CB-CG	5.67	118.27	112.60
3	K	38	ILE	N-CA-CB	5.66	117.82	110.57
3	L	241	ASP	CA-CB-CG	5.65	118.25	112.60
1	E	589	GLY	N-CA-C	-5.64	107.40	115.64
1	G	441	LYS	CA-C-N	5.64	127.87	120.60
1	G	441	LYS	C-N-CA	5.64	127.87	120.60
1	C	712	ALA	CA-C-N	5.63	127.82	120.28
1	C	712	ALA	C-N-CA	5.63	127.82	120.28
1	E	981	SER	N-CA-C	-5.63	102.58	110.35
2	B	457	LEU	N-CA-C	5.62	118.70	109.76
1	E	656	GLU	N-CA-C	5.62	118.73	110.30
1	G	258	ASP	N-CA-C	-5.62	106.38	113.18
2	F	702	ILE	CA-C-N	5.62	128.26	120.29
2	F	702	ILE	C-N-CA	5.62	128.26	120.29
1	E	570	ASP	CA-CB-CG	5.61	118.21	112.60
3	J	211	ASP	CA-C-N	5.61	129.23	120.82
3	J	211	ASP	C-N-CA	5.61	129.23	120.82
1	A	258	ASP	N-CA-C	-5.60	106.40	113.18
2	F	913	SER	N-CA-C	5.59	117.89	109.23
3	I	340	ASN	CB-CA-C	5.58	118.10	110.06
3	J	237	THR	CB-CA-C	5.58	120.10	111.28
1	C	950	VAL	N-CA-C	5.57	116.21	110.36
2	D	891	VAL	N-CA-CB	-5.57	103.08	112.44
3	I	324	TYR	CA-C-N	5.57	130.28	121.09
3	I	324	TYR	C-N-CA	5.57	130.28	121.09
1	C	175	SER	N-CA-C	5.57	117.44	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	333	ASP	CA-CB-CG	5.56	118.16	112.60
2	H	134	VAL	N-CA-C	-5.55	104.28	112.04
2	H	913	SER	N-CA-C	5.55	117.83	109.23
3	I	257	LEU	N-CA-C	-5.54	105.14	111.07
3	I	68	ASP	CA-CB-CG	5.53	118.13	112.60
3	L	85	PHE	CA-CB-CG	5.53	119.33	113.80
1	A	441	LYS	CA-C-N	5.52	127.72	120.60
1	A	441	LYS	C-N-CA	5.52	127.72	120.60
2	F	552	ASN	CA-CB-CG	5.51	118.11	112.60
2	D	552	ASN	CA-CB-CG	5.51	118.11	112.60
1	G	902	ASN	CA-CB-CG	5.51	118.11	112.60
3	K	340	ASN	CA-CB-CG	5.49	118.09	112.60
1	A	361	ASP	CA-C-N	5.48	130.63	122.74
1	A	361	ASP	C-N-CA	5.48	130.63	122.74
2	B	8	ASN	N-CA-C	5.47	118.01	111.71
2	H	854	SER	CA-C-N	5.47	127.93	120.54
2	H	854	SER	C-N-CA	5.47	127.93	120.54
1	G	712	ALA	CA-C-N	5.47	127.61	120.28
1	G	712	ALA	C-N-CA	5.47	127.61	120.28
1	G	343	GLU	CA-C-N	5.47	127.87	120.38
1	G	343	GLU	C-N-CA	5.47	127.87	120.38
3	K	201	LYS	CA-C-N	5.46	127.53	120.44
3	K	201	LYS	C-N-CA	5.46	127.53	120.44
1	C	70	GLU	N-CA-C	5.46	118.01	108.52
3	L	74	TYR	N-CA-C	5.45	116.91	110.97
3	J	91	PHE	CA-CB-CG	5.45	119.25	113.80
1	C	676	ASP	CA-CB-CG	5.45	118.05	112.60
2	F	134	VAL	N-CA-C	-5.44	104.42	112.04
1	G	361	ASP	CA-C-N	5.44	130.57	122.74
1	G	361	ASP	C-N-CA	5.44	130.57	122.74
3	L	247	ASN	CA-CB-CG	5.43	118.03	112.60
2	D	81	ASN	CA-C-N	5.42	129.64	121.40
2	D	81	ASN	C-N-CA	5.42	129.64	121.40
1	C	343	GLU	CA-C-N	5.42	127.80	120.38
1	C	343	GLU	C-N-CA	5.42	127.80	120.38
1	G	728	VAL	CA-C-N	5.42	128.08	120.28
1	G	728	VAL	C-N-CA	5.42	128.08	120.28
2	H	891	VAL	N-CA-CB	-5.41	103.35	112.44
1	E	361	ASP	CA-C-N	5.41	130.53	122.74
1	E	361	ASP	C-N-CA	5.41	130.53	122.74
3	K	316	ASN	CA-C-N	5.40	131.86	121.54
3	K	316	ASN	C-N-CA	5.40	131.86	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	255	ASN	CA-CB-CG	5.40	118.00	112.60
1	C	728	VAL	CA-C-N	5.40	128.05	120.28
1	C	728	VAL	C-N-CA	5.40	128.05	120.28
1	C	258	ASP	N-CA-C	-5.39	106.65	113.18
2	B	134	VAL	N-CA-C	-5.39	104.49	112.04
3	J	254	ASN	CA-C-N	5.39	129.00	121.02
3	J	254	ASN	C-N-CA	5.39	129.00	121.02
1	A	509	THR	CB-CA-C	5.39	119.41	110.90
3	L	215	ASP	N-CA-C	5.39	117.96	109.39
2	F	181	ARG	CA-C-N	5.39	129.34	121.31
2	F	181	ARG	C-N-CA	5.39	129.34	121.31
3	J	90	GLY	CA-C-N	5.39	131.02	122.94
3	J	90	GLY	C-N-CA	5.39	131.02	122.94
2	B	552	ASN	CA-CB-CG	5.39	117.99	112.60
2	H	81	ASN	CA-C-N	5.38	129.58	121.40
2	H	81	ASN	C-N-CA	5.38	129.58	121.40
3	J	114	SER	N-CA-C	5.38	118.83	110.17
2	F	891	VAL	N-CA-CB	-5.37	103.41	112.44
2	B	146	PHE	CA-C-N	5.37	129.94	121.56
2	B	146	PHE	C-N-CA	5.37	129.94	121.56
1	A	728	VAL	CA-C-N	5.37	128.01	120.28
1	A	728	VAL	C-N-CA	5.37	128.01	120.28
2	B	706	VAL	N-CA-C	5.37	113.18	107.76
1	E	405	ARG	N-CA-C	5.35	117.19	111.36
2	B	891	VAL	N-CA-CB	-5.35	103.45	112.44
2	D	784	SER	CA-C-N	5.35	127.39	120.44
2	D	784	SER	C-N-CA	5.35	127.39	120.44
1	A	534	LEU	CA-C-N	-5.34	114.44	122.24
1	A	534	LEU	C-N-CA	-5.34	114.44	122.24
1	C	589	GLY	N-CA-C	-5.34	107.84	115.64
2	B	561	HIS	N-CA-C	5.33	118.62	112.97
3	L	41	VAL	N-CA-CB	5.33	117.40	110.57
1	A	981	SER	N-CA-C	-5.33	102.99	110.35
1	A	570	ASP	CA-CB-CG	5.33	117.93	112.60
3	I	238	LYS	N-CA-C	-5.32	100.56	109.24
3	I	199	CYS	CA-C-N	5.32	127.41	120.28
3	I	199	CYS	C-N-CA	5.32	127.41	120.28
2	F	333	ASP	CA-CB-CG	5.32	117.92	112.60
3	K	294	GLU	CB-CG-CD	5.32	121.64	112.60
3	J	109	SER	CA-C-N	5.31	127.66	120.38
3	J	109	SER	C-N-CA	5.31	127.66	120.38
1	G	361	ASP	CA-CB-CG	5.31	117.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	570	ASP	CA-CB-CG	5.31	117.91	112.60
2	F	854	SER	CA-C-N	5.31	127.71	120.54
2	F	854	SER	C-N-CA	5.31	127.71	120.54
1	C	361	ASP	CA-C-N	5.30	130.38	122.74
1	C	361	ASP	C-N-CA	5.30	130.38	122.74
3	K	41	VAL	N-CA-CB	5.30	117.36	110.57
1	G	405	ARG	N-CA-C	5.30	117.14	111.36
1	A	361	ASP	CA-CB-CG	5.29	117.89	112.60
2	B	705	ASN	CA-CB-CG	5.29	117.89	112.60
1	E	736	GLU	N-CA-C	-5.28	107.01	113.50
2	B	854	SER	CA-C-N	5.28	127.66	120.54
2	B	854	SER	C-N-CA	5.28	127.66	120.54
1	E	434	ASN	N-CA-C	5.28	118.84	111.56
3	J	33	SER	CA-C-N	5.27	127.88	120.28
3	J	33	SER	C-N-CA	5.27	127.88	120.28
2	D	705	ASN	CA-CB-CG	5.26	117.86	112.60
3	K	292	TYR	CA-C-N	5.25	127.38	120.60
3	K	292	TYR	C-N-CA	5.25	127.38	120.60
1	C	570	ASP	CA-CB-CG	5.25	117.85	112.60
2	D	854	SER	CA-C-N	5.25	127.62	120.54
2	D	854	SER	C-N-CA	5.25	127.62	120.54
1	C	361	ASP	CA-CB-CG	5.25	117.85	112.60
3	L	202	THR	CA-C-N	5.25	127.31	120.28
3	L	202	THR	C-N-CA	5.25	127.31	120.28
1	E	70	GLU	N-CA-C	5.25	117.65	108.52
2	D	865	GLU	CA-C-N	5.24	127.30	120.28
2	D	865	GLU	C-N-CA	5.24	127.30	120.28
1	C	736	GLU	N-CA-C	-5.24	107.05	113.50
1	G	70	GLU	N-CA-C	5.24	117.63	108.52
1	A	343	GLU	CA-C-N	5.23	127.55	120.38
1	A	343	GLU	C-N-CA	5.23	127.55	120.38
1	E	892	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	645	GLY	CA-C-N	5.22	131.52	121.54
1	A	645	GLY	C-N-CA	5.22	131.52	121.54
2	F	554	ILE	N-CA-CB	5.22	117.64	110.54
2	D	706	VAL	N-CA-C	5.22	113.03	107.76
1	E	591	TYR	CA-C-N	5.22	128.51	121.05
1	E	591	TYR	C-N-CA	5.22	128.51	121.05
3	L	59	SER	CA-C-N	5.21	127.52	120.38
3	L	59	SER	C-N-CA	5.21	127.52	120.38
3	I	325	VAL	N-CA-C	5.21	120.16	113.07
1	A	66	PHE	N-CA-C	5.21	115.58	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	357	VAL	N-CA-CB	5.20	117.59	111.66
2	H	865	GLU	CA-C-N	5.20	127.25	120.28
2	H	865	GLU	C-N-CA	5.20	127.25	120.28
1	A	70	GLU	N-CA-C	5.20	117.57	108.52
1	C	509	THR	CB-CA-C	5.20	119.12	110.90
2	B	738	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	711	ARG	CA-C-N	5.19	127.50	120.65
1	A	711	ARG	C-N-CA	5.19	127.50	120.65
1	C	798	PRO	N-CA-C	5.19	119.24	111.14
1	C	79	GLU	CA-C-N	5.19	128.14	120.82
1	C	79	GLU	C-N-CA	5.19	128.14	120.82
1	A	97	GLY	N-CA-C	5.18	122.54	112.64
1	E	258	ASP	N-CA-C	-5.18	106.91	113.18
1	C	145	GLY	N-CA-C	5.18	119.07	112.13
1	C	405	ARG	N-CA-C	5.18	117.00	111.36
2	F	81	ASN	CA-C-N	5.18	129.27	121.40
2	F	81	ASN	C-N-CA	5.18	129.27	121.40
1	A	798	PRO	N-CA-C	5.18	119.22	111.14
1	A	736	GLU	N-CA-C	-5.17	107.13	113.50
2	B	839	VAL	CA-C-N	5.17	128.96	120.63
2	B	839	VAL	C-N-CA	5.17	128.96	120.63
1	C	950	VAL	N-CA-CB	5.17	116.25	110.51
2	D	287	GLY	CA-C-N	5.17	127.46	120.38
2	D	287	GLY	C-N-CA	5.17	127.46	120.38
2	B	894	GLY	N-CA-C	5.17	120.44	111.14
2	D	181	ARG	CA-C-N	5.17	129.01	121.31
2	D	181	ARG	C-N-CA	5.17	129.01	121.31
3	L	309	LYS	CA-C-N	5.17	127.72	120.28
3	L	309	LYS	C-N-CA	5.17	127.72	120.28
1	C	981	SER	N-CA-C	-5.17	103.22	110.35
1	E	588	ASP	CA-CB-CG	5.16	117.76	112.60
2	D	554	ILE	N-CA-CB	5.15	117.55	110.54
1	E	728	VAL	CA-C-N	5.15	127.70	120.28
1	E	728	VAL	C-N-CA	5.15	127.70	120.28
3	L	194	THR	CA-C-N	5.15	129.45	122.19
3	L	194	THR	C-N-CA	5.15	129.45	122.19
1	E	66	PHE	N-CA-C	5.14	115.52	109.60
1	G	588	ASP	CA-CB-CG	5.14	117.75	112.60
3	J	119	PRO	N-CA-C	5.14	119.39	111.21
1	A	86	GLU	CA-C-N	5.14	130.10	120.95
1	A	86	GLU	C-N-CA	5.14	130.10	120.95
2	F	615	ALA	N-CA-C	5.14	116.57	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	361	ASP	CA-CB-CG	5.13	117.73	112.60
3	J	144	GLU	CA-C-N	5.13	127.16	120.28
3	J	144	GLU	C-N-CA	5.13	127.16	120.28
1	G	645	GLY	CA-C-N	5.13	131.34	121.54
1	G	645	GLY	C-N-CA	5.13	131.34	121.54
1	G	434	ASN	N-CA-C	5.13	118.64	111.56
3	K	307	PHE	N-CA-C	-5.13	105.38	111.69
3	J	329	ASN	CA-CB-CG	5.12	117.72	112.60
1	G	509	THR	CB-CA-C	5.12	119.00	110.90
1	A	676	ASP	CA-CB-CG	5.12	117.72	112.60
2	B	181	ARG	CA-C-N	5.12	128.94	121.31
2	B	181	ARG	C-N-CA	5.12	128.94	121.31
2	B	911	PHE	N-CA-C	5.12	120.00	113.55
2	H	705	ASN	CA-CB-CG	5.11	117.71	112.60
1	G	145	GLY	N-CA-C	5.11	118.98	112.13
2	H	911	PHE	N-CA-C	5.11	119.98	113.55
1	C	591	TYR	CA-C-N	5.11	128.35	121.05
1	C	591	TYR	C-N-CA	5.11	128.35	121.05
2	D	463	THR	CB-CA-C	5.10	118.63	110.16
2	D	517	VAL	N-CA-CB	5.10	116.17	110.51
2	B	149	PRO	CA-C-N	5.09	131.27	121.54
2	B	149	PRO	C-N-CA	5.09	131.27	121.54
1	E	712	ALA	CA-C-N	5.09	127.11	120.28
1	E	712	ALA	C-N-CA	5.09	127.11	120.28
2	D	894	GLY	N-CA-C	5.09	120.31	111.14
1	G	943	SER	CA-C-N	5.09	128.44	120.75
1	G	943	SER	C-N-CA	5.09	128.44	120.75
3	L	10	ASP	CA-CB-CG	5.09	117.69	112.60
3	L	94	ASP	CA-CB-CG	5.08	117.68	112.60
1	G	589	GLY	N-CA-C	-5.08	108.23	115.64
1	C	97	GLY	N-CA-C	5.08	122.33	112.64
3	I	178	ASN	CA-C-N	5.08	130.54	122.62
3	I	178	ASN	C-N-CA	5.08	130.54	122.62
2	D	351	ARG	CA-C-N	5.07	126.95	120.56
2	D	351	ARG	C-N-CA	5.07	126.95	120.56
1	E	711	ARG	CA-C-N	5.07	127.35	120.65
1	E	711	ARG	C-N-CA	5.07	127.35	120.65
2	D	134	VAL	N-CA-C	-5.07	104.95	112.04
1	C	588	ASP	CA-CB-CG	5.06	117.66	112.60
1	E	950	VAL	N-CA-CB	5.06	116.12	110.51
2	H	615	ALA	N-CA-C	5.06	116.48	111.07
2	F	705	ASN	CA-CB-CG	5.05	117.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	432	GLU	CA-C-N	5.05	127.00	120.44
1	G	432	GLU	C-N-CA	5.05	127.00	120.44
1	C	749	SER	CA-C-N	5.05	125.54	119.94
1	C	749	SER	C-N-CA	5.05	125.54	119.94
1	A	79	GLU	CA-C-N	5.04	127.93	120.82
1	A	79	GLU	C-N-CA	5.04	127.93	120.82
1	G	591	TYR	CA-C-N	5.04	128.25	121.05
1	G	591	TYR	C-N-CA	5.04	128.25	121.05
1	A	405	ARG	N-CA-C	5.03	116.84	111.36
2	B	351	ARG	CA-C-N	5.02	126.89	120.56
2	B	351	ARG	C-N-CA	5.02	126.89	120.56
2	D	206	ALA	CA-C-N	5.02	125.55	119.98
2	D	206	ALA	C-N-CA	5.02	125.55	119.98
3	L	47	THR	CB-CA-C	5.02	118.43	109.29
3	K	224	VAL	N-CA-CB	5.02	116.08	110.51
1	C	432	GLU	CA-C-N	5.02	126.96	120.44
1	C	432	GLU	C-N-CA	5.02	126.96	120.44
1	E	137	LEU	CA-C-N	5.01	126.96	120.44
1	E	137	LEU	C-N-CA	5.01	126.96	120.44
3	L	277	ASP	N-CA-C	5.01	116.23	109.11
2	F	146	PHE	CA-C-N	5.01	129.37	121.56
2	F	146	PHE	C-N-CA	5.01	129.37	121.56
2	D	911	PHE	N-CA-C	5.00	119.86	113.55
1	E	357	VAL	N-CA-CB	5.00	117.37	111.66

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	915	VAL	Mainchain
2	D	915	VAL	Mainchain
1	E	123	LEU	Mainchain
2	F	915	VAL	Mainchain
2	H	915	VAL	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	7008	0	6692	86	0
1	C	7008	0	6692	85	0
1	E	7008	0	6692	86	0
1	G	7008	0	6692	81	0
2	B	6546	0	6253	73	0
2	D	6546	0	6253	75	0
2	F	6546	0	6253	72	0
2	H	6546	0	6253	73	0
3	I	2590	0	2509	41	0
3	J	2590	0	2509	54	0
3	K	2590	0	2509	40	0
3	L	2590	0	2509	46	0
4	A	65	0	0	1	0
4	B	10	0	0	0	0
4	C	50	0	0	3	0
4	D	15	0	0	0	0
4	E	40	0	0	2	0
4	F	15	0	0	0	0
4	G	40	0	0	0	0
4	H	20	0	0	0	0
4	I	25	0	0	0	0
4	J	15	0	0	0	0
4	K	15	0	0	0	0
4	L	15	0	0	0	0
5	B	31	0	12	0	0
5	D	31	0	12	0	0
5	F	31	0	12	1	0
5	H	31	0	12	1	0
All	All	65025	0	61864	750	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (750) 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)
2:B:650:ASP:CB	2:D:148:ASN:HB2	2.01	0.90
2:F:148:ASN:HB2	2:H:650:ASP:CB	2.06	0.85
1:C:622:LEU:HD21	1:C:655:VAL:HG11	1.59	0.84
1:E:216:ILE:HG22	1:E:246:CYS:HB3	1.60	0.84
3:I:255:ASN:O	3:I:259:GLN:HG3	1.78	0.84
1:C:216:ILE:HG22	1:C:246:CYS:HB3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:216:ILE:HG22	1:G:246:CYS:HB3	1.60	0.83
1:A:216:ILE:HG22	1:A:246:CYS:HB3	1.60	0.82
1:A:622:LEU:HD21	1:A:655:VAL:HG11	1.62	0.81
1:G:622:LEU:HD21	1:G:655:VAL:HG11	1.65	0.79
2:B:148:ASN:HB2	2:D:650:ASP:CB	2.13	0.79
1:E:622:LEU:HD21	1:E:655:VAL:HG11	1.65	0.78
3:K:225:THR:HG22	3:K:320:LEU:HD22	1.68	0.75
3:J:86:VAL:HG22	3:J:242:LEU:HB3	1.67	0.74
1:G:467:LEU:HD23	1:G:560:LYS:HG2	1.70	0.73
1:E:467:LEU:HD23	1:E:560:LYS:HG2	1.71	0.73
1:A:467:LEU:HD23	1:A:560:LYS:HG2	1.71	0.73
1:G:393:SER:HB2	1:G:396:ARG:HG3	1.70	0.73
1:A:393:SER:HB2	1:A:396:ARG:HG3	1.70	0.72
1:E:445:ARG:HE	1:E:587:ASP:HB2	1.55	0.72
2:H:122:SER:HB3	2:H:123:PRO:HD3	1.72	0.72
2:D:780:MET:CE	3:J:265:SER:HB3	2.20	0.72
1:G:445:ARG:HE	1:G:587:ASP:HB2	1.54	0.71
1:E:393:SER:HB2	1:E:396:ARG:HG3	1.70	0.71
2:B:122:SER:HB3	2:B:123:PRO:HD3	1.72	0.71
1:C:393:SER:HB2	1:C:396:ARG:HG3	1.73	0.71
1:C:445:ARG:HE	1:C:587:ASP:HB2	1.56	0.70
2:F:650:ASP:CB	2:H:148:ASN:HB2	2.20	0.70
1:C:467:LEU:HD23	1:C:560:LYS:HG2	1.73	0.70
2:F:122:SER:HB3	2:F:123:PRO:HD3	1.72	0.70
1:A:445:ARG:HE	1:A:587:ASP:HB2	1.56	0.70
3:J:282:VAL:HG22	3:J:340:ASN:HD21	1.57	0.70
3:J:218:MET:HE3	3:J:226:LEU:HD12	1.74	0.69
3:L:225:THR:HG22	3:L:320:LEU:HD22	1.74	0.69
3:J:282:VAL:HG22	3:J:340:ASN:ND2	2.07	0.69
2:D:122:SER:HB3	2:D:123:PRO:HD3	1.73	0.68
1:C:390:THR:HG23	2:D:470:GLY:HA2	1.74	0.68
2:H:189:SER:HB3	2:H:288:SER:HB3	1.75	0.68
2:F:189:SER:HB3	2:F:288:SER:HB3	1.74	0.68
3:L:75:TYR:HB3	3:L:79:GLU:HB2	1.74	0.68
1:A:294:LEU:HD11	1:A:331:ILE:HD12	1.75	0.66
3:K:228:LEU:HD22	3:K:320:LEU:HD21	1.77	0.66
3:I:264:GLU:HG2	3:I:330:ILE:HD12	1.78	0.66
3:J:307:PHE:HD2	3:J:308:LEU:HD12	1.59	0.66
2:B:189:SER:HB3	2:B:288:SER:HB3	1.77	0.66
3:I:329:ASN:HD22	3:I:329:ASN:H	1.42	0.65
1:A:390:THR:HG23	2:B:470:GLY:HA2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:709:THR:CG2	2:D:894:GLY:HA2	2.27	0.65
1:G:728:VAL:HG22	1:G:744:CYS:HB2	1.78	0.64
3:I:123:TYR:HD1	3:I:198:LEU:HD11	1.62	0.64
2:H:709:THR:CG2	2:H:894:GLY:HA2	2.27	0.64
2:D:189:SER:HB3	2:D:288:SER:HB3	1.78	0.64
2:F:709:THR:CG2	2:F:894:GLY:HA2	2.28	0.64
3:I:290:ASN:O	3:I:294:GLU:HB2	1.96	0.64
1:C:728:VAL:HG22	1:C:744:CYS:HB2	1.78	0.63
1:G:390:THR:HG23	2:H:470:GLY:HA2	1.79	0.63
3:I:247:ASN:HD22	3:I:247:ASN:H	1.47	0.63
1:A:728:VAL:HG22	1:A:744:CYS:HB2	1.80	0.63
2:F:290:THR:HG22	2:F:520:VAL:HG13	1.81	0.63
2:B:412:CYS:SG	2:B:454:ARG:HD2	2.38	0.63
1:E:728:VAL:HG22	1:E:744:CYS:HB2	1.81	0.63
3:I:257:LEU:HG	3:I:261:LYS:HD2	1.81	0.63
2:B:709:THR:CG2	2:B:894:GLY:HA2	2.29	0.62
3:L:221:ARG:HG3	3:L:253:MET:HB3	1.80	0.62
1:E:294:LEU:HD11	1:E:331:ILE:HD12	1.82	0.62
1:G:294:LEU:HD11	1:G:331:ILE:HD12	1.79	0.62
3:J:125:VAL:HG22	3:J:198:LEU:HD12	1.82	0.62
2:H:412:CYS:SG	2:H:454:ARG:HD2	2.40	0.61
3:I:120:LEU:HD23	3:I:193:ILE:HD12	1.82	0.61
3:I:95:LEU:HB3	3:I:99:LEU:HD23	1.83	0.61
2:F:412:CYS:SG	2:F:454:ARG:HD2	2.42	0.60
2:B:577:ILE:HD11	2:B:666:LEU:HD21	1.83	0.60
1:G:412:LEU:HD21	1:G:577:TYR:HA	1.84	0.60
3:J:11:LEU:HD22	3:J:16:VAL:HG11	1.84	0.60
3:K:307:PHE:HD2	3:K:308:LEU:HD12	1.66	0.60
1:C:762:SER:HB3	2:D:643:ARG:HG3	1.84	0.60
2:F:577:ILE:HD11	2:F:666:LEU:HD21	1.84	0.60
2:D:188:THR:OG1	2:D:249:THR:HG21	2.02	0.59
1:C:294:LEU:HD11	1:C:331:ILE:HD12	1.83	0.59
2:F:188:THR:OG1	2:F:249:THR:HG21	2.02	0.59
3:K:228:LEU:HD21	3:K:266:LEU:HD11	1.83	0.59
2:B:290:THR:HG22	2:B:520:VAL:HG13	1.83	0.59
2:H:286:ASP:O	2:H:290:THR:HG23	2.03	0.59
2:F:286:ASP:O	2:F:290:THR:HG23	2.03	0.59
2:H:918:ARG:HD2	2:H:920:ARG:HH21	1.68	0.59
2:B:286:ASP:O	2:B:290:THR:HG23	2.03	0.59
3:I:90:GLY:HA2	3:I:125:VAL:O	2.02	0.59
2:B:188:THR:OG1	2:B:249:THR:HG21	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:411:MET:HE1	2:H:447:VAL:HG13	1.84	0.58
2:H:577:ILE:HD11	2:H:666:LEU:HD21	1.84	0.58
2:D:577:ILE:HD11	2:D:666:LEU:HD21	1.84	0.58
1:C:412:LEU:HD21	1:C:577:TYR:HA	1.85	0.58
1:E:412:LEU:HD21	1:E:577:TYR:HA	1.84	0.58
3:L:179:ARG:HG3	3:L:202:THR:HG23	1.85	0.58
2:D:780:MET:HE1	3:J:265:SER:HB3	1.84	0.58
2:D:411:MET:HE1	2:D:447:VAL:HG13	1.85	0.58
1:E:390:THR:HG23	2:F:470:GLY:HA2	1.85	0.58
2:B:918:ARG:HD2	2:B:920:ARG:HH21	1.67	0.57
2:D:286:ASP:O	2:D:290:THR:HG23	2.04	0.57
2:D:412:CYS:SG	2:D:454:ARG:HD2	2.45	0.57
2:F:411:MET:HE1	2:F:447:VAL:HG13	1.86	0.57
3:I:320:LEU:HG	3:I:324:TYR:HD2	1.69	0.57
3:K:218:MET:HE3	3:K:226:LEU:HD12	1.86	0.57
2:H:188:THR:OG1	2:H:249:THR:HG21	2.03	0.57
1:A:412:LEU:HD21	1:A:577:TYR:HA	1.85	0.57
1:C:686:GLN:HE21	1:G:685:GLN:HE21	1.51	0.57
3:J:247:ASN:HD22	3:J:247:ASN:H	1.53	0.57
2:D:918:ARG:HD2	2:D:920:ARG:HH21	1.68	0.57
1:A:129:PHE:HD1	2:D:10:THR:HG23	1.70	0.56
2:D:290:THR:HG22	2:D:520:VAL:HG13	1.87	0.56
2:F:709:THR:HG22	2:F:894:GLY:HA2	1.88	0.56
2:H:903:THR:HB	2:H:908:LEU:HD11	1.87	0.56
3:K:69:LYS:O	3:K:73:ASN:HB2	2.05	0.56
1:A:762:SER:HB3	2:B:643:ARG:HG3	1.87	0.56
2:B:411:MET:HE1	2:B:447:VAL:HG13	1.87	0.56
3:J:69:LYS:O	3:J:73:ASN:ND2	2.39	0.56
2:F:918:ARG:HD2	2:F:920:ARG:HH21	1.68	0.56
3:J:307:PHE:HZ	3:J:321:ILE:HD12	1.70	0.56
3:K:312:LYS:HE3	3:K:317:ALA:HA	1.88	0.56
1:A:130:PHE:HD1	1:A:170:PHE:HA	1.70	0.56
2:D:211:GLY:HA3	3:J:296:ILE:HG21	1.88	0.56
1:G:247:TYR:HE2	1:G:261:LYS:HB2	1.71	0.56
1:G:668:THR:O	2:H:736:THR:HG22	2.06	0.56
3:L:178:ASN:HB3	3:L:205:MET:HE1	1.87	0.56
3:L:247:ASN:HD22	3:L:247:ASN:H	1.53	0.55
1:E:130:PHE:HD1	1:E:170:PHE:HA	1.72	0.55
1:A:668:THR:O	2:B:736:THR:HG22	2.07	0.55
2:F:903:THR:HB	2:F:908:LEU:HD11	1.88	0.55
1:A:247:TYR:HE2	1:A:261:LYS:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:PHE:HD1	1:G:170:PHE:HA	1.70	0.55
2:H:709:THR:HG22	2:H:894:GLY:HA2	1.87	0.55
1:A:427:GLU:HG3	1:A:573:PHE:CZ	2.42	0.55
1:G:427:GLU:HG3	1:G:573:PHE:CZ	2.41	0.55
3:J:307:PHE:CD2	3:J:308:LEU:HD12	2.40	0.55
2:D:123:PRO:HD2	2:D:126:ILE:HA	1.89	0.55
1:E:427:GLU:HG3	1:E:573:PHE:CZ	2.41	0.55
3:K:51:LEU:HD11	3:K:98:PRO:HB2	1.87	0.55
2:B:709:THR:HG22	2:B:894:GLY:HA2	1.88	0.55
2:D:709:THR:HG22	2:D:894:GLY:HA2	1.88	0.55
1:A:686:GLN:HE21	1:E:685:GLN:HE21	1.55	0.54
1:C:427:GLU:HG3	1:C:573:PHE:CZ	2.42	0.54
2:H:290:THR:HG22	2:H:520:VAL:HG13	1.88	0.54
3:J:51:LEU:HD21	3:J:98:PRO:HB2	1.90	0.54
1:C:592:LEU:CD1	1:C:598:ARG:HH12	2.20	0.54
2:F:123:PRO:HD2	2:F:126:ILE:HA	1.89	0.54
2:D:903:THR:HB	2:D:908:LEU:HD11	1.89	0.54
1:E:592:LEU:CD1	1:E:598:ARG:HH12	2.20	0.54
2:F:182:LYS:HB2	2:F:278:ASP:HB2	1.89	0.54
2:F:267:LYS:HA	2:F:270:LYS:HD2	1.90	0.54
3:J:69:LYS:HB2	3:J:72:THR:HB	1.90	0.54
2:B:903:THR:HB	2:B:908:LEU:HD11	1.90	0.54
3:L:127:ASN:HD21	3:L:248:ASN:CG	2.15	0.54
2:D:182:LYS:HB2	2:D:278:ASP:HB2	1.90	0.54
2:D:384:LEU:HD13	2:D:550:MET:HE2	1.89	0.54
2:B:123:PRO:HD2	2:B:126:ILE:HA	1.89	0.54
1:G:592:LEU:CD1	1:G:598:ARG:HH12	2.20	0.54
3:J:310:LYS:HD3	3:J:311:ARG:HG3	1.89	0.54
2:D:709:THR:HG23	2:D:894:GLY:HA2	1.89	0.54
3:J:178:ASN:HB3	3:J:205:MET:HE1	1.90	0.54
1:C:130:PHE:HD1	1:C:170:PHE:HA	1.72	0.53
1:E:226:ASN:HD22	1:E:275:GLY:H	1.56	0.53
1:E:383:LEU:HD13	2:F:467:VAL:HG21	1.89	0.53
2:H:123:PRO:HD2	2:H:126:ILE:HA	1.89	0.53
2:H:182:LYS:HB2	2:H:278:ASP:HB2	1.90	0.53
1:A:123:LEU:HD22	2:D:136:PRO:HD2	1.90	0.53
1:C:383:LEU:HD13	2:D:467:VAL:HG21	1.89	0.53
1:E:247:TYR:HE2	1:E:261:LYS:HB2	1.72	0.53
3:J:66:PRO:HG2	3:J:73:ASN:ND2	2.22	0.53
3:K:276:LEU:HG	3:K:343:ILE:HG12	1.90	0.53
2:B:780:MET:HE1	3:I:265:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:TYR:HE2	1:C:261:LYS:HB2	1.72	0.53
1:E:826:LYS:HZ2	1:E:827:ILE:H	1.56	0.53
1:G:882:LEU:HD11	1:G:940:ILE:HD11	1.90	0.53
1:A:826:LYS:HZ2	1:A:827:ILE:H	1.56	0.53
2:B:363:ALA:O	2:B:365:SER:N	2.42	0.53
2:B:474:VAL:HG13	2:B:720:ASN:HD21	1.73	0.53
1:G:226:ASN:HD22	1:G:275:GLY:H	1.56	0.53
3:L:83:LEU:HD22	3:L:242:LEU:HB2	1.91	0.53
1:G:148:ILE:HB	1:G:159:SER:HB3	1.91	0.53
3:K:71:LEU:HD11	3:K:107:MET:HG3	1.90	0.53
3:K:97:ILE:O	3:K:101:VAL:HG23	2.09	0.53
1:G:826:LYS:HZ2	1:G:827:ILE:H	1.57	0.52
2:F:709:THR:HG23	2:F:894:GLY:HA2	1.91	0.52
2:H:709:THR:HG23	2:H:894:GLY:HA2	1.90	0.52
3:I:92:SER:HB2	3:I:246:THR:OG1	2.10	0.52
3:J:292:TYR:HD1	3:J:303:GLU:HG2	1.74	0.52
1:A:148:ILE:HB	1:A:159:SER:HB3	1.92	0.52
1:A:420:ALA:HB2	1:A:457:ILE:HD12	1.91	0.52
2:D:193:SER:O	2:D:196:MET:HG3	2.10	0.52
1:C:770:GLU:HB3	1:C:861:VAL:HG13	1.92	0.52
1:A:592:LEU:CD1	1:A:598:ARG:HH12	2.23	0.52
1:C:530:VAL:HG23	1:C:543:LEU:HA	1.91	0.52
1:C:615:PRO:HG3	1:C:871:PRO:HG3	1.92	0.52
1:A:78:ARG:HE	2:B:571:ARG:HH12	1.58	0.52
2:D:267:LYS:HA	2:D:270:LYS:HD2	1.92	0.52
2:H:577:ILE:HG23	2:H:607:ILE:HB	1.90	0.52
2:B:193:SER:O	2:B:196:MET:HG3	2.09	0.52
1:C:882:LEU:HD11	1:C:940:ILE:HD11	1.92	0.52
1:C:439:LEU:HD11	1:C:475:VAL:HG13	1.92	0.52
1:E:78:ARG:HE	2:F:571:ARG:HH12	1.58	0.52
1:C:826:LYS:HZ2	1:C:827:ILE:H	1.58	0.52
1:E:530:VAL:HG23	1:E:543:LEU:HA	1.92	0.52
3:I:307:PHE:HZ	3:I:321:ILE:HD12	1.74	0.52
2:B:267:LYS:HA	2:B:270:LYS:HD2	1.91	0.52
2:B:566:LEU:HD12	2:B:600:ARG:HB3	1.92	0.52
1:G:420:ALA:HB2	1:G:457:ILE:HD12	1.92	0.52
2:H:363:ALA:O	2:H:365:SER:N	2.43	0.52
2:B:182:LYS:HB2	2:B:278:ASP:HB2	1.92	0.51
1:E:148:ILE:HB	1:E:159:SER:HB3	1.90	0.51
2:H:631:TRP:HA	2:H:634:LEU:HD12	1.92	0.51
1:E:439:LEU:HD11	1:E:475:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:ARG:HB2	2:F:463:THR:HG23	1.92	0.51
4:E:991:SO4:O3	2:F:739:ARG:NH2	2.43	0.51
2:H:780:MET:HE1	3:L:265:SER:HB3	1.91	0.51
1:A:530:VAL:HG23	1:A:543:LEU:HA	1.91	0.51
1:E:444:LEU:HD11	1:E:482:ILE:HD12	1.92	0.51
2:F:363:ALA:O	2:F:365:SER:N	2.43	0.51
1:A:226:ASN:HD22	1:A:275:GLY:H	1.57	0.51
3:L:66:PRO:HB2	3:L:73:ASN:HD21	1.76	0.51
2:D:363:ALA:O	2:D:365:SER:N	2.44	0.51
2:F:566:LEU:HD12	2:F:600:ARG:HB3	1.93	0.51
1:G:606:VAL:O	1:G:696:GLY:HA3	2.11	0.51
3:K:333:GLN:HB2	3:K:347:SER:HB3	1.92	0.51
1:A:606:VAL:O	1:A:696:GLY:HA3	2.11	0.51
1:E:420:ALA:HB2	1:E:457:ILE:HD12	1.93	0.51
1:G:599:LEU:HB3	1:G:690:ASP:HB2	1.93	0.51
2:H:193:SER:O	2:H:196:MET:HG3	2.11	0.51
2:H:566:LEU:HD12	2:H:600:ARG:HB3	1.92	0.51
3:I:320:LEU:HG	3:I:324:TYR:CD2	2.46	0.51
1:E:790:LEU:HG	1:E:826:LYS:HE3	1.93	0.51
1:G:444:LEU:HD11	1:G:482:ILE:HD12	1.92	0.51
3:L:95:LEU:HD22	3:L:99:LEU:HD23	1.93	0.51
2:B:577:ILE:HG23	2:B:607:ILE:HB	1.92	0.51
3:I:88:GLN:HE22	3:I:104:VAL:HG22	1.75	0.51
3:J:19:GLU:CD	3:J:19:GLU:H	2.18	0.51
3:J:273:CYS:HB3	3:J:346:ILE:HD12	1.93	0.51
3:L:81:ASN:ND2	3:L:114:SER:H	2.08	0.51
2:B:384:LEU:HD13	2:B:550:MET:HE2	1.91	0.51
1:C:599:LEU:HB3	1:C:690:ASP:HB2	1.93	0.51
1:E:615:PRO:HG3	1:E:871:PRO:HG3	1.92	0.51
2:F:193:SER:O	2:F:196:MET:HG3	2.11	0.51
2:F:631:TRP:HA	2:F:634:LEU:HD12	1.92	0.51
1:G:615:PRO:HG3	1:G:871:PRO:HG3	1.92	0.51
2:D:474:VAL:HG13	2:D:720:ASN:HD21	1.74	0.50
2:D:566:LEU:HD12	2:D:600:ARG:HB3	1.92	0.50
2:H:267:LYS:HA	2:H:270:LYS:HD2	1.93	0.50
3:I:11:LEU:HD22	3:I:16:VAL:HG11	1.93	0.50
2:B:709:THR:HG23	2:B:894:GLY:HA2	1.92	0.50
2:D:780:MET:HE1	3:J:324:TYR:HA	1.93	0.50
1:G:383:LEU:HD13	2:H:467:VAL:HG21	1.93	0.50
1:A:595:GLU:HG3	1:A:598:ARG:HH21	1.76	0.50
3:J:24:LEU:HD22	3:J:140:TYR:HD2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:VAL:O	1:C:696:GLY:HA3	2.11	0.50
2:D:299:TRP:O	2:D:301:SER:N	2.44	0.50
1:G:530:VAL:HG23	1:G:543:LEU:HA	1.92	0.50
1:C:949:PRO:HB2	1:C:952:GLN:HE21	1.77	0.50
2:D:659:GLU:HB2	2:D:690:SER:HB3	1.93	0.50
2:H:576:ILE:CG2	2:H:593:MET:HE2	2.41	0.50
1:A:898:LYS:HG2	3:K:117:ASP:O	2.12	0.50
3:I:38:ILE:HD11	3:I:105:LEU:O	2.11	0.50
3:I:245:LEU:O	3:I:277:ASP:HA	2.11	0.50
2:D:577:ILE:HG23	2:D:607:ILE:HB	1.92	0.50
1:E:668:THR:O	2:F:736:THR:HG22	2.12	0.50
1:E:762:SER:HB3	2:F:643:ARG:HG3	1.94	0.50
2:F:577:ILE:HG23	2:F:607:ILE:HB	1.93	0.50
2:H:659:GLU:HB2	2:H:690:SER:HB3	1.94	0.50
1:A:882:LEU:HD11	1:A:940:ILE:HD11	1.94	0.50
1:C:420:ALA:HB2	1:C:457:ILE:HD12	1.94	0.50
2:F:384:LEU:HD13	2:F:550:MET:HE2	1.94	0.50
1:G:674:SER:HG	1:G:706:GLU:CD	2.20	0.50
3:L:218:MET:HE3	3:L:226:LEU:HD12	1.94	0.50
2:B:257:LYS:HA	2:B:260:ARG:HE	1.77	0.50
1:C:226:ASN:HD22	1:C:275:GLY:H	1.59	0.50
2:D:396:LEU:HD13	2:D:430:VAL:HG22	1.94	0.50
1:E:882:LEU:HD11	1:E:940:ILE:HD11	1.93	0.50
1:G:541:GLN:HE21	1:G:541:GLN:HA	1.77	0.49
3:K:292:TYR:HD1	3:K:303:GLU:HG2	1.77	0.49
1:A:444:LEU:HD11	1:A:482:ILE:HD12	1.93	0.49
1:C:790:LEU:HG	1:C:826:LYS:HE3	1.94	0.49
2:F:356:ILE:HG12	2:F:372:VAL:HG21	1.94	0.49
2:F:659:GLU:HB2	2:F:690:SER:HB3	1.95	0.49
1:A:439:LEU:HD11	1:A:475:VAL:HG13	1.93	0.49
2:F:474:VAL:HG13	2:F:720:ASN:HD21	1.76	0.49
2:H:299:TRP:O	2:H:301:SER:N	2.45	0.49
3:I:78:TYR:CZ	3:I:82:VAL:HG21	2.47	0.49
3:K:41:VAL:HG11	3:K:145:ALA:HB2	1.93	0.49
1:A:513:VAL:HG21	1:A:976:VAL:HG13	1.95	0.49
1:A:599:LEU:HB3	1:A:690:ASP:HB2	1.95	0.49
2:D:356:ILE:HG12	2:D:372:VAL:HG21	1.94	0.49
1:G:790:LEU:HG	1:G:826:LYS:HE3	1.93	0.49
3:J:292:TYR:CD1	3:J:303:GLU:HG2	2.47	0.49
3:L:81:ASN:HD21	3:L:114:SER:H	1.60	0.49
2:H:474:VAL:HG13	2:H:720:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:PRO:HG3	1:A:871:PRO:HG3	1.94	0.49
2:B:631:TRP:HA	2:B:634:LEU:HD12	1.95	0.49
1:C:148:ILE:HB	1:C:159:SER:HB3	1.93	0.49
1:G:595:GLU:HG3	1:G:598:ARG:HH21	1.78	0.49
3:I:255:ASN:HB3	3:I:258:GLN:HB2	1.94	0.49
3:K:83:LEU:HD22	3:K:242:LEU:HB2	1.95	0.49
1:A:129:PHE:CD1	2:D:10:THR:HG23	2.48	0.49
1:A:383:LEU:HD13	2:B:467:VAL:HG21	1.95	0.49
1:G:439:LEU:HD11	1:G:475:VAL:HG13	1.94	0.49
1:C:444:LEU:HD11	1:C:482:ILE:HD12	1.94	0.49
1:E:599:LEU:HB3	1:E:690:ASP:HB2	1.94	0.49
2:H:205:ARG:HG2	2:H:237:TRP:CD2	2.48	0.49
3:L:107:MET:HG2	3:L:244:LEU:HD11	1.95	0.49
3:L:207:LEU:HD11	3:L:226:LEU:HD13	1.95	0.49
1:A:949:PRO:HB2	1:A:952:GLN:HE21	1.78	0.48
2:H:739:ARG:HD3	2:H:741:PHE:CE2	2.48	0.48
2:B:780:MET:O	3:I:327:ARG:NH2	2.45	0.48
2:D:780:MET:HE2	3:J:265:SER:HB3	1.95	0.48
2:F:257:LYS:HA	2:F:260:ARG:HE	1.78	0.48
2:F:396:LEU:HD13	2:F:430:VAL:HG22	1.94	0.48
1:G:762:SER:HB3	2:H:643:ARG:HG3	1.95	0.48
1:G:949:PRO:HB2	1:G:952:GLN:HE21	1.79	0.48
1:E:949:PRO:HB2	1:E:952:GLN:HE21	1.78	0.48
2:B:396:LEU:HD13	2:B:430:VAL:HG22	1.94	0.48
1:C:361:ASP:HB2	4:C:991:SO4:O3	2.13	0.48
1:G:919:LYS:HE2	1:G:929:VAL:HG21	1.95	0.48
2:H:384:LEU:HD13	2:H:550:MET:HE2	1.94	0.48
3:I:71:LEU:HD12	3:I:110:GLN:HB2	1.95	0.48
1:A:490:ARG:HB2	2:B:463:THR:HG23	1.96	0.48
1:C:592:LEU:HD13	1:C:598:ARG:HH12	1.78	0.48
2:D:576:ILE:CG2	2:D:593:MET:HE2	2.43	0.48
2:D:739:ARG:HD3	2:D:741:PHE:CE2	2.49	0.48
3:I:264:GLU:HG2	3:I:330:ILE:CD1	2.42	0.48
3:J:62:ASN:ND2	3:J:340:ASN:HB2	2.29	0.48
2:F:205:ARG:HG2	2:F:237:TRP:CD2	2.49	0.48
2:F:739:ARG:HD3	2:F:741:PHE:CE2	2.48	0.48
3:L:90:GLY:HA2	3:L:125:VAL:O	2.14	0.48
2:B:356:ILE:HG12	2:B:372:VAL:HG21	1.95	0.48
2:D:631:TRP:HA	2:D:634:LEU:HD12	1.94	0.48
2:F:299:TRP:O	2:F:301:SER:N	2.45	0.48
2:H:356:ILE:HG12	2:H:372:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:558:SER:O	2:F:560:ASP:N	2.47	0.48
1:E:95:LEU:HB3	1:E:96:LEU:H	1.61	0.48
1:E:513:VAL:HG21	1:E:976:VAL:HG13	1.96	0.48
1:G:490:ARG:HB2	2:H:463:THR:HG23	1.96	0.48
3:J:5:ASP:HA	3:J:8:ILE:HD12	1.96	0.48
2:B:659:GLU:HB2	2:B:690:SER:HB3	1.95	0.48
1:C:541:GLN:HE21	1:C:541:GLN:HA	1.79	0.48
1:C:901:ALA:HB2	3:L:118:LEU:HD13	1.96	0.48
2:D:257:LYS:HA	2:D:260:ARG:HE	1.78	0.48
2:D:397:ILE:HD11	2:D:550:MET:HE3	1.94	0.48
2:F:576:ILE:CG2	2:F:593:MET:HE2	2.44	0.48
1:G:60:GLU:HG2	1:G:109:LYS:HA	1.96	0.47
2:H:257:LYS:HA	2:H:260:ARG:HE	1.79	0.47
2:H:878:ILE:HG22	2:H:879:SER:H	1.79	0.47
3:I:81:ASN:ND2	3:I:117:ASP:OD2	2.47	0.47
3:J:78:TYR:CE2	3:J:82:VAL:HG21	2.49	0.47
3:K:107:MET:HE2	3:K:244:LEU:HD21	1.95	0.47
3:L:255:ASN:O	3:L:259:GLN:HB2	2.14	0.47
1:A:592:LEU:HD13	1:A:598:ARG:HH12	1.79	0.47
1:A:635:ARG:NH2	4:A:993:SO4:O1	2.47	0.47
1:A:790:LEU:HG	1:A:826:LYS:HE3	1.95	0.47
1:E:869:LYS:HA	2:F:731:GLN:HE22	1.79	0.47
1:G:592:LEU:HD13	1:G:598:ARG:HH12	1.80	0.47
2:D:205:ARG:HG2	2:D:237:TRP:CD2	2.50	0.47
2:D:558:SER:O	2:D:560:ASP:N	2.47	0.47
3:J:126:LEU:HG	3:J:197:LEU:HD11	1.95	0.47
2:F:815:GLU:O	2:F:819:THR:HG23	2.14	0.47
3:I:272:ASN:HB2	3:I:345:GLN:NE2	2.29	0.47
3:J:73:ASN:OD1	3:J:74:TYR:N	2.48	0.47
2:B:576:ILE:CG2	2:B:593:MET:HE2	2.45	0.47
1:E:541:GLN:HA	1:E:541:GLN:HE21	1.79	0.47
2:F:576:ILE:HD13	2:F:593:MET:HG2	1.97	0.47
1:G:133:SER:HB3	1:G:136:LYS:HB2	1.94	0.47
3:L:97:ILE:HD11	3:L:131:THR:HG22	1.95	0.47
1:A:15:VAL:HG22	1:A:109:LYS:HB2	1.97	0.47
1:A:60:GLU:HG2	1:A:109:LYS:HA	1.97	0.47
1:C:95:LEU:HB3	1:C:96:LEU:H	1.61	0.47
1:E:133:SER:HB3	1:E:136:LYS:HB2	1.97	0.47
1:E:510:VAL:HG12	1:E:538:ILE:HG13	1.96	0.47
1:G:234:ARG:HD2	1:G:268:VAL:HG23	1.97	0.47
3:J:74:TYR:OH	3:J:335:LYS:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:606:VAL:O	1:E:696:GLY:HA3	2.15	0.47
1:G:150:PRO:HG3	1:G:157:GLU:O	2.15	0.47
2:H:396:LEU:HD13	2:H:430:VAL:HG22	1.95	0.47
3:K:80:VAL:HA	3:K:83:LEU:HD12	1.97	0.47
3:L:307:PHE:HZ	3:L:321:ILE:HD12	1.79	0.47
2:B:205:ARG:HG2	2:B:237:TRP:CD2	2.50	0.47
2:B:739:ARG:HD3	2:B:741:PHE:CE2	2.49	0.47
1:C:510:VAL:HG12	1:C:538:ILE:HG13	1.97	0.47
1:G:15:VAL:HG22	1:G:109:LYS:HB2	1.97	0.47
3:J:244:LEU:HD22	3:J:276:LEU:HD22	1.97	0.47
1:A:541:GLN:HE21	1:A:541:GLN:HA	1.80	0.47
1:A:770:GLU:HB3	1:A:861:VAL:HG13	1.96	0.47
1:A:851:GLY:HA3	1:A:854:ARG:HB2	1.97	0.47
1:C:513:VAL:HG21	1:C:976:VAL:HG13	1.97	0.47
2:D:211:GLY:HA3	3:J:296:ILE:CG2	2.45	0.47
1:A:133:SER:HB3	1:A:136:LYS:HB2	1.97	0.46
2:B:558:SER:O	2:B:560:ASP:N	2.48	0.46
1:E:770:GLU:HB3	1:E:861:VAL:HG13	1.97	0.46
2:F:257:LYS:H	2:F:257:LYS:HD3	1.81	0.46
2:H:908:LEU:HA	2:H:912:GLU:HB2	1.97	0.46
1:A:403:MET:HA	1:A:460:GLU:HB2	1.97	0.46
1:E:60:GLU:HG2	1:E:109:LYS:HA	1.97	0.46
2:B:908:LEU:HA	2:B:912:GLU:HB2	1.98	0.46
2:D:848:MET:HE2	2:D:852:ARG:NH2	2.30	0.46
2:H:576:ILE:HD13	2:H:593:MET:HG2	1.96	0.46
3:J:244:LEU:HD23	3:J:276:LEU:HB3	1.96	0.46
1:G:757:GLN:OE1	2:H:843:GLY:HA2	2.15	0.46
3:L:21:GLY:HA2	3:L:24:LEU:HD12	1.97	0.46
1:C:133:SER:HB3	1:C:136:LYS:HB2	1.97	0.46
2:F:908:LEU:HA	2:F:912:GLU:HB2	1.98	0.46
1:G:513:VAL:HG21	1:G:976:VAL:HG13	1.97	0.46
1:G:838:TYR:HB3	1:G:843:ILE:HD11	1.98	0.46
2:H:558:SER:O	2:H:560:ASP:N	2.49	0.46
3:L:179:ARG:HD2	3:L:206:ILE:HG13	1.98	0.46
2:D:576:ILE:HD13	2:D:593:MET:HG2	1.98	0.46
1:E:592:LEU:HD13	1:E:598:ARG:HH12	1.80	0.46
2:F:249:THR:HG22	2:F:252:GLY:H	1.81	0.46
1:G:510:VAL:HG12	1:G:538:ILE:HG13	1.96	0.46
1:G:851:GLY:HA3	1:G:854:ARG:HB2	1.98	0.46
1:G:770:GLU:HB3	1:G:861:VAL:HG13	1.96	0.46
2:H:397:ILE:HD11	2:H:550:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:134:TYR:O	3:I:138:VAL:HG23	2.16	0.46
3:L:86:VAL:HG23	3:L:120:LEU:HD11	1.97	0.46
1:A:233:THR:HA	1:A:243:VAL:HG21	1.98	0.46
3:J:183:ARG:HG2	3:J:194:THR:HB	1.97	0.46
3:K:255:ASN:O	3:K:259:GLN:HG3	2.15	0.46
1:A:798:PRO:HG2	3:J:233:ARG:HA	1.98	0.46
1:G:233:THR:HA	1:G:243:VAL:HG21	1.98	0.46
1:E:15:VAL:HG22	1:E:109:LYS:HB2	1.97	0.46
3:I:27:LEU:HD21	3:I:41:VAL:HG23	1.98	0.46
3:L:39:GLU:HA	3:L:42:LYS:HB2	1.97	0.46
1:C:60:GLU:HG2	1:C:109:LYS:HA	1.96	0.45
2:F:811:VAL:HG13	1:G:845:ALA:HB1	1.98	0.45
2:H:897:LYS:O	2:H:899:GLN:N	2.49	0.45
3:K:220:ASP:HB2	3:K:253:MET:HE3	1.97	0.45
2:B:576:ILE:HD13	2:B:593:MET:HG2	1.98	0.45
3:J:37:PRO:O	3:J:41:VAL:HG12	2.15	0.45
2:H:127:SER:CB	2:H:128:PRO:HD3	2.47	0.45
2:H:815:GLU:O	2:H:819:THR:HG23	2.16	0.45
3:K:74:TYR:CE1	3:K:335:LYS:HB3	2.51	0.45
3:L:85:PHE:CD2	3:L:238:LYS:HB3	2.51	0.45
1:A:685:GLN:HE21	1:E:686:GLN:HE21	1.64	0.45
1:A:838:TYR:HB3	1:A:843:ILE:HD11	1.99	0.45
1:C:86:GLU:HG2	2:D:621:ARG:HH21	1.80	0.45
1:C:233:THR:HA	1:C:243:VAL:HG21	1.97	0.45
1:C:851:GLY:HA3	1:C:854:ARG:HB2	1.97	0.45
2:D:187:MET:HB3	2:D:217:ILE:HB	1.98	0.45
2:D:257:LYS:H	2:D:257:LYS:HD3	1.82	0.45
2:D:815:GLU:O	2:D:819:THR:HG23	2.17	0.45
3:L:243:LEU:HD22	3:L:245:LEU:HD13	1.98	0.45
1:E:423:ILE:HG22	1:E:457:ILE:HB	1.99	0.45
1:G:70:GLU:HB2	1:G:181:ILE:HA	1.99	0.45
2:B:249:THR:HG22	2:B:252:GLY:H	1.82	0.45
2:B:257:LYS:H	2:B:257:LYS:HD3	1.81	0.45
3:J:71:LEU:HD11	3:J:107:MET:HG3	1.99	0.45
2:B:299:TRP:O	2:B:301:SER:N	2.48	0.45
1:G:34:PHE:HB3	1:G:63:LEU:HB3	1.99	0.45
3:L:125:VAL:HG22	3:L:198:LEU:HD12	1.98	0.45
1:C:403:MET:HA	1:C:460:GLU:HB2	1.98	0.45
2:H:78:ASN:HA	2:H:81:ASN:HD22	1.82	0.45
3:L:220:ASP:HB2	3:L:253:MET:HG3	1.98	0.45
2:B:127:SER:CB	2:B:128:PRO:HD3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:MET:HB3	2:B:217:ILE:HB	1.98	0.45
1:C:15:VAL:HG22	1:C:109:LYS:HB2	1.98	0.45
1:C:800:ASN:ND2	1:C:803:THR:HG23	2.31	0.45
3:I:81:ASN:HB3	3:I:117:ASP:OD1	2.17	0.45
3:K:87:LEU:HB3	3:K:243:LEU:HD23	1.99	0.45
1:A:510:VAL:HG12	1:A:538:ILE:HG13	1.98	0.45
2:B:136:PRO:HD2	1:C:123:LEU:HD22	1.99	0.45
2:B:918:ARG:HB3	2:B:920:ARG:HE	1.82	0.45
1:C:595:GLU:HG3	1:C:598:ARG:HH21	1.82	0.45
1:E:595:GLU:HG3	1:E:598:ARG:HH21	1.82	0.45
2:H:918:ARG:HB3	2:H:920:ARG:HE	1.82	0.45
2:B:397:ILE:HD11	2:B:550:MET:HE3	1.99	0.44
1:C:838:TYR:HB3	1:C:843:ILE:HD11	1.99	0.44
2:F:187:MET:HB3	2:F:217:ILE:HB	1.99	0.44
1:C:234:ARG:HD2	1:C:268:VAL:HG23	1.98	0.44
1:E:233:THR:HA	1:E:243:VAL:HG21	1.99	0.44
1:E:272:LEU:H	1:E:272:LEU:HD23	1.82	0.44
1:E:403:MET:HA	1:E:460:GLU:HB2	1.98	0.44
1:G:403:MET:HA	1:G:460:GLU:HB2	1.98	0.44
3:L:5:ASP:HA	3:L:8:ILE:HD12	1.98	0.44
1:C:423:ILE:HG22	1:C:457:ILE:HB	1.99	0.44
3:K:308:LEU:HD21	3:K:325:VAL:HG11	1.99	0.44
3:K:327:ARG:HB2	3:K:330:ILE:CD1	2.48	0.44
3:L:120:LEU:HB2	3:L:191:ARG:CZ	2.47	0.44
2:B:143:PHE:CE1	2:B:148:ASN:O	2.71	0.44
1:C:417:ALA:O	1:C:876:ARG:HD3	2.17	0.44
1:C:685:GLN:HE21	1:G:686:GLN:HE21	1.64	0.44
1:E:851:GLY:HA3	1:E:854:ARG:HB2	1.98	0.44
2:F:414:ILE:HG12	5:F:942:ATP:H3'	1.99	0.44
2:H:249:THR:HG22	2:H:252:GLY:H	1.83	0.44
1:A:84:LEU:HD11	2:B:605:TYR:CE1	2.53	0.44
2:B:187:MET:HE2	2:B:282:VAL:HG13	2.00	0.44
2:B:939:THR:HG21	3:I:326:GLY:O	2.18	0.44
1:C:919:LYS:HE2	1:C:929:VAL:HG21	2.00	0.44
2:H:604:PRO:HB2	2:H:623:ILE:HD12	2.00	0.44
3:I:76:ASN:O	3:I:80:VAL:HG12	2.18	0.44
3:K:320:LEU:HG	3:K:324:TYR:HD2	1.82	0.44
2:D:897:LYS:O	2:D:899:GLN:N	2.51	0.44
2:F:780:MET:HE1	3:K:324:TYR:HA	1.98	0.44
3:J:90:GLY:HA2	3:J:125:VAL:O	2.18	0.44
1:A:423:ILE:HG22	1:A:457:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:815:GLU:O	2:B:819:THR:HG23	2.17	0.44
1:C:245:ALA:HB1	1:C:279:ILE:HG12	1.99	0.44
1:C:800:ASN:H	1:C:803:THR:HG1	1.65	0.44
1:G:247:TYR:O	1:G:252:GLY:HA3	2.18	0.44
3:K:126:LEU:HD12	3:K:197:LEU:HD11	2.00	0.44
1:C:272:LEU:HD23	1:C:272:LEU:H	1.83	0.44
1:C:377:LEU:HA	1:C:380:ILE:HD12	1.99	0.44
2:D:878:ILE:HG22	2:D:879:SER:H	1.82	0.44
1:E:123:LEU:HD22	2:H:136:PRO:HD2	2.00	0.44
1:E:735:THR:HB	1:E:939:GLY:HA3	2.00	0.44
2:H:257:LYS:HD3	2:H:257:LYS:H	1.81	0.44
3:I:329:ASN:HB2	3:I:350:LEU:HB2	2.00	0.44
3:L:88:GLN:HA	3:L:244:LEU:HB2	1.99	0.44
1:C:396:ARG:NH1	4:C:996:SO4:O2	2.50	0.44
2:D:127:SER:CB	2:D:128:PRO:HD3	2.48	0.44
2:D:249:THR:HG22	2:D:252:GLY:H	1.83	0.44
2:F:918:ARG:HB3	2:F:920:ARG:HE	1.82	0.44
3:L:147:GLY:C	3:L:149:GLU:H	2.26	0.44
3:L:221:ARG:H	3:L:253:MET:HE3	1.82	0.44
2:D:908:LEU:HA	2:D:912:GLU:HB2	2.00	0.43
1:E:377:LEU:HA	1:E:380:ILE:HD12	1.99	0.43
2:F:78:ASN:HA	2:F:81:ASN:HD22	1.82	0.43
2:F:878:ILE:HG22	2:F:879:SER:H	1.83	0.43
3:K:23:PHE:O	3:K:27:LEU:HB2	2.18	0.43
1:A:34:PHE:HB3	1:A:63:LEU:HB3	1.99	0.43
1:E:346:GLU:HG3	1:E:349:ARG:HH21	1.83	0.43
1:E:838:TYR:HB3	1:E:843:ILE:HD11	2.00	0.43
3:J:320:LEU:HG	3:J:324:TYR:HD2	1.82	0.43
1:A:417:ALA:O	1:A:876:ARG:HD3	2.18	0.43
2:D:78:ASN:HA	2:D:81:ASN:HD22	1.83	0.43
1:E:150:PRO:HG3	1:E:157:GLU:O	2.18	0.43
2:H:848:MET:HE2	2:H:852:ARG:NH2	2.33	0.43
3:I:35:LYS:HE2	3:I:39:GLU:HB3	1.99	0.43
2:D:399:GLU:O	2:D:535:PHE:HB3	2.19	0.43
2:D:604:PRO:HB2	2:D:623:ILE:HD12	1.99	0.43
1:E:919:LYS:HE2	1:E:929:VAL:HG21	2.00	0.43
1:G:272:LEU:HD23	1:G:272:LEU:H	1.82	0.43
2:H:375:MET:HE1	2:H:465:GLY:HA2	2.00	0.43
3:L:80:VAL:HA	3:L:83:LEU:HD12	1.99	0.43
1:A:763:ARG:HH11	1:A:763:ARG:HA	1.83	0.43
2:F:848:MET:HE2	2:F:852:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:187:MET:HE2	2:H:282:VAL:HG13	2.01	0.43
1:A:800:ASN:ND2	1:A:803:THR:HG23	2.33	0.43
1:G:140:LYS:HB2	1:G:140:LYS:HE3	1.83	0.43
3:I:179:ARG:HG2	3:I:202:THR:HG23	2.01	0.43
3:I:332:TYR:CE1	3:I:346:ILE:HG12	2.53	0.43
2:D:741:PHE:HA	2:D:832:LYS:O	2.18	0.43
2:F:897:LYS:O	2:F:899:GLN:N	2.52	0.43
1:G:797:ASN:HA	1:G:798:PRO:HD3	1.91	0.43
2:H:187:MET:HB3	2:H:217:ILE:HB	2.00	0.43
3:J:255:ASN:HB3	3:J:258:GLN:HB2	2.00	0.43
3:K:126:LEU:HD22	3:K:131:THR:HB	2.01	0.43
3:K:208:VAL:HG23	3:K:211:ASP:H	1.84	0.43
1:C:140:LYS:HB2	1:C:140:LYS:HE3	1.83	0.43
1:E:417:ALA:O	1:E:876:ARG:HD3	2.18	0.43
1:G:156:VAL:HA	1:G:169:SER:HB3	2.01	0.43
1:G:614:ASN:ND2	1:G:665:GLU:HG2	2.34	0.43
3:J:78:TYR:CZ	3:J:82:VAL:HG21	2.53	0.43
1:A:377:LEU:HA	1:A:380:ILE:HD12	2.01	0.43
1:A:614:ASN:ND2	1:A:665:GLU:HG2	2.33	0.43
1:C:70:GLU:HB2	1:C:181:ILE:HA	2.01	0.43
3:L:60:ARG:HH21	3:L:61:LYS:HE2	1.84	0.43
1:A:14:PHE:CE1	1:A:164:MET:HE2	2.53	0.43
2:B:604:PRO:HB2	2:B:623:ILE:HD12	2.01	0.43
2:B:783:ASN:HA	2:B:786:LYS:HD3	2.01	0.43
2:D:682:GLU:HA	2:D:685:ARG:HD3	2.01	0.43
1:E:70:GLU:HB2	1:E:181:ILE:HA	2.01	0.43
1:E:162:ASP:CG	1:E:163:PRO:HD2	2.44	0.43
1:G:423:ILE:HG22	1:G:457:ILE:HB	2.00	0.43
3:J:97:ILE:O	3:J:101:VAL:HG23	2.19	0.43
1:C:556:ALA:HB2	1:C:564:LYS:HD3	2.00	0.42
3:J:128:ASN:ND2	3:J:131:THR:H	2.17	0.42
3:K:179:ARG:HG3	3:K:205:MET:SD	2.58	0.42
1:E:779:LEU:HD23	1:E:779:LEU:HA	1.94	0.42
2:F:682:GLU:HA	2:F:685:ARG:HD3	2.01	0.42
1:G:14:PHE:CE1	1:G:164:MET:HE2	2.54	0.42
1:G:800:ASN:ND2	1:G:803:THR:HG23	2.35	0.42
1:A:346:GLU:HG3	1:A:349:ARG:HH21	1.83	0.42
2:B:78:ASN:HA	2:B:81:ASN:HD22	1.84	0.42
1:G:417:ALA:O	1:G:876:ARG:HD3	2.19	0.42
1:G:423:ILE:HG12	1:G:580:PHE:CE2	2.55	0.42
1:A:150:PRO:HG3	1:A:157:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HD2	1:A:268:VAL:HG23	2.00	0.42
1:G:162:ASP:CG	1:G:163:PRO:HD2	2.44	0.42
2:H:403:SER:HB3	5:H:942:ATP:O3G	2.19	0.42
3:K:292:TYR:CD1	3:K:303:GLU:HG2	2.54	0.42
3:L:273:CYS:HB3	3:L:346:ILE:HD12	2.00	0.42
1:A:156:VAL:HA	1:A:169:SER:HB3	2.01	0.42
1:A:162:ASP:CG	1:A:163:PRO:HD2	2.45	0.42
1:A:272:LEU:HD23	1:A:272:LEU:H	1.84	0.42
1:A:430:PRO:HB2	1:A:435:TRP:HB3	2.02	0.42
1:A:476:LYS:HG2	1:A:486:THR:HB	2.01	0.42
1:C:34:PHE:HB3	1:C:63:LEU:HB3	2.00	0.42
1:C:346:GLU:HG3	1:C:349:ARG:HH21	1.84	0.42
1:C:614:ASN:ND2	1:C:665:GLU:HG2	2.34	0.42
1:E:234:ARG:HD2	1:E:268:VAL:HG23	2.01	0.42
1:E:247:TYR:O	1:E:252:GLY:HA3	2.19	0.42
1:E:423:ILE:HG12	1:E:580:PHE:CE2	2.55	0.42
1:E:800:ASN:ND2	1:E:803:THR:HG23	2.34	0.42
2:F:127:SER:CB	2:F:128:PRO:HD3	2.49	0.42
3:J:8:ILE:HG12	3:J:21:GLY:HA2	2.02	0.42
2:B:356:ILE:HB	2:B:390:THR:HG21	2.02	0.42
2:B:758:GLN:HG3	2:B:763:ALA:HB3	2.00	0.42
2:B:848:MET:HE2	2:B:852:ARG:NH2	2.33	0.42
2:D:787:GLU:HG3	3:J:267:ASN:HB2	2.01	0.42
1:E:428:ARG:HD3	1:E:566:LEU:HD13	2.02	0.42
2:H:127:SER:HB3	2:H:128:PRO:HD3	2.02	0.42
2:H:356:ILE:HB	2:H:390:THR:HG21	2.01	0.42
1:A:735:THR:HB	1:A:939:GLY:HA3	2.01	0.42
1:A:793:TYR:HE2	1:A:828:PHE:HD2	1.67	0.42
1:A:984:LEU:HD21	3:J:207:LEU:HB3	2.00	0.42
2:B:768:VAL:HA	2:B:769:PRO:HD3	1.96	0.42
1:C:988:THR:O	3:I:218:MET:HA	2.19	0.42
1:E:364:MET:HE3	1:E:546:SER:HB3	2.02	0.42
1:E:614:ASN:ND2	1:E:665:GLU:HG2	2.35	0.42
2:F:187:MET:HE2	2:F:282:VAL:HG13	2.00	0.42
2:F:397:ILE:HD11	2:F:550:MET:HE3	2.01	0.42
2:F:741:PHE:HA	2:F:832:LYS:O	2.20	0.42
2:H:143:PHE:CE1	2:H:148:ASN:O	2.73	0.42
3:K:250:ASP:OD1	3:K:253:MET:HG3	2.20	0.42
1:A:797:ASN:HA	1:A:798:PRO:HD3	1.92	0.42
2:B:741:PHE:HA	2:B:832:LYS:O	2.19	0.42
2:F:596:TYR:CZ	2:F:600:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:913:PHE:CE1	1:G:915:ASP:HB2	2.55	0.42
2:H:195:GLY:C	2:H:198:PRO:HD2	2.45	0.42
3:L:51:LEU:HD22	3:L:99:LEU:HB2	2.00	0.42
1:A:245:ALA:HB1	1:A:279:ILE:HG12	2.01	0.42
1:C:247:TYR:O	1:C:252:GLY:HA3	2.20	0.42
1:C:428:ARG:HD3	1:C:566:LEU:HD13	2.02	0.42
1:E:245:ALA:HB1	1:E:279:ILE:HG12	2.01	0.42
4:E:990:SO4:S	2:F:828:ARG:NH2	2.92	0.42
1:G:346:GLU:HG3	1:G:349:ARG:HH21	1.84	0.42
1:G:377:LEU:HA	1:G:380:ILE:HD12	2.02	0.42
3:J:247:ASN:H	3:J:247:ASN:ND2	2.16	0.42
1:A:762:SER:HB3	2:B:643:ARG:H	1.84	0.42
1:C:162:ASP:CG	1:C:163:PRO:HD2	2.45	0.42
1:C:763:ARG:HH11	1:C:763:ARG:HA	1.84	0.42
2:D:218:HIS:HA	2:D:251:ILE:HG23	2.02	0.42
1:E:430:PRO:HB2	1:E:435:TRP:HB3	2.01	0.42
2:F:204:VAL:HA	2:F:214:VAL:HG11	2.01	0.42
2:H:204:VAL:HA	2:H:214:VAL:HG11	2.02	0.42
2:H:682:GLU:HA	2:H:685:ARG:HD3	2.02	0.42
3:I:224:VAL:HA	3:I:227:LEU:HD12	2.01	0.42
3:L:243:LEU:HD11	3:L:263:LEU:HD12	2.01	0.42
1:A:70:GLU:HB2	1:A:181:ILE:HA	2.02	0.41
1:C:156:VAL:HA	1:C:169:SER:HB3	2.02	0.41
1:E:14:PHE:CE1	1:E:164:MET:HE2	2.55	0.41
2:F:143:PHE:CE1	2:F:148:ASN:O	2.72	0.41
2:F:356:ILE:HA	2:F:359:ILE:HD12	2.01	0.41
2:F:604:PRO:HB2	2:F:623:ILE:HD12	2.01	0.41
1:G:735:THR:HB	1:G:939:GLY:HA3	2.01	0.41
2:B:897:LYS:O	2:B:899:GLN:N	2.53	0.41
1:C:938:ILE:HG12	1:C:947:PHE:CD1	2.54	0.41
1:E:757:GLN:OE1	2:F:843:GLY:HA2	2.20	0.41
1:A:18:ASP:HB3	1:A:21:LEU:HB2	2.02	0.41
2:B:375:MET:HE1	2:B:465:GLY:HA2	2.03	0.41
1:C:67:PRO:HB3	1:C:102:GLN:HA	2.01	0.41
1:E:34:PHE:HB3	1:E:63:LEU:HB3	2.01	0.41
1:E:913:PHE:CE1	1:E:915:ASP:HB2	2.55	0.41
1:G:430:PRO:HB2	1:G:435:TRP:HB3	2.03	0.41
3:K:95:LEU:HB3	3:K:99:LEU:HD23	2.02	0.41
1:C:735:THR:HB	1:C:939:GLY:HA3	2.02	0.41
2:D:143:PHE:CE1	2:D:148:ASN:O	2.72	0.41
2:D:918:ARG:HB3	2:D:920:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:LYS:HG2	1:E:486:THR:HB	2.01	0.41
2:F:218:HIS:HA	2:F:251:ILE:HG23	2.03	0.41
1:G:78:ARG:HB3	1:G:79:GLU:H	1.77	0.41
3:J:218:MET:CE	3:J:226:LEU:HD12	2.47	0.41
1:C:793:TYR:HE2	1:C:828:PHE:HD2	1.68	0.41
1:G:401:GLU:HB3	1:G:490:ARG:HG2	2.03	0.41
2:H:218:HIS:HA	2:H:251:ILE:HG23	2.02	0.41
3:J:38:ILE:O	3:J:42:LYS:HB2	2.21	0.41
3:L:87:LEU:O	3:L:243:LEU:HD23	2.20	0.41
3:L:101:VAL:HG11	3:L:141:LEU:HD12	2.01	0.41
1:A:423:ILE:HG12	1:A:580:PHE:CE2	2.56	0.41
1:C:423:ILE:HG12	1:C:580:PHE:CE2	2.56	0.41
1:C:476:LYS:HG2	1:C:486:THR:HB	2.02	0.41
1:G:763:ARG:HH11	1:G:763:ARG:HA	1.85	0.41
3:I:329:ASN:H	3:I:329:ASN:ND2	2.14	0.41
3:J:278:TYR:O	3:J:279:GLN:HB3	2.20	0.41
1:A:401:GLU:HB3	1:A:490:ARG:HG2	2.03	0.41
1:A:751:TYR:OH	2:B:836:PRO:O	2.39	0.41
1:C:762:SER:N	2:D:642:ASN:HA	2.35	0.41
1:E:797:ASN:HA	1:E:798:PRO:HD3	1.94	0.41
1:G:245:ALA:HB1	1:G:279:ILE:HG12	2.01	0.41
1:G:428:ARG:HD3	1:G:566:LEU:HD13	2.03	0.41
3:I:93:ARG:HG2	3:I:247:ASN:OD1	2.19	0.41
1:A:924:SER:HB2	1:A:926:LYS:HG3	2.03	0.41
1:E:18:ASP:HB3	1:E:21:LEU:HB2	2.03	0.41
1:E:156:VAL:HA	1:E:169:SER:HB3	2.02	0.41
2:F:336:MET:SD	2:F:523:THR:HG21	2.61	0.41
1:G:556:ALA:HB2	1:G:564:LYS:HD3	2.02	0.41
1:G:869:LYS:HA	2:H:731:GLN:HE22	1.86	0.41
2:H:741:PHE:HA	2:H:832:LYS:O	2.20	0.41
3:K:35:LYS:HE2	3:K:39:GLU:HB3	2.02	0.41
1:A:428:ARG:HD3	1:A:566:LEU:HD13	2.02	0.41
1:A:912:PHE:CD1	1:A:919:LYS:HE3	2.56	0.41
1:A:919:LYS:HE2	1:A:929:VAL:HG21	2.03	0.41
2:B:590:VAL:HG21	2:B:639:ILE:HD12	2.03	0.41
2:B:878:ILE:HG22	2:B:879:SER:H	1.85	0.41
1:C:360:ILE:N	4:C:991:SO4:O1	2.51	0.41
1:C:430:PRO:HB2	1:C:435:TRP:HB3	2.01	0.41
1:C:490:ARG:HB2	2:D:463:THR:HG23	2.03	0.41
1:C:720:PRO:HB2	1:C:890:ILE:HA	2.03	0.41
2:D:356:ILE:HA	2:D:359:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:707:PRO:HG3	2:D:913:SER:HB3	2.02	0.41
2:F:356:ILE:HB	2:F:390:THR:HG21	2.03	0.41
1:G:324:ARG:HB3	1:G:353:ILE:HG21	2.02	0.41
2:H:596:TYR:CZ	2:H:600:ARG:HD3	2.56	0.41
3:J:66:PRO:HG2	3:J:73:ASN:HD21	1.86	0.41
3:K:203:ALA:O	3:K:207:LEU:HG	2.21	0.41
3:L:179:ARG:HD3	3:L:205:MET:HB2	2.03	0.41
2:D:193:SER:N	2:D:196:MET:HE2	2.36	0.41
1:E:793:TYR:HE2	1:E:828:PHE:HD2	1.69	0.41
1:E:798:PRO:HG2	3:L:233:ARG:HA	2.03	0.41
2:F:105:LEU:HD11	2:F:142:GLY:HA3	2.03	0.41
2:H:218:HIS:O	2:H:223:GLY:HA3	2.21	0.41
3:J:301:ARG:HD2	3:J:328:TRP:CE2	2.56	0.41
3:K:218:MET:HE2	3:K:223:PHE:HA	2.02	0.41
3:K:301:ARG:HD2	3:K:328:TRP:CE2	2.56	0.41
1:A:247:TYR:O	1:A:252:GLY:HA3	2.21	0.40
1:C:14:PHE:CE1	1:C:164:MET:HE2	2.57	0.40
1:E:482:ILE:HD13	1:E:482:ILE:HA	1.99	0.40
3:L:87:LEU:HD11	3:L:89:MET:HE2	2.02	0.40
3:L:179:ARG:CG	3:L:202:THR:HG23	2.49	0.40
2:D:187:MET:HE2	2:D:282:VAL:HG13	2.01	0.40
2:D:573:LYS:HG2	2:D:605:TYR:HE2	1.86	0.40
1:E:556:ALA:HB2	1:E:564:LYS:HD3	2.02	0.40
2:H:356:ILE:HA	2:H:359:ILE:HD12	2.03	0.40
2:H:399:GLU:O	2:H:535:PHE:HB3	2.21	0.40
3:I:85:PHE:C	3:I:85:PHE:CD1	2.99	0.40
3:K:24:LEU:HD22	3:K:140:TYR:HD2	1.86	0.40
1:A:25:THR:HA	1:A:162:ASP:OD1	2.21	0.40
2:B:127:SER:HB3	2:B:128:PRO:HD3	2.03	0.40
2:B:682:GLU:HA	2:B:685:ARG:HD3	2.03	0.40
2:D:596:TYR:CZ	2:D:600:ARG:HD3	2.56	0.40
1:E:401:GLU:HB3	1:E:490:ARG:HG2	2.03	0.40
1:E:763:ARG:HA	1:E:763:ARG:HH11	1.85	0.40
3:I:186:VAL:HB	3:I:193:ILE:HG21	2.03	0.40
3:K:218:MET:CE	3:K:226:LEU:HD12	2.50	0.40
3:L:337:HIS:HD2	3:L:342:SER:HB3	1.86	0.40
2:B:105:LEU:HD11	2:B:142:GLY:HA3	2.03	0.40
1:E:25:THR:HA	1:E:162:ASP:OD1	2.22	0.40
1:E:162:ASP:C	1:E:164:MET:N	2.80	0.40
1:G:38:ARG:HH12	1:G:50:LEU:CB	2.34	0.40
1:G:476:LYS:HG2	1:G:486:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:O	1:C:100:PRO:HA	2.22	0.40
1:C:779:LEU:HD23	1:C:779:LEU:HA	1.93	0.40
1:C:913:PHE:CE1	1:C:915:ASP:HB2	2.56	0.40
1:E:924:SER:HB2	1:E:926:LYS:HG3	2.03	0.40
1:G:364:MET:HE3	1:G:546:SER:HB3	2.02	0.40
2:H:783:ASN:HA	2:H:786:LYS:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	908/989 (92%)	840 (92%)	58 (6%)	10 (1%)	11	34
1	C	908/989 (92%)	841 (93%)	57 (6%)	10 (1%)	11	34
1	E	908/989 (92%)	841 (93%)	57 (6%)	10 (1%)	11	34
1	G	908/989 (92%)	843 (93%)	55 (6%)	10 (1%)	11	34
2	B	859/941 (91%)	800 (93%)	46 (5%)	13 (2%)	8	28
2	D	859/941 (91%)	803 (94%)	45 (5%)	11 (1%)	9	31
2	F	859/941 (91%)	803 (94%)	45 (5%)	11 (1%)	9	31
2	H	859/941 (91%)	800 (93%)	46 (5%)	13 (2%)	8	28
3	I	319/351 (91%)	296 (93%)	21 (7%)	2 (1%)	21	48
3	J	319/351 (91%)	285 (89%)	29 (9%)	5 (2%)	7	26
3	K	319/351 (91%)	286 (90%)	31 (10%)	2 (1%)	21	48
3	L	319/351 (91%)	283 (89%)	33 (10%)	3 (1%)	14	39
All	All	8344/9124 (92%)	7721 (92%)	523 (6%)	100 (1%)	10	32

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	646	ALA
2	B	127	SER
2	B	150	PHE
2	B	303	ILE
1	C	646	ALA
2	D	127	SER
2	D	150	PHE
2	D	303	ILE
1	E	646	ALA
2	F	127	SER
2	F	150	PHE
2	F	303	ILE
1	G	646	ALA
2	H	127	SER
2	H	150	PHE
2	H	303	ILE
3	J	339	GLY
3	K	317	ALA
1	A	162	ASP
1	A	179	LYS
1	C	162	ASP
1	C	179	LYS
1	E	162	ASP
1	E	179	LYS
1	G	162	ASP
1	G	179	LYS
3	I	317	ALA
3	I	339	GLY
3	J	279	GLN
3	K	339	GLY
3	L	64	ASN
3	L	339	GLY
1	A	171	SER
1	A	256	GLY
2	B	315	GLN
2	D	315	GLN
2	D	917	ARG
1	E	171	SER
2	F	315	GLN
1	G	78	ARG
1	G	171	SER
2	H	315	GLN
2	H	917	ARG

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Mol	Chain	Res	Type
3	J	31	LEU
3	J	317	ALA
2	B	122	SER
2	B	840	GLN
2	B	917	ARG
2	B	925	TRP
1	C	78	ARG
1	C	171	SER
1	C	256	GLY
2	D	122	SER
1	E	78	ARG
1	E	256	GLY
2	F	122	SER
2	F	840	GLN
2	F	917	ARG
1	G	256	GLY
2	H	122	SER
2	H	840	GLN
3	J	236	THR
1	A	52	GLY
1	A	78	ARG
2	B	793	GLN
2	B	878	ILE
1	C	52	GLY
2	D	840	GLN
2	D	925	TRP
2	F	286	ASP
2	F	925	TRP
2	H	286	ASP
2	H	925	TRP
3	L	148	ALA
2	B	438	ASP
2	D	878	ILE
1	E	52	GLY
2	F	878	ILE
1	G	52	GLY
2	H	438	ASP
2	H	878	ILE
1	A	83	PRO
1	A	274	ILE
1	C	274	ILE
1	E	274	ILE

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Mol	Chain	Res	Type
1	G	274	ILE
1	C	83	PRO
1	E	83	PRO
1	G	83	PRO
2	H	376	GLY
2	B	376	GLY
1	C	257	GLY
1	E	257	GLY
2	F	376	GLY
1	A	257	GLY
2	D	300	PRO
2	D	376	GLY
1	G	257	GLY
2	B	300	PRO
2	H	300	PRO

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	725/835 (87%)	637 (88%)	88 (12%)	5	17
1	C	725/835 (87%)	638 (88%)	87 (12%)	5	17
1	E	725/835 (87%)	643 (89%)	82 (11%)	5	20
1	G	725/835 (87%)	642 (89%)	83 (11%)	5	20
2	B	670/799 (84%)	588 (88%)	82 (12%)	5	17
2	D	670/799 (84%)	588 (88%)	82 (12%)	5	17
2	F	670/799 (84%)	587 (88%)	83 (12%)	4	16
2	H	670/799 (84%)	587 (88%)	83 (12%)	4	16
3	I	282/322 (88%)	238 (84%)	44 (16%)	2	10
3	J	282/322 (88%)	239 (85%)	43 (15%)	3	10
3	K	282/322 (88%)	237 (84%)	45 (16%)	2	10
3	L	282/322 (88%)	238 (84%)	44 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6708/7824 (86%)	5862 (87%)	846 (13%)	4 16

All (846) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	10	SER
1	A	47	ASP
1	A	69	SER
1	A	70	GLU
1	A	71	VAL
1	A	79	GLU
1	A	88	VAL
1	A	92	SER
1	A	95	LEU
1	A	96	LEU
1	A	112	LEU
1	A	120	ASN
1	A	121	ASN
1	A	123	LEU
1	A	127	VAL
1	A	135	ASP
1	A	143	GLU
1	A	167	VAL
1	A	168	ILE
1	A	185	ASP
1	A	215	ILE
1	A	216	ILE
1	A	234	ARG
1	A	260	LEU
1	A	262	GLU
1	A	279	ILE
1	A	306	ASP
1	A	322	LEU
1	A	324	ARG
1	A	346	GLU
1	A	357	VAL
1	A	359	SER
1	A	382	GLU
1	A	383	LEU
1	A	390	THR
1	A	412	LEU

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Mol	Chain	Res	Type
1	A	427	GLU
1	A	439	LEU
1	A	447	ARG
1	A	482	ILE
1	A	505	ARG
1	A	509	THR
1	A	537	LYS
1	A	541	GLN
1	A	543	LEU
1	A	544	VAL
1	A	553	VAL
1	A	566	LEU
1	A	568	LEU
1	A	579	ASN
1	A	581	LEU
1	A	592	LEU
1	A	595	GLU
1	A	596	SER
1	A	599	LEU
1	A	641	LEU
1	A	648	ARG
1	A	655	VAL
1	A	660	ASN
1	A	704	LEU
1	A	716	ILE
1	A	728	VAL
1	A	730	ASN
1	A	745	LEU
1	A	749	SER
1	A	757	GLN
1	A	763	ARG
1	A	779	LEU
1	A	826	LYS
1	A	827	ILE
1	A	832	GLU
1	A	833	LYS
1	A	855	PHE
1	A	861	VAL
1	A	865	VAL
1	A	867	GLN
1	A	898	LYS
1	A	916	ASP

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Mol	Chain	Res	Type
1	A	936	VAL
1	A	941	GLN
1	A	950	VAL
1	A	954	TRP
1	A	955	GLU
1	A	956	ASN
1	A	972	GLN
1	A	985	SER
1	A	986	ILE
2	B	6	LEU
2	B	10	THR
2	B	13	ILE
2	B	14	THR
2	B	58	VAL
2	B	59	SER
2	B	98	ILE
2	B	106	SER
2	B	119	VAL
2	B	186	VAL
2	B	189	SER
2	B	233	LYS
2	B	234	GLU
2	B	246	GLU
2	B	257	LYS
2	B	286	ASP
2	B	302	LEU
2	B	329	VAL
2	B	365	SER
2	B	375	MET
2	B	400	LYS
2	B	425	LYS
2	B	435	ILE
2	B	437	ASN
2	B	444	CYS
2	B	457	LEU
2	B	459	THR
2	B	463	THR
2	B	472	THR
2	B	474	VAL
2	B	492	VAL
2	B	495	CYS
2	B	496	ASP

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Mol	Chain	Res	Type
2	B	508	GLU
2	B	510	GLN
2	B	511	ILE
2	B	513	ARG
2	B	517	VAL
2	B	522	LEU
2	B	525	GLN
2	B	547	VAL
2	B	550	MET
2	B	554	ILE
2	B	561	HIS
2	B	562	VAL
2	B	568	LEU
2	B	569	GLU
2	B	577	ILE
2	B	593	MET
2	B	599	SER
2	B	639	ILE
2	B	678	LEU
2	B	679	HIS
2	B	685	ARG
2	B	686	ILE
2	B	690	SER
2	B	693	ILE
2	B	701	THR
2	B	705	ASN
2	B	709	THR
2	B	713	LEU
2	B	719	LEU
2	B	729	ILE
2	B	739	ARG
2	B	740	VAL
2	B	745	VAL
2	B	753	ILE
2	B	768	VAL
2	B	780	MET
2	B	793	GLN
2	B	795	LYS
2	B	806	GLU
2	B	815	GLU
2	B	824	GLU
2	B	844	ILE

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Mol	Chain	Res	Type
2	B	854	SER
2	B	885	GLU
2	B	891	VAL
2	B	915	VAL
2	B	923	ILE
2	B	926	SER
2	B	932	SER
1	C	8	ASP
1	C	10	SER
1	C	47	ASP
1	C	69	SER
1	C	70	GLU
1	C	71	VAL
1	C	79	GLU
1	C	88	VAL
1	C	92	SER
1	C	95	LEU
1	C	96	LEU
1	C	112	LEU
1	C	121	ASN
1	C	123	LEU
1	C	127	VAL
1	C	135	ASP
1	C	143	GLU
1	C	167	VAL
1	C	168	ILE
1	C	185	ASP
1	C	215	ILE
1	C	216	ILE
1	C	234	ARG
1	C	260	LEU
1	C	262	GLU
1	C	272	LEU
1	C	279	ILE
1	C	306	ASP
1	C	322	LEU
1	C	324	ARG
1	C	346	GLU
1	C	357	VAL
1	C	359	SER
1	C	382	GLU
1	C	383	LEU

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Mol	Chain	Res	Type
1	C	390	THR
1	C	393	SER
1	C	412	LEU
1	C	427	GLU
1	C	439	LEU
1	C	447	ARG
1	C	482	ILE
1	C	505	ARG
1	C	509	THR
1	C	537	LYS
1	C	541	GLN
1	C	543	LEU
1	C	544	VAL
1	C	553	VAL
1	C	566	LEU
1	C	568	LEU
1	C	579	ASN
1	C	581	LEU
1	C	592	LEU
1	C	595	GLU
1	C	596	SER
1	C	599	LEU
1	C	641	LEU
1	C	648	ARG
1	C	655	VAL
1	C	660	ASN
1	C	704	LEU
1	C	716	ILE
1	C	728	VAL
1	C	730	ASN
1	C	745	LEU
1	C	749	SER
1	C	757	GLN
1	C	763	ARG
1	C	779	LEU
1	C	826	LYS
1	C	827	ILE
1	C	832	GLU
1	C	833	LYS
1	C	855	PHE
1	C	861	VAL
1	C	865	VAL

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Mol	Chain	Res	Type
1	C	867	GLN
1	C	898	LYS
1	C	916	ASP
1	C	936	VAL
1	C	941	GLN
1	C	950	VAL
1	C	954	TRP
1	C	955	GLU
1	C	956	ASN
1	C	972	GLN
2	D	6	LEU
2	D	10	THR
2	D	13	ILE
2	D	14	THR
2	D	58	VAL
2	D	59	SER
2	D	98	ILE
2	D	106	SER
2	D	119	VAL
2	D	186	VAL
2	D	189	SER
2	D	233	LYS
2	D	234	GLU
2	D	246	GLU
2	D	257	LYS
2	D	286	ASP
2	D	302	LEU
2	D	329	VAL
2	D	365	SER
2	D	375	MET
2	D	400	LYS
2	D	425	LYS
2	D	435	ILE
2	D	437	ASN
2	D	444	CYS
2	D	457	LEU
2	D	459	THR
2	D	463	THR
2	D	472	THR
2	D	474	VAL
2	D	492	VAL
2	D	495	CYS

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Mol	Chain	Res	Type
2	D	496	ASP
2	D	508	GLU
2	D	510	GLN
2	D	511	ILE
2	D	513	ARG
2	D	517	VAL
2	D	522	LEU
2	D	525	GLN
2	D	547	VAL
2	D	550	MET
2	D	554	ILE
2	D	561	HIS
2	D	562	VAL
2	D	568	LEU
2	D	569	GLU
2	D	577	ILE
2	D	593	MET
2	D	599	SER
2	D	639	ILE
2	D	678	LEU
2	D	679	HIS
2	D	685	ARG
2	D	686	ILE
2	D	690	SER
2	D	693	ILE
2	D	701	THR
2	D	705	ASN
2	D	709	THR
2	D	713	LEU
2	D	719	LEU
2	D	729	ILE
2	D	739	ARG
2	D	740	VAL
2	D	745	VAL
2	D	753	ILE
2	D	768	VAL
2	D	780	MET
2	D	793	GLN
2	D	795	LYS
2	D	806	GLU
2	D	815	GLU
2	D	824	GLU

Continued on next page...

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Mol	Chain	Res	Type
2	D	844	ILE
2	D	854	SER
2	D	885	GLU
2	D	891	VAL
2	D	915	VAL
2	D	923	ILE
2	D	926	SER
2	D	932	SER
1	E	8	ASP
1	E	10	SER
1	E	69	SER
1	E	70	GLU
1	E	71	VAL
1	E	79	GLU
1	E	88	VAL
1	E	95	LEU
1	E	96	LEU
1	E	112	LEU
1	E	121	ASN
1	E	123	LEU
1	E	127	VAL
1	E	135	ASP
1	E	143	GLU
1	E	167	VAL
1	E	168	ILE
1	E	185	ASP
1	E	215	ILE
1	E	216	ILE
1	E	234	ARG
1	E	260	LEU
1	E	262	GLU
1	E	279	ILE
1	E	306	ASP
1	E	322	LEU
1	E	324	ARG
1	E	346	GLU
1	E	357	VAL
1	E	359	SER
1	E	382	GLU
1	E	383	LEU
1	E	390	THR
1	E	412	LEU

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Mol	Chain	Res	Type
1	E	427	GLU
1	E	439	LEU
1	E	447	ARG
1	E	482	ILE
1	E	509	THR
1	E	537	LYS
1	E	541	GLN
1	E	543	LEU
1	E	544	VAL
1	E	553	VAL
1	E	566	LEU
1	E	568	LEU
1	E	579	ASN
1	E	581	LEU
1	E	592	LEU
1	E	595	GLU
1	E	596	SER
1	E	599	LEU
1	E	641	LEU
1	E	648	ARG
1	E	655	VAL
1	E	660	ASN
1	E	704	LEU
1	E	716	ILE
1	E	728	VAL
1	E	730	ASN
1	E	745	LEU
1	E	749	SER
1	E	757	GLN
1	E	763	ARG
1	E	779	LEU
1	E	826	LYS
1	E	827	ILE
1	E	832	GLU
1	E	833	LYS
1	E	855	PHE
1	E	861	VAL
1	E	865	VAL
1	E	867	GLN
1	E	898	LYS
1	E	916	ASP
1	E	936	VAL

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Mol	Chain	Res	Type
1	E	941	GLN
1	E	950	VAL
1	E	954	TRP
1	E	955	GLU
1	E	956	ASN
1	E	972	GLN
2	F	6	LEU
2	F	10	THR
2	F	13	ILE
2	F	14	THR
2	F	58	VAL
2	F	59	SER
2	F	98	ILE
2	F	106	SER
2	F	119	VAL
2	F	186	VAL
2	F	189	SER
2	F	196	MET
2	F	233	LYS
2	F	234	GLU
2	F	246	GLU
2	F	257	LYS
2	F	286	ASP
2	F	302	LEU
2	F	329	VAL
2	F	365	SER
2	F	375	MET
2	F	400	LYS
2	F	425	LYS
2	F	435	ILE
2	F	437	ASN
2	F	444	CYS
2	F	457	LEU
2	F	459	THR
2	F	463	THR
2	F	472	THR
2	F	474	VAL
2	F	492	VAL
2	F	495	CYS
2	F	496	ASP
2	F	508	GLU
2	F	510	GLN

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Mol	Chain	Res	Type
2	F	511	ILE
2	F	513	ARG
2	F	517	VAL
2	F	522	LEU
2	F	525	GLN
2	F	547	VAL
2	F	550	MET
2	F	554	ILE
2	F	561	HIS
2	F	562	VAL
2	F	568	LEU
2	F	569	GLU
2	F	577	ILE
2	F	593	MET
2	F	599	SER
2	F	639	ILE
2	F	678	LEU
2	F	679	HIS
2	F	685	ARG
2	F	686	ILE
2	F	690	SER
2	F	693	ILE
2	F	701	THR
2	F	705	ASN
2	F	709	THR
2	F	713	LEU
2	F	719	LEU
2	F	729	ILE
2	F	739	ARG
2	F	740	VAL
2	F	745	VAL
2	F	753	ILE
2	F	768	VAL
2	F	780	MET
2	F	793	GLN
2	F	795	LYS
2	F	806	GLU
2	F	815	GLU
2	F	824	GLU
2	F	844	ILE
2	F	854	SER
2	F	885	GLU

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Mol	Chain	Res	Type
2	F	891	VAL
2	F	915	VAL
2	F	923	ILE
2	F	926	SER
2	F	932	SER
1	G	8	ASP
1	G	10	SER
1	G	69	SER
1	G	70	GLU
1	G	71	VAL
1	G	79	GLU
1	G	88	VAL
1	G	95	LEU
1	G	96	LEU
1	G	112	LEU
1	G	121	ASN
1	G	123	LEU
1	G	127	VAL
1	G	135	ASP
1	G	143	GLU
1	G	167	VAL
1	G	168	ILE
1	G	185	ASP
1	G	215	ILE
1	G	216	ILE
1	G	234	ARG
1	G	260	LEU
1	G	262	GLU
1	G	279	ILE
1	G	286	GLU
1	G	306	ASP
1	G	322	LEU
1	G	324	ARG
1	G	346	GLU
1	G	357	VAL
1	G	359	SER
1	G	382	GLU
1	G	383	LEU
1	G	390	THR
1	G	412	LEU
1	G	427	GLU
1	G	439	LEU

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Mol	Chain	Res	Type
1	G	447	ARG
1	G	482	ILE
1	G	509	THR
1	G	537	LYS
1	G	541	GLN
1	G	543	LEU
1	G	544	VAL
1	G	553	VAL
1	G	566	LEU
1	G	568	LEU
1	G	579	ASN
1	G	581	LEU
1	G	592	LEU
1	G	595	GLU
1	G	596	SER
1	G	599	LEU
1	G	641	LEU
1	G	648	ARG
1	G	655	VAL
1	G	660	ASN
1	G	704	LEU
1	G	716	ILE
1	G	728	VAL
1	G	730	ASN
1	G	745	LEU
1	G	749	SER
1	G	757	GLN
1	G	763	ARG
1	G	779	LEU
1	G	826	LYS
1	G	827	ILE
1	G	832	GLU
1	G	833	LYS
1	G	855	PHE
1	G	861	VAL
1	G	865	VAL
1	G	867	GLN
1	G	898	LYS
1	G	916	ASP
1	G	936	VAL
1	G	941	GLN
1	G	950	VAL

Continued on next page...

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Mol	Chain	Res	Type
1	G	954	TRP
1	G	955	GLU
1	G	956	ASN
1	G	972	GLN
2	H	6	LEU
2	H	10	THR
2	H	13	ILE
2	H	14	THR
2	H	58	VAL
2	H	59	SER
2	H	98	ILE
2	H	106	SER
2	H	119	VAL
2	H	186	VAL
2	H	189	SER
2	H	233	LYS
2	H	234	GLU
2	H	246	GLU
2	H	257	LYS
2	H	286	ASP
2	H	302	LEU
2	H	329	VAL
2	H	365	SER
2	H	375	MET
2	H	400	LYS
2	H	425	LYS
2	H	435	ILE
2	H	437	ASN
2	H	444	CYS
2	H	457	LEU
2	H	459	THR
2	H	463	THR
2	H	472	THR
2	H	474	VAL
2	H	492	VAL
2	H	495	CYS
2	H	496	ASP
2	H	508	GLU
2	H	510	GLN
2	H	511	ILE
2	H	513	ARG
2	H	517	VAL

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Mol	Chain	Res	Type
2	H	522	LEU
2	H	525	GLN
2	H	547	VAL
2	H	550	MET
2	H	554	ILE
2	H	561	HIS
2	H	562	VAL
2	H	568	LEU
2	H	569	GLU
2	H	577	ILE
2	H	593	MET
2	H	599	SER
2	H	639	ILE
2	H	678	LEU
2	H	679	HIS
2	H	685	ARG
2	H	686	ILE
2	H	690	SER
2	H	693	ILE
2	H	701	THR
2	H	705	ASN
2	H	709	THR
2	H	713	LEU
2	H	719	LEU
2	H	729	ILE
2	H	739	ARG
2	H	740	VAL
2	H	745	VAL
2	H	753	ILE
2	H	768	VAL
2	H	780	MET
2	H	793	GLN
2	H	795	LYS
2	H	806	GLU
2	H	815	GLU
2	H	824	GLU
2	H	828	ARG
2	H	844	ILE
2	H	854	SER
2	H	885	GLU
2	H	891	VAL
2	H	915	VAL

Continued on next page...

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Mol	Chain	Res	Type
2	H	923	ILE
2	H	926	SER
2	H	932	SER
3	I	6	SER
3	I	13	ARG
3	I	27	LEU
3	I	39	GLU
3	I	56	GLN
3	I	73	ASN
3	I	87	LEU
3	I	95	LEU
3	I	97	ILE
3	I	105	LEU
3	I	118	LEU
3	I	133	LYS
3	I	141	LEU
3	I	142	ILE
3	I	146	VAL
3	I	179	ARG
3	I	186	VAL
3	I	194	THR
3	I	197	LEU
3	I	211	ASP
3	I	217	GLU
3	I	220	ASP
3	I	225	THR
3	I	228	LEU
3	I	237	THR
3	I	238	LYS
3	I	239	LYS
3	I	241	ASP
3	I	242	LEU
3	I	243	LEU
3	I	245	LEU
3	I	247	ASN
3	I	253	MET
3	I	286	THR
3	I	294	GLU
3	I	303	GLU
3	I	308	LEU
3	I	320	LEU
3	I	327	ARG

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Mol	Chain	Res	Type
3	I	329	ASN
3	I	333	GLN
3	I	338	GLN
3	I	340	ASN
3	I	342	SER
3	J	6	SER
3	J	13	ARG
3	J	27	LEU
3	J	38	ILE
3	J	41	VAL
3	J	42	LYS
3	J	44	GLN
3	J	95	LEU
3	J	97	ILE
3	J	111	LEU
3	J	118	LEU
3	J	121	ASP
3	J	127	ASN
3	J	128	ASN
3	J	141	LEU
3	J	142	ILE
3	J	178	ASN
3	J	186	VAL
3	J	190	ASP
3	J	194	THR
3	J	198	LEU
3	J	217	GLU
3	J	224	VAL
3	J	225	THR
3	J	228	LEU
3	J	236	THR
3	J	237	THR
3	J	238	LYS
3	J	239	LYS
3	J	242	LEU
3	J	243	LEU
3	J	245	LEU
3	J	247	ASN
3	J	253	MET
3	J	259	GLN
3	J	265	SER
3	J	270	LYS

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Mol	Chain	Res	Type
3	J	286	THR
3	J	303	GLU
3	J	329	ASN
3	J	333	GLN
3	J	342	SER
3	J	350	LEU
3	K	19	GLU
3	K	27	LEU
3	K	39	GLU
3	K	45	LEU
3	K	56	GLN
3	K	64	ASN
3	K	68	ASP
3	K	70	LEU
3	K	72	THR
3	K	82	VAL
3	K	87	LEU
3	K	105	LEU
3	K	107	MET
3	K	121	ASP
3	K	142	ILE
3	K	149	GLU
3	K	186	VAL
3	K	194	THR
3	K	197	LEU
3	K	198	LEU
3	K	206	ILE
3	K	215	ASP
3	K	217	GLU
3	K	224	VAL
3	K	228	LEU
3	K	236	THR
3	K	237	THR
3	K	238	LYS
3	K	242	LEU
3	K	243	LEU
3	K	245	LEU
3	K	247	ASN
3	K	250	ASP
3	K	253	MET
3	K	256	LYS
3	K	275	VAL

Continued on next page...

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Mol	Chain	Res	Type
3	K	282	VAL
3	K	291	SER
3	K	303	GLU
3	K	313	THR
3	K	320	LEU
3	K	329	ASN
3	K	340	ASN
3	K	342	SER
3	K	350	LEU
3	L	6	SER
3	L	27	LEU
3	L	29	THR
3	L	38	ILE
3	L	39	GLU
3	L	41	VAL
3	L	44	GLN
3	L	47	THR
3	L	72	THR
3	L	85	PHE
3	L	87	LEU
3	L	97	ILE
3	L	105	LEU
3	L	107	MET
3	L	121	ASP
3	L	133	LYS
3	L	142	ILE
3	L	149	GLU
3	L	176	LEU
3	L	178	ASN
3	L	186	VAL
3	L	193	ILE
3	L	194	THR
3	L	196	HIS
3	L	197	LEU
3	L	217	GLU
3	L	225	THR
3	L	228	LEU
3	L	236	THR
3	L	237	THR
3	L	238	LYS
3	L	242	LEU
3	L	243	LEU

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Mol	Chain	Res	Type
3	L	245	LEU
3	L	247	ASN
3	L	251	THR
3	L	253	MET
3	L	259	GLN
3	L	260	LEU
3	L	270	LYS
3	L	281	THR
3	L	282	VAL
3	L	303	GLU
3	L	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (201) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	44	ASN
1	A	266	GLN
1	A	303	ASN
1	A	394	HIS
1	A	466	GLN
1	A	541	GLN
1	A	571	GLN
1	A	644	HIS
1	A	659	HIS
1	A	686	GLN
1	A	831	ASN
1	A	867	GLN
1	A	952	GLN
1	A	972	GLN
2	B	24	GLN
2	B	81	ASN
2	B	121	GLN
2	B	148	ASN
2	B	250	ASN
2	B	378	HIS
2	B	453	ASN
2	B	490	ASN
2	B	534	ASN
2	B	552	ASN
2	B	557	ASN
2	B	705	ASN

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Mol	Chain	Res	Type
2	B	720	ASN
2	B	758	GLN
2	B	764	GLN
2	B	777	GLN
2	B	793	GLN
2	B	807	ASN
2	B	872	GLN
2	B	907	GLN
2	B	922	ASN
1	C	44	ASN
1	C	85	GLN
1	C	266	GLN
1	C	303	ASN
1	C	344	GLN
1	C	394	HIS
1	C	466	GLN
1	C	541	GLN
1	C	571	GLN
1	C	686	GLN
1	C	772	GLN
1	C	831	ASN
1	C	864	HIS
1	C	867	GLN
1	C	902	ASN
1	C	952	GLN
1	C	972	GLN
2	D	81	ASN
2	D	121	GLN
2	D	148	ASN
2	D	250	ASN
2	D	378	HIS
2	D	490	ASN
2	D	510	GLN
2	D	534	ASN
2	D	552	ASN
2	D	557	ASN
2	D	561	HIS
2	D	705	ASN
2	D	720	ASN
2	D	758	GLN
2	D	764	GLN
2	D	777	GLN

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Mol	Chain	Res	Type
2	D	807	ASN
2	D	872	GLN
2	D	907	GLN
2	D	922	ASN
1	E	44	ASN
1	E	85	GLN
1	E	266	GLN
1	E	303	ASN
1	E	344	GLN
1	E	394	HIS
1	E	466	GLN
1	E	541	GLN
1	E	623	ASN
1	E	686	GLN
1	E	831	ASN
1	E	867	GLN
1	E	899	HIS
1	E	902	ASN
1	E	952	GLN
1	E	972	GLN
2	F	24	GLN
2	F	81	ASN
2	F	121	GLN
2	F	148	ASN
2	F	250	ASN
2	F	378	HIS
2	F	410	GLN
2	F	490	ASN
2	F	534	ASN
2	F	552	ASN
2	F	557	ASN
2	F	561	HIS
2	F	705	ASN
2	F	720	ASN
2	F	731	GLN
2	F	758	GLN
2	F	764	GLN
2	F	777	GLN
2	F	807	ASN
2	F	872	GLN
2	F	907	GLN
2	F	922	ASN

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Mol	Chain	Res	Type
1	G	27	ASN
1	G	44	ASN
1	G	266	GLN
1	G	303	ASN
1	G	344	GLN
1	G	394	HIS
1	G	541	GLN
1	G	571	GLN
1	G	644	HIS
1	G	686	GLN
1	G	772	GLN
1	G	802	GLN
1	G	831	ASN
1	G	867	GLN
1	G	900	ASN
1	G	902	ASN
1	G	952	GLN
1	G	972	GLN
2	H	24	GLN
2	H	81	ASN
2	H	121	GLN
2	H	148	ASN
2	H	250	ASN
2	H	378	HIS
2	H	410	GLN
2	H	453	ASN
2	H	490	ASN
2	H	534	ASN
2	H	552	ASN
2	H	557	ASN
2	H	561	HIS
2	H	705	ASN
2	H	720	ASN
2	H	731	GLN
2	H	758	GLN
2	H	764	GLN
2	H	777	GLN
2	H	793	GLN
2	H	807	ASN
2	H	872	GLN
2	H	907	GLN
3	I	25	ASN

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Mol	Chain	Res	Type
3	I	62	ASN
3	I	73	ASN
3	I	128	ASN
3	I	247	ASN
3	I	267	ASN
3	I	284	GLN
3	I	329	ASN
3	I	333	GLN
3	I	338	GLN
3	J	25	ASN
3	J	44	GLN
3	J	48	HIS
3	J	62	ASN
3	J	81	ASN
3	J	128	ASN
3	J	247	ASN
3	J	255	ASN
3	J	267	ASN
3	J	284	GLN
3	J	290	ASN
3	J	306	ASN
3	J	329	ASN
3	J	333	GLN
3	J	338	GLN
3	J	340	ASN
3	K	62	ASN
3	K	77	ASN
3	K	81	ASN
3	K	185	ASN
3	K	247	ASN
3	K	252	ASN
3	K	267	ASN
3	K	329	ASN
3	K	337	HIS
3	L	25	ASN
3	L	73	ASN
3	L	81	ASN
3	L	127	ASN
3	L	247	ASN
3	L	248	ASN
3	L	252	ASN
3	L	255	ASN

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Mol	Chain	Res	Type
3	L	284	GLN
3	L	329	ASN
3	L	333	GLN
3	L	337	HIS
3	L	338	GLN
3	L	340	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 ⓘ

69 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	$\# Z > 2$
4	SO4	I	352	-	4,4,4	0.65	0	6,6,6	0.51	0
4	SO4	G	996	-	4,4,4	0.28	0	6,6,6	0.09	0
5	ATP	B	942	-	32,33,33	1.31	5 (15%)	48,52,52	1.15	4 (8%)
4	SO4	A	990	-	4,4,4	0.71	0	6,6,6	0.33	0
4	SO4	E	995	-	4,4,4	0.35	0	6,6,6	0.21	0
4	SO4	C	998	-	4,4,4	0.30	0	6,6,6	0.21	0
4	SO4	F	944	-	4,4,4	0.45	0	6,6,6	0.27	0
4	SO4	F	945	-	4,4,4	0.30	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	G	991	-	4,4,4	0.53	0	6,6,6	0.49	0
4	SO4	K	353	-	4,4,4	0.34	0	6,6,6	0.15	0
4	SO4	A	999	-	4,4,4	0.81	0	6,6,6	0.19	0
4	SO4	A	1002	-	4,4,4	0.35	0	6,6,6	0.16	0
4	SO4	C	992	-	4,4,4	1.21	0	6,6,6	0.23	0
4	SO4	A	994	-	4,4,4	0.22	0	6,6,6	0.38	0
4	SO4	C	995	-	4,4,4	0.37	0	6,6,6	0.18	0
4	SO4	A	995	-	4,4,4	0.60	0	6,6,6	0.26	0
4	SO4	C	991	-	4,4,4	0.62	0	6,6,6	0.25	0
4	SO4	A	992	-	4,4,4	0.39	0	6,6,6	0.18	0
4	SO4	G	995	-	4,4,4	0.19	0	6,6,6	0.26	0
4	SO4	J	352	-	4,4,4	0.32	0	6,6,6	0.22	0
4	SO4	A	1001	-	4,4,4	0.59	0	6,6,6	0.23	0
4	SO4	D	944	-	4,4,4	0.39	0	6,6,6	0.35	0
4	SO4	F	943	-	4,4,4	0.49	0	6,6,6	0.23	0
4	SO4	E	990	-	4,4,4	0.37	0	6,6,6	0.14	0
5	ATP	F	942	-	32,33,33	1.16	3 (9%)	48,52,52	1.19	2 (4%)
4	SO4	D	945	-	4,4,4	0.22	0	6,6,6	0.38	0
4	SO4	C	993	-	4,4,4	0.24	0	6,6,6	0.41	0
4	SO4	A	996	-	4,4,4	0.57	0	6,6,6	0.29	0
4	SO4	E	996	-	4,4,4	0.25	0	6,6,6	0.12	0
4	SO4	E	991	-	4,4,4	0.83	0	6,6,6	0.27	0
4	SO4	C	997	-	4,4,4	0.36	0	6,6,6	0.21	0
4	SO4	E	993	-	4,4,4	0.28	0	6,6,6	0.41	0
4	SO4	G	992	-	4,4,4	0.57	0	6,6,6	0.13	0
4	SO4	A	991	-	4,4,4	0.96	0	6,6,6	0.28	0
4	SO4	L	352	-	4,4,4	0.20	0	6,6,6	0.12	0
4	SO4	A	998	-	4,4,4	0.68	0	6,6,6	0.37	0
4	SO4	E	997	-	4,4,4	0.19	0	6,6,6	0.19	0
5	ATP	H	942	-	32,33,33	1.44	7 (21%)	48,52,52	1.35	6 (12%)
4	SO4	B	943	-	4,4,4	0.63	0	6,6,6	0.30	0
4	SO4	K	354	-	4,4,4	0.28	0	6,6,6	0.19	0
4	SO4	G	993	-	4,4,4	0.38	0	6,6,6	0.26	0
4	SO4	D	943	-	4,4,4	0.92	0	6,6,6	0.42	0
4	SO4	A	1000	-	4,4,4	0.32	0	6,6,6	0.21	0
4	SO4	I	355	-	4,4,4	0.42	0	6,6,6	0.16	0
4	SO4	J	353	-	4,4,4	0.39	0	6,6,6	0.16	0
4	SO4	C	994	-	4,4,4	0.50	0	6,6,6	0.30	0
4	SO4	A	997	-	4,4,4	0.32	0	6,6,6	0.24	0
5	ATP	D	942	-	32,33,33	1.41	5 (15%)	48,52,52	1.40	8 (16%)
4	SO4	H	943	-	4,4,4	0.26	0	6,6,6	0.34	0
4	SO4	H	944	-	4,4,4	0.20	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	944	-	4,4,4	0.62	0	6,6,6	0.57	0
4	SO4	E	992	-	4,4,4	0.28	0	6,6,6	0.26	0
4	SO4	E	994	-	4,4,4	0.41	0	6,6,6	0.12	0
4	SO4	G	990	-	4,4,4	0.44	0	6,6,6	0.41	0
4	SO4	I	354	-	4,4,4	0.26	0	6,6,6	0.05	0
4	SO4	H	945	-	4,4,4	0.37	0	6,6,6	0.38	0
4	SO4	C	990	-	4,4,4	0.86	0	6,6,6	0.39	0
4	SO4	G	994	-	4,4,4	0.39	0	6,6,6	0.26	0
4	SO4	J	354	-	4,4,4	0.39	0	6,6,6	0.14	0
4	SO4	L	353	-	4,4,4	0.34	0	6,6,6	0.15	0
4	SO4	C	996	-	4,4,4	0.63	0	6,6,6	0.44	0
4	SO4	G	997	-	4,4,4	0.19	0	6,6,6	0.21	0
4	SO4	I	353	-	4,4,4	0.34	0	6,6,6	0.32	0
4	SO4	C	999	-	4,4,4	0.32	0	6,6,6	0.08	0
4	SO4	H	946	-	4,4,4	0.32	0	6,6,6	0.26	0
4	SO4	L	354	-	4,4,4	0.27	0	6,6,6	0.14	0
4	SO4	A	993	-	4,4,4	0.33	0	6,6,6	0.19	0
4	SO4	K	352	-	4,4,4	0.34	0	6,6,6	0.35	0
4	SO4	I	356	-	4,4,4	0.36	0	6,6,6	0.13	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
5	ATP	D	942	-	-	1/22/38/38	0/3/3/3
5	ATP	F	942	-	-	4/22/38/38	0/3/3/3
5	ATP	H	942	-	-	1/22/38/38	0/3/3/3
5	ATP	B	942	-	-	0/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	942	ATP	O2'-C2'	4.04	1.53	1.43
5	H	942	ATP	C4-N3	3.10	1.40	1.34
5	F	942	ATP	C2-N1	2.94	1.39	1.33
5	H	942	ATP	C2-N1	2.85	1.39	1.33
5	H	942	ATP	C6-N6	2.73	1.41	1.34
5	B	942	ATP	PB-O3B	-2.58	1.56	1.59
5	D	942	ATP	C4-N3	2.55	1.39	1.34
5	H	942	ATP	C4-N9	2.53	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	942	ATP	PA-O1A	2.40	1.59	1.50
5	H	942	ATP	C5-C6	2.26	1.47	1.41
5	F	942	ATP	O4'-C1'	2.24	1.47	1.42
5	H	942	ATP	C5-C4	2.24	1.43	1.39
5	D	942	ATP	C2-N1	2.16	1.37	1.33
5	B	942	ATP	C4-N3	2.16	1.38	1.34
5	B	942	ATP	O4'-C4'	-2.15	1.40	1.45
5	D	942	ATP	PB-O3B	2.13	1.61	1.59
5	B	942	ATP	O2'-C2'	2.10	1.48	1.43
5	F	942	ATP	C5-C4	2.04	1.42	1.39
5	H	942	ATP	PG-O1G	2.03	1.56	1.50
5	B	942	ATP	PA-O1A	2.02	1.57	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	942	ATP	O2'-C2'-C1'	3.88	123.48	110.10
5	F	942	ATP	O2G-PG-O3B	3.71	117.06	104.64
5	F	942	ATP	C2'-C1'-N9	3.69	122.47	113.30
5	D	942	ATP	O3A-PA-O1A	3.38	120.89	110.70
5	H	942	ATP	O2G-PG-O3B	3.14	115.18	104.64
5	D	942	ATP	C2'-C1'-N9	3.14	121.10	113.30
5	B	942	ATP	N3-C2-N1	-2.84	124.28	128.58
5	H	942	ATP	O2A-PA-O3A	2.84	114.94	107.27
5	D	942	ATP	O2B-PB-O3A	2.70	114.56	107.27
5	D	942	ATP	C3'-C2'-C1'	-2.54	96.66	101.46
5	H	942	ATP	C5-N7-C8	2.52	107.41	103.45
5	B	942	ATP	O2B-PB-O3A	2.46	113.94	107.27
5	D	942	ATP	N3-C2-N1	-2.43	124.91	128.58
5	D	942	ATP	C4-N9-C8	2.37	108.23	105.74
5	H	942	ATP	O3B-PB-O1B	-2.22	104.03	110.70
5	H	942	ATP	O3'-C3'-C4'	2.19	117.37	111.08
5	D	942	ATP	O5'-C5'-C4'	-2.13	101.73	108.99
5	D	942	ATP	O4'-C1'-N9	2.12	112.17	108.09
5	H	942	ATP	O3A-PB-O1B	-2.12	104.33	110.70
5	B	942	ATP	O3'-C3'-C4'	2.02	116.87	111.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	942	ATP	PB-O3A-PA-O5'

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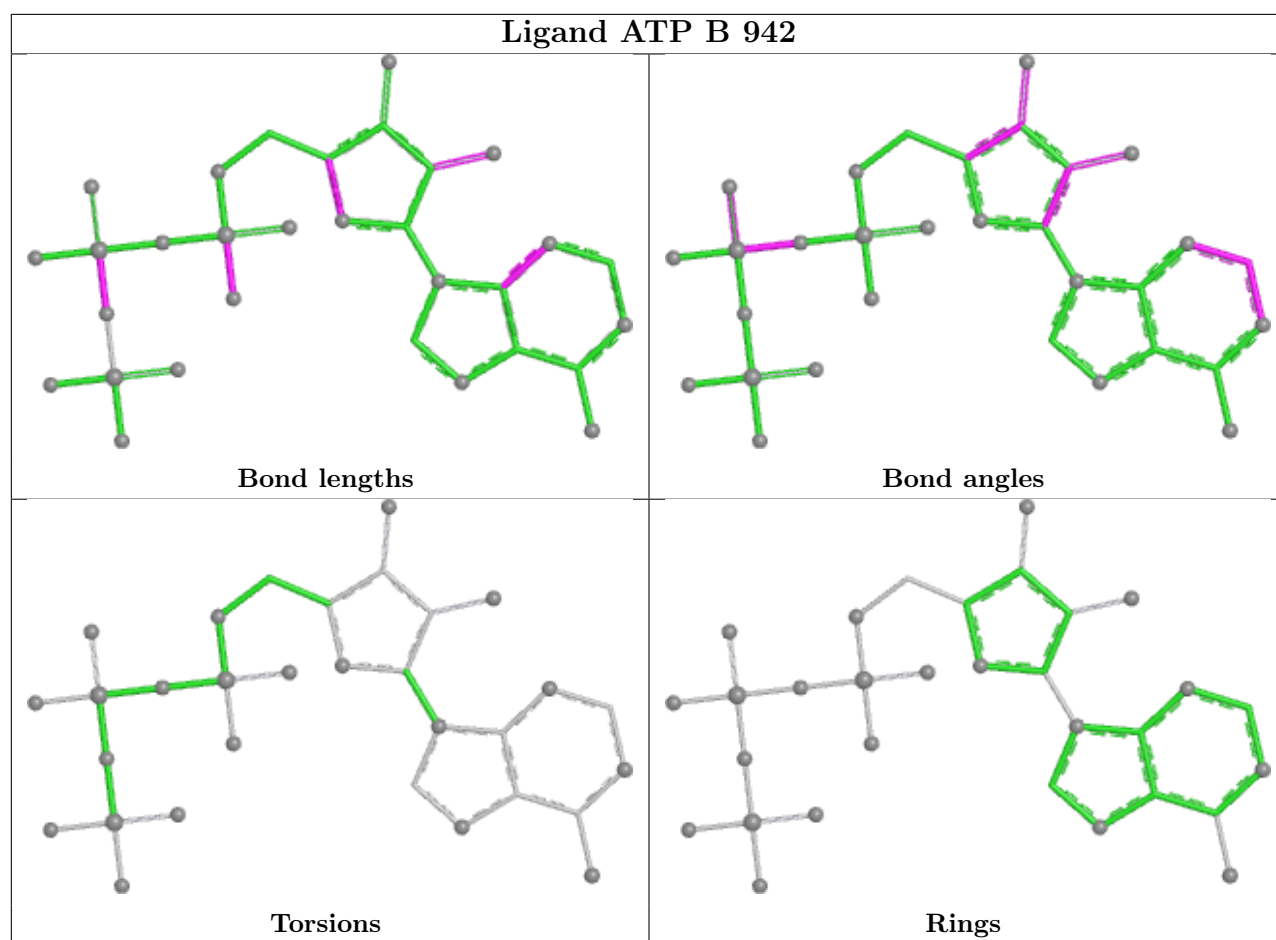
Mol	Chain	Res	Type	Atoms
5	H	942	ATP	PB-O3A-PA-O5'
5	F	942	ATP	O4'-C4'-C5'-O5'
5	F	942	ATP	C5'-O5'-PA-O1A
5	D	942	ATP	PG-O3B-PB-O2B
5	F	942	ATP	C3'-C4'-C5'-O5'

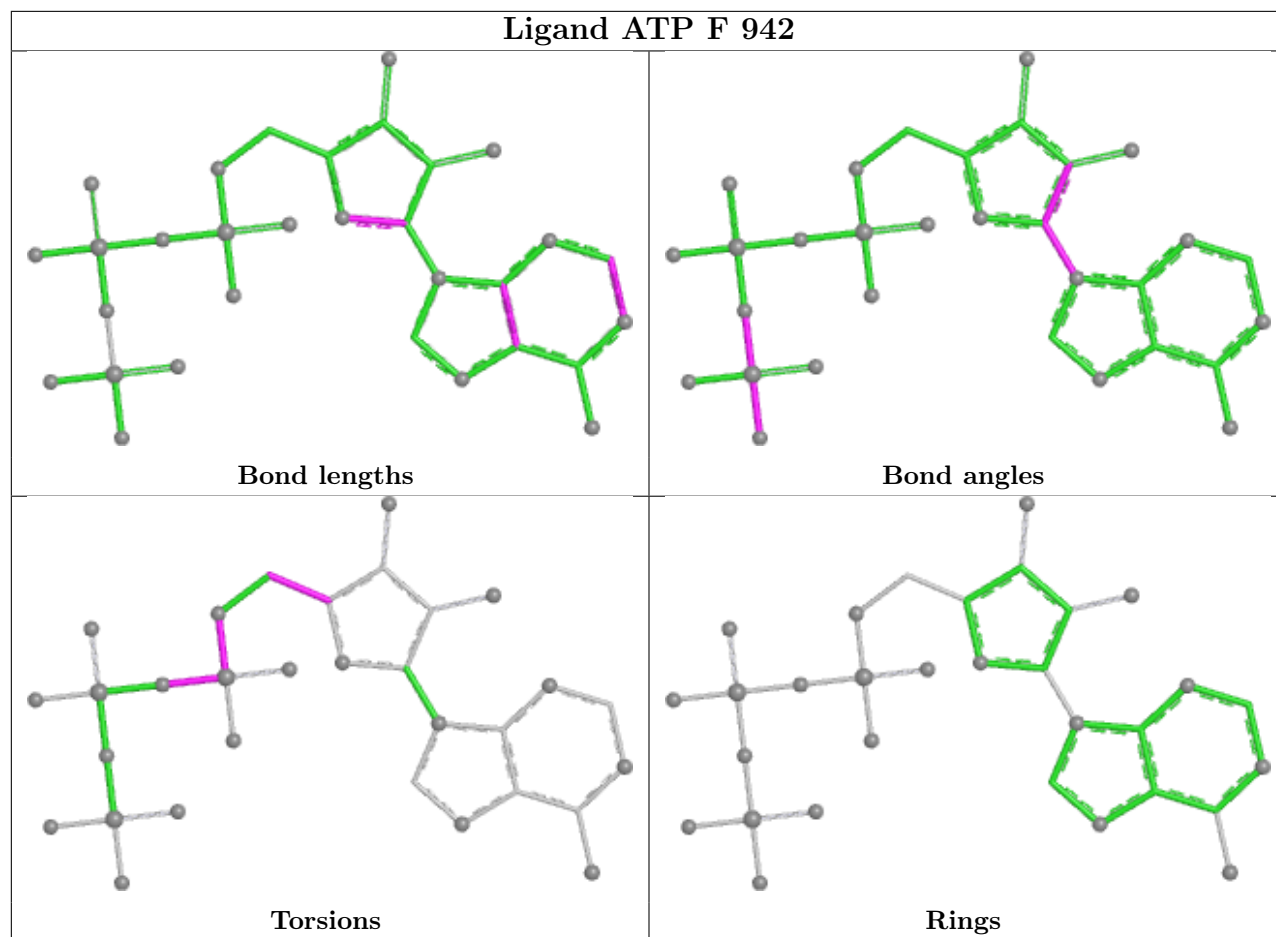
There are no ring outliers.

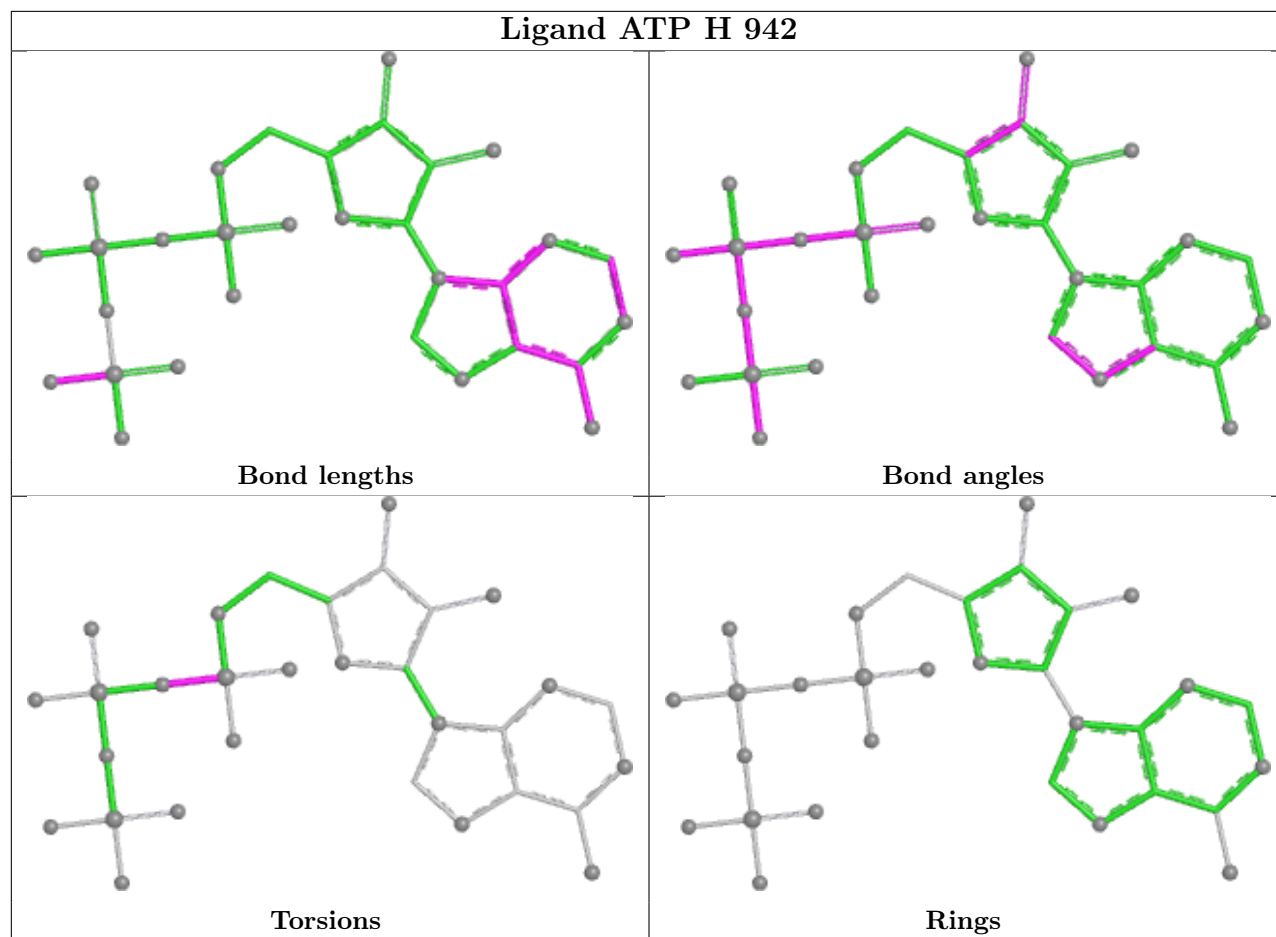
7 monomers are involved in 8 short contacts:

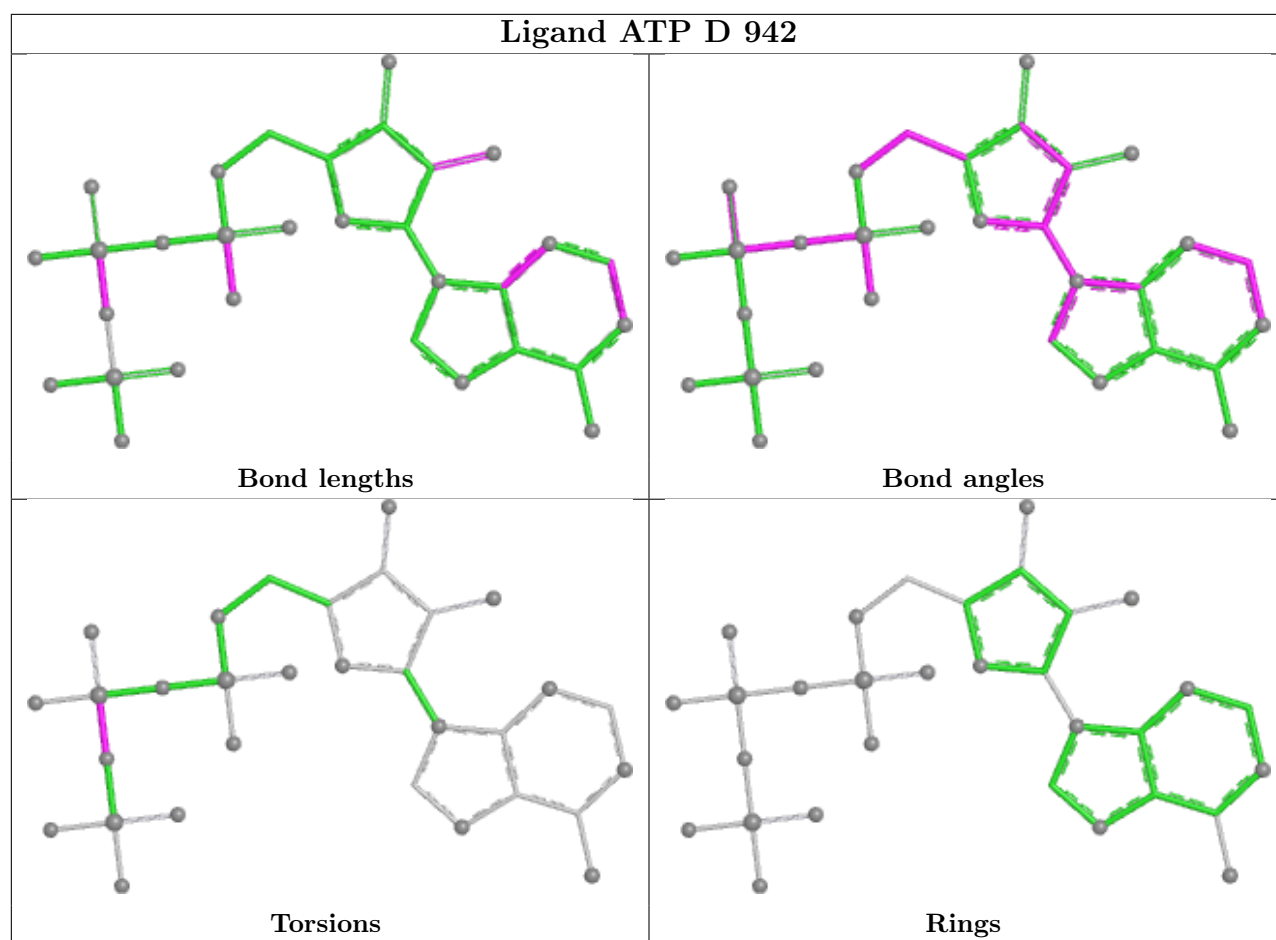
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	991	SO4	2	0
4	E	990	SO4	1	0
5	F	942	ATP	1	0
4	E	991	SO4	1	0
5	H	942	ATP	1	0
4	C	996	SO4	1	0
4	A	993	SO4	1	0

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.









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	936/989 (94%)	-1.26	0 100 100	19, 52, 102, 146	0
1	C	936/989 (94%)	-1.27	0 100 100	21, 53, 107, 163	0
1	E	936/989 (94%)	-1.06	0 100 100	31, 75, 120, 163	0
1	G	936/989 (94%)	-1.10	1 (0%) 92 86	31, 70, 114, 160	0
2	B	884/941 (93%)	-1.22	0 100 100	20, 52, 109, 162	0
2	D	884/941 (93%)	-1.21	1 (0%) 92 86	20, 51, 113, 186	0
2	F	884/941 (93%)	-0.84	1 (0%) 92 86	43, 83, 126, 191	0
2	H	884/941 (93%)	-0.98	0 100 100	38, 72, 133, 184	0
3	I	323/351 (92%)	-1.42	0 100 100	22, 47, 84, 106	0
3	J	323/351 (92%)	-1.43	0 100 100	17, 47, 84, 113	0
3	K	323/351 (92%)	-1.26	0 100 100	38, 66, 96, 121	0
3	L	323/351 (92%)	-1.11	0 100 100	47, 72, 104, 125	0
All	All	8572/9124 (93%)	-1.15	3 (0%) 100 100	17, 64, 116, 191	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	19	ASN	2.3
1	G	173	TYR	2.2
2	F	528	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	E	996	5/5	0.95	0.08	123,127,128,129	0
4	SO4	I	355	5/5	0.95	0.08	131,135,136,137	0
4	SO4	J	354	5/5	0.95	0.06	140,144,145,145	0
4	SO4	L	353	5/5	0.95	0.07	165,169,170,170	0
4	SO4	K	354	5/5	0.96	0.07	136,141,141,142	0
4	SO4	I	354	5/5	0.96	0.06	160,164,165,166	0
4	SO4	G	996	5/5	0.97	0.06	133,137,138,139	0
4	SO4	C	999	5/5	0.97	0.07	147,152,152,153	0
4	SO4	L	352	5/5	0.97	0.04	122,127,128,128	0
4	SO4	A	1002	5/5	0.97	0.06	131,136,136,137	0
4	SO4	G	997	5/5	0.98	0.05	135,139,139,140	0
4	SO4	H	944	5/5	0.98	0.05	94,99,99,100	0
4	SO4	H	946	5/5	0.98	0.07	116,120,121,121	0
4	SO4	I	353	5/5	0.98	0.05	91,95,97,97	0
4	SO4	A	992	5/5	0.98	0.04	76,80,80,82	0
4	SO4	A	997	5/5	0.98	0.05	102,106,107,108	0
4	SO4	I	356	5/5	0.98	0.05	125,129,130,130	0
4	SO4	J	352	5/5	0.98	0.07	104,108,109,109	0
4	SO4	E	992	5/5	0.98	0.05	94,99,100,100	0
4	SO4	K	353	5/5	0.98	0.05	95,100,100,100	0
4	SO4	A	1000	5/5	0.98	0.05	105,109,110,110	0
4	SO4	E	997	5/5	0.98	0.05	124,128,129,129	0
4	SO4	A	1001	5/5	0.98	0.05	90,94,95,96	0
4	SO4	L	354	5/5	0.98	0.05	129,133,134,135	0
5	ATP	F	942	31/31	0.98	0.05	83,87,104,105	0
4	SO4	A	993	5/5	0.99	0.03	82,87,88,88	0
4	SO4	A	994	5/5	0.99	0.04	61,65,66,68	0
4	SO4	F	943	5/5	0.99	0.04	68,73,74,74	0
4	SO4	F	944	5/5	0.99	0.03	79,84,84,85	0
4	SO4	F	945	5/5	0.99	0.04	113,118,118,119	0
4	SO4	G	991	5/5	0.99	0.03	55,58,60,61	0
4	SO4	G	992	5/5	0.99	0.03	79,83,84,85	0

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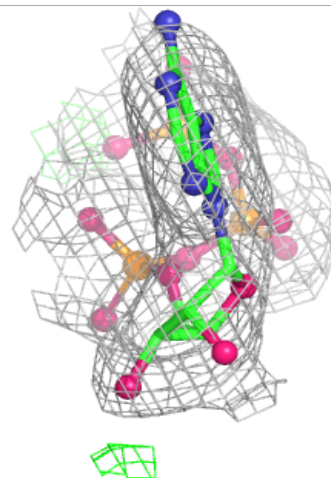
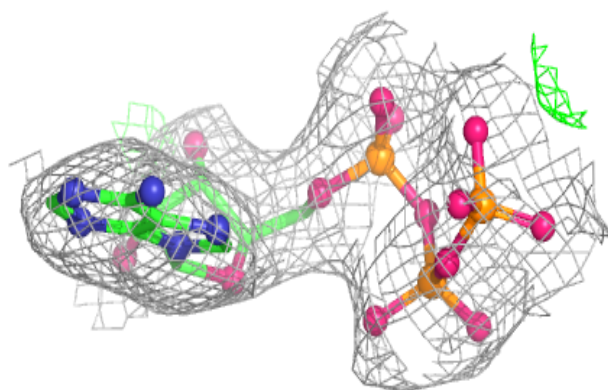
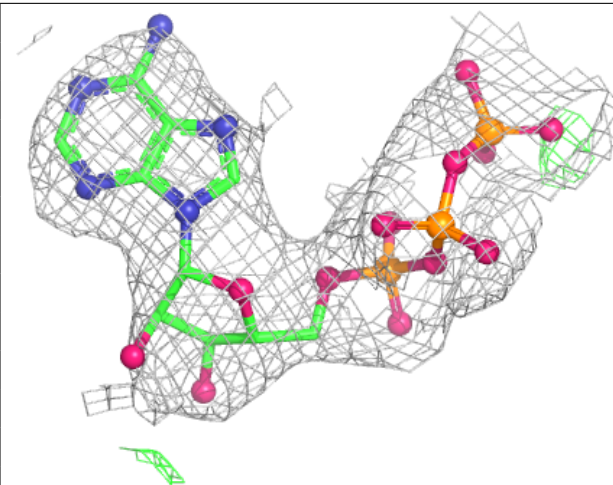
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	G	993	5/5	0.99	0.03	97,101,102,103	0
4	SO4	G	995	5/5	0.99	0.05	96,101,101,102	0
4	SO4	A	995	5/5	0.99	0.06	116,120,121,122	0
4	SO4	B	943	5/5	0.99	0.05	45,49,50,50	0
4	SO4	H	943	5/5	0.99	0.04	69,73,74,75	0
4	SO4	C	990	5/5	0.99	0.03	43,45,48,50	0
4	SO4	C	992	5/5	0.99	0.03	61,65,65,66	0
4	SO4	I	352	5/5	0.99	0.04	66,69,71,71	0
4	SO4	C	994	5/5	0.99	0.04	87,91,92,92	0
4	SO4	C	995	5/5	0.99	0.04	85,89,90,90	0
4	SO4	C	997	5/5	0.99	0.04	113,117,118,118	0
4	SO4	C	998	5/5	0.99	0.06	119,123,124,125	0
4	SO4	A	990	5/5	0.99	0.03	70,74,75,76	0
4	SO4	J	353	5/5	0.99	0.06	83,87,88,88	0
4	SO4	D	944	5/5	0.99	0.03	79,83,83,85	0
4	SO4	K	352	5/5	0.99	0.06	88,92,93,94	0
4	SO4	E	990	5/5	0.99	0.05	110,114,115,115	0
4	SO4	E	991	5/5	0.99	0.04	66,70,72,72	0
4	SO4	A	998	5/5	0.99	0.04	84,87,89,90	0
4	SO4	E	993	5/5	0.99	0.04	93,97,99,99	0
4	SO4	E	994	5/5	0.99	0.04	118,122,123,124	0
5	ATP	D	942	31/31	0.99	0.03	38,42,53,56	0
4	SO4	E	995	5/5	0.99	0.04	95,99,100,100	0
5	ATP	H	942	31/31	0.99	0.04	69,70,102,104	0
4	SO4	A	999	5/5	1.00	0.03	46,50,51,52	0
4	SO4	D	943	5/5	1.00	0.02	33,36,38,40	0
4	SO4	C	993	5/5	1.00	0.02	57,60,61,64	0
4	SO4	D	945	5/5	1.00	0.02	49,53,55,55	0
4	SO4	A	991	5/5	1.00	0.02	57,61,62,64	0
4	SO4	H	945	5/5	1.00	0.03	59,64,65,66	0
4	SO4	B	944	5/5	1.00	0.02	36,40,41,42	0
4	SO4	G	990	5/5	1.00	0.03	63,66,69,70	0
4	SO4	C	996	5/5	1.00	0.02	46,49,51,53	0
5	ATP	B	942	31/31	1.00	0.03	34,36,55,57	0
4	SO4	A	996	5/5	1.00	0.03	45,48,50,53	0
4	SO4	C	991	5/5	1.00	0.02	58,61,63,65	0
4	SO4	G	994	5/5	1.00	0.04	86,89,92,92	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

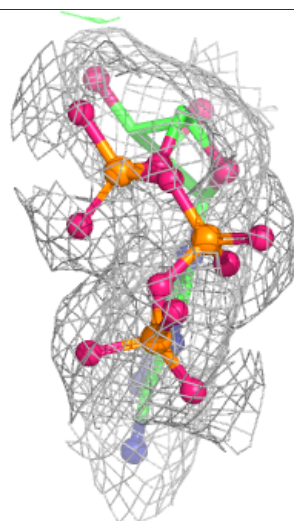
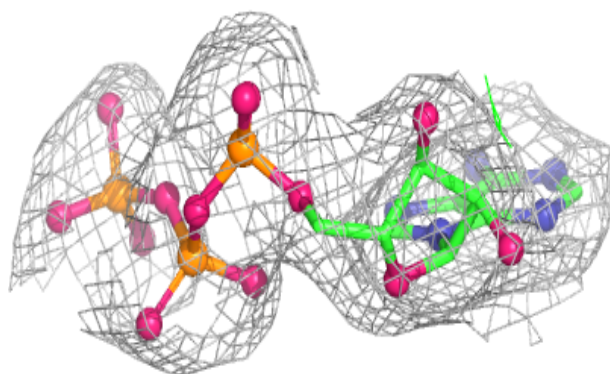
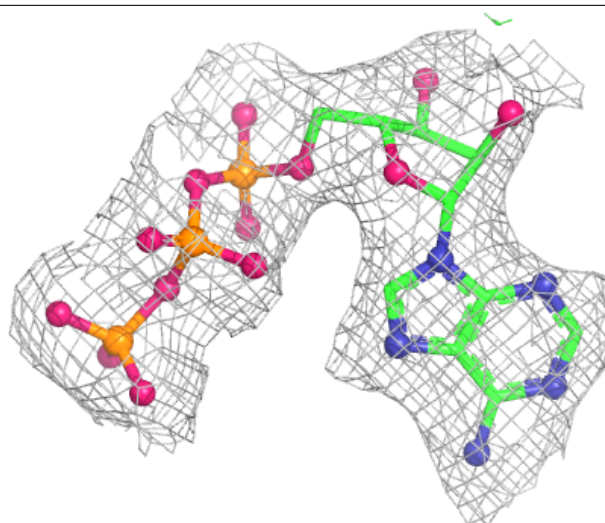
Electron density around ATP F 942:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



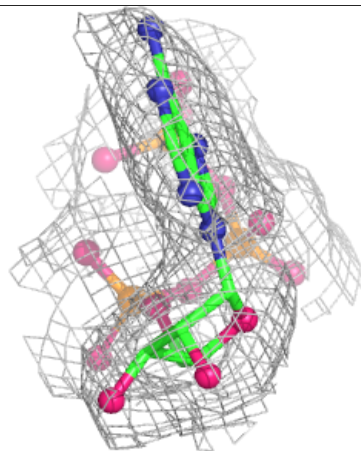
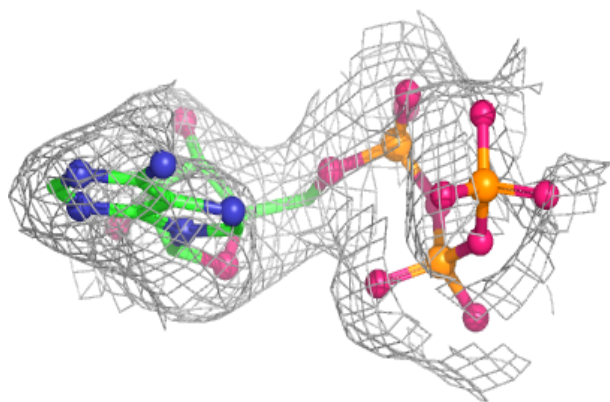
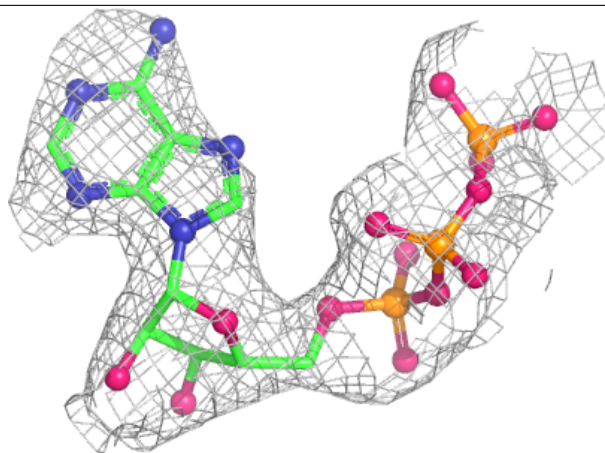
Electron density around ATP D 942:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



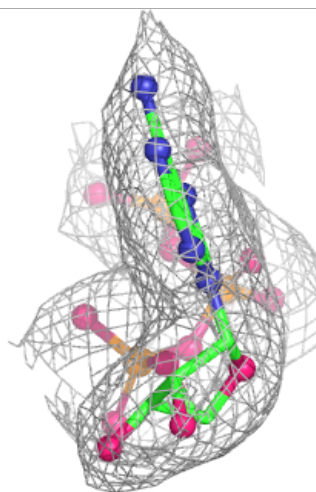
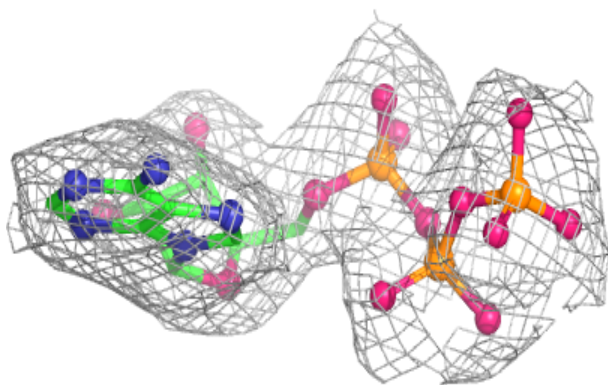
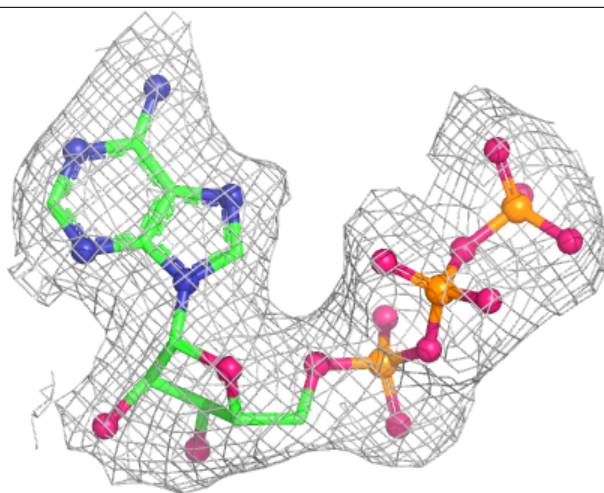
Electron density around ATP H 942:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP B 942:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.