



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:58 am GMT

PDB ID : 4LNI
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of the transition state complex
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on : 2013-07-11
Resolution : 2.58 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

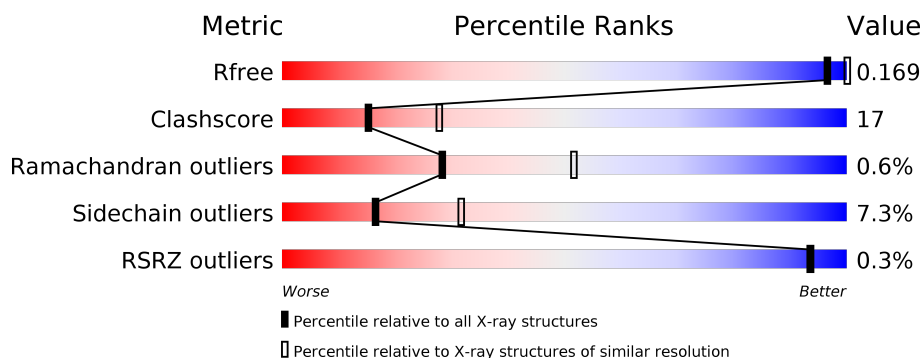
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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}	100719	2899 (2.60-2.56)
Clashscore	112137	3268 (2.60-2.56)
Ramachandran outliers	110173	3218 (2.60-2.56)
Sidechain outliers	110143	3218 (2.60-2.56)
RSRZ outliers	101464	2907 (2.60-2.56)

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

Mol	Chain	Length	Quality of chain
1	A	443	 67% 28% 5%
1	B	443	 67% 27% 6%
1	C	443	 68% 27% 5% .
1	D	443	 65% 29% 5% .
1	E	443	 68% 27% 5%
1	F	443	 63% 33% .

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Mol	Chain	Length	Quality of chain
1	G	443	
1	H	443	
1	I	443	
1	J	443	
1	K	443	
1	L	443	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P3S	A	501	-	-	-	X
2	P3S	D	501	-	-	X	X
2	P3S	F	601	-	-	X	X
2	P3S	G	601	-	-	X	-
2	P3S	K	501	-	-	-	X
4	MG	A	503	-	-	-	X
4	MG	B	503	-	-	-	X
4	MG	B	504	-	-	-	X
4	MG	C	503	-	-	-	X
4	MG	C	505	-	-	-	X
4	MG	D	503	-	-	-	X
4	MG	D	505	-	-	-	X
4	MG	E	503	-	-	-	X
4	MG	H	603	-	-	-	X
4	MG	I	503	-	-	-	X
4	MG	K	503	-	-	-	X
4	MG	L	503	-	-	-	X

2 Entry composition

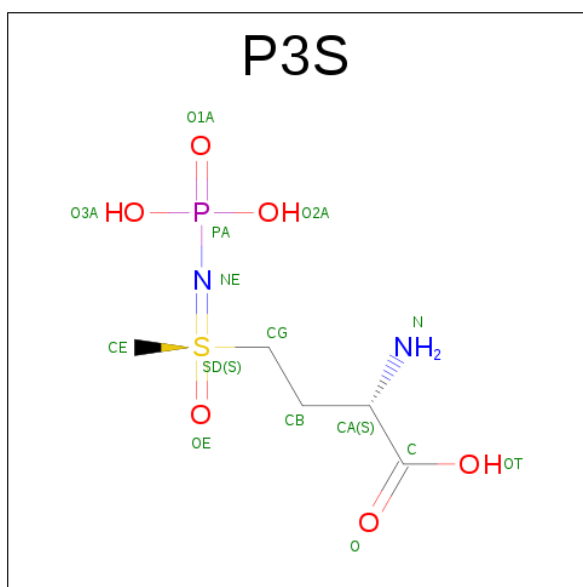
There are 5 unique types of molecules in this entry. The entry contains 86960 atoms, of which 41847 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

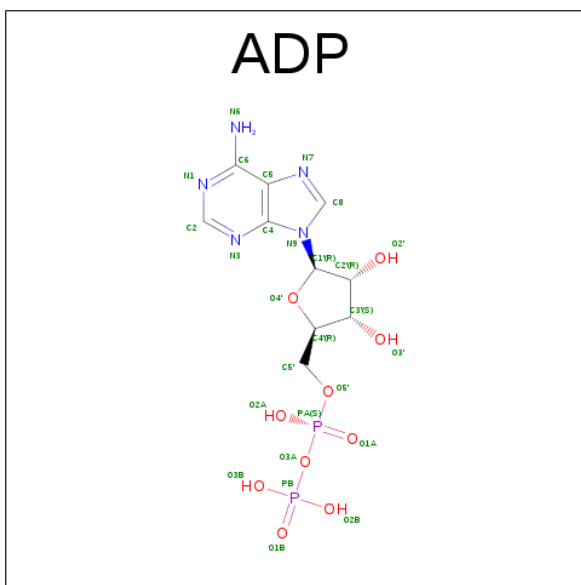
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	B	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	C	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	D	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	E	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	F	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	G	443	Total	C	H	N	O	S	0	0	0
			7009	2259	3474	590	670	16			
1	H	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	I	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	J	441	Total	C	H	N	O	S	0	0	0
			6980	2250	3459	587	668	16			
1	K	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			
1	L	443	Total	C	H	N	O	S	0	0	0
			7012	2259	3477	590	670	16			

- Molecule 2 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: C₅H₁₃N₂O₆PS).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	I	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	J	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	K	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		
2	L	1	Total	C	H	N	O	P	S	0	0
			27	5	12	2	6	1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	3	Total Mg 3 3	0	0
4	J	3	Total Mg 3 3	0	0
4	D	3	Total Mg 3 3	0	0
4	K	3	Total Mg 3 3	0	0
4	E	3	Total Mg 3 3	0	0
4	H	3	Total Mg 3 3	0	0
4	B	3	Total Mg 3 3	0	0
4	I	3	Total Mg 3 3	0	0
4	C	3	Total Mg 3 3	0	0
4	A	3	Total Mg 3 3	0	0
4	L	3	Total Mg 3 3	0	0
4	F	3	Total Mg 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	177	Total O 177 177	0	0
5	B	178	Total O 178 178	0	0
5	C	183	Total O 183 183	0	0
5	D	200	Total O 200 200	0	0
5	E	168	Total O 168 168	0	0
5	F	166	Total O 166 166	0	0
5	G	184	Total O 184 184	0	0
5	H	174	Total O 174 174	0	0

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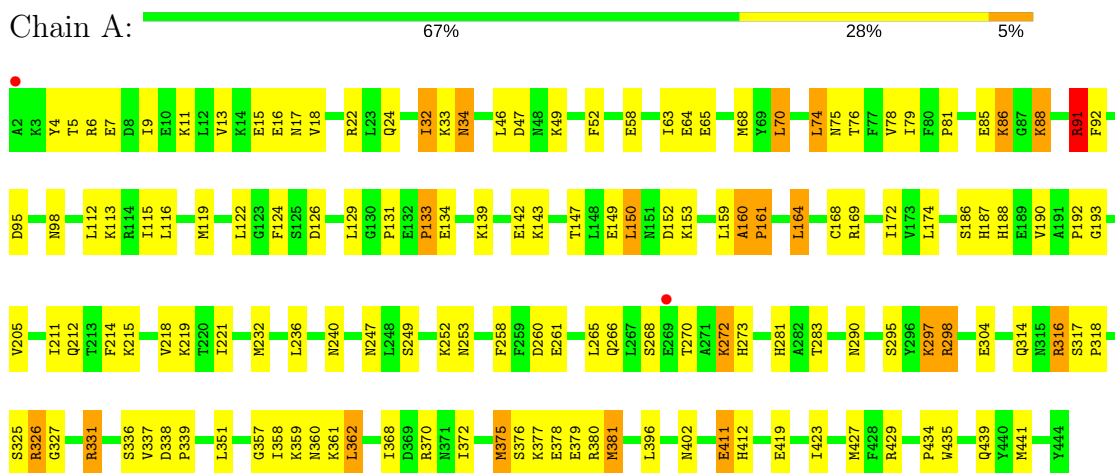
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	189	Total 189	O 189	0	0
5	J	194	Total 194	O 194	0	0
5	K	191	Total 191	O 191	0	0
5	L	163	Total 163	O 163	0	0

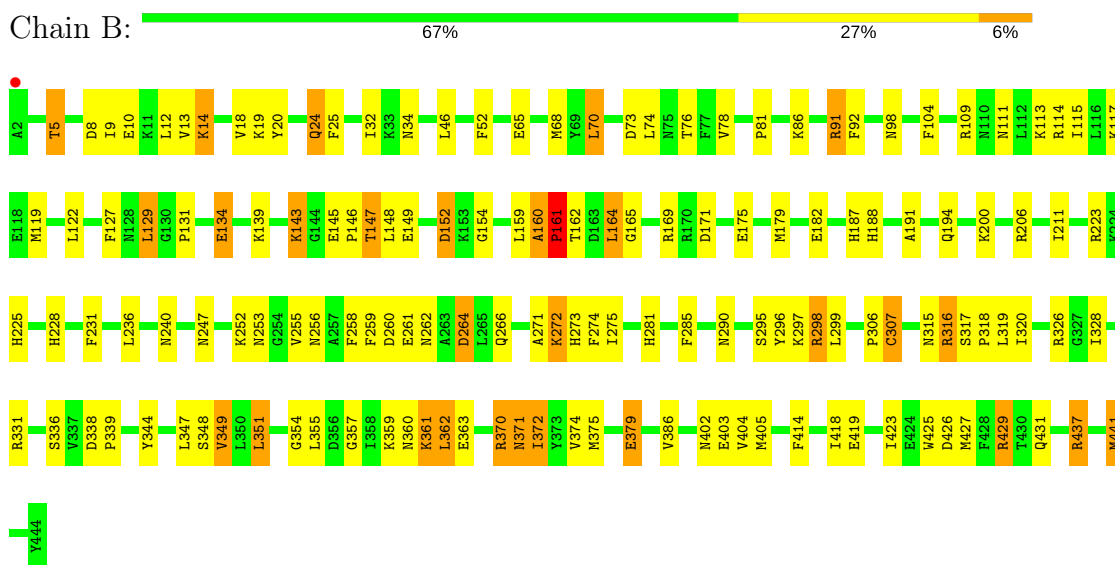
3 Residue-property plots

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

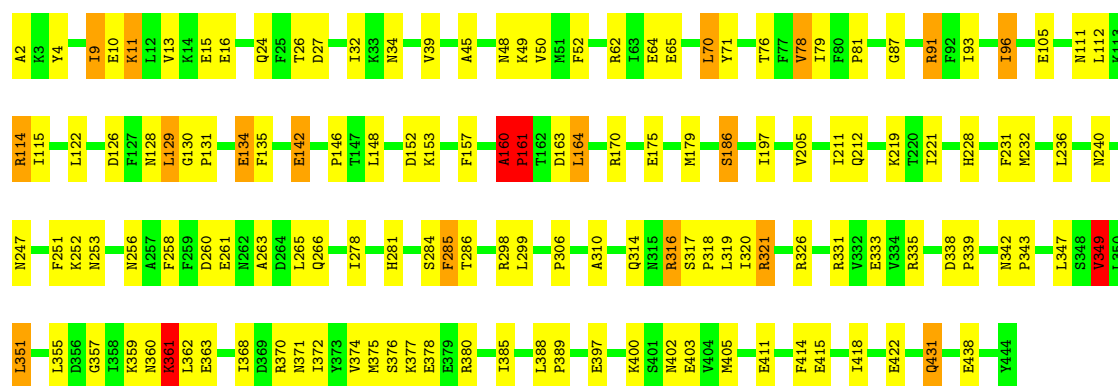


• Molecule 1: Glutamine synthetase



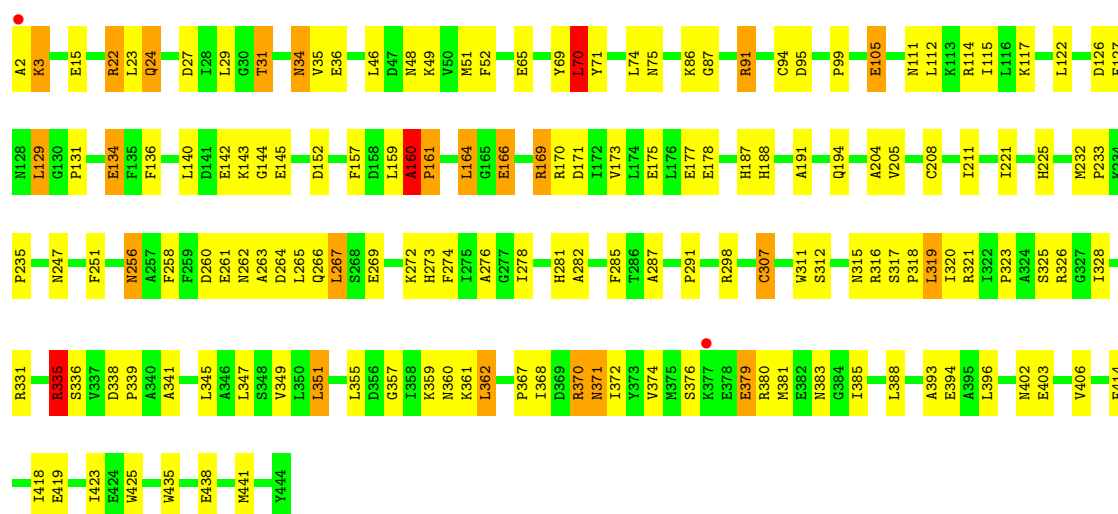
• Molecule 1: Glutamine synthetase





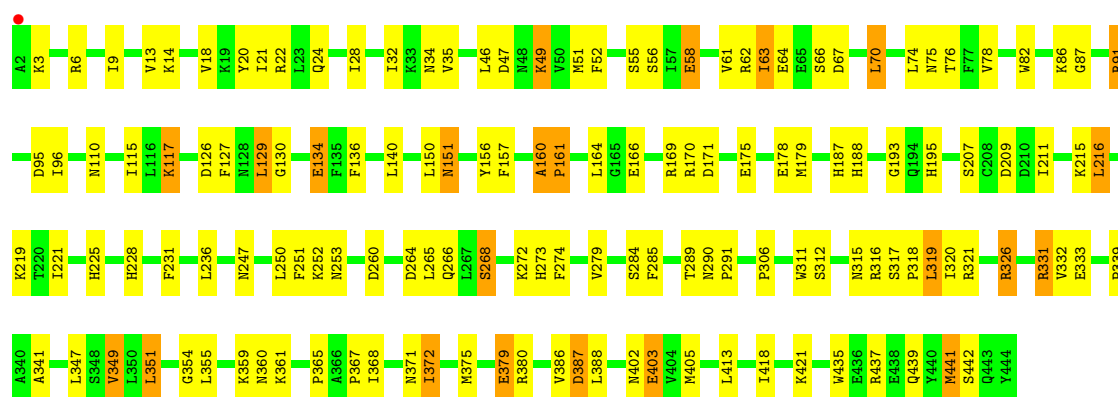
• Molecule 1: Glutamine synthetase

Chain D: 65% 29% 5% •



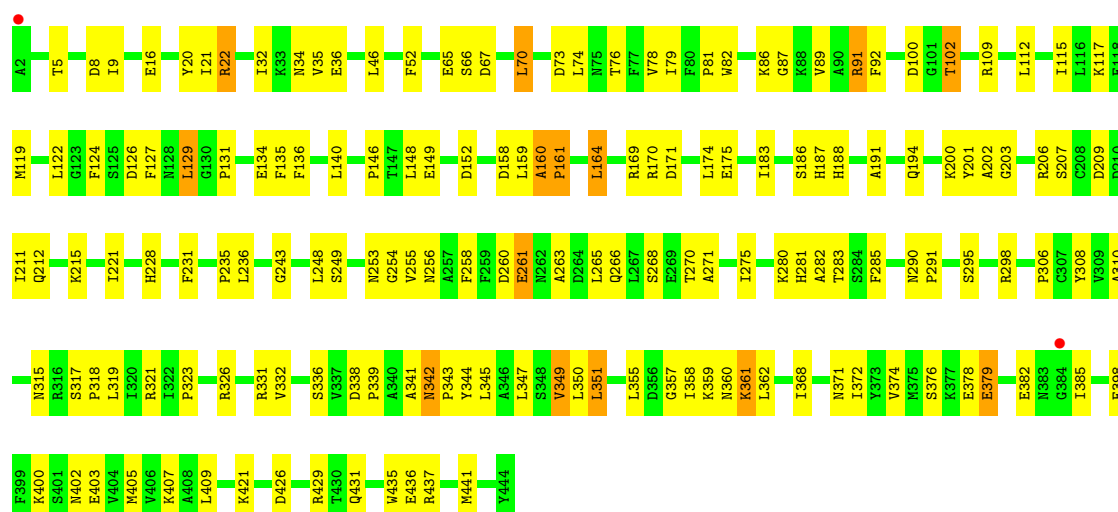
• Molecule 1: Glutamine synthetase

Chain E: 68% 27% 5% •

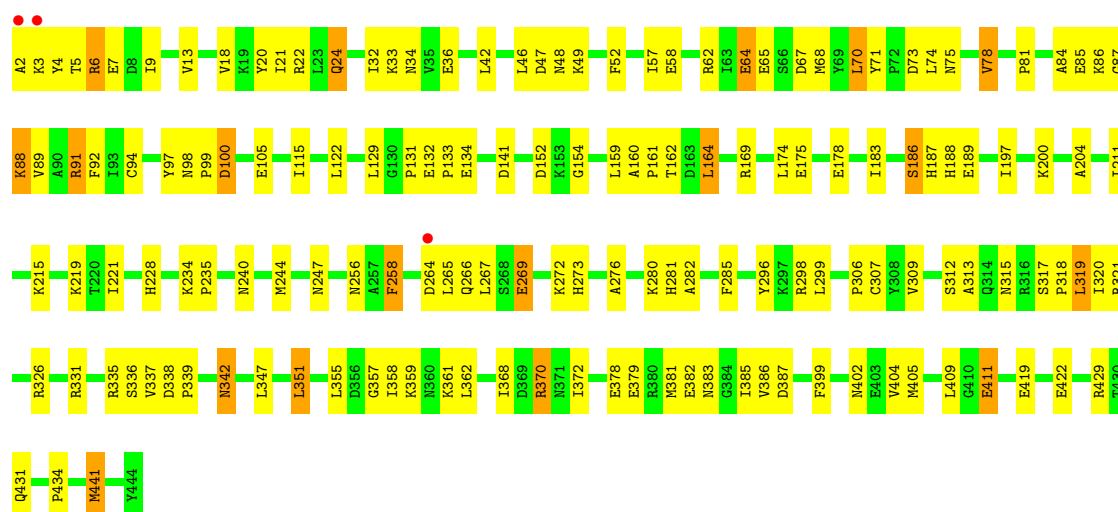


• Molecule 1: Glutamine synthetase

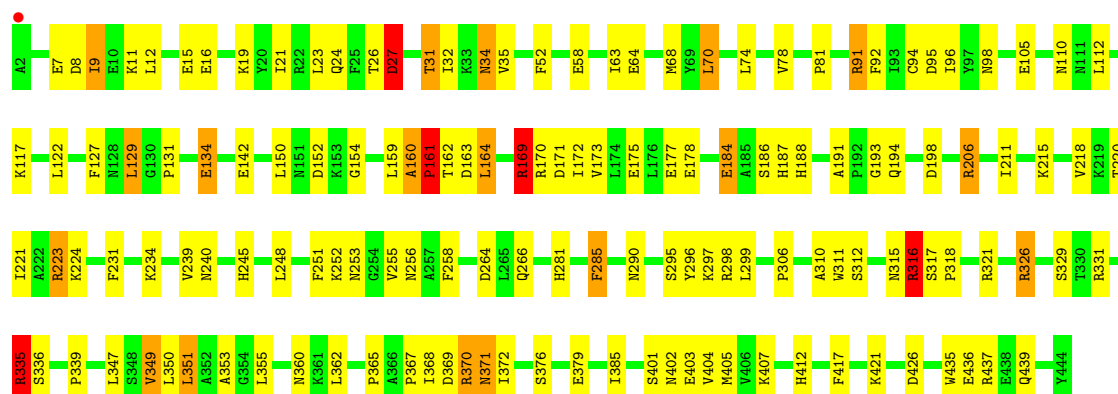
Chain F: 63% 33% 4% •



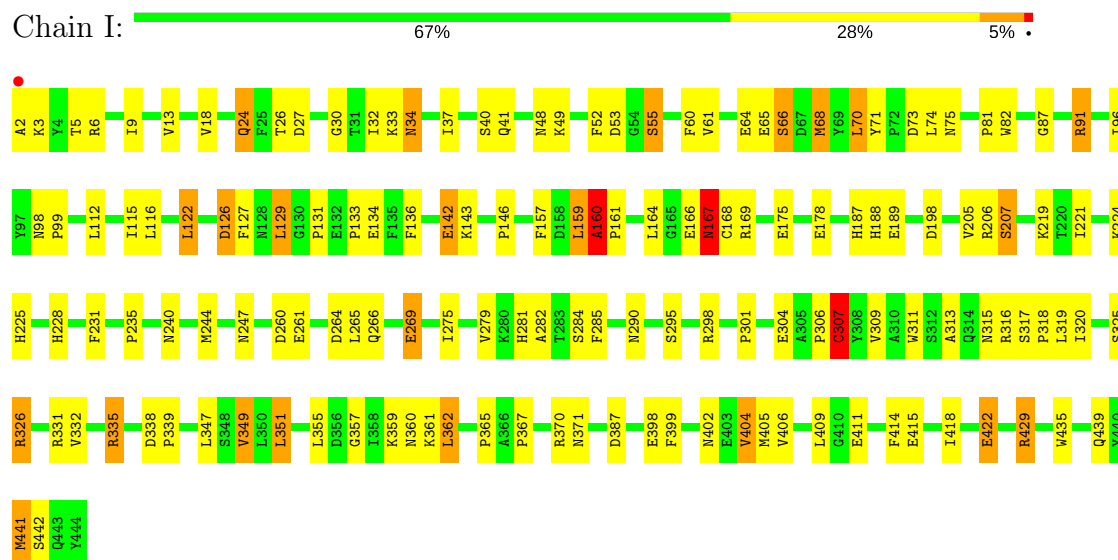
• Molecule 1: Glutamine synthetase



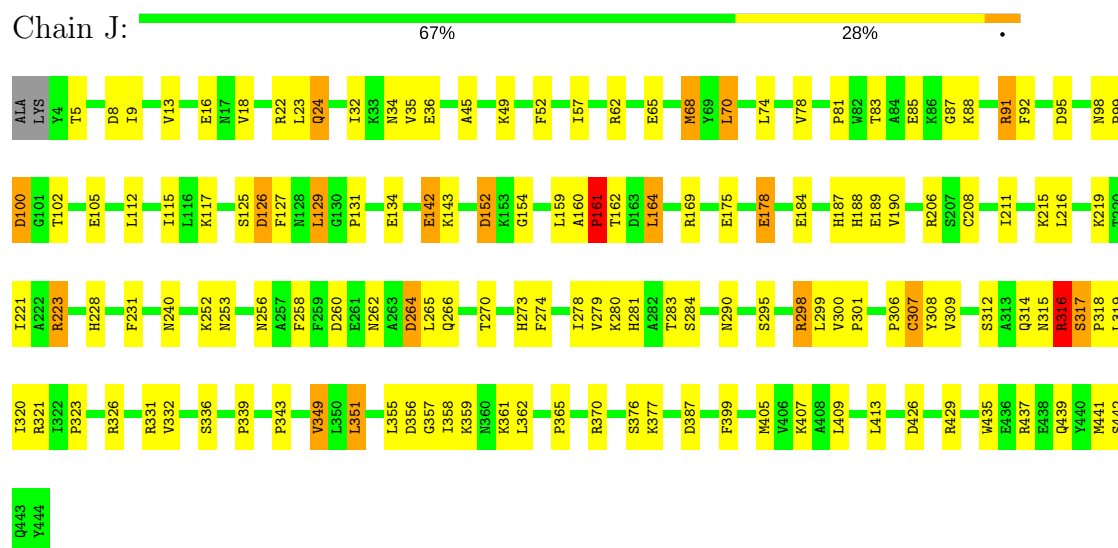
• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase

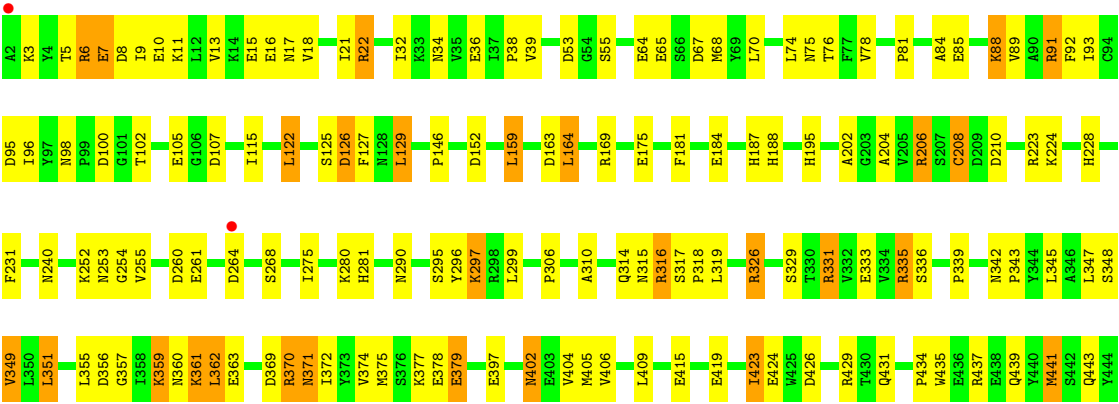


• Molecule 1: Glutamine synthetase





● Molecule 1: Glutamine synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.20Å 141.60Å 142.10Å 60.29° 67.38° 76.20°	Depositor
Resolution (Å)	117.10 – 2.58 117.10 – 2.58	Depositor EDS
% Data completeness (in resolution range)	90.8 (117.10-2.58) 77.8 (117.10-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.165 , 0.223 0.166 , 0.169	Depositor DCC
R_{free} test set	21985 reflections (12.59%)	DCC
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	1.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	86960	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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: P3S, MG, ADP

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	0.96	0/3618	0.95	6/4895 (0.1%)
1	B	0.98	3/3618 (0.1%)	0.97	10/4895 (0.2%)
1	C	0.98	4/3618 (0.1%)	1.02	10/4895 (0.2%)
1	D	0.97	4/3618 (0.1%)	0.96	9/4895 (0.2%)
1	E	0.97	3/3618 (0.1%)	1.03	14/4895 (0.3%)
1	F	0.95	1/3618 (0.0%)	0.96	5/4895 (0.1%)
1	G	0.95	3/3618 (0.1%)	0.92	6/4895 (0.1%)
1	H	0.97	2/3618 (0.1%)	0.99	9/4895 (0.2%)
1	I	0.96	2/3618 (0.1%)	0.99	11/4895 (0.2%)
1	J	0.98	6/3604 (0.2%)	1.01	10/4877 (0.2%)
1	K	1.01	2/3618 (0.1%)	1.00	8/4895 (0.2%)
1	L	0.96	2/3618 (0.1%)	0.89	2/4895 (0.0%)
All	All	0.97	32/43402 (0.1%)	0.98	100/58722 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
1	I	0	1
All	All	0	9

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	161	PRO	N-CD	7.91	1.58	1.47
1	D	166	GLU	CG-CD	7.69	1.63	1.51
1	C	134	GLU	CG-CD	7.57	1.63	1.51
1	I	307	CYS	CB-SG	-6.89	1.70	1.82
1	J	105	GLU	CG-CD	6.76	1.62	1.51
1	D	307	CYS	CB-SG	-6.51	1.71	1.82
1	G	269	GLU	CG-CD	6.22	1.61	1.51
1	B	307	CYS	CB-SG	-6.22	1.71	1.82
1	F	134	GLU	CG-CD	6.08	1.61	1.51
1	K	134	GLU	CG-CD	5.93	1.60	1.51
1	E	134	GLU	CG-CD	5.90	1.60	1.51
1	G	36	GLU	CD-OE2	5.87	1.32	1.25
1	H	134	GLU	CG-CD	5.83	1.60	1.51
1	B	264	ASP	CB-CG	5.79	1.63	1.51
1	K	307	CYS	CB-SG	-5.77	1.72	1.81
1	C	15	GLU	CG-CD	5.72	1.60	1.51
1	B	134	GLU	CG-CD	5.69	1.60	1.51
1	D	169	ARG	CB-CG	-5.68	1.37	1.52
1	I	167	ASN	CB-CG	5.60	1.64	1.51
1	G	94	CYS	CB-SG	-5.54	1.72	1.81
1	J	178	GLU	CG-CD	5.50	1.60	1.51
1	J	316	ARG	CB-CG	-5.50	1.37	1.52
1	J	78	VAL	CB-CG2	-5.50	1.41	1.52
1	C	349	VAL	CB-CG2	-5.40	1.41	1.52
1	L	208	CYS	CB-SG	-5.29	1.73	1.81
1	D	134	GLU	CG-CD	5.21	1.59	1.51
1	E	403	GLU	CG-CD	5.17	1.59	1.51
1	L	36	GLU	CG-CD	5.09	1.59	1.51
1	J	105	GLU	CB-CG	5.07	1.61	1.52
1	J	169	ARG	CB-CG	-5.07	1.38	1.52
1	H	169	ARG	CB-CG	-5.05	1.39	1.52
1	C	105	GLU	CG-CD	5.03	1.59	1.51

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	160	ALA	C-N-CD	-26.90	61.42	120.60
1	K	160	ALA	C-N-CD	-23.72	68.41	120.60
1	C	160	ALA	C-N-CD	-22.46	71.20	120.60
1	H	160	ALA	C-N-CD	-22.29	71.56	120.60
1	J	160	ALA	C-N-CD	-22.20	71.76	120.60
1	I	160	ALA	C-N-CD	-19.28	78.18	120.60
1	F	160	ALA	C-N-CD	-17.43	82.25	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	ALA	C-N-CD	-17.21	82.73	120.60
1	B	160	ALA	C-N-CD	-15.41	86.70	120.60
1	H	160	ALA	C-N-CA	12.74	175.50	122.00
1	J	160	ALA	C-N-CA	12.70	175.33	122.00
1	A	160	ALA	C-N-CD	-12.32	93.49	120.60
1	A	298	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	K	160	ALA	C-N-CA	11.45	170.10	122.00
1	A	298	ARG	NE-CZ-NH2	-10.65	114.97	120.30
1	E	326	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	E	326	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	B	316	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	I	160	ALA	C-N-CA	9.46	161.73	122.00
1	G	160	ALA	C-N-CD	-9.45	99.81	120.60
1	E	161	PRO	CA-N-CD	-8.74	99.27	111.50
1	D	298	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	I	169	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	C	160	ALA	C-N-CA	8.33	156.99	122.00
1	E	160	ALA	C-N-CA	8.26	156.71	122.00
1	C	321	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	C	298	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	316	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	B	298	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	C	161	PRO	CA-N-CD	-7.75	100.64	111.50
1	B	298	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	I	298	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	J	298	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	I	206	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	96	ILE	CG1-CB-CG2	-7.15	95.67	111.40
1	K	223	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	C	298	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	I	169	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	169	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	G	47	ASP	CB-CG-OD2	6.82	124.44	118.30
1	H	335	ARG	NE-CZ-NH1	-6.73	116.94	120.30
1	A	91	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	E	326	ARG	CG-CD-NE	-6.71	97.70	111.80
1	H	316	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	E	161	PRO	N-CA-CB	6.61	111.23	103.30
1	K	161	PRO	CA-N-CD	-6.50	102.41	111.50
1	K	96	ILE	CG1-CB-CG2	-6.49	97.12	111.40
1	F	437	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	152	ASP	CB-CG-OD1	6.43	124.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	152	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	K	27	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	264	ASP	CB-CG-OD1	6.31	123.98	118.30
1	H	169	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	D	298	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	J	316	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	335	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	E	160	ALA	O-C-N	6.03	132.56	121.10
1	D	160	ALA	C-N-CA	6.01	147.23	122.00
1	A	150	LEU	CA-CB-CG	-5.97	101.57	115.30
1	E	161	PRO	N-CA-C	-5.95	96.63	112.10
1	H	437	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	F	298	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	I	326	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	223	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	F	209	ASP	CB-CG-OD2	5.84	123.56	118.30
1	D	70	LEU	CB-CG-CD2	-5.80	101.15	111.00
1	G	47	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	H	95	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	70	LEU	CA-CB-CG	5.76	128.55	115.30
1	H	27	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	437	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	C	114	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	95	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	J	161	PRO	CA-N-CD	-5.61	103.64	111.50
1	J	316	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	K	95	ASP	CB-CG-OD1	5.58	123.32	118.30
1	J	152	ASP	CB-CG-OD2	5.56	123.30	118.30
1	G	160	ALA	C-N-CA	5.52	145.19	122.00
1	I	429	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	I	387	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	114	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	J	95	ASP	CB-CG-OD2	5.45	123.20	118.30
1	I	298	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	K	198	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	E	70	LEU	CA-CB-CG	5.38	127.68	115.30
1	E	95	ASP	CB-CG-OD1	5.38	123.14	118.30
1	G	258	PHE	CB-CG-CD1	-5.36	117.05	120.80
1	H	335	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	G	405	MET	CG-SD-CE	5.34	108.75	100.20
1	D	95	ASP	CB-CG-OD1	5.29	123.07	118.30
1	F	298	ARG	NE-CZ-NH1	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	370	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	I	189	GLU	CB-CA-C	5.21	120.82	110.40
1	L	95	ASP	CB-CG-OD1	5.20	122.98	118.30
1	J	22	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	D	335	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	E	150	LEU	CA-CB-CG	-5.04	103.70	115.30
1	L	159	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	E	209	ASP	CB-CG-OD2	5.02	122.81	118.30
1	E	134	GLU	OE1-CD-OE2	-5.02	117.28	123.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ALA	Peptide
1	B	160	ALA	Peptide
1	C	160	ALA	Mainchain,Peptide
1	D	160	ALA	Peptide
1	E	160	ALA	Peptide
1	F	160	ALA	Peptide
1	H	160	ALA	Peptide
1	I	160	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3535	3477	3466	118	0
1	B	3535	3477	3466	113	0
1	C	3535	3477	3466	114	0
1	D	3535	3477	3466	128	0
1	E	3535	3477	3466	117	0
1	F	3535	3477	3466	140	0
1	G	3535	3474	3466	141	0
1	H	3535	3477	3466	126	0
1	I	3535	3477	3466	129	0
1	J	3521	3459	3448	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3535	3477	3466	111	0
1	L	3535	3477	3466	129	0
2	A	15	12	10	4	0
2	B	15	12	10	1	0
2	C	15	12	10	4	0
2	D	15	12	10	6	0
2	E	15	12	10	1	0
2	F	15	12	10	6	0
2	G	15	12	10	8	0
2	H	15	12	10	5	0
2	I	15	12	10	2	0
2	J	15	12	10	3	0
2	K	15	12	10	2	0
2	L	15	12	10	1	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	1	0
3	F	27	0	12	1	0
3	G	27	0	12	0	0
3	H	27	0	12	0	0
3	I	27	0	12	0	0
3	J	27	0	12	0	0
3	K	27	0	12	0	0
3	L	27	0	12	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
4	I	3	0	0	0	0
4	J	3	0	0	0	0
4	K	3	0	0	0	0
4	L	3	0	0	0	0
5	A	177	0	0	11	0
5	B	178	0	0	14	0
5	C	183	0	0	13	0
5	D	200	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	168	0	0	11	0
5	F	166	0	0	15	0
5	G	184	0	0	19	0
5	H	174	0	0	17	0
5	I	189	0	0	16	0
5	J	194	0	0	20	0
5	K	191	0	0	19	0
5	L	163	0	0	11	0
All	All	45113	41847	41838	1414	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 17.

All (1414) 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:H:601:P3S:SD	2:H:601:P3S:CE	2.01	1.48
2:G:601:P3S:CE	2:G:601:P3S:SD	2.01	1.46
2:F:601:P3S:CE	2:F:601:P3S:SD	2.02	1.45
2:D:501:P3S:CE	2:D:501:P3S:SD	2.03	1.43
1:I:357:GLY:HA2	1:I:362:LEU:CD1	1.64	1.27
1:I:357:GLY:HA2	1:I:362:LEU:HD13	1.16	1.15
2:G:601:P3S:CG	2:G:601:P3S:CE	2.24	1.14
1:K:211:ILE:HG13	5:K:635:HOH:O	1.49	1.13
2:F:601:P3S:CG	2:F:601:P3S:CE	2.34	1.05
1:F:100:ASP:OD1	1:F:102:THR:CG2	2.06	1.03
1:B:147:THR:HG22	1:B:149:GLU:H	1.24	1.01
2:G:601:P3S:CG	2:G:601:P3S:HEC2	1.89	1.00
1:I:2:ALA:HB2	5:I:766:HOH:O	1.63	0.97
1:C:321:ARG:NH1	5:C:602:HOH:O	1.98	0.97
1:L:22:ARG:HH11	1:L:89:VAL:HG11	1.30	0.97
1:G:3:LYS:NZ	1:G:4:TYR:CE2	2.33	0.96
1:F:100:ASP:OD1	1:F:102:THR:HG22	1.63	0.96
1:G:3:LYS:NZ	1:G:4:TYR:CD2	2.34	0.96
2:D:501:P3S:CE	2:D:501:P3S:CG	2.44	0.94
1:D:266:GLN:HB2	1:D:326:ARG:HD2	1.48	0.94
1:D:326:ARG:CZ	5:D:712:HOH:O	2.18	0.92
2:F:601:P3S:HEC2	2:F:601:P3S:CG	1.99	0.92
1:G:269:GLU:HG2	5:G:745:HOH:O	1.71	0.90
2:H:601:P3S:CG	2:H:601:P3S:CE	2.50	0.89
1:L:224:LYS:HE2	5:L:642:HOH:O	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:ASP:O	1:H:11:LYS:HG2	1.72	0.88
1:L:223:ARG:HG3	5:L:700:HOH:O	1.74	0.88
1:F:206:ARG:NH1	5:F:748:HOH:O	2.07	0.88
1:J:252:LYS:HE3	5:J:749:HOH:O	1.75	0.86
1:H:31:THR:HG21	5:H:811:HOH:O	1.75	0.86
1:G:3:LYS:NZ	1:G:4:TYR:CZ	2.44	0.85
1:K:429:ARG:HD3	5:K:697:HOH:O	1.75	0.85
1:J:16:GLU:O	1:J:88:LYS:HE3	1.77	0.84
1:G:3:LYS:NZ	1:G:4:TYR:CG	2.46	0.84
1:G:411:GLU:HG2	5:G:824:HOH:O	1.78	0.84
1:L:11:LYS:HE2	1:L:15:GLU:OE2	1.79	0.83
1:C:411:GLU:O	1:C:415:GLU:HG2	1.77	0.83
1:I:357:GLY:CA	1:I:362:LEU:HD13	2.06	0.83
1:J:264:ASP:OD1	5:J:763:HOH:O	1.96	0.83
1:I:357:GLY:CA	1:I:362:LEU:CD1	2.54	0.82
1:D:122:LEU:HD21	1:D:359:LYS:HG2	1.62	0.82
2:G:601:P3S:HGC2	2:G:601:P3S:HEC2	1.61	0.82
1:I:81:PRO:HG2	1:I:175:GLU:OE2	1.80	0.81
1:L:254:GLY:O	1:L:255:VAL:HG23	1.80	0.81
1:G:13:VAL:HG13	1:G:18:VAL:HB	1.63	0.81
1:H:266:GLN:HB2	1:H:326:ARG:HD2	1.62	0.81
1:C:349:VAL:HG22	1:C:405:MET:SD	2.21	0.81
1:F:131:PRO:CB	1:F:211:ILE:HD11	2.12	0.80
1:H:81:PRO:HG2	1:H:175:GLU:OE1	1.81	0.80
1:B:357:GLY:HA2	1:B:362:LEU:HD22	1.64	0.80
1:L:65:GLU:HA	1:L:65:GLU:OE1	1.80	0.80
1:D:326:ARG:NH2	5:D:712:HOH:O	2.15	0.79
1:I:362:LEU:HD12	1:I:362:LEU:H	1.47	0.79
1:J:83:THR:HB	1:K:170:ARG:HH22	1.48	0.78
1:C:380:ARG:HB2	1:C:385:ILE:HB	1.65	0.78
1:L:423:ILE:C	1:L:423:ILE:HD12	2.03	0.78
1:J:83:THR:HB	1:K:170:ARG:NH2	1.98	0.78
1:K:429:ARG:CD	5:K:697:HOH:O	2.30	0.78
1:K:370:ARG:HD2	5:K:700:HOH:O	1.83	0.77
1:L:357:GLY:HA2	1:L:362:LEU:HD22	1.66	0.77
1:F:9:ILE:HG13	1:F:74:LEU:HD12	1.64	0.77
1:E:13:VAL:HG13	1:E:18:VAL:HB	1.65	0.77
1:A:52:PHE:CE1	1:A:70:LEU:HD13	2.20	0.77
2:D:501:P3S:HEC3	2:D:501:P3S:CG	2.14	0.76
1:H:223:ARG:HG2	1:H:223:ARG:HH11	1.50	0.76
1:A:150:LEU:HD23	1:A:193:GLY:HA3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLU:CD	1:D:142:GLU:H	1.88	0.76
1:L:22:ARG:NH1	1:L:89:VAL:HG11	1.98	0.76
1:G:3:LYS:NZ	1:G:4:TYR:CD1	2.54	0.76
1:L:68:MET:HE3	1:L:98:ASN:HA	1.66	0.76
1:B:351:LEU:HD22	1:B:355:LEU:HG	1.68	0.76
5:A:693:HOH:O	1:B:143:LYS:HD3	1.84	0.75
1:K:131:PRO:CG	1:K:211:ILE:HD11	2.16	0.75
1:F:403:GLU:OE2	1:F:407:LYS:HE2	1.86	0.75
1:L:13:VAL:HG13	1:L:18:VAL:HB	1.69	0.75
1:G:399:PHE:HZ	1:G:409:LEU:HD22	1.52	0.75
1:G:368:ILE:CD1	1:G:385:ILE:HD11	2.16	0.74
1:B:9:ILE:O	1:B:13:VAL:HG23	1.86	0.74
1:D:256:ASN:HD22	1:D:258:PHE:H	1.35	0.74
1:I:357:GLY:HA2	1:I:362:LEU:HD11	1.66	0.74
1:H:105:GLU:OE1	5:H:866:HOH:O	2.04	0.73
1:G:3:LYS:NZ	1:G:4:TYR:CE1	2.54	0.73
1:F:16:GLU:HG2	1:F:79:ILE:CD1	2.18	0.73
1:K:122:LEU:CD2	1:K:124:PHE:HE1	2.02	0.73
1:I:9:ILE:HG13	1:I:74:LEU:HD12	1.69	0.73
1:F:271:ALA:O	1:F:275:ILE:HG12	1.89	0.73
1:J:211:ILE:HG22	1:J:215:LYS:HE2	1.71	0.73
1:F:131:PRO:HB2	1:F:211:ILE:HD11	1.72	0.72
2:H:601:P3S:CG	2:H:601:P3S:HEC2	2.18	0.72
1:K:122:LEU:CD2	1:K:124:PHE:CE1	2.72	0.72
1:G:5:THR:HB	5:G:850:HOH:O	1.89	0.71
1:I:351:LEU:HD22	1:I:355:LEU:HG	1.71	0.71
1:C:316:ARG:HD3	2:C:501:P3S:OE	1.90	0.71
1:H:152:ASP:HB3	1:H:164:LEU:HB2	1.70	0.71
1:J:265:LEU:O	1:J:326:ARG:NH1	2.24	0.71
1:J:407:LYS:HG2	5:J:671:HOH:O	1.89	0.71
1:J:68:MET:HE2	1:J:98:ASN:HA	1.71	0.71
1:H:68:MET:HE3	1:H:98:ASN:HA	1.71	0.71
1:C:321:ARG:CZ	5:C:602:HOH:O	2.32	0.71
1:C:368:ILE:HG12	1:C:385:ILE:HD11	1.71	0.71
1:D:319:LEU:CD2	1:D:336:SER:HB2	2.21	0.70
1:I:24:GLN:NE2	1:I:91:ARG:HH11	1.89	0.70
1:J:300:VAL:HG13	1:J:301:PRO:HD2	1.73	0.70
1:H:368:ILE:HD12	1:H:385:ILE:HD11	1.72	0.70
1:A:52:PHE:CD1	1:A:70:LEU:HD13	2.26	0.70
1:J:266:GLN:HB2	1:J:326:ARG:HD2	1.74	0.70
1:K:131:PRO:HG3	1:K:211:ILE:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:357:GLY:HA2	1:J:362:LEU:HD12	1.74	0.70
1:F:372:ILE:HD11	1:F:385:ILE:HG21	1.73	0.70
1:F:5:THR:HG23	1:F:8:ASP:H	1.57	0.70
1:G:265:LEU:O	1:G:326:ARG:NH1	2.25	0.70
1:H:285:PHE:HB2	1:H:349:VAL:HG11	1.74	0.70
1:G:3:LYS:CE	1:G:4:TYR:CE2	2.75	0.69
1:I:335:ARG:HD3	5:I:647:HOH:O	1.92	0.69
1:J:24:GLN:HE21	1:J:91:ARG:HD3	1.57	0.69
1:D:115:ILE:HG22	1:D:351:LEU:HD13	1.73	0.69
1:K:115:ILE:HG22	1:K:351:LEU:HD13	1.73	0.69
1:L:351:LEU:HD22	1:L:355:LEU:HG	1.74	0.69
1:D:262:ASN:ND2	5:D:764:HOH:O	2.17	0.69
1:K:281:HIS:HD2	1:K:402:ASN:HD21	1.40	0.69
1:F:5:THR:HG22	1:F:8:ASP:OD2	1.91	0.69
1:B:379:GLU:HG3	5:B:673:HOH:O	1.90	0.69
1:H:187:HIS:HD2	1:H:188:HIS:O	1.76	0.69
1:I:96:ILE:N	1:I:96:ILE:HD12	2.07	0.69
1:K:99:PRO:HG2	1:L:314:GLN:HE22	1.56	0.69
1:C:65:GLU:OE2	5:C:750:HOH:O	2.11	0.69
1:B:370:ARG:NE	5:B:686:HOH:O	2.26	0.69
1:L:152:ASP:HB3	1:L:164:LEU:HB2	1.75	0.69
1:G:351:LEU:HD22	1:G:355:LEU:HG	1.75	0.69
1:F:345:LEU:HD22	1:F:409:LEU:HD22	1.75	0.68
1:C:24:GLN:HE21	1:C:34:ASN:HD22	1.40	0.68
1:A:150:LEU:CD2	1:A:192:PRO:O	2.42	0.68
1:D:126:ASP:HB2	1:D:251:PHE:HB2	1.76	0.68
1:C:232:MET:HE1	1:I:441:MET:HB2	1.74	0.68
1:E:9:ILE:O	1:E:13:VAL:HG23	1.94	0.68
1:D:2:ALA:HB3	1:D:75:ASN:HD21	1.59	0.68
1:F:169:ARG:CD	1:F:186:SER:OG	2.42	0.68
1:C:351:LEU:HD22	1:C:355:LEU:HG	1.76	0.67
1:C:377:LYS:HG3	1:C:378:GLU:N	2.09	0.67
1:E:175:GLU:HG3	1:E:221:ILE:HD11	1.75	0.67
1:J:161:PRO:O	1:J:164:LEU:HD13	1.94	0.67
1:J:24:GLN:NE2	1:J:91:ARG:HH11	1.92	0.67
1:A:265:LEU:O	1:A:326:ARG:NH1	2.28	0.67
1:D:131:PRO:HB3	1:D:211:ILE:HD11	1.76	0.67
1:J:252:LYS:CE	5:J:749:HOH:O	2.39	0.67
1:L:423:ILE:HD12	1:L:423:ILE:O	1.94	0.67
1:F:115:ILE:HG22	1:F:351:LEU:HD13	1.75	0.67
1:G:152:ASP:HB3	1:G:164:LEU:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LYS:O	1:B:147:THR:HB	1.95	0.67
1:F:281:HIS:HD2	1:F:402:ASN:HD21	1.42	0.67
1:F:429:ARG:HD2	5:F:799:HOH:O	1.94	0.67
1:B:315:ASN:O	1:B:318:PRO:HD2	1.95	0.66
1:A:16:GLU:HG2	1:A:79:ILE:HD13	1.76	0.66
1:L:163:ASP:OD2	1:L:169:ARG:NH2	2.28	0.66
1:G:399:PHE:CZ	1:G:409:LEU:HD22	2.30	0.66
1:C:131:PRO:HB3	1:C:211:ILE:HD11	1.77	0.66
1:E:3:LYS:HB3	1:E:75:ASN:ND2	2.11	0.66
1:J:274:PHE:CE2	1:J:278:ILE:HD11	2.30	0.66
1:B:187:HIS:HD2	1:B:188:HIS:O	1.78	0.66
1:D:27:ASP:OD1	1:D:31:THR:HG23	1.95	0.66
1:F:285:PHE:HB2	1:F:349:VAL:HG11	1.78	0.66
1:F:359:LYS:CE	5:F:737:HOH:O	2.43	0.66
1:H:360:ASN:HB2	1:H:362:LEU:CD1	2.25	0.66
1:H:376:SER:OG	1:H:379:GLU:HB2	1.96	0.66
1:A:187:HIS:HD2	1:A:188:HIS:O	1.78	0.66
1:B:161:PRO:HG2	1:C:219:LYS:HB3	1.77	0.66
1:G:6:ARG:HD2	1:G:46:LEU:HD13	1.78	0.65
1:J:62:ARG:NH1	5:J:790:HOH:O	2.29	0.65
1:L:81:PRO:HG2	1:L:175:GLU:OE2	1.95	0.65
1:F:285:PHE:HB2	1:F:349:VAL:CG1	2.26	0.65
1:H:52:PHE:CE1	1:H:70:LEU:HD13	2.32	0.65
1:L:5:THR:HG22	1:L:8:ASP:CG	2.16	0.65
1:F:100:ASP:OD1	1:F:102:THR:HG23	1.92	0.65
1:D:24:GLN:HE21	1:D:91:ARG:HD3	1.61	0.65
1:D:204:ALA:HB1	1:D:347:LEU:HD13	1.78	0.65
1:A:172:ILE:HD12	1:A:218:VAL:HA	1.78	0.65
1:B:281:HIS:HD2	1:B:402:ASN:HD21	1.45	0.65
1:H:19:LYS:HD3	5:H:863:HOH:O	1.96	0.65
1:K:110:ASN:ND2	5:K:745:HOH:O	2.30	0.65
1:K:170:ARG:HB3	5:K:636:HOH:O	1.96	0.65
1:G:169:ARG:HG3	1:G:197:ILE:HD11	1.78	0.65
1:H:206:ARG:NH1	5:H:731:HOH:O	2.30	0.65
1:C:377:LYS:HG3	1:C:378:GLU:H	1.62	0.64
1:D:351:LEU:HD22	1:D:355:LEU:HG	1.80	0.64
1:K:338:ASP:HB2	1:K:339:PRO:HD2	1.78	0.64
1:K:378:GLU:O	1:K:382:GLU:HG2	1.98	0.64
1:B:285:PHE:HB2	1:B:349:VAL:CG1	2.27	0.64
1:G:7:GLU:OE1	1:G:7:GLU:HA	1.97	0.64
1:G:20:TYR:HB2	1:G:89:VAL:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:407:LYS:CG	5:J:671:HOH:O	2.45	0.64
1:K:261:GLU:HG2	5:K:680:HOH:O	1.96	0.64
1:C:142:GLU:H	1:C:142:GLU:CD	2.00	0.64
1:H:142:GLU:OE1	1:H:142:GLU:HA	1.97	0.64
1:H:150:LEU:HD22	1:H:193:GLY:HA3	1.79	0.64
1:J:351:LEU:HD22	1:J:355:LEU:HG	1.80	0.64
1:A:427:MET:HE1	5:G:869:HOH:O	1.98	0.64
1:F:357:GLY:HA2	1:F:362:LEU:HD22	1.79	0.64
1:I:142:GLU:OE1	1:I:143:LYS:HG3	1.98	0.64
1:I:167:ASN:ND2	1:I:168:CYS:H	1.96	0.64
1:J:429:ARG:HD3	5:J:750:HOH:O	1.97	0.64
1:J:98:ASN:HD22	1:J:102:THR:HG22	1.63	0.64
1:B:290:ASN:HB3	1:B:295:SER:HB3	1.79	0.64
1:F:306:PRO:HB3	1:F:319:LEU:HA	1.80	0.64
1:L:306:PRO:HB3	1:L:319:LEU:HA	1.78	0.64
1:D:357:GLY:HA2	1:D:362:LEU:HD22	1.79	0.64
1:G:68:MET:CE	1:G:98:ASN:HA	2.28	0.64
1:I:167:ASN:HA	5:I:617:HOH:O	1.97	0.64
1:I:68:MET:CE	1:I:98:ASN:HA	2.28	0.64
1:J:52:PHE:CE1	1:J:70:LEU:HD13	2.33	0.64
1:E:359:LYS:HE2	5:E:626:HOH:O	1.98	0.63
1:J:32:ILE:HG23	1:K:159:LEU:HG	1.79	0.63
1:B:231:PHE:O	1:B:339:PRO:HG2	1.98	0.63
1:G:32:ILE:HG23	1:H:159:LEU:HD13	1.79	0.63
1:A:131:PRO:HB3	1:A:211:ILE:HD11	1.79	0.63
1:A:338:ASP:HB2	1:A:339:PRO:HD2	1.80	0.63
1:G:21:ILE:HD13	1:G:42:LEU:HD13	1.80	0.63
1:K:17:ASN:HA	5:K:703:HOH:O	1.98	0.63
1:G:68:MET:HE2	1:G:98:ASN:HA	1.80	0.63
1:A:281:HIS:HD2	1:A:402:ASN:HD21	1.47	0.63
1:F:148:LEU:HD21	1:L:437:ARG:HD3	1.79	0.63
1:E:285:PHE:HB2	1:E:349:VAL:HG11	1.80	0.63
1:K:357:GLY:HA2	1:K:362:LEU:HD22	1.81	0.63
1:D:136:PHE:CD1	1:D:235:PRO:HG2	2.33	0.63
1:D:22:ARG:HD2	1:D:34:ASN:OD1	1.99	0.63
1:G:368:ILE:HG21	1:G:372:ILE:HD12	1.81	0.63
1:L:402:ASN:HD22	1:L:402:ASN:C	2.01	0.63
1:L:419:GLU:O	1:L:423:ILE:HG23	1.99	0.63
1:A:134:GLU:OE1	2:A:501:P3S:N	2.32	0.62
1:E:351:LEU:HD22	1:E:355:LEU:HG	1.80	0.62
1:L:378:GLU:HG3	1:L:379:GLU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ILE:HD13	1:A:221:ILE:HB	1.81	0.62
1:A:316:ARG:NH1	2:A:501:P3S:O2A	2.31	0.62
1:H:351:LEU:HD22	1:H:355:LEU:HG	1.81	0.62
1:J:206:ARG:NH2	5:J:672:HOH:O	2.32	0.62
1:B:111:ASN:OD1	1:B:114:ARG:NH1	2.31	0.62
1:E:349:VAL:HG22	1:E:405:MET:SD	2.39	0.62
1:L:231:PHE:HB3	1:L:339:PRO:HB2	1.82	0.62
1:B:425:TRP:O	1:B:429:ARG:HG2	1.98	0.62
1:F:400:LYS:HE3	5:F:776:HOH:O	1.98	0.62
1:G:24:GLN:NE2	1:G:91:ARG:HH11	1.96	0.62
1:L:281:HIS:HE1	1:L:356:ASP:OD2	1.83	0.62
1:L:84:ALA:HA	1:L:88:LYS:HB3	1.81	0.62
1:L:96:ILE:N	1:L:96:ILE:HD12	2.14	0.62
1:I:269:GLU:CD	1:I:269:GLU:H	2.03	0.62
1:J:115:ILE:HG22	1:J:351:LEU:HD13	1.82	0.62
1:L:377:LYS:HG3	5:L:726:HOH:O	1.99	0.62
1:A:419:GLU:O	1:A:423:ILE:HG12	2.00	0.62
1:C:65:GLU:HG3	1:C:65:GLU:O	1.99	0.62
1:D:178:GLU:HG3	5:D:798:HOH:O	2.00	0.62
1:D:24:GLN:NE2	1:D:91:ARG:HH11	1.98	0.62
1:H:318:PRO:HB3	1:H:372:ILE:HD11	1.80	0.62
1:H:360:ASN:HB2	1:H:362:LEU:HD11	1.82	0.62
1:G:187:HIS:HD2	1:G:188:HIS:O	1.83	0.62
1:J:273:HIS:HB3	1:J:358:ILE:HA	1.82	0.62
1:D:311:TRP:CZ2	1:D:367:PRO:HG3	2.35	0.62
1:E:110:ASN:ND2	5:E:640:HOH:O	2.31	0.62
1:I:65:GLU:O	1:I:65:GLU:HG3	2.00	0.62
1:K:26:THR:HG21	1:K:344:TYR:HE1	1.65	0.62
1:E:9:ILE:HG13	1:E:74:LEU:HD22	1.81	0.61
1:H:32:ILE:HG23	1:I:159:LEU:HG	1.82	0.61
1:K:86:LYS:HG3	5:K:714:HOH:O	2.00	0.61
1:B:273:HIS:CE1	1:B:361:LYS:HB3	2.36	0.61
1:J:290:ASN:HB3	1:J:295:SER:HB3	1.82	0.61
1:G:313:ALA:HB1	5:G:735:HOH:O	1.99	0.61
1:J:231:PHE:HB3	1:J:339:PRO:HB2	1.83	0.61
1:C:129:LEU:HD22	1:C:130:GLY:N	2.15	0.61
1:D:394:GLU:HB2	5:D:660:HOH:O	2.00	0.61
1:G:115:ILE:HG22	1:G:351:LEU:HD13	1.82	0.61
1:J:24:GLN:HB3	1:J:34:ASN:HB3	1.83	0.61
1:A:357:GLY:HA2	1:A:362:LEU:HD22	1.83	0.61
1:B:143:LYS:HE2	1:B:145:GLU:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:ILE:HG22	1:E:215:LYS:HE2	1.83	0.61
1:H:91:ARG:HD2	1:H:91:ARG:C	2.21	0.61
1:E:311:TRP:CZ2	1:E:367:PRO:HG3	2.36	0.61
1:G:273:HIS:O	1:G:276:ALA:HB3	2.00	0.61
1:G:68:MET:HE3	1:G:99:PRO:HD3	1.83	0.61
1:F:270:THR:HG23	1:F:358:ILE:HD12	1.82	0.61
1:H:285:PHE:HB2	1:H:349:VAL:CG1	2.31	0.61
1:I:357:GLY:O	1:I:362:LEU:HD12	1.99	0.61
1:D:256:ASN:HD21	1:D:258:PHE:HB2	1.66	0.61
1:F:261:GLU:CD	1:F:261:GLU:H	2.04	0.61
1:L:317:SER:N	1:L:318:PRO:CD	2.64	0.61
1:I:167:ASN:HB3	5:I:617:HOH:O	2.00	0.60
1:D:111:ASN:OD1	1:D:114:ARG:NH1	2.34	0.60
1:E:117:LYS:HD2	5:E:630:HOH:O	2.02	0.60
1:G:4:TYR:H	1:G:75:ASN:ND2	1.99	0.60
1:K:411:GLU:O	1:K:415:GLU:HG2	2.02	0.60
1:C:236:LEU:HD12	5:C:710:HOH:O	2.02	0.60
1:L:426:ASP:HB2	5:L:671:HOH:O	2.02	0.60
1:D:208:CYS:SG	1:D:347:LEU:HD12	2.41	0.60
1:J:34:ASN:CG	1:K:159:LEU:CD2	2.70	0.60
1:J:219:LYS:HB3	1:K:161:PRO:HG2	1.82	0.60
1:D:318:PRO:HB3	1:D:372:ILE:HD11	1.84	0.60
1:E:170:ARG:NH1	1:F:86:LYS:HD3	2.17	0.60
1:C:52:PHE:CE1	1:C:70:LEU:HD13	2.37	0.60
1:H:335:ARG:HD3	5:H:766:HOH:O	2.02	0.60
1:I:315:ASN:OD1	1:I:318:PRO:HD3	2.01	0.60
1:B:298:ARG:NH2	1:B:336:SER:O	2.35	0.59
1:G:247:ASN:HB3	1:G:331:ARG:HD2	1.83	0.59
1:I:205:VAL:HB	5:I:625:HOH:O	2.00	0.59
1:I:349:VAL:HG22	1:I:405:MET:SD	2.42	0.59
1:D:70:LEU:HD23	1:D:94:CYS:SG	2.42	0.59
1:K:317:SER:OG	1:K:372:ILE:HG12	2.01	0.59
1:C:357:GLY:HA2	1:C:362:LEU:HD12	1.82	0.59
1:F:175:GLU:HG3	1:F:221:ILE:HD11	1.84	0.59
1:G:211:ILE:HG22	1:G:215:LYS:HE2	1.85	0.59
1:C:170:ARG:HG2	5:C:713:HOH:O	2.02	0.59
1:G:122:LEU:HD11	1:G:359:LYS:HG3	1.84	0.59
1:L:204:ALA:HB1	1:L:347:LEU:HD13	1.84	0.59
1:D:2:ALA:HB1	5:D:791:HOH:O	2.02	0.59
1:F:129:LEU:HG	1:F:347:LEU:HD11	1.83	0.59
1:H:223:ARG:CG	1:H:223:ARG:HH11	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:187:HIS:HD2	1:I:188:HIS:O	1.85	0.59
1:K:333:GLU:OE2	1:K:335:ARG:HD2	2.01	0.59
2:F:601:P3S:HEC2	2:F:601:P3S:HGC2	1.85	0.59
1:E:170:ARG:CZ	1:F:86:LYS:HD3	2.33	0.59
1:H:317:SER:N	1:H:318:PRO:CD	2.66	0.59
1:F:117:LYS:HG3	5:F:818:HOH:O	2.02	0.59
1:I:53:ASP:OD2	1:I:55:SER:HB3	2.02	0.59
1:K:252:LYS:O	1:K:253:ASN:HB2	2.03	0.59
1:A:142:GLU:CD	1:A:142:GLU:N	2.56	0.59
1:G:342:ASN:C	1:G:342:ASN:HD22	2.06	0.59
1:H:170:ARG:NH1	1:H:171:ASP:OD2	2.36	0.59
1:L:91:ARG:C	1:L:91:ARG:HD2	2.22	0.58
1:C:131:PRO:CB	1:C:211:ILE:HD11	2.33	0.58
1:L:402:ASN:ND2	1:L:405:MET:H	2.00	0.58
1:A:150:LEU:HD23	1:A:192:PRO:O	2.02	0.58
1:B:306:PRO:HB3	1:B:319:LEU:HA	1.84	0.58
1:C:316:ARG:NH1	2:C:501:P3S:O3A	2.36	0.58
1:I:68:MET:HE3	1:I:98:ASN:HA	1.86	0.58
1:L:349:VAL:HG22	1:L:405:MET:SD	2.44	0.58
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.86	0.58
1:B:127:PHE:CD2	1:B:351:LEU:HG	2.38	0.58
1:D:317:SER:N	1:D:318:PRO:CD	2.66	0.58
1:F:169:ARG:HD3	1:F:186:SER:OG	2.03	0.58
1:H:316:ARG:HD3	2:H:601:P3S:OE	2.04	0.58
1:B:154:GLY:HA2	1:B:162:THR:HG22	1.86	0.58
1:E:63:ILE:HG22	1:E:64:GLU:OE2	2.03	0.58
1:I:261:GLU:HB2	1:I:266:GLN:HE21	1.69	0.58
1:L:169:ARG:HD3	1:L:195:HIS:HB3	1.84	0.58
1:A:112:LEU:HD12	1:A:205:VAL:HG22	1.85	0.58
1:E:96:ILE:N	1:E:96:ILE:HD12	2.18	0.58
1:H:127:PHE:CD2	1:H:351:LEU:HG	2.39	0.58
1:H:27:ASP:OD2	1:H:31:THR:HG23	2.04	0.58
1:H:281:HIS:NE2	1:H:404:VAL:HG11	2.19	0.58
1:A:368:ILE:HG21	1:A:372:ILE:HD12	1.86	0.58
1:A:316:ARG:HD2	2:A:501:P3S:OE	2.03	0.58
1:I:429:ARG:NH2	5:I:687:HOH:O	2.37	0.58
1:J:9:ILE:O	1:J:13:VAL:HG23	2.04	0.58
1:B:129:LEU:HG	1:B:347:LEU:HD11	1.86	0.57
1:D:23:LEU:HB3	1:D:70:LEU:CD2	2.35	0.57
1:F:152:ASP:HB3	1:F:164:LEU:HB2	1.86	0.57
1:A:290:ASN:HB3	1:A:295:SER:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:GLU:HG3	1:C:221:ILE:HD11	1.86	0.57
1:E:317:SER:N	1:E:318:PRO:CD	2.67	0.57
1:J:154:GLY:HA2	1:J:162:THR:HG22	1.85	0.57
1:J:279:VAL:HG11	1:J:365:PRO:HG2	1.86	0.57
1:A:52:PHE:CE1	1:A:70:LEU:CD1	2.88	0.57
1:B:25:PHE:CD2	1:B:70:LEU:HD11	2.39	0.57
1:J:134:GLU:OE2	2:J:501:P3S:N	2.38	0.57
1:J:34:ASN:ND2	1:K:159:LEU:HD22	2.19	0.57
1:L:402:ASN:O	1:L:406:VAL:HG23	2.04	0.57
1:I:261:GLU:HA	1:I:266:GLN:HG2	1.87	0.57
1:J:161:PRO:O	1:J:164:LEU:CD1	2.53	0.57
1:K:131:PRO:CB	1:K:211:ILE:HD11	2.34	0.57
1:K:122:LEU:HD23	1:K:122:LEU:O	2.05	0.57
1:B:285:PHE:HB2	1:B:349:VAL:HG11	1.85	0.57
1:B:91:ARG:C	1:B:91:ARG:HD2	2.25	0.57
1:B:115:ILE:HD12	1:B:348:SER:HB3	1.86	0.57
1:C:338:ASP:HB2	1:C:339:PRO:HD2	1.86	0.57
1:C:418:ILE:O	1:C:422:GLU:HG3	2.05	0.57
1:D:170:ARG:NH1	1:D:171:ASP:OD2	2.38	0.57
1:G:368:ILE:HD11	1:G:385:ILE:HD11	1.85	0.57
1:A:139:LYS:HD2	1:A:149:GLU:HG2	1.86	0.57
1:D:159:LEU:HD22	1:E:32:ILE:CG2	2.35	0.57
1:F:253:ASN:ND2	5:F:766:HOH:O	2.38	0.57
1:F:79:ILE:O	1:F:81:PRO:HD3	2.05	0.57
1:G:86:LYS:HG2	1:H:170:ARG:CZ	2.35	0.57
1:I:99:PRO:HG2	1:J:314:GLN:NE2	2.19	0.57
1:K:187:HIS:HD2	1:K:188:HIS:O	1.87	0.57
1:B:386:VAL:HG12	5:B:618:HOH:O	2.05	0.56
1:D:117:LYS:NZ	5:D:689:HOH:O	2.38	0.56
1:H:7:GLU:HG3	5:H:860:HOH:O	2.05	0.56
1:C:122:LEU:HD11	1:C:359:LYS:HB3	1.87	0.56
1:E:285:PHE:HB2	1:E:349:VAL:CG1	2.34	0.56
1:H:329:SER:O	1:H:331:ARG:HD3	2.05	0.56
1:L:415:GLU:HB2	5:L:669:HOH:O	2.04	0.56
1:C:16:GLU:HG2	1:C:79:ILE:CD1	2.35	0.56
1:H:173:VAL:O	1:H:177:GLU:HG3	2.05	0.56
1:J:5:THR:HG22	1:J:8:ASP:OD1	2.05	0.56
1:L:252:LYS:O	1:L:253:ASN:HB2	2.05	0.56
1:D:160:ALA:HB2	1:D:166:GLU:OE2	2.06	0.56
1:F:349:VAL:HG22	1:F:405:MET:SD	2.45	0.56
1:G:281:HIS:HD2	1:G:402:ASN:HD21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:24:GLN:NE2	1:K:91:ARG:HH11	2.03	0.56
1:E:170:ARG:HG2	5:E:753:HOH:O	2.04	0.56
1:L:360:ASN:HB2	1:L:362:LEU:HD13	1.88	0.56
1:C:317:SER:N	1:C:318:PRO:CD	2.68	0.56
1:F:202:ALA:HB1	1:F:206:ARG:NE	2.21	0.56
1:D:419:GLU:O	1:D:423:ILE:HD13	2.06	0.56
1:F:211:ILE:HG22	1:F:215:LYS:HE2	1.87	0.56
1:K:403:GLU:OE1	1:K:403:GLU:HA	2.04	0.56
1:L:125:SER:HB3	1:L:126:ASP:OD1	2.05	0.56
1:D:264:ASP:OD2	1:D:265:LEU:N	2.39	0.56
1:D:269:GLU:HG2	5:D:703:HOH:O	2.06	0.56
1:J:52:PHE:CD1	1:J:70:LEU:HD13	2.41	0.56
1:B:117:LYS:HE2	5:B:681:HOH:O	2.05	0.56
1:H:368:ILE:CD1	1:H:385:ILE:HD11	2.36	0.56
1:I:37:ILE:HD12	1:I:41:GLN:HB2	1.88	0.56
1:L:317:SER:H	1:L:318:PRO:CD	2.18	0.56
1:D:105:GLU:CD	1:D:105:GLU:H	2.08	0.56
1:G:2:ALA:HA	5:G:796:HOH:O	2.06	0.56
2:G:601:P3S:HGC1	2:G:601:P3S:CE	2.31	0.56
1:H:426:ASP:HB2	5:H:794:HOH:O	2.04	0.56
1:K:211:ILE:CG1	5:K:635:HOH:O	2.27	0.56
1:A:5:THR:O	1:A:6:ARG:C	2.45	0.56
1:C:48:ASN:HB3	1:C:71:TYR:CD1	2.41	0.56
1:J:126:ASP:HB3	5:J:718:HOH:O	2.06	0.56
1:E:20:TYR:C	1:E:21:ILE:HD12	2.27	0.55
1:F:265:LEU:O	1:F:326:ARG:NH1	2.39	0.55
1:G:306:PRO:HB3	1:G:319:LEU:HA	1.88	0.55
1:G:338:ASP:HB2	1:G:339:PRO:HD2	1.88	0.55
1:A:427:MET:HE2	5:G:823:HOH:O	2.05	0.55
1:B:122:LEU:HD11	1:B:359:LYS:HG3	1.88	0.55
1:E:306:PRO:HB3	1:E:319:LEU:HA	1.87	0.55
1:I:167:ASN:CA	5:I:617:HOH:O	2.53	0.55
1:J:45:ALA:HA	5:J:663:HOH:O	2.04	0.55
1:B:317:SER:N	1:B:318:PRO:CD	2.69	0.55
1:L:9:ILE:HG13	1:L:74:LEU:HD12	1.87	0.55
1:A:115:ILE:HG22	1:A:351:LEU:HD23	1.87	0.55
1:B:319:LEU:HD13	1:B:320:ILE:HG13	1.88	0.55
1:D:161:PRO:O	1:D:164:LEU:HD13	2.06	0.55
1:I:112:LEU:HD12	1:I:205:VAL:HG22	1.88	0.55
1:G:159:LEU:HD13	1:L:32:ILE:HG23	1.88	0.55
1:G:3:LYS:HE2	1:G:4:TYR:CE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:265:LEU:O	1:I:326:ARG:NH1	2.40	0.55
1:E:134:GLU:OE1	2:E:501:P3S:N	2.40	0.55
1:E:311:TRP:CH2	1:E:367:PRO:HG3	2.41	0.55
1:G:105:GLU:O	1:G:105:GLU:HG2	2.05	0.55
1:I:142:GLU:H	1:I:142:GLU:CD	2.10	0.55
1:B:113:LYS:HG2	5:B:750:HOH:O	2.05	0.55
1:F:342:ASN:HD22	1:F:342:ASN:C	2.10	0.55
1:L:316:ARG:HD3	2:L:501:P3S:OE	2.07	0.55
1:C:112:LEU:HD12	1:C:205:VAL:HG22	1.89	0.55
1:D:27:ASP:OD2	1:D:27:ASP:C	2.44	0.55
1:J:429:ARG:CD	5:J:750:HOH:O	2.51	0.55
1:A:32:ILE:HD13	1:A:33:LYS:N	2.22	0.54
1:E:272:LYS:NZ	1:E:311:TRP:CH2	2.76	0.54
1:G:7:GLU:OE1	1:G:7:GLU:CA	2.54	0.54
1:D:2:ALA:O	1:D:3:LYS:C	2.45	0.54
1:E:3:LYS:HB3	1:E:75:ASN:HD21	1.71	0.54
1:G:3:LYS:CE	1:G:4:TYR:CD2	2.90	0.54
1:D:441:MET:O	1:J:228:HIS:HE1	1.89	0.54
1:L:443:GLN:NE2	5:L:734:HOH:O	2.39	0.54
1:A:232:MET:HE1	1:G:441:MET:HB2	1.88	0.54
1:C:231:PHE:HB3	1:C:339:PRO:HB2	1.90	0.54
1:D:311:TRP:CH2	1:D:367:PRO:HG3	2.42	0.54
1:E:319:LEU:HD13	1:E:320:ILE:HG13	1.88	0.54
1:G:154:GLY:HA2	1:G:162:THR:HG22	1.88	0.54
1:G:58:GLU:HB2	5:G:705:HOH:O	2.07	0.54
1:H:231:PHE:HB3	1:H:339:PRO:HB2	1.88	0.54
1:A:32:ILE:HG23	1:F:159:LEU:HD13	1.88	0.54
1:C:129:LEU:HG	1:C:347:LEU:HD11	1.88	0.54
1:C:2:ALA:HB3	5:C:783:HOH:O	2.07	0.54
1:E:169:ARG:HE	1:E:195:HIS:HD2	1.54	0.54
1:F:16:GLU:HG2	1:F:79:ILE:HD13	1.90	0.54
1:G:321:ARG:NH2	1:L:67:ASP:OD2	2.41	0.54
1:H:24:GLN:HE21	1:H:91:ARG:HD3	1.70	0.54
1:K:175:GLU:HG3	1:K:221:ILE:HD11	1.89	0.54
1:G:281:HIS:NE2	1:G:404:VAL:HG11	2.22	0.54
1:G:9:ILE:HD13	1:G:74:LEU:HG	1.90	0.54
1:J:24:GLN:NE2	1:J:91:ARG:HD3	2.20	0.54
1:L:370:ARG:HD2	1:L:375:MET:SD	2.46	0.54
1:C:333:GLU:CD	5:C:602:HOH:O	2.46	0.54
1:F:261:GLU:CD	1:F:261:GLU:N	2.60	0.54
1:A:435:TRP:CD1	1:G:431:GLN:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ARG:N	5:G:850:HOH:O	2.41	0.54
1:J:407:LYS:HD3	5:J:678:HOH:O	2.07	0.54
1:C:306:PRO:HB3	1:C:319:LEU:HA	1.90	0.54
1:E:236:LEU:HD12	5:E:708:HOH:O	2.07	0.54
1:E:24:GLN:NE2	1:E:91:ARG:HD3	2.23	0.54
1:L:85:GLU:O	1:L:85:GLU:HG2	2.07	0.54
1:C:256:ASN:OD1	1:C:258:PHE:HB2	2.08	0.54
1:C:62:ARG:HG2	1:C:62:ARG:HH11	1.73	0.54
1:F:140:LEU:HD21	1:F:228:HIS:HB2	1.89	0.54
1:L:76:THR:HG21	1:L:93:ILE:HB	1.88	0.54
1:C:9:ILE:O	1:C:13:VAL:HG13	2.09	0.54
1:D:393:ALA:HB2	1:D:425:TRP:CE2	2.43	0.54
1:E:127:PHE:CD2	1:E:351:LEU:HG	2.43	0.54
1:E:386:VAL:HG22	5:E:604:HOH:O	2.07	0.54
1:G:86:LYS:HD3	5:H:716:HOH:O	2.07	0.54
1:J:152:ASP:HB3	1:J:164:LEU:HB2	1.90	0.54
1:A:247:ASN:OD1	1:A:331:ARG:HD2	2.07	0.53
1:E:187:HIS:HD2	1:E:188:HIS:O	1.90	0.53
1:L:3:LYS:HB3	1:L:75:ASN:OD1	2.08	0.53
1:L:74:LEU:N	1:L:74:LEU:HD22	2.22	0.53
1:D:282:ALA:HA	1:D:285:PHE:CZ	2.44	0.53
1:E:164:LEU:HA	5:E:764:HOH:O	2.08	0.53
1:F:315:ASN:OD1	1:F:318:PRO:HD3	2.07	0.53
1:I:167:ASN:CB	5:I:617:HOH:O	2.55	0.53
1:I:65:GLU:O	1:I:65:GLU:CG	2.57	0.53
1:K:170:ARG:CB	5:K:636:HOH:O	2.55	0.53
1:L:208:CYS:SG	1:L:347:LEU:HD12	2.48	0.53
1:L:78:VAL:HG12	1:L:91:ARG:HG3	1.90	0.53
1:F:131:PRO:O	5:F:731:HOH:O	2.19	0.53
1:H:191:ALA:H	1:H:194:GLN:HE21	1.55	0.53
1:H:369:ASP:O	1:H:370:ARG:HG3	2.07	0.53
1:B:68:MET:HE3	1:B:98:ASN:HA	1.90	0.53
1:F:148:LEU:HD21	1:L:437:ARG:CD	2.38	0.53
1:A:16:GLU:HG2	1:A:79:ILE:CD1	2.38	0.53
1:B:5:THR:HG23	1:B:8:ASP:OD2	2.09	0.53
1:C:403:GLU:HG3	5:C:674:HOH:O	2.08	0.53
1:F:16:GLU:HG3	1:F:16:GLU:O	2.09	0.53
1:I:311:TRP:CZ2	1:I:367:PRO:HD3	2.44	0.53
1:I:219:LYS:HB3	1:J:161:PRO:HG2	1.90	0.53
1:A:232:MET:HE2	1:G:441:MET:HA	1.89	0.53
1:B:147:THR:HG22	1:B:149:GLU:N	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:VAL:HG12	1:G:91:ARG:HG3	1.91	0.53
1:A:372:ILE:HA	1:A:375:MET:HE3	1.90	0.53
1:E:268:SER:O	1:E:272:LYS:HG2	2.09	0.53
1:G:378:GLU:OE1	1:G:378:GLU:HA	2.09	0.53
1:I:282:ALA:HA	1:I:285:PHE:CZ	2.44	0.53
1:J:306:PRO:HB3	1:J:319:LEU:HA	1.91	0.53
1:A:6:ARG:NH2	1:A:47:ASP:OD1	2.41	0.53
1:D:159:LEU:HD22	1:E:32:ILE:HG21	1.90	0.53
1:F:202:ALA:HB1	1:F:206:ARG:CZ	2.39	0.53
1:F:249:SER:HA	1:F:258:PHE:CE1	2.44	0.53
1:H:24:GLN:NE2	1:H:91:ARG:HH11	2.06	0.53
1:H:256:ASN:OD1	1:H:258:PHE:HB2	2.09	0.53
1:L:129:LEU:HG	1:L:347:LEU:HD21	1.89	0.53
1:B:427:MET:O	1:B:431:GLN:HG2	2.09	0.53
1:C:252:LYS:O	1:C:253:ASN:HB2	2.09	0.53
1:E:76:THR:O	1:E:78:VAL:HG23	2.09	0.53
1:F:5:THR:HG22	1:F:8:ASP:CG	2.28	0.53
1:G:22:ARG:HG3	1:G:89:VAL:CG1	2.38	0.53
1:D:281:HIS:HD2	1:D:402:ASN:HD21	1.58	0.52
1:E:22:ARG:HD2	1:E:34:ASN:ND2	2.25	0.52
1:E:372:ILE:O	1:E:375:MET:HB3	2.09	0.52
1:B:76:THR:O	1:B:78:VAL:HG23	2.09	0.52
1:D:131:PRO:CB	1:D:211:ILE:HD11	2.39	0.52
1:E:252:LYS:O	1:E:253:ASN:HB2	2.10	0.52
1:G:235:PRO:HG2	5:G:726:HOH:O	2.09	0.52
1:I:231:PHE:HB3	1:I:339:PRO:HB2	1.91	0.52
1:G:2:ALA:CA	5:G:796:HOH:O	2.58	0.52
1:I:30:GLY:HA3	5:I:691:HOH:O	2.09	0.52
1:G:183:ILE:HB	1:L:38:PRO:HG2	1.90	0.52
1:D:91:ARG:HD2	1:D:91:ARG:C	2.30	0.52
1:G:312:SER:HB2	1:G:368:ILE:O	2.09	0.52
1:K:154:GLY:HA2	1:K:162:THR:HG22	1.91	0.52
1:A:298:ARG:NH2	1:A:336:SER:O	2.42	0.52
1:B:317:SER:H	1:B:318:PRO:CD	2.23	0.52
1:C:260:ASP:OD1	1:C:263:ALA:HB2	2.10	0.52
1:E:317:SER:N	1:E:318:PRO:HD2	2.24	0.52
1:F:308:TYR:HB2	1:F:372:ILE:HD13	1.90	0.52
1:F:52:PHE:CE1	1:F:70:LEU:HD13	2.44	0.52
1:H:129:LEU:HG	1:H:347:LEU:HD11	1.90	0.52
1:B:104:PHE:HA	5:B:668:HOH:O	2.08	0.52
1:D:383:ASN:HB2	1:D:385:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:SER:OG	1:F:379:GLU:HB2	2.09	0.52
1:H:311:TRP:CZ2	1:H:367:PRO:HD3	2.44	0.52
1:J:298:ARG:NH2	1:J:336:SER:O	2.42	0.52
1:D:112:LEU:HD12	1:D:205:VAL:HG22	1.91	0.52
1:C:48:ASN:HB3	1:C:71:TYR:CE1	2.45	0.52
1:H:9:ILE:HG12	1:H:92:PHE:HZ	1.74	0.52
1:J:187:HIS:HD2	1:J:188:HIS:O	1.92	0.52
1:L:53:ASP:OD2	1:L:55:SER:HB3	2.10	0.52
1:A:76:THR:O	1:A:91:ARG:NH1	2.43	0.52
1:B:13:VAL:HG13	1:B:18:VAL:HB	1.92	0.52
1:J:142:GLU:OE1	1:J:143:LYS:HD2	2.10	0.52
1:J:413:LEU:HD23	5:J:735:HOH:O	2.10	0.52
1:E:321:ARG:NH2	1:F:67:ASP:OD2	2.43	0.51
1:E:52:PHE:CE1	1:E:70:LEU:HD13	2.45	0.51
1:J:34:ASN:CG	1:K:159:LEU:HD21	2.31	0.51
1:L:280:LYS:HE2	1:L:281:HIS:CE1	2.45	0.51
1:A:304:GLU:OE1	1:A:316:ARG:HG2	2.10	0.51
1:B:252:LYS:O	1:B:253:ASN:HB2	2.08	0.51
1:B:370:ARG:HA	1:C:64:GLU:HG2	1.92	0.51
1:K:122:LEU:HD22	1:K:124:PHE:CE1	2.44	0.51
1:G:370:ARG:HA	1:L:64:GLU:HG2	1.92	0.51
1:E:170:ARG:NH1	1:E:171:ASP:OD2	2.44	0.51
1:E:311:TRP:CB	1:E:320:ILE:HB	2.40	0.51
1:G:169:ARG:HG3	1:G:197:ILE:CD1	2.41	0.51
1:J:57:ILE:N	1:J:57:ILE:HD12	2.26	0.51
1:K:64:GLU:HG2	1:L:370:ARG:HA	1.91	0.51
1:L:100:ASP:OD1	1:L:102:THR:HG23	2.10	0.51
1:L:202:ALA:HB1	1:L:206:ARG:HG2	1.92	0.51
1:L:369:ASP:O	1:L:370:ARG:HB3	2.11	0.51
1:C:81:PRO:HB2	1:C:175:GLU:OE1	2.10	0.51
1:D:152:ASP:HB3	1:D:164:LEU:HB2	1.92	0.51
1:H:63:ILE:HD11	1:I:304:GLU:HG2	1.93	0.51
1:B:349:VAL:HG22	1:B:405:MET:SD	2.51	0.51
1:C:400:LYS:HE2	1:C:418:ILE:HD13	1.92	0.51
1:D:319:LEU:HD13	1:D:320:ILE:HG13	1.92	0.51
1:I:362:LEU:HD12	1:I:362:LEU:N	2.19	0.51
1:J:437:ARG:O	1:J:441:MET:HB3	2.10	0.51
1:B:191:ALA:H	1:B:194:GLN:HE21	1.58	0.51
1:A:232:MET:CE	1:G:441:MET:HA	2.41	0.51
1:I:347:LEU:HD22	1:I:347:LEU:N	2.24	0.51
1:J:223:ARG:HG2	5:J:638:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:216:LEU:HD13	1:L:159:LEU:HD23	1.92	0.51
1:L:317:SER:N	1:L:318:PRO:HD2	2.26	0.51
1:C:285:PHE:HB2	1:C:349:VAL:CG1	2.40	0.51
1:E:157:PHE:CE2	1:F:35:VAL:HB	2.46	0.51
1:H:220:THR:HG22	1:H:224:LYS:NZ	2.26	0.51
1:H:34:ASN:ND2	1:I:159:LEU:HD22	2.25	0.51
1:J:24:GLN:HE22	1:J:91:ARG:HH11	1.56	0.51
1:K:396:LEU:HD11	1:K:421:LYS:HB2	1.92	0.51
1:L:5:THR:HG22	1:L:8:ASP:OD2	2.11	0.51
1:A:325:SER:HB3	5:B:766:HOH:O	2.09	0.51
1:D:51:MET:HG2	1:D:69:TYR:CE2	2.46	0.51
1:F:368:ILE:HG12	1:F:385:ILE:HD11	1.93	0.51
1:G:319:LEU:HD13	1:G:320:ILE:HG13	1.92	0.51
1:I:285:PHE:HB2	1:I:349:VAL:HG11	1.92	0.51
1:K:317:SER:N	1:K:318:PRO:CD	2.73	0.51
1:B:317:SER:N	1:B:318:PRO:HD2	2.26	0.51
1:B:431:GLN:NE2	5:B:685:HOH:O	2.43	0.51
1:E:115:ILE:HG22	1:E:351:LEU:HD13	1.93	0.51
1:I:338:ASP:HB2	1:I:339:PRO:HD2	1.92	0.51
1:J:316:ARG:HD2	2:J:501:P3S:OE	2.11	0.51
1:K:172:ILE:HD13	1:K:221:ILE:HB	1.91	0.51
1:K:426:ASP:HB2	5:K:652:HOH:O	2.11	0.51
1:A:24:GLN:HB3	1:A:32:ILE:HD11	1.93	0.51
1:A:377:LYS:HD3	1:A:380:ARG:HH22	1.76	0.51
1:D:86:LYS:NZ	5:D:674:HOH:O	2.43	0.51
1:H:402:ASN:OD1	1:H:404:VAL:HG12	2.11	0.51
1:K:52:PHE:CE1	1:K:70:LEU:HD13	2.45	0.51
1:A:152:ASP:HB3	1:A:164:LEU:HB2	1.94	0.50
1:D:48:ASN:HB3	1:D:71:TYR:CE1	2.46	0.50
1:F:22:ARG:HG3	1:F:89:VAL:HG11	1.92	0.50
1:G:419:GLU:HA	5:G:793:HOH:O	2.11	0.50
1:A:427:MET:CE	5:G:823:HOH:O	2.58	0.50
1:B:171:ASP:OD2	1:B:225:HIS:NE2	2.44	0.50
1:C:186:SER:HB2	1:C:197:ILE:HG12	1.92	0.50
1:D:256:ASN:ND2	1:D:258:PHE:HB2	2.26	0.50
1:E:272:LYS:HE3	1:E:272:LYS:HA	1.92	0.50
1:I:306:PRO:HB3	1:I:319:LEU:HA	1.93	0.50
1:L:74:LEU:H	1:L:74:LEU:CD2	2.24	0.50
1:L:91:ARG:HD2	1:L:92:PHE:N	2.26	0.50
1:B:5:THR:CG2	1:B:8:ASP:OD2	2.59	0.50
1:C:10:GLU:O	1:C:13:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLU:HG2	1:C:79:ILE:HD13	1.92	0.50
1:D:374:VAL:HG12	1:D:374:VAL:O	2.12	0.50
1:G:64:GLU:O	1:G:65:GLU:HG2	2.10	0.50
1:G:86:LYS:HG2	1:H:170:ARG:NH1	2.26	0.50
1:H:403:GLU:O	1:H:407:LYS:HG2	2.11	0.50
1:B:159:LEU:HD11	1:C:34:ASN:CG	2.32	0.50
1:F:187:HIS:HD2	1:F:188:HIS:O	1.95	0.50
1:G:175:GLU:HG3	1:G:221:ILE:HD11	1.92	0.50
1:K:296:TYR:CD1	1:K:296:TYR:N	2.77	0.50
1:C:314:GLN:NE2	1:D:99:PRO:HG3	2.27	0.50
1:E:24:GLN:HE22	1:E:91:ARG:HH11	1.59	0.50
1:E:437:ARG:O	1:E:441:MET:HB3	2.12	0.50
1:F:203:GLY:H	1:F:206:ARG:NH2	2.09	0.50
1:J:317:SER:H	1:J:318:PRO:HD2	1.77	0.50
1:C:310:ALA:HA	5:C:695:HOH:O	2.10	0.50
1:E:272:LYS:NZ	1:E:311:TRP:CZ2	2.80	0.50
2:F:601:P3S:HGC2	2:F:601:P3S:CE	2.37	0.50
1:H:281:HIS:HD2	1:H:402:ASN:HD21	1.58	0.50
1:D:403:GLU:HA	1:D:403:GLU:OE1	2.12	0.50
1:G:234:LYS:HD3	1:G:298:ARG:HA	1.93	0.50
1:I:129:LEU:HD13	1:I:131:PRO:HG3	1.92	0.50
1:K:284:SER:CB	1:K:402:ASN:HD22	2.24	0.50
1:A:261:GLU:H	1:A:261:GLU:CD	2.14	0.50
1:A:336:SER:O	1:A:337:VAL:C	2.46	0.50
1:B:256:ASN:OD1	1:B:258:PHE:HB2	2.11	0.50
1:C:128:ASN:ND2	5:C:775:HOH:O	2.44	0.50
1:F:360:ASN:O	1:F:361:LYS:C	2.48	0.50
1:H:8:ASP:C	1:H:11:LYS:HG2	2.33	0.50
1:H:154:GLY:HA2	1:H:162:THR:HG22	1.93	0.50
1:L:127:PHE:CE2	1:L:351:LEU:HG	2.47	0.50
1:L:315:ASN:OD1	1:L:318:PRO:HD3	2.12	0.50
1:G:215:LYS:O	1:G:219:LYS:HD3	2.12	0.50
1:G:282:ALA:HA	1:G:285:PHE:CZ	2.47	0.50
1:K:81:PRO:HG2	1:K:175:GLU:OE2	2.12	0.50
1:K:351:LEU:HD22	1:K:355:LEU:HG	1.94	0.50
1:K:402:ASN:O	1:K:406:VAL:HG23	2.12	0.50
1:F:441:MET:O	1:L:228:HIS:HE1	1.94	0.50
1:L:310:ALA:HA	5:L:741:HOH:O	2.11	0.50
1:A:161:PRO:O	1:A:164:LEU:HD13	2.12	0.49
1:F:169:ARG:HD2	1:F:186:SER:OG	2.11	0.49
1:F:109:ARG:HG3	1:F:344:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:PHE:CE2	1:H:351:LEU:HG	2.46	0.49
1:B:274:PHE:CE1	1:B:354:GLY:HA3	2.47	0.49
1:I:281:HIS:O	1:I:284:SER:HB2	2.11	0.49
1:I:290:ASN:HB3	1:I:295:SER:HB3	1.93	0.49
1:I:317:SER:N	1:I:318:PRO:CD	2.76	0.49
1:I:96:ILE:N	1:I:96:ILE:CD1	2.75	0.49
1:C:228:HIS:HE1	1:I:441:MET:O	1.95	0.49
1:H:223:ARG:CG	1:H:223:ARG:NH1	2.74	0.49
1:H:35:VAL:HB	1:I:157:PHE:CE2	2.47	0.49
1:I:133:PRO:HB3	1:I:244:MET:HG3	1.94	0.49
1:A:372:ILE:HA	1:A:375:MET:CE	2.42	0.49
1:B:285:PHE:HB2	1:B:349:VAL:HG13	1.94	0.49
1:D:129:LEU:HG	1:D:347:LEU:HD21	1.94	0.49
2:F:601:P3S:HEC2	2:F:601:P3S:HGC1	1.87	0.49
1:H:175:GLU:HG3	1:H:221:ILE:HD11	1.94	0.49
1:B:264:ASP:OD2	1:B:272:LYS:HE3	2.12	0.49
1:C:314:GLN:HE22	1:D:99:PRO:HG3	1.76	0.49
1:F:343:PRO:O	1:F:347:LEU:HD23	2.12	0.49
1:G:357:GLY:HA2	1:G:362:LEU:HD12	1.94	0.49
1:H:163:ASP:CG	1:H:169:ARG:HH22	2.15	0.49
1:H:122:LEU:HD12	1:H:355:LEU:HD22	1.93	0.49
1:G:62:ARG:HD2	5:G:866:HOH:O	2.12	0.49
1:B:131:PRO:CB	1:B:211:ILE:HD11	2.42	0.49
1:B:247:ASN:HB3	1:B:331:ARG:HD2	1.93	0.49
1:D:319:LEU:HD23	1:D:336:SER:HB2	1.94	0.49
1:H:23:LEU:HD22	1:H:94:CYS:SG	2.53	0.49
1:F:202:ALA:HA	1:F:206:ARG:HH21	1.78	0.49
1:G:131:PRO:HB3	1:G:211:ILE:HD11	1.95	0.49
1:H:63:ILE:HG23	1:H:64:GLU:N	2.28	0.49
1:L:439:GLN:HA	1:L:439:GLN:HE21	1.77	0.49
1:D:380:ARG:O	1:D:383:ASN:O	2.30	0.49
1:E:20:TYR:O	1:E:21:ILE:HD12	2.13	0.49
1:G:351:LEU:HD22	1:G:355:LEU:CG	2.42	0.49
1:L:187:HIS:HD2	1:L:188:HIS:O	1.95	0.49
5:F:849:HOH:O	1:L:297:LYS:HD2	2.12	0.49
1:G:141:ASP:C	1:G:141:ASP:OD2	2.51	0.49
1:H:252:LYS:O	1:H:253:ASN:HB2	2.13	0.49
1:I:317:SER:N	1:I:318:PRO:HD2	2.27	0.49
1:I:34:ASN:CG	1:J:159:LEU:HD11	2.34	0.49
1:J:189:GLU:OE2	2:J:501:P3S:HEC2	2.13	0.49
1:A:314:GLN:NE2	5:A:705:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:727:HOH:O	1:B:86:LYS:HE3	2.12	0.48
1:D:326:ARG:NE	5:D:712:HOH:O	2.37	0.48
1:E:62:ARG:NH1	1:E:64:GLU:OE1	2.43	0.48
1:F:260:ASP:HB2	1:F:268:SER:HA	1.95	0.48
1:G:256:ASN:OD1	1:G:258:PHE:HB2	2.13	0.48
1:H:206:ARG:NH2	5:H:738:HOH:O	2.46	0.48
1:J:317:SER:N	1:J:318:PRO:HD2	2.27	0.48
1:K:133:PRO:HG2	1:K:214:PHE:CE2	2.48	0.48
1:B:431:GLN:HG3	1:H:435:TRP:CD1	2.48	0.48
1:C:414:PHE:CZ	1:C:418:ILE:HD12	2.48	0.48
1:E:231:PHE:HB3	1:E:339:PRO:HB2	1.94	0.48
1:B:81:PRO:HG2	1:B:175:GLU:OE2	2.14	0.48
1:D:335:ARG:NH1	2:D:501:P3S:O1A	2.46	0.48
1:G:386:VAL:HG22	5:G:714:HOH:O	2.12	0.48
1:C:126:ASP:HB2	1:C:251:PHE:HB2	1.95	0.48
1:E:372:ILE:HG23	1:E:375:MET:HE2	1.94	0.48
1:F:136:PHE:CD1	1:F:235:PRO:HG2	2.49	0.48
1:L:349:VAL:HB	5:L:628:HOH:O	2.12	0.48
1:B:372:ILE:O	1:B:375:MET:HB2	2.14	0.48
1:B:437:ARG:O	1:B:441:MET:HB3	2.13	0.48
1:C:285:PHE:HB2	1:C:349:VAL:HG11	1.95	0.48
1:D:161:PRO:HG2	1:E:219:LYS:HB3	1.96	0.48
1:J:320:ILE:CG2	1:J:332:VAL:HG13	2.43	0.48
1:D:316:ARG:HH11	1:E:66:SER:HB2	1.78	0.48
1:F:282:ALA:HA	1:F:285:PHE:CE2	2.48	0.48
1:H:215:LYS:HG2	1:H:231:PHE:CE2	2.48	0.48
1:I:32:ILE:O	1:I:33:LYS:HD2	2.13	0.48
1:I:402:ASN:OD1	1:I:404:VAL:HG13	2.14	0.48
1:L:127:PHE:CD2	1:L:351:LEU:HG	2.49	0.48
1:D:414:PHE:CZ	1:D:418:ILE:HD12	2.49	0.48
1:E:63:ILE:O	1:E:66:SER:OG	2.32	0.48
1:I:9:ILE:HG13	1:I:74:LEU:CD1	2.42	0.48
5:D:724:HOH:O	1:J:219:LYS:HE2	2.12	0.48
1:J:34:ASN:ND2	1:K:159:LEU:CD2	2.76	0.48
1:K:103:PRO:HG2	5:K:667:HOH:O	2.14	0.48
1:B:134:GLU:OE1	2:B:501:P3S:N	2.47	0.48
1:B:24:GLN:HB3	1:B:34:ASN:HB3	1.95	0.48
1:C:281:HIS:HD2	1:C:402:ASN:HD21	1.62	0.48
1:H:105:GLU:N	5:H:780:HOH:O	2.45	0.48
1:H:245:HIS:CD2	1:H:335:ARG:HB3	2.48	0.48
1:J:281:HIS:HE1	1:J:356:ASP:OD1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:65:GLU:CD	5:K:653:HOH:O	2.52	0.48
1:B:147:THR:CG2	1:B:148:LEU:N	2.77	0.48
1:C:78:VAL:HG12	1:C:91:ARG:CG	2.43	0.48
1:I:74:LEU:HD22	1:I:74:LEU:N	2.29	0.48
1:K:6:ARG:HG3	1:K:46:LEU:HD13	1.96	0.48
1:L:5:THR:HG21	1:L:7:GLU:OE2	2.14	0.48
1:A:297:LYS:HD3	1:A:297:LYS:N	2.27	0.48
1:C:161:PRO:O	1:C:164:LEU:HD13	2.14	0.48
1:D:265:LEU:O	1:D:326:ARG:NH1	2.46	0.48
1:D:52:PHE:CE1	1:D:70:LEU:HD12	2.49	0.48
1:G:115:ILE:HG22	1:G:351:LEU:CD1	2.43	0.48
1:I:399:PHE:HZ	1:I:409:LEU:HD22	1.78	0.48
1:L:146:PRO:HG3	1:L:228:HIS:CD2	2.49	0.48
1:A:252:LYS:O	1:A:253:ASN:HB2	2.13	0.47
1:A:429:ARG:HD2	5:A:647:HOH:O	2.13	0.47
1:E:127:PHE:CE2	1:E:351:LEU:HG	2.49	0.47
1:J:9:ILE:HG13	1:J:74:LEU:HD22	1.95	0.47
1:L:74:LEU:N	1:L:74:LEU:CD2	2.77	0.47
1:A:150:LEU:HD11	1:A:236:LEU:HD11	1.95	0.47
1:C:431:GLN:HG2	1:I:435:TRP:CD1	2.49	0.47
1:E:216:LEU:CD2	1:E:216:LEU:C	2.83	0.47
1:I:247:ASN:HB3	1:I:331:ARG:HD2	1.95	0.47
1:K:316:ARG:HD3	2:K:501:P3S:OE	2.15	0.47
1:F:436:GLU:OE2	1:L:297:LYS:HE3	2.14	0.47
1:G:64:GLU:HG2	1:H:371:ASN:N	2.29	0.47
1:H:296:TYR:CD1	1:H:296:TYR:N	2.81	0.47
1:A:11:LYS:HE3	1:A:15:GLU:OE1	2.14	0.47
1:B:191:ALA:H	1:B:194:GLN:NE2	2.12	0.47
1:I:48:ASN:HB3	1:I:71:TYR:CE1	2.49	0.47
1:I:52:PHE:CE1	1:I:70:LEU:HD13	2.49	0.47
1:J:216:LEU:HD13	1:K:159:LEU:HD12	1.96	0.47
1:L:125:SER:CB	1:L:126:ASP:OD1	2.61	0.47
1:B:371:ASN:HD22	1:B:371:ASN:C	2.18	0.47
1:C:134:GLU:OE1	2:C:501:P3S:N	2.47	0.47
1:D:287:ALA:HB1	1:D:396:LEU:HD23	1.97	0.47
1:D:376:SER:O	1:D:379:GLU:HB2	2.14	0.47
1:E:311:TRP:HB3	1:E:320:ILE:HB	1.95	0.47
1:I:160:ALA:HB2	1:I:166:GLU:CD	2.35	0.47
1:J:256:ASN:OD1	1:J:258:PHE:HB2	2.14	0.47
1:L:441:MET:HG3	1:L:441:MET:O	2.14	0.47
1:A:150:LEU:H	1:A:150:LEU:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:ASP:HB2	1:D:339:PRO:HD2	1.95	0.47
1:D:362:LEU:HA	5:D:756:HOH:O	2.14	0.47
1:E:272:LYS:CA	1:E:272:LYS:HE3	2.43	0.47
1:F:127:PHE:CZ	1:F:248:LEU:HD22	2.49	0.47
1:F:319:LEU:CD1	1:F:336:SER:HB2	2.45	0.47
1:H:34:ASN:OD1	1:I:159:LEU:HD13	2.14	0.47
1:H:376:SER:OG	1:H:379:GLU:CB	2.63	0.47
1:J:407:LYS:NZ	5:J:787:HOH:O	2.42	0.47
1:K:429:ARG:NH2	5:K:664:HOH:O	2.47	0.47
1:L:360:ASN:O	1:L:361:LYS:C	2.51	0.47
1:A:4:TYR:H	1:A:75:ASN:ND2	2.13	0.47
1:D:247:ASN:HB3	1:D:331:ARG:HD2	1.96	0.47
1:D:266:GLN:CB	1:D:326:ARG:HD2	2.32	0.47
1:H:312:SER:HB2	1:H:368:ILE:O	2.15	0.47
1:A:283:THR:HG23	5:A:612:HOH:O	2.15	0.47
1:B:131:PRO:HB3	1:B:211:ILE:HD11	1.97	0.47
1:J:317:SER:H	1:J:318:PRO:CD	2.27	0.47
1:J:399:PHE:HZ	1:J:409:LEU:HD22	1.80	0.47
1:J:349:VAL:HG22	1:J:405:MET:SD	2.55	0.47
1:K:91:ARG:HD2	1:K:91:ARG:C	2.35	0.47
1:B:19:LYS:HB3	1:B:20:TYR:CE2	2.50	0.47
1:B:260:ASP:O	1:B:266:GLN:HA	2.14	0.47
1:E:24:GLN:NE2	1:E:91:ARG:HH11	2.13	0.47
1:F:91:ARG:HD2	1:F:92:PHE:N	2.30	0.47
1:F:200:LYS:HG3	1:F:201:TYR:N	2.30	0.47
1:F:359:LYS:HE2	5:F:737:HOH:O	2.11	0.47
1:G:317:SER:N	1:G:318:PRO:CD	2.78	0.47
1:G:73:ASP:OD1	1:G:73:ASP:C	2.54	0.47
1:G:68:MET:CE	1:G:99:PRO:HD3	2.44	0.47
1:H:318:PRO:HA	1:H:372:ILE:HD12	1.97	0.47
1:G:67:ASP:OD2	1:H:321:ARG:NH2	2.48	0.47
1:H:435:TRP:O	1:H:439:GLN:HG2	2.15	0.47
1:I:285:PHE:HB2	1:I:349:VAL:CG1	2.45	0.47
1:J:312:SER:HB3	1:J:315:ASN:HB3	1.96	0.47
1:J:65:GLU:OE1	1:J:65:GLU:HA	2.14	0.47
1:A:232:MET:HE1	1:G:441:MET:CB	2.45	0.47
1:F:161:PRO:O	1:F:164:LEU:HD13	2.14	0.47
1:F:243:GLY:C	1:F:339:PRO:HD3	2.35	0.47
1:G:161:PRO:O	1:G:164:LEU:HD13	2.15	0.47
1:H:184:GLU:HB3	1:H:198:ASP:HB2	1.97	0.47
1:I:27:ASP:OD2	1:I:27:ASP:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:317:SER:N	1:J:318:PRO:CD	2.78	0.47
1:J:91:ARG:HD2	1:J:91:ARG:C	2.35	0.47
1:A:270:THR:HG23	1:A:358:ILE:HD12	1.97	0.46
1:J:100:ASP:OD2	1:J:102:THR:HB	2.15	0.46
1:K:312:SER:HB3	1:K:315:ASN:HB3	1.97	0.46
1:K:328:ILE:O	1:K:328:ILE:HG12	2.15	0.46
1:A:372:ILE:HG23	1:A:375:MET:HE3	1.97	0.46
1:A:376:SER:OG	1:A:379:GLU:HB2	2.15	0.46
1:A:427:MET:CE	5:G:869:HOH:O	2.59	0.46
1:H:234:LYS:HD3	1:H:298:ARG:HA	1.97	0.46
1:F:435:TRP:CD1	1:L:431:GLN:HG2	2.49	0.46
1:B:296:TYR:CD1	1:B:296:TYR:N	2.83	0.46
1:B:338:ASP:HB2	1:B:339:PRO:HD2	1.97	0.46
1:F:371:ASN:O	1:F:374:VAL:HG22	2.16	0.46
1:G:204:ALA:HB1	1:G:347:LEU:CD2	2.46	0.46
1:H:172:ILE:HD13	1:H:218:VAL:HG22	1.96	0.46
1:I:275:ILE:O	1:I:279:VAL:HG23	2.15	0.46
1:K:65:GLU:OE2	5:K:653:HOH:O	2.20	0.46
1:L:434:PRO:HD2	5:L:719:HOH:O	2.16	0.46
1:A:434:PRO:HG2	1:G:434:PRO:HG2	1.96	0.46
1:H:169:ARG:HD2	1:H:186:SER:OG	2.16	0.46
1:K:375:MET:CE	1:K:379:GLU:HG2	2.46	0.46
1:E:435:TRP:O	1:E:439:GLN:HG2	2.15	0.46
1:F:117:LYS:HE3	5:F:818:HOH:O	2.15	0.46
1:F:403:GLU:OE2	1:F:407:LYS:CE	2.61	0.46
1:G:186:SER:HB2	1:G:197:ILE:HD13	1.96	0.46
1:I:313:ALA:HB1	5:I:634:HOH:O	2.15	0.46
1:I:115:ILE:HG22	1:I:351:LEU:HD13	1.96	0.46
1:J:306:PRO:HG2	1:J:336:SER:N	2.30	0.46
1:J:361:LYS:HE2	5:J:677:HOH:O	2.16	0.46
1:A:159:LEU:HD13	1:B:32:ILE:HG23	1.98	0.46
1:A:172:ILE:CD1	1:A:221:ILE:HB	2.45	0.46
1:B:414:PHE:O	1:B:418:ILE:HG12	2.15	0.46
1:B:423:ILE:HG13	5:B:737:HOH:O	2.15	0.46
1:C:355:LEU:O	1:C:359:LYS:HG2	2.15	0.46
1:H:117:LYS:NZ	5:H:740:HOH:O	2.43	0.46
1:H:131:PRO:HB3	1:H:211:ILE:HD11	1.96	0.46
1:I:136:PHE:CD1	1:I:235:PRO:HG2	2.50	0.46
1:I:175:GLU:HG3	1:I:221:ILE:HD11	1.97	0.46
1:L:296:TYR:CD1	1:L:296:TYR:N	2.83	0.46
1:L:306:PRO:HG2	1:L:336:SER:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:CYS:O	1:A:172:ILE:HG12	2.16	0.46
1:E:140:LEU:HD21	1:E:228:HIS:HB2	1.96	0.46
1:F:280:LYS:NZ	5:F:836:HOH:O	2.45	0.46
1:H:306:PRO:HG2	1:H:336:SER:CA	2.45	0.46
1:H:8:ASP:O	1:H:11:LYS:CG	2.55	0.46
1:J:129:LEU:O	1:J:131:PRO:HD3	2.15	0.46
1:K:285:PHE:CD1	1:K:285:PHE:C	2.89	0.46
1:B:165:GLY:O	1:B:169:ARG:HB2	2.16	0.46
1:D:187:HIS:HD2	1:D:188:HIS:O	1.99	0.46
1:D:260:ASP:O	1:D:266:GLN:HA	2.15	0.46
1:D:291:PRO:HG3	1:D:341:ALA:HA	1.98	0.46
1:G:134:GLU:OE2	2:G:601:P3S:N	2.49	0.46
1:G:204:ALA:HB1	1:G:347:LEU:HD23	1.98	0.46
1:G:91:ARG:HD2	1:G:91:ARG:C	2.36	0.46
1:J:264:ASP:OD1	1:J:264:ASP:O	2.34	0.46
1:L:125:SER:C	1:L:126:ASP:OD1	2.54	0.46
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.88	0.46
1:F:378:GLU:O	1:F:382:GLU:HG2	2.16	0.46
1:G:267:LEU:HG	1:G:326:ARG:HH12	1.81	0.46
1:H:191:ALA:H	1:H:194:GLN:NE2	2.13	0.46
1:K:16:GLU:HB2	1:K:18:VAL:HG23	1.97	0.46
1:A:133:PRO:HG2	1:A:214:PHE:CE2	2.51	0.46
1:E:225:HIS:HD2	5:E:663:HOH:O	1.99	0.46
1:E:58:GLU:HB2	5:E:609:HOH:O	2.16	0.46
1:G:48:ASN:OD1	1:G:71:TYR:HA	2.16	0.46
1:H:248:LEU:HD11	1:H:350:LEU:HD13	1.98	0.46
1:K:150:LEU:HD22	1:K:193:GLY:HA3	1.97	0.46
1:L:202:ALA:CB	1:L:206:ARG:HG2	2.45	0.46
1:A:435:TRP:CH2	1:A:439:GLN:HG3	2.52	0.45
1:C:372:ILE:H	1:C:372:ILE:HG13	1.48	0.45
1:C:377:LYS:CG	1:C:378:GLU:N	2.76	0.45
1:E:136:PHE:HA	1:E:193:GLY:O	2.16	0.45
1:A:64:GLU:OE2	1:F:371:ASN:HB2	2.16	0.45
1:H:198:ASP:HA	5:H:842:HOH:O	2.15	0.45
1:I:435:TRP:O	1:I:439:GLN:HG2	2.16	0.45
1:L:423:ILE:HG13	1:L:424:GLU:N	2.31	0.45
1:A:68:MET:HE3	1:A:98:ASN:HA	1.98	0.45
1:D:171:ASP:OD1	1:D:225:HIS:HE1	1.98	0.45
1:E:82:TRP:HZ3	1:E:179:MET:HE2	1.81	0.45
1:H:11:LYS:HG3	1:H:12:LEU:N	2.31	0.45
1:H:105:GLU:HG3	1:H:412:HIS:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:LYS:NZ	1:H:436:GLU:OE1	2.46	0.45
1:I:13:VAL:HG13	1:I:18:VAL:HB	1.98	0.45
1:I:99:PRO:HG2	1:J:314:GLN:HE22	1.81	0.45
1:L:6:ARG:HD2	1:L:10:GLU:OE2	2.16	0.45
1:L:409:LEU:HA	1:L:409:LEU:HD23	1.73	0.45
1:C:2:ALA:CB	5:C:783:HOH:O	2.65	0.45
1:E:273:HIS:CE1	1:E:361:LYS:HB3	2.51	0.45
1:G:132:GLU:O	1:G:244:MET:HA	2.16	0.45
1:G:368:ILE:CG2	1:G:372:ILE:HD12	2.45	0.45
1:H:31:THR:CG2	5:H:811:HOH:O	2.46	0.45
1:I:301:PRO:HD3	1:I:307:CYS:SG	2.57	0.45
1:J:260:ASP:C	1:J:260:ASP:OD1	2.55	0.45
1:A:249:SER:HA	1:A:258:PHE:CE1	2.51	0.45
1:A:317:SER:N	1:A:318:PRO:CD	2.79	0.45
1:A:270:THR:CG2	1:A:358:ILE:HD12	2.47	0.45
1:D:24:GLN:HE21	1:D:91:ARG:HH11	1.63	0.45
1:D:321:ARG:NH2	1:E:67:ASP:OD2	2.50	0.45
1:D:328:ILE:O	1:D:328:ILE:HG12	2.16	0.45
1:E:247:ASN:OD1	1:E:331:ARG:HD2	2.17	0.45
1:G:379:GLU:HA	1:G:382:GLU:HG2	1.98	0.45
1:H:24:GLN:HE22	1:H:91:ARG:HH11	1.64	0.45
1:J:315:ASN:OD1	1:J:318:PRO:HD3	2.16	0.45
1:A:13:VAL:HG13	1:A:18:VAL:HB	1.97	0.45
1:A:6:ARG:HG3	1:A:46:LEU:HD13	1.98	0.45
1:C:160:ALA:HA	1:C:163:ASP:O	2.17	0.45
1:A:88:LYS:HE2	5:A:666:HOH:O	2.16	0.45
1:D:360:ASN:O	1:D:361:LYS:C	2.55	0.45
1:A:86:LYS:HG2	1:F:170:ARG:CZ	2.47	0.45
1:K:183:ILE:N	1:K:183:ILE:HD12	2.31	0.45
1:L:281:HIS:CE1	1:L:356:ASP:OD2	2.67	0.45
1:A:159:LEU:HG	1:B:34:ASN:ND2	2.31	0.45
1:C:372:ILE:HA	1:C:375:MET:HG2	1.98	0.45
1:D:173:VAL:O	1:D:177:GLU:HG3	2.16	0.45
1:G:99:PRO:O	1:G:100:ASP:O	2.34	0.45
1:I:26:THR:HG22	1:I:27:ASP:O	2.16	0.45
1:A:317:SER:N	1:A:318:PRO:HD2	2.31	0.45
1:A:378:GLU:HG2	1:A:381:MET:HE2	1.99	0.45
1:C:39:VAL:HG22	1:C:39:VAL:O	2.17	0.45
1:C:438:GLU:HG3	5:C:703:HOH:O	2.16	0.45
1:D:435:TRP:HA	1:D:438:GLU:OE2	2.16	0.45
1:D:159:LEU:HD23	1:E:216:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LYS:NZ	5:E:627:HOH:O	2.50	0.45
1:L:329:SER:O	1:L:331:ARG:HD3	2.17	0.45
1:C:278:ILE:CG2	1:C:320:ILE:HD11	2.46	0.45
1:E:129:LEU:HG	1:E:347:LEU:HD21	1.99	0.45
1:I:398:GLU:HG2	5:I:755:HOH:O	2.16	0.45
1:I:134:GLU:OE1	2:I:501:P3S:N	2.50	0.45
1:K:389:PRO:HA	1:K:394:GLU:OE1	2.17	0.45
1:A:412:HIS:HA	5:A:634:HOH:O	2.16	0.45
1:E:291:PRO:HG3	1:E:341:ALA:HA	1.98	0.45
1:E:6:ARG:HD3	1:E:46:LEU:HD13	1.98	0.45
1:F:131:PRO:CG	1:F:211:ILE:HD11	2.47	0.45
1:G:62:ARG:CG	5:G:866:HOH:O	2.64	0.45
1:H:134:GLU:OE1	2:H:601:P3S:N	2.50	0.45
1:J:208:CYS:SG	1:J:343:PRO:HB2	2.56	0.45
1:D:273:HIS:O	1:D:276:ALA:HB3	2.17	0.44
1:D:282:ALA:HA	1:D:285:PHE:CE2	2.52	0.44
1:E:264:ASP:O	1:E:265:LEU:HB2	2.17	0.44
1:E:47:ASP:O	1:E:49:LYS:HD2	2.18	0.44
1:G:306:PRO:HG2	1:G:336:SER:N	2.32	0.44
1:L:122:LEU:HD11	1:L:359:LYS:HD3	1.99	0.44
1:C:78:VAL:HG12	1:C:91:ARG:HG2	1.99	0.44
1:D:371:ASN:C	1:D:371:ASN:HD22	2.19	0.44
1:E:375:MET:HG3	1:E:379:GLU:HB3	2.00	0.44
1:A:143:LYS:HE3	1:F:149:GLU:OE1	2.18	0.44
1:I:122:LEU:HD21	1:I:359:LYS:HG3	1.98	0.44
1:I:61:VAL:HB	1:I:65:GLU:OE1	2.17	0.44
1:J:321:ARG:O	1:J:323:PRO:HD3	2.17	0.44
1:K:282:ALA:HA	1:K:285:PHE:CZ	2.52	0.44
1:B:328:ILE:O	1:B:328:ILE:HG12	2.17	0.44
1:D:345:LEU:O	1:D:349:VAL:HG22	2.17	0.44
1:E:55:SER:HA	1:E:61:VAL:O	2.18	0.44
1:F:202:ALA:HB3	1:F:207:SER:HB2	1.99	0.44
1:F:283:THR:O	1:F:398:GLU:HG2	2.17	0.44
1:H:131:PRO:CB	1:H:211:ILE:HD11	2.47	0.44
1:H:290:ASN:HB3	1:H:295:SER:HB3	1.99	0.44
1:J:399:PHE:CZ	1:J:409:LEU:HD22	2.52	0.44
1:A:63:ILE:HG22	1:A:64:GLU:OE2	2.17	0.44
1:C:388:LEU:HB3	1:C:389:PRO:HD2	1.99	0.44
1:F:317:SER:N	1:F:318:PRO:CD	2.81	0.44
1:H:52:PHE:CD1	1:H:70:LEU:HD13	2.53	0.44
1:C:152:ASP:HB3	1:C:164:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:ASN:O	1:E:321:ARG:HB2	2.18	0.44
1:J:117:LYS:HD2	5:J:675:HOH:O	2.17	0.44
1:K:291:PRO:HG3	1:K:341:ALA:HA	1.99	0.44
1:B:306:PRO:CB	1:B:319:LEU:HA	2.48	0.44
1:B:9:ILE:HG21	1:B:92:PHE:HZ	1.82	0.44
1:C:170:ARG:HG3	5:D:648:HOH:O	2.17	0.44
1:C:317:SER:N	1:C:318:PRO:HD2	2.33	0.44
1:C:247:ASN:HB3	1:C:331:ARG:HD2	1.99	0.44
1:C:368:ILE:N	1:C:368:ILE:HD12	2.33	0.44
1:C:45:ALA:HA	1:C:50:VAL:HG23	1.98	0.44
1:F:321:ARG:NH1	3:F:602:ADP:O1B	2.51	0.44
1:H:74:LEU:HD22	1:H:74:LEU:N	2.33	0.44
1:K:176:LEU:O	1:K:181:PHE:HB2	2.17	0.44
1:L:223:ARG:HG3	1:L:223:ARG:HH11	1.83	0.44
1:A:441:MET:O	1:G:228:HIS:HE1	2.00	0.44
1:B:236:LEU:HD12	5:B:773:HOH:O	2.18	0.44
1:D:307:CYS:HA	1:D:388:LEU:HD12	2.00	0.44
1:E:24:GLN:HE21	1:E:91:ARG:HD3	1.83	0.44
1:F:140:LEU:HD23	1:F:146:PRO:HA	2.00	0.44
1:F:82:TRP:HE3	1:F:175:GLU:OE1	2.01	0.44
1:H:8:ASP:CA	1:H:11:LYS:HE2	2.48	0.44
1:I:221:ILE:O	1:I:225:HIS:HD2	1.99	0.44
1:J:5:THR:HG23	1:J:8:ASP:H	1.83	0.44
1:D:127:PHE:CD2	1:D:351:LEU:HG	2.53	0.44
1:F:270:THR:HG23	1:F:358:ILE:CD1	2.47	0.44
1:F:32:ILE:HD13	1:F:212:GLN:HB3	2.00	0.44
1:G:296:TYR:N	1:G:296:TYR:CD1	2.86	0.44
1:I:282:ALA:HA	1:I:285:PHE:CE2	2.53	0.44
1:J:68:MET:CE	1:J:99:PRO:HD3	2.46	0.44
1:K:3:LYS:HB3	1:K:75:ASN:OD1	2.17	0.44
1:L:181:PHE:CE2	1:L:210:ASP:HB3	2.53	0.44
1:A:150:LEU:HD12	1:A:150:LEU:N	2.33	0.44
1:A:153:LYS:HA	1:A:192:PRO:HB3	2.00	0.44
1:E:375:MET:HG2	1:E:380:ARG:HG3	1.99	0.44
1:F:171:ASP:HA	1:F:174:LEU:HD12	2.00	0.44
1:G:81:PRO:HG2	1:G:175:GLU:OE2	2.18	0.44
1:H:317:SER:H	1:H:318:PRO:CD	2.30	0.44
1:I:360:ASN:O	1:I:361:LYS:C	2.57	0.44
1:I:55:SER:HB3	1:I:66:SER:HB3	1.99	0.44
1:J:281:HIS:O	1:J:284:SER:HB2	2.17	0.44
1:J:34:ASN:CG	1:K:159:LEU:HD22	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:248:LEU:HD11	1:K:350:LEU:HD13	2.00	0.44
1:K:67:ASP:CG	1:L:314:GLN:HB2	2.39	0.44
1:L:378:GLU:HG3	1:L:379:GLU:H	1.81	0.44
1:A:273:HIS:HB2	1:A:358:ILE:HD13	1.99	0.43
1:A:33:LYS:O	1:A:34:ASN:HB3	2.18	0.43
1:D:143:LYS:O	1:D:145:GLU:HG2	2.17	0.43
1:D:161:PRO:O	1:D:164:LEU:CD1	2.66	0.43
1:D:351:LEU:O	1:D:355:LEU:HG	2.17	0.43
1:D:134:GLU:OE1	2:D:501:P3S:N	2.50	0.43
1:E:126:ASP:HB2	1:E:251:PHE:HB2	1.99	0.43
1:F:290:ASN:HB3	1:F:295:SER:HB3	2.00	0.43
1:F:76:THR:O	1:F:78:VAL:HG23	2.17	0.43
1:G:306:PRO:HG3	1:G:335:ARG:HB2	2.00	0.43
1:I:24:GLN:NE2	1:I:91:ARG:HD3	2.32	0.43
1:I:9:ILE:CG1	1:I:74:LEU:HD12	2.44	0.43
1:J:307:CYS:HB3	1:J:308:TYR:CD1	2.53	0.43
1:J:279:VAL:HG13	1:J:309:VAL:HG12	2.00	0.43
1:K:287:ALA:HB1	1:K:396:LEU:HD23	2.00	0.43
1:A:147:THR:HB	5:A:641:HOH:O	2.18	0.43
1:A:317:SER:H	1:A:318:PRO:CD	2.31	0.43
1:D:52:PHE:CD1	1:D:70:LEU:HD12	2.53	0.43
1:E:169:ARG:HE	1:E:195:HIS:CD2	2.36	0.43
1:F:275:ILE:HD11	1:F:332:VAL:HG22	2.00	0.43
1:F:122:LEU:HD12	1:F:355:LEU:HD22	1.99	0.43
1:F:426:ASP:CG	5:F:855:HOH:O	2.56	0.43
1:G:9:ILE:HG21	1:G:92:PHE:HZ	1.83	0.43
1:H:26:THR:HG22	1:H:27:ASP:O	2.18	0.43
1:H:34:ASN:CG	1:I:159:LEU:HD22	2.38	0.43
1:I:441:MET:O	1:I:441:MET:HG3	2.18	0.43
1:L:402:ASN:ND2	1:L:402:ASN:C	2.71	0.43
1:D:325:SER:HB3	1:E:51:MET:HE1	1.99	0.43
1:F:256:ASN:OD1	1:F:258:PHE:HB2	2.19	0.43
1:F:260:ASP:HB3	1:F:263:ALA:HB3	2.00	0.43
1:F:315:ASN:O	1:F:318:PRO:HD2	2.17	0.43
1:G:273:HIS:HB3	1:G:358:ILE:HA	2.00	0.43
1:G:68:MET:HE3	1:G:68:MET:HA	2.00	0.43
1:K:122:LEU:HD22	1:K:124:PHE:CD1	2.53	0.43
1:A:260:ASP:O	1:A:266:GLN:HA	2.18	0.43
1:D:402:ASN:O	1:D:406:VAL:HG23	2.18	0.43
1:E:360:ASN:O	1:E:361:LYS:C	2.57	0.43
1:F:310:ALA:HB1	1:F:368:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:110:ASN:OD1	5:H:723:HOH:O	2.21	0.43
1:H:96:ILE:HD12	1:H:96:ILE:N	2.33	0.43
1:A:370:ARG:NH1	1:A:379:GLU:OE2	2.50	0.43
1:C:96:ILE:N	1:C:96:ILE:HD12	2.33	0.43
1:D:370:ARG:HH11	1:D:370:ARG:HB3	1.81	0.43
1:E:387:ASP:N	1:E:387:ASP:OD1	2.51	0.43
1:G:219:LYS:HB3	1:H:161:PRO:HG2	2.00	0.43
1:K:26:THR:HG21	1:K:344:TYR:CE1	2.51	0.43
1:C:135:PHE:HB3	1:C:231:PHE:CE1	2.54	0.43
1:C:212:GLN:HA	1:C:212:GLN:OE1	2.18	0.43
1:D:157:PHE:CZ	1:E:35:VAL:HB	2.53	0.43
1:G:351:LEU:HD22	1:G:355:LEU:CD1	2.48	0.43
1:G:387:ASP:OD2	1:G:387:ASP:N	2.51	0.43
1:H:142:GLU:CA	1:H:142:GLU:OE1	2.67	0.43
1:L:351:LEU:HD22	1:L:355:LEU:CG	2.45	0.43
1:A:219:LYS:NZ	5:A:654:HOH:O	2.50	0.43
1:F:291:PRO:HG3	1:F:341:ALA:HA	2.00	0.43
1:I:279:VAL:HG13	1:I:309:VAL:HG12	2.01	0.43
1:K:421:LYS:HA	1:K:421:LYS:HD3	1.94	0.43
1:F:321:ARG:O	1:F:323:PRO:HD3	2.18	0.43
1:G:189:GLU:OE2	2:G:601:P3S:HEC2	2.19	0.43
1:H:317:SER:N	1:H:318:PRO:HD2	2.33	0.43
1:I:40:SER:HB3	5:I:736:HOH:O	2.18	0.43
1:K:129:LEU:HD22	1:K:347:LEU:HD11	2.01	0.43
1:K:281:HIS:CD2	1:K:402:ASN:HD21	2.27	0.43
1:L:402:ASN:ND2	1:L:404:VAL:N	2.67	0.43
1:B:10:GLU:O	1:B:14:LYS:HE2	2.19	0.43
1:C:360:ASN:O	1:C:361:LYS:C	2.57	0.43
1:D:191:ALA:H	1:D:194:GLN:HE21	1.65	0.43
1:E:289:THR:OG1	1:E:290:ASN:ND2	2.51	0.43
1:F:285:PHE:HB2	1:F:349:VAL:HG13	1.98	0.43
1:I:415:GLU:HB2	5:I:681:HOH:O	2.17	0.43
1:I:55:SER:CB	1:I:66:SER:HB3	2.48	0.43
1:J:175:GLU:HG3	1:J:221:ILE:HD11	2.00	0.43
1:K:315:ASN:OD1	1:K:317:SER:HB3	2.19	0.43
1:L:68:MET:HE3	1:L:98:ASN:CA	2.43	0.43
1:A:79:ILE:O	1:A:81:PRO:HD3	2.19	0.43
1:A:74:LEU:HA	1:A:92:PHE:HE2	1.84	0.43
1:C:380:ARG:HB2	1:C:385:ILE:CB	2.44	0.43
1:D:159:LEU:HD22	1:E:32:ILE:HG23	2.01	0.43
1:D:22:ARG:NH1	1:D:36:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:PHE:CZ	1:D:418:ILE:CD1	3.02	0.43
1:F:282:ALA:HA	1:F:285:PHE:CZ	2.54	0.43
1:I:129:LEU:HD12	1:I:207:SER:HB3	2.00	0.43
1:I:146:PRO:HB3	1:I:228:HIS:CG	2.54	0.43
1:H:63:ILE:CD1	1:I:304:GLU:HG2	2.47	0.43
1:L:439:GLN:HA	1:L:439:GLN:NE2	2.34	0.43
1:A:316:ARG:CD	2:A:501:P3S:OE	2.67	0.42
1:B:255:VAL:HG12	1:B:256:ASN:N	2.34	0.42
1:C:175:GLU:O	1:C:179:MET:HG3	2.18	0.42
1:C:24:GLN:HE21	1:C:34:ASN:ND2	2.11	0.42
1:C:321:ARG:NE	5:C:602:HOH:O	2.45	0.42
1:F:202:ALA:HB1	1:F:206:ARG:NH2	2.34	0.42
1:F:254:GLY:O	1:F:255:VAL:HG23	2.19	0.42
1:G:115:ILE:N	1:G:115:ILE:HD12	2.33	0.42
2:G:601:P3S:HGC1	2:G:601:P3S:HEC2	1.91	0.42
1:H:27:ASP:OD1	1:H:58:GLU:HB2	2.19	0.42
1:H:315:ASN:OD1	1:H:318:PRO:HD3	2.19	0.42
1:I:320:ILE:CG2	1:I:332:VAL:HG13	2.49	0.42
1:I:127:PHE:CE2	1:I:347:LEU:HD12	2.53	0.42
1:J:129:LEU:HD13	1:J:131:PRO:HG3	2.00	0.42
1:L:326:ARG:HD3	1:L:326:ARG:HA	1.96	0.42
1:L:316:ARG:HG2	1:L:335:ARG:CZ	2.49	0.42
1:B:52:PHE:CD1	1:B:52:PHE:N	2.86	0.42
1:E:316:ARG:HB2	1:F:66:SER:OG	2.19	0.42
1:E:279:VAL:HG11	1:E:365:PRO:HG2	2.00	0.42
1:F:260:ASP:HB2	1:F:268:SER:CA	2.49	0.42
1:I:82:TRP:HB2	1:I:224:LYS:NZ	2.33	0.42
1:J:81:PRO:HB2	5:J:720:HOH:O	2.19	0.42
1:K:46:LEU:HD23	1:K:46:LEU:HA	1.78	0.42
1:L:115:ILE:HG13	1:L:348:SER:HB2	2.00	0.42
1:L:316:ARG:HG2	1:L:335:ARG:NH2	2.34	0.42
1:L:371:ASN:O	1:L:374:VAL:HG22	2.19	0.42
1:B:152:ASP:HB3	1:B:164:LEU:HB2	2.01	0.42
1:A:33:LYS:HE2	1:F:158:ASP:OD2	2.19	0.42
1:F:421:LYS:HA	1:F:421:LYS:HD3	1.85	0.42
1:H:306:PRO:HG2	1:H:336:SER:HA	1.99	0.42
1:H:8:ASP:CB	1:H:11:LYS:HE2	2.49	0.42
1:I:347:LEU:HD13	1:I:347:LEU:HA	1.84	0.42
1:I:52:PHE:CD1	1:I:70:LEU:HD13	2.54	0.42
1:J:35:VAL:HG22	1:J:36:GLU:N	2.33	0.42
1:K:234:LYS:HD3	1:K:298:ARG:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:368:ILE:HD11	1:K:385:ILE:HD11	2.01	0.42
1:B:360:ASN:HB2	1:B:362:LEU:HD13	2.01	0.42
1:C:335:ARG:HH21	1:C:335:ARG:HD3	1.70	0.42
1:D:263:ALA:CB	1:D:267:LEU:O	2.68	0.42
1:E:260:ASP:C	1:E:260:ASP:OD2	2.57	0.42
1:E:317:SER:H	1:E:318:PRO:CD	2.30	0.42
1:A:32:ILE:HD12	1:F:159:LEU:CD2	2.49	0.42
1:F:319:LEU:HD12	1:F:336:SER:HB2	2.01	0.42
1:G:368:ILE:CG2	1:G:372:ILE:CD1	2.97	0.42
1:G:71:TYR:CE1	1:G:97:TYR:HB2	2.53	0.42
1:H:365:PRO:HB2	5:H:807:HOH:O	2.18	0.42
1:I:429:ARG:HD3	5:I:773:HOH:O	2.19	0.42
1:I:3:LYS:HB3	1:I:75:ASN:OD1	2.19	0.42
1:K:178:GLU:OE1	1:K:178:GLU:HA	2.20	0.42
1:A:368:ILE:CG2	1:A:372:ILE:HD12	2.49	0.42
1:B:146:PRO:HG3	1:B:228:HIS:CD2	2.54	0.42
1:B:360:ASN:O	1:B:361:LYS:C	2.58	0.42
1:C:157:PHE:CE2	1:D:35:VAL:HB	2.54	0.42
1:D:317:SER:N	1:D:318:PRO:HD2	2.34	0.42
1:H:164:LEU:HD12	1:H:164:LEU:HA	1.77	0.42
1:A:112:LEU:HD13	1:A:116:LEU:CD1	2.50	0.42
1:B:119:MET:SD	1:B:127:PHE:HB2	2.60	0.42
1:B:317:SER:H	1:B:318:PRO:HD2	1.82	0.42
1:B:5:THR:CG2	1:B:8:ASP:CG	2.87	0.42
1:E:316:ARG:HH21	1:F:66:SER:HB3	1.84	0.42
1:F:20:TYR:HB2	1:F:89:VAL:HG22	2.01	0.42
1:K:33:LYS:O	1:K:34:ASN:HB3	2.19	0.42
1:A:65:GLU:HB2	5:A:667:HOH:O	2.19	0.42
1:C:377:LYS:CG	1:C:378:GLU:H	2.28	0.42
1:E:284:SER:CB	1:E:402:ASN:HD22	2.33	0.42
1:E:320:ILE:CG2	1:E:332:VAL:HG13	2.50	0.42
1:G:115:ILE:HD12	1:G:115:ILE:H	1.85	0.42
1:G:68:MET:HE1	5:G:742:HOH:O	2.20	0.42
1:H:215:LYS:HG2	1:H:231:PHE:CZ	2.54	0.42
1:I:48:ASN:HB3	1:I:71:TYR:CD1	2.54	0.42
1:J:283:THR:HG23	5:J:659:HOH:O	2.20	0.42
1:K:13:VAL:HG13	1:K:18:VAL:HB	2.00	0.42
1:A:16:GLU:O	1:A:17:ASN:HB2	2.20	0.42
1:C:146:PRO:HG3	1:C:228:HIS:CD2	2.55	0.42
1:C:347:LEU:O	1:C:351:LEU:HB2	2.19	0.42
1:C:76:THR:HG21	1:C:93:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLU:N	1:D:142:GLU:CD	2.64	0.42
1:E:130:GLY:HA3	3:E:502:ADP:H1'	2.02	0.42
1:E:129:LEU:HD13	1:E:207:SER:OG	2.20	0.42
1:F:22:ARG:NH1	1:F:36:GLU:OE2	2.53	0.42
1:H:9:ILE:HD13	1:H:74:LEU:HD12	2.02	0.42
1:J:23:LEU:HA	1:J:23:LEU:HD23	1.85	0.42
1:K:136:PHE:CZ	5:K:766:HOH:O	2.69	0.42
1:K:371:ASN:HD21	1:K:373:TYR:HB2	1.85	0.42
1:A:317:SER:H	1:A:318:PRO:HD2	1.85	0.42
1:B:127:PHE:CE2	1:B:351:LEU:HG	2.55	0.42
1:C:371:ASN:O	1:C:374:VAL:HG22	2.20	0.42
1:D:175:GLU:HG3	1:D:221:ILE:HD11	2.02	0.42
1:D:232:MET:HA	1:D:233:PRO:HD3	1.91	0.42
1:E:171:ASP:OD1	1:E:225:HIS:CE1	2.73	0.42
1:E:368:ILE:HG21	1:E:375:MET:HE3	2.02	0.42
1:G:9:ILE:O	1:G:13:VAL:HG23	2.20	0.42
1:L:107:ASP:OD1	1:L:107:ASP:C	2.56	0.42
1:A:9:ILE:HD13	1:A:92:PHE:CZ	2.55	0.42
1:C:319:LEU:O	1:C:319:LEU:HD22	2.20	0.42
1:E:166:GLU:HB3	5:E:764:HOH:O	2.20	0.42
1:E:266:GLN:HB2	1:E:326:ARG:HD2	2.02	0.42
1:K:240:ASN:HD22	1:K:303:TYR:HD2	1.67	0.42
1:A:49:LYS:HD3	1:A:49:LYS:HA	1.80	0.41
1:B:175:GLU:O	1:B:179:MET:HG3	2.20	0.41
1:B:426:ASP:HB2	5:B:687:HOH:O	2.20	0.41
1:C:115:ILE:HG22	1:C:351:LEU:HD13	2.02	0.41
1:C:299:LEU:HD22	1:C:306:PRO:O	2.19	0.41
1:C:351:LEU:O	1:C:355:LEU:HG	2.20	0.41
1:D:272:LYS:HZ3	1:D:311:TRP:HH2	1.62	0.41
1:D:368:ILE:HG13	1:D:385:ILE:HD11	2.01	0.41
1:D:48:ASN:HB3	1:D:71:TYR:CD1	2.55	0.41
1:E:216:LEU:HD23	1:E:216:LEU:O	2.20	0.41
1:E:421:LYS:HD3	1:E:421:LYS:HA	1.88	0.41
1:I:279:VAL:HG11	1:I:365:PRO:HG2	2.02	0.41
1:K:134:GLU:OE1	2:K:501:P3S:N	2.53	0.41
1:L:105:GLU:CG	1:L:105:GLU:O	2.68	0.41
1:B:259:PHE:CE1	1:B:326:ARG:HG3	2.55	0.41
1:B:73:ASP:OD2	1:B:73:ASP:C	2.57	0.41
1:C:111:ASN:OD1	1:C:114:ARG:NH1	2.53	0.41
1:C:11:LYS:HB3	1:C:11:LYS:HE3	1.83	0.41
1:E:274:PHE:CE1	1:E:354:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:SER:HB3	1:E:315:ASN:HB3	2.02	0.41
1:F:281:HIS:CD2	1:F:402:ASN:HD21	2.30	0.41
1:I:112:LEU:HD13	1:I:116:LEU:HD12	2.01	0.41
1:I:260:ASP:O	1:I:266:GLN:HA	2.20	0.41
1:K:122:LEU:HD23	1:K:124:PHE:CE1	2.55	0.41
1:K:177:GLU:HG3	1:K:183:ILE:HD13	2.00	0.41
1:K:273:HIS:O	1:K:276:ALA:HB3	2.19	0.41
1:L:345:LEU:HD22	1:L:409:LEU:HD22	2.02	0.41
1:L:402:ASN:HD22	1:L:404:VAL:N	2.17	0.41
1:C:286:THR:HG21	1:C:389:PRO:HG2	2.02	0.41
1:C:4:TYR:HB3	1:C:9:ILE:HD13	2.02	0.41
1:D:22:ARG:O	1:D:91:ARG:HA	2.20	0.41
1:F:310:ALA:O	1:F:318:PRO:HB2	2.20	0.41
1:J:262:ASN:HA	5:J:706:HOH:O	2.19	0.41
1:K:172:ILE:CD1	1:K:218:VAL:HA	2.49	0.41
1:K:78:VAL:HG12	1:K:91:ARG:HG3	2.02	0.41
1:L:402:ASN:ND2	1:L:404:VAL:H	2.18	0.41
1:B:371:ASN:N	1:C:64:GLU:HG2	2.35	0.41
1:C:342:ASN:O	1:C:343:PRO:C	2.58	0.41
1:F:429:ARG:CD	5:F:799:HOH:O	2.62	0.41
1:G:22:ARG:HG3	1:G:89:VAL:HG11	2.02	0.41
1:G:264:ASP:C	1:G:266:GLN:N	2.73	0.41
1:G:6:ARG:CD	1:G:46:LEU:HD13	2.49	0.41
1:J:376:SER:O	1:J:377:LYS:C	2.59	0.41
1:J:437:ARG:O	1:J:441:MET:CB	2.68	0.41
1:J:435:TRP:O	1:J:439:GLN:HG2	2.20	0.41
1:J:91:ARG:HD2	1:J:92:PHE:N	2.35	0.41
1:K:211:ILE:CD1	5:K:635:HOH:O	2.61	0.41
1:K:317:SER:N	1:K:318:PRO:HD2	2.35	0.41
1:A:411:GLU:HA	1:A:411:GLU:OE1	2.20	0.41
1:B:109:ARG:HG3	1:B:344:TYR:CE2	2.56	0.41
1:G:309:VAL:CG2	1:G:386:VAL:HG23	2.50	0.41
1:H:353:ALA:HB2	1:H:405:MET:HE3	2.01	0.41
1:H:417:PHE:O	1:H:421:LYS:HG2	2.20	0.41
1:I:126:ASP:HB3	5:I:671:HOH:O	2.20	0.41
1:I:418:ILE:O	1:I:422:GLU:HB2	2.19	0.41
1:K:125:SER:C	1:K:126:ASP:OD2	2.57	0.41
1:K:23:LEU:HD22	1:K:94:CYS:SG	2.61	0.41
1:L:333:GLU:OE2	1:L:335:ARG:HD2	2.21	0.41
1:D:321:ARG:O	1:D:323:PRO:HD3	2.20	0.41
1:F:22:ARG:HG3	1:F:89:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:PHE:HB3	1:F:231:PHE:CE1	2.56	0.41
1:F:260:ASP:O	1:F:266:GLN:HA	2.21	0.41
1:G:273:HIS:ND1	1:G:362:LEU:O	2.52	0.41
1:H:187:HIS:HE1	5:H:840:HOH:O	2.02	0.41
1:H:52:PHE:CE1	1:H:70:LEU:CD1	3.04	0.41
1:I:5:THR:O	1:I:6:ARG:C	2.59	0.41
1:K:300:VAL:HG23	1:K:300:VAL:O	2.19	0.41
1:L:370:ARG:HD3	5:L:702:HOH:O	2.19	0.41
1:A:63:ILE:HG23	1:A:64:GLU:N	2.36	0.41
1:B:403:GLU:HG2	5:B:615:HOH:O	2.20	0.41
1:D:171:ASP:OD1	1:D:225:HIS:CE1	2.74	0.41
1:D:312:SER:HB3	1:D:315:ASN:HB3	2.03	0.41
1:F:119:MET:HG2	1:F:124:PHE:HB2	2.03	0.41
1:F:338:ASP:HB2	1:F:339:PRO:HD2	2.01	0.41
1:G:78:VAL:HG12	1:G:91:ARG:CG	2.51	0.41
1:I:167:ASN:HD22	1:I:168:CYS:H	1.67	0.41
1:I:221:ILE:HA	1:I:221:ILE:HD13	1.81	0.41
1:I:402:ASN:O	1:I:406:VAL:HG23	2.21	0.41
1:K:107:ASP:C	1:K:107:ASP:OD1	2.58	0.41
1:A:212:GLN:OE1	1:A:215:LYS:NZ	2.53	0.41
1:B:52:PHE:CE1	1:B:70:LEU:HD13	2.56	0.41
1:E:156:TYR:CZ	1:E:157:PHE:CE1	3.08	0.41
1:G:381:MET:O	1:G:383:ASN:O	2.39	0.41
1:G:429:ARG:HD3	5:G:862:HOH:O	2.20	0.41
1:G:62:ARG:HE	1:G:62:ARG:HB3	1.73	0.41
1:G:52:PHE:CE1	1:G:70:LEU:HD13	2.55	0.41
1:H:251:PHE:HA	1:H:255:VAL:O	2.21	0.41
1:B:403:GLU:HG3	1:B:404:VAL:N	2.35	0.41
1:B:8:ASP:O	1:B:12:LEU:HB2	2.20	0.41
1:D:122:LEU:HD11	1:D:359:LYS:CG	2.51	0.41
1:E:413:LEU:HD23	1:E:413:LEU:HA	1.91	0.41
1:F:129:LEU:HD13	1:F:131:PRO:HD3	2.01	0.41
1:F:351:LEU:HD22	1:F:355:LEU:HG	2.03	0.41
1:G:336:SER:O	1:G:337:VAL:C	2.58	0.41
1:H:234:LYS:HE3	1:H:239:VAL:O	2.21	0.41
1:H:371:ASN:C	1:H:371:ASN:HD22	2.23	0.41
1:A:190:VAL:HA	5:A:602:HOH:O	2.20	0.41
1:A:261:GLU:N	1:A:261:GLU:CD	2.74	0.41
1:A:268:SER:O	1:A:272:LYS:HG2	2.20	0.41
1:A:95:ASP:OD2	1:A:113:LYS:NZ	2.53	0.41
1:B:319:LEU:CD1	1:B:320:ILE:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:GLU:HG3	5:B:737:HOH:O	2.21	0.41
1:B:46:LEU:HD22	1:B:74:LEU:HD21	2.01	0.41
1:C:278:ILE:HG21	1:C:320:ILE:HD11	2.02	0.41
1:C:351:LEU:HD22	1:C:355:LEU:CG	2.46	0.41
1:D:274:PHE:CE2	1:D:278:ILE:HD11	2.56	0.41
1:E:388:LEU:HA	1:E:388:LEU:HD23	1.79	0.41
1:E:52:PHE:CD1	1:E:70:LEU:HD13	2.56	0.41
1:F:248:LEU:HD11	1:F:350:LEU:HD13	2.02	0.41
1:F:431:GLN:HG2	1:L:435:TRP:CD1	2.56	0.41
1:F:73:ASP:HA	5:F:800:HOH:O	2.20	0.41
1:G:49:LYS:HA	1:G:49:LYS:HD3	1.86	0.41
1:I:316:ARG:HD3	2:I:501:P3S:OE	2.20	0.41
1:I:52:PHE:CE1	1:I:68:MET:HB3	2.56	0.41
1:I:73:ASP:C	1:I:73:ASP:OD1	2.59	0.41
1:J:280:LYS:HG3	1:J:281:HIS:N	2.36	0.41
1:K:22:ARG:HD3	1:K:34:ASN:OD1	2.21	0.41
1:L:426:ASP:HA	1:L:429:ARG:HG2	2.03	0.41
1:B:182:GLU:HB2	1:B:200:LYS:HB2	2.02	0.41
1:C:266:GLN:HB2	1:C:326:ARG:HD2	2.02	0.41
1:F:359:LYS:NZ	5:F:737:HOH:O	2.26	0.41
1:G:312:SER:HB3	1:G:315:ASN:HB3	2.03	0.41
1:G:315:ASN:O	1:G:318:PRO:HD2	2.21	0.41
1:G:368:ILE:HG22	1:G:372:ILE:CD1	2.51	0.41
1:I:64:GLU:HG2	1:J:370:ARG:C	2.41	0.41
1:L:342:ASN:O	1:L:343:PRO:C	2.60	0.41
1:L:347:LEU:HA	1:L:347:LEU:HD23	1.79	0.41
1:L:397:GLU:HA	1:L:397:GLU:OE1	2.21	0.41
1:A:326:ARG:HB3	1:A:327:GLY:H	1.71	0.40
1:A:5:THR:O	1:A:7:GLU:N	2.54	0.40
1:C:26:THR:HG22	1:C:27:ASP:O	2.21	0.40
1:D:140:LEU:HD22	1:D:144:GLY:O	2.21	0.40
1:E:151:ASN:OD1	1:E:195:HIS:HE1	2.03	0.40
1:F:191:ALA:H	1:F:194:GLN:HE21	1.68	0.40
1:G:402:ASN:C	1:G:402:ASN:OD1	2.59	0.40
1:I:409:LEU:HD23	1:I:414:PHE:HA	2.03	0.40
1:K:282:ALA:HA	1:K:285:PHE:CE2	2.57	0.40
1:L:275:ILE:HG21	1:L:275:ILE:HD13	1.87	0.40
1:L:439:GLN:HE21	1:L:439:GLN:CA	2.33	0.40
1:B:115:ILE:HD12	1:B:348:SER:CB	2.48	0.40
1:C:129:LEU:C	1:C:129:LEU:HD22	2.42	0.40
1:C:335:ARG:NH1	2:C:501:P3S:OE	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLU:O	1:C:65:GLU:CG	2.65	0.40
2:D:501:P3S:HEC3	2:D:501:P3S:HGC1	1.97	0.40
1:E:250:LEU:HD23	1:E:250:LEU:HA	1.81	0.40
1:F:266:GLN:HB2	1:F:326:ARG:HH11	1.86	0.40
1:F:46:LEU:HD23	1:F:46:LEU:HA	1.78	0.40
1:F:74:LEU:H	1:F:74:LEU:HD22	1.85	0.40
1:G:84:ALA:CB	1:G:88:LYS:HG3	2.52	0.40
1:H:310:ALA:HA	5:H:823:HOH:O	2.21	0.40
1:J:435:TRP:CH2	1:J:439:GLN:HG3	2.56	0.40
1:J:18:VAL:HA	1:J:88:LYS:HG2	2.03	0.40
1:L:290:ASN:HB3	1:L:295:SER:HB3	2.03	0.40
1:L:306:PRO:HG2	1:L:336:SER:CA	2.50	0.40
1:B:371:ASN:O	1:B:374:VAL:HG22	2.20	0.40
1:D:46:LEU:HD22	1:D:74:LEU:HD21	2.03	0.40
1:E:170:ARG:NH2	1:F:86:LYS:HD3	2.35	0.40
1:G:57:ILE:HD12	1:G:57:ILE:N	2.37	0.40
1:I:142:GLU:N	1:I:142:GLU:CD	2.73	0.40
1:I:74:LEU:CD2	1:I:74:LEU:N	2.84	0.40
1:J:9:ILE:HG21	1:J:92:PHE:HZ	1.86	0.40
1:K:403:GLU:OE2	1:K:407:LYS:HE2	2.21	0.40
1:K:429:ARG:NH2	5:K:732:HOH:O	2.54	0.40
1:K:71:TYR:CE1	1:K:97:TYR:HB2	2.57	0.40
1:A:360:ASN:O	1:A:361:LYS:C	2.60	0.40
1:B:271:ALA:O	1:B:275:ILE:HG13	2.20	0.40
1:D:27:ASP:OD2	1:D:29:LEU:N	2.54	0.40
1:I:198:ASP:HA	5:I:601:HOH:O	2.21	0.40
1:J:315:ASN:O	1:J:318:PRO:HD2	2.20	0.40
1:L:21:ILE:HD11	1:L:39:VAL:HG23	2.03	0.40
1:L:402:ASN:HB2	5:L:720:HOH:O	2.20	0.40
1:A:119:MET:HG2	1:A:124:PHE:HB2	2.04	0.40
1:B:143:LYS:O	1:B:143:LYS:CG	2.69	0.40
1:B:331:ARG:N	5:B:666:HOH:O	2.50	0.40
1:D:129:LEU:HD12	1:D:347:LEU:HD11	2.03	0.40
1:G:309:VAL:HG21	1:G:386:VAL:HG23	2.04	0.40
1:J:127:PHE:CD2	1:J:351:LEU:HG	2.57	0.40
1:L:260:ASP:HB2	1:L:268:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/443 (100%)	407 (92%)	32 (7%)	2 (0%)	32	56
1	B	441/443 (100%)	417 (95%)	22 (5%)	2 (0%)	32	56
1	C	441/443 (100%)	414 (94%)	22 (5%)	5 (1%)	17	33
1	D	441/443 (100%)	407 (92%)	31 (7%)	3 (1%)	25	47
1	E	441/443 (100%)	417 (95%)	21 (5%)	3 (1%)	25	47
1	F	441/443 (100%)	410 (93%)	28 (6%)	3 (1%)	25	47
1	G	441/443 (100%)	403 (91%)	34 (8%)	4 (1%)	20	39
1	H	441/443 (100%)	420 (95%)	20 (4%)	1 (0%)	51	74
1	I	441/443 (100%)	414 (94%)	24 (5%)	3 (1%)	25	47
1	J	439/443 (99%)	413 (94%)	23 (5%)	3 (1%)	25	47
1	K	441/443 (100%)	416 (94%)	23 (5%)	2 (0%)	32	56
1	L	441/443 (100%)	416 (94%)	24 (5%)	1 (0%)	51	74
All	All	5290/5316 (100%)	4954 (94%)	304 (6%)	32 (1%)	28	52

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	B	161	PRO
1	C	161	PRO
1	C	361	LYS
1	D	161	PRO
1	E	161	PRO
1	F	161	PRO
1	G	100	ASP
1	H	161	PRO
1	I	161	PRO
1	J	161	PRO
1	K	161	PRO

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Mol	Chain	Res	Type
1	C	261	GLU
1	D	3	LYS
1	L	361	LYS
1	F	361	LYS
1	B	361	LYS
1	C	265	LEU
1	E	268	SER
1	G	361	LYS
1	I	60	PHE
1	D	87	GLY
1	E	87	GLY
1	G	133	PRO
1	A	133	PRO
1	J	87	GLY
1	K	87	GLY
1	C	87	GLY
1	F	87	GLY
1	I	87	GLY
1	J	317	SER
1	G	87	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	382/382 (100%)	353 (92%)	29 (8%)	15	29
1	B	382/382 (100%)	354 (93%)	28 (7%)	16	32
1	C	382/382 (100%)	358 (94%)	24 (6%)	21	40
1	D	382/382 (100%)	358 (94%)	24 (6%)	21	40
1	E	382/382 (100%)	357 (94%)	25 (6%)	20	38
1	F	382/382 (100%)	363 (95%)	19 (5%)	28	52
1	G	382/382 (100%)	354 (93%)	28 (7%)	16	32
1	H	382/382 (100%)	350 (92%)	32 (8%)	13	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	382/382 (100%)	349 (91%)	33 (9%)	12	23
1	J	381/382 (100%)	349 (92%)	32 (8%)	13	24
1	K	382/382 (100%)	359 (94%)	23 (6%)	22	43
1	L	382/382 (100%)	346 (91%)	36 (9%)	10	18
All	All	4583/4584 (100%)	4250 (93%)	333 (7%)	16	32

All (333) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	32	ILE
1	A	34	ASN
1	A	58	GLU
1	A	70	LEU
1	A	74	LEU
1	A	78	VAL
1	A	85	GLU
1	A	86	LYS
1	A	88	LYS
1	A	91	ARG
1	A	122	LEU
1	A	126	ASP
1	A	129	LEU
1	A	164	LEU
1	A	174	LEU
1	A	186	SER
1	A	240	ASN
1	A	272	LYS
1	A	297	LYS
1	A	316	ARG
1	A	326	ARG
1	A	331	ARG
1	A	359	LYS
1	A	362	LEU
1	A	375	MET
1	A	381	MET
1	A	396	LEU
1	A	411	GLU
1	B	5	THR
1	B	14	LYS
1	B	24	GLN

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Mol	Chain	Res	Type
1	B	65	GLU
1	B	91	ARG
1	B	129	LEU
1	B	143	LYS
1	B	147	THR
1	B	161	PRO
1	B	164	LEU
1	B	206	ARG
1	B	240	ASN
1	B	261	GLU
1	B	262	ASN
1	B	272	LYS
1	B	299	LEU
1	B	307	CYS
1	B	316	ARG
1	B	349	VAL
1	B	351	LEU
1	B	362	LEU
1	B	363	GLU
1	B	370	ARG
1	B	371	ASN
1	B	372	ILE
1	B	379	GLU
1	B	429	ARG
1	B	441	MET
1	C	9	ILE
1	C	11	LYS
1	C	32	ILE
1	C	49	LYS
1	C	70	LEU
1	C	78	VAL
1	C	91	ARG
1	C	129	LEU
1	C	142	GLU
1	C	148	LEU
1	C	153	LYS
1	C	164	LEU
1	C	186	SER
1	C	240	ASN
1	C	284	SER
1	C	285	PHE
1	C	316	ARG

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Mol	Chain	Res	Type
1	C	349	VAL
1	C	351	LEU
1	C	361	LYS
1	C	363	GLU
1	C	376	SER
1	C	397	GLU
1	C	431	GLN
1	D	15	GLU
1	D	22	ARG
1	D	24	GLN
1	D	31	THR
1	D	34	ASN
1	D	49	LYS
1	D	65	GLU
1	D	70	LEU
1	D	91	ARG
1	D	105	GLU
1	D	129	LEU
1	D	164	LEU
1	D	169	ARG
1	D	256	ASN
1	D	261	GLU
1	D	267	LEU
1	D	319	LEU
1	D	335	ARG
1	D	351	LEU
1	D	362	LEU
1	D	370	ARG
1	D	371	ASN
1	D	379	GLU
1	D	381	MET
1	E	14	LYS
1	E	28	ILE
1	E	49	LYS
1	E	56	SER
1	E	58	GLU
1	E	63	ILE
1	E	91	ARG
1	E	117	LYS
1	E	129	LEU
1	E	151	ASN
1	E	178	GLU

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Mol	Chain	Res	Type
1	E	216	LEU
1	E	319	LEU
1	E	331	ARG
1	E	333	GLU
1	E	349	VAL
1	E	351	LEU
1	E	371	ASN
1	E	372	ILE
1	E	379	GLU
1	E	387	ASP
1	E	403	GLU
1	E	418	ILE
1	E	441	MET
1	E	442	SER
1	F	21	ILE
1	F	22	ARG
1	F	34	ASN
1	F	65	GLU
1	F	70	LEU
1	F	91	ARG
1	F	102	THR
1	F	112	LEU
1	F	126	ASP
1	F	129	LEU
1	F	164	LEU
1	F	183	ILE
1	F	236	LEU
1	F	261	GLU
1	F	331	ARG
1	F	342	ASN
1	F	349	VAL
1	F	351	LEU
1	F	379	GLU
1	G	6	ARG
1	G	24	GLN
1	G	33	LYS
1	G	34	ASN
1	G	64	GLU
1	G	70	LEU
1	G	78	VAL
1	G	85	GLU
1	G	88	LYS

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Mol	Chain	Res	Type
1	G	91	ARG
1	G	129	LEU
1	G	164	LEU
1	G	174	LEU
1	G	178	GLU
1	G	186	SER
1	G	200	LYS
1	G	240	ASN
1	G	272	LYS
1	G	280	LYS
1	G	299	LEU
1	G	307	CYS
1	G	319	LEU
1	G	342	ASN
1	G	351	LEU
1	G	370	ARG
1	G	411	GLU
1	G	422	GLU
1	G	441	MET
1	H	9	ILE
1	H	15	GLU
1	H	16	GLU
1	H	21	ILE
1	H	27	ASP
1	H	31	THR
1	H	34	ASN
1	H	70	LEU
1	H	78	VAL
1	H	91	ARG
1	H	112	LEU
1	H	129	LEU
1	H	161	PRO
1	H	164	LEU
1	H	169	ARG
1	H	178	GLU
1	H	184	GLU
1	H	206	ARG
1	H	223	ARG
1	H	240	ASN
1	H	264	ASP
1	H	285	PHE
1	H	297	LYS

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Mol	Chain	Res	Type
1	H	299	LEU
1	H	316	ARG
1	H	326	ARG
1	H	335	ARG
1	H	349	VAL
1	H	351	LEU
1	H	370	ARG
1	H	371	ASN
1	H	401	SER
1	I	24	GLN
1	I	34	ASN
1	I	49	LYS
1	I	55	SER
1	I	66	SER
1	I	68	MET
1	I	70	LEU
1	I	91	ARG
1	I	122	LEU
1	I	126	ASP
1	I	129	LEU
1	I	142	GLU
1	I	159	LEU
1	I	164	LEU
1	I	167	ASN
1	I	178	GLU
1	I	207	SER
1	I	240	ASN
1	I	264	ASP
1	I	269	GLU
1	I	307	CYS
1	I	325	SER
1	I	335	ARG
1	I	349	VAL
1	I	351	LEU
1	I	362	LEU
1	I	370	ARG
1	I	371	ASN
1	I	404	VAL
1	I	411	GLU
1	I	422	GLU
1	I	441	MET
1	I	442	SER

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Mol	Chain	Res	Type
1	J	24	GLN
1	J	49	LYS
1	J	68	MET
1	J	70	LEU
1	J	85	GLU
1	J	91	ARG
1	J	100	ASP
1	J	112	LEU
1	J	125	SER
1	J	126	ASP
1	J	129	LEU
1	J	142	GLU
1	J	161	PRO
1	J	164	LEU
1	J	178	GLU
1	J	184	GLU
1	J	190	VAL
1	J	223	ARG
1	J	240	ASN
1	J	253	ASN
1	J	264	ASP
1	J	270	THR
1	J	299	LEU
1	J	307	CYS
1	J	316	ARG
1	J	331	ARG
1	J	349	VAL
1	J	351	LEU
1	J	359	LYS
1	J	387	ASP
1	J	426	ASP
1	J	442	SER
1	K	24	GLN
1	K	26	THR
1	K	33	LYS
1	K	34	ASN
1	K	65	GLU
1	K	66	SER
1	K	70	LEU
1	K	74	LEU
1	K	78	VAL
1	K	86	LYS

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Mol	Chain	Res	Type
1	K	88	LYS
1	K	91	ARG
1	K	112	LEU
1	K	161	PRO
1	K	255	VAL
1	K	285	PHE
1	K	299	LEU
1	K	307	CYS
1	K	351	LEU
1	K	362	LEU
1	K	370	ARG
1	K	371	ASN
1	K	372	ILE
1	L	6	ARG
1	L	7	GLU
1	L	16	GLU
1	L	17	ASN
1	L	22	ARG
1	L	34	ASN
1	L	70	LEU
1	L	88	LYS
1	L	91	ARG
1	L	122	LEU
1	L	126	ASP
1	L	129	LEU
1	L	164	LEU
1	L	184	GLU
1	L	206	ARG
1	L	240	ASN
1	L	261	GLU
1	L	264	ASP
1	L	297	LYS
1	L	299	LEU
1	L	316	ARG
1	L	326	ARG
1	L	331	ARG
1	L	335	ARG
1	L	349	VAL
1	L	351	LEU
1	L	359	LYS
1	L	362	LEU
1	L	363	GLU

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Mol	Chain	Res	Type
1	L	370	ARG
1	L	371	ASN
1	L	372	ILE
1	L	379	GLU
1	L	402	ASN
1	L	423	ILE
1	L	441	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	167	ASN
1	A	187	HIS
1	A	240	ASN
1	A	266	GLN
1	A	281	HIS
1	A	314	GLN
1	A	443	GLN
1	B	24	GLN
1	B	34	ASN
1	B	167	ASN
1	B	187	HIS
1	B	194	GLN
1	B	228	HIS
1	B	240	ASN
1	B	281	HIS
1	B	290	ASN
1	B	314	GLN
1	B	371	ASN
1	B	412	HIS
1	B	416	HIS
1	B	431	GLN
1	C	34	ASN
1	C	128	ASN
1	C	167	ASN
1	C	187	HIS
1	C	194	GLN
1	C	228	HIS
1	C	240	ASN
1	C	281	HIS
1	C	290	ASN

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Mol	Chain	Res	Type
1	C	314	GLN
1	D	24	GLN
1	D	75	ASN
1	D	110	ASN
1	D	167	ASN
1	D	187	HIS
1	D	194	GLN
1	D	225	HIS
1	D	228	HIS
1	D	240	ASN
1	D	245	HIS
1	D	256	ASN
1	D	281	HIS
1	D	290	ASN
1	D	314	GLN
1	D	371	ASN
1	D	443	GLN
1	E	24	GLN
1	E	34	ASN
1	E	41	GLN
1	E	75	ASN
1	E	110	ASN
1	E	187	HIS
1	E	195	HIS
1	E	225	HIS
1	E	228	HIS
1	E	240	ASN
1	E	290	ASN
1	E	314	GLN
1	E	371	ASN
1	F	128	ASN
1	F	167	ASN
1	F	187	HIS
1	F	194	GLN
1	F	228	HIS
1	F	240	ASN
1	F	247	ASN
1	F	253	ASN
1	F	281	HIS
1	F	290	ASN
1	F	314	GLN
1	F	342	ASN

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Mol	Chain	Res	Type
1	G	24	GLN
1	G	41	GLN
1	G	167	ASN
1	G	187	HIS
1	G	194	GLN
1	G	228	HIS
1	G	240	ASN
1	G	281	HIS
1	G	314	GLN
1	G	342	ASN
1	G	360	ASN
1	G	431	GLN
1	G	443	GLN
1	H	24	GLN
1	H	128	ASN
1	H	167	ASN
1	H	187	HIS
1	H	194	GLN
1	H	228	HIS
1	H	240	ASN
1	H	281	HIS
1	H	290	ASN
1	H	314	GLN
1	H	371	ASN
1	I	24	GLN
1	I	34	ASN
1	I	128	ASN
1	I	167	ASN
1	I	187	HIS
1	I	225	HIS
1	I	240	ASN
1	I	266	GLN
1	I	290	ASN
1	I	314	GLN
1	I	371	ASN
1	J	24	GLN
1	J	34	ASN
1	J	128	ASN
1	J	167	ASN
1	J	187	HIS
1	J	194	GLN
1	J	228	HIS

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Mol	Chain	Res	Type
1	J	240	ASN
1	J	281	HIS
1	J	290	ASN
1	J	314	GLN
1	J	412	HIS
1	J	431	GLN
1	K	24	GLN
1	K	110	ASN
1	K	167	ASN
1	K	187	HIS
1	K	194	GLN
1	K	212	GLN
1	K	240	ASN
1	K	281	HIS
1	K	290	ASN
1	K	314	GLN
1	K	371	ASN
1	K	412	HIS
1	L	41	GLN
1	L	110	ASN
1	L	128	ASN
1	L	167	ASN
1	L	187	HIS
1	L	194	GLN
1	L	228	HIS
1	L	240	ASN
1	L	281	HIS
1	L	290	ASN
1	L	314	GLN
1	L	371	ASN
1	L	402	ASN
1	L	439	GLN
1	L	443	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 36 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	P3S	A	501	4	8,14,14	5.70	4 (50%)	7,21,21	7.37	3 (42%)
3	ADP	A	502	4	25,29,29	1.01	1 (4%)	24,45,45	2.21	4 (16%)
2	P3S	B	501	4	8,14,14	6.03	4 (50%)	7,21,21	6.49	5 (71%)
3	ADP	B	502	4	25,29,29	0.94	1 (4%)	24,45,45	2.44	7 (29%)
2	P3S	C	501	4	8,14,14	6.26	4 (50%)	7,21,21	10.45	4 (57%)
3	ADP	C	502	4	25,29,29	0.90	1 (4%)	24,45,45	2.90	7 (29%)
2	P3S	D	501	4	8,14,14	5.75	5 (62%)	7,21,21	9.53	3 (42%)
3	ADP	D	502	4	25,29,29	0.96	1 (4%)	24,45,45	2.48	7 (29%)
2	P3S	E	501	4	8,14,14	6.27	4 (50%)	7,21,21	6.78	4 (57%)
3	ADP	E	502	4	25,29,29	0.92	1 (4%)	24,45,45	3.15	7 (29%)
2	P3S	F	601	4	8,14,14	5.30	5 (62%)	7,21,21	9.39	3 (42%)
3	ADP	F	602	4	25,29,29	1.08	3 (12%)	24,45,45	2.80	9 (37%)
2	P3S	G	601	4	8,14,14	6.17	4 (50%)	7,21,21	7.83	4 (57%)
3	ADP	G	602	4	25,29,29	0.97	1 (4%)	24,45,45	2.01	9 (37%)
2	P3S	H	601	4	8,14,14	5.96	6 (75%)	7,21,21	6.74	3 (42%)
3	ADP	H	602	4	25,29,29	1.10	3 (12%)	24,45,45	2.39	4 (16%)
2	P3S	I	501	4	8,14,14	5.36	4 (50%)	7,21,21	5.59	4 (57%)
3	ADP	I	502	4	25,29,29	1.13	2 (8%)	24,45,45	2.34	7 (29%)
2	P3S	J	501	4	8,14,14	5.34	3 (37%)	7,21,21	7.33	3 (42%)
3	ADP	J	502	4	25,29,29	0.88	1 (4%)	24,45,45	2.11	5 (20%)
2	P3S	K	501	4	8,14,14	5.64	4 (50%)	7,21,21	6.20	3 (42%)
3	ADP	K	502	4	25,29,29	0.99	2 (8%)	24,45,45	2.89	8 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P3S	L	501	4	8,14,14	5.89	4 (50%)	7,21,21	7.90	3 (42%)
3	ADP	L	502	4	25,29,29	1.15	2 (8%)	24,45,45	2.04	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P3S	A	501	4	-	0/5/16/16	0/0/0/0
3	ADP	A	502	4	-	0/12/32/32	0/3/3/3
2	P3S	B	501	4	-	0/5/16/16	0/0/0/0
3	ADP	B	502	4	-	0/12/32/32	0/3/3/3
2	P3S	C	501	4	-	0/5/16/16	0/0/0/0
3	ADP	C	502	4	-	0/12/32/32	0/3/3/3
2	P3S	D	501	4	-	0/5/16/16	0/0/0/0
3	ADP	D	502	4	-	0/12/32/32	0/3/3/3
2	P3S	E	501	4	-	0/5/16/16	0/0/0/0
3	ADP	E	502	4	-	0/12/32/32	0/3/3/3
2	P3S	F	601	4	-	0/5/16/16	0/0/0/0
3	ADP	F	602	4	-	0/12/32/32	0/3/3/3
2	P3S	G	601	4	-	0/5/16/16	0/0/0/0
3	ADP	G	602	4	-	0/12/32/32	0/3/3/3
2	P3S	H	601	4	-	0/5/16/16	0/0/0/0
3	ADP	H	602	4	-	0/12/32/32	0/3/3/3
2	P3S	I	501	4	-	0/5/16/16	0/0/0/0
3	ADP	I	502	4	-	0/12/32/32	0/3/3/3
2	P3S	J	501	4	-	0/5/16/16	0/0/0/0
3	ADP	J	502	4	-	0/12/32/32	0/3/3/3
2	P3S	K	501	4	-	0/5/16/16	0/0/0/0
3	ADP	K	502	4	-	0/12/32/32	0/3/3/3
2	P3S	L	501	4	-	0/5/16/16	0/0/0/0
3	ADP	L	502	4	-	0/12/32/32	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	P3S	CB-CG	-4.00	1.48	1.52
3	F	602	ADP	PB-O2B	-2.70	1.43	1.54
2	I	501	P3S	PA-O2A	-2.54	1.49	1.54
3	F	602	ADP	C2'-C1'	-2.32	1.50	1.53
3	D	502	ADP	PB-O2B	-2.25	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	P3S	CB-CG	-2.24	1.50	1.52
3	K	502	ADP	C2'-C1'	-2.15	1.50	1.53
3	H	602	ADP	C2'-C1'	-2.12	1.50	1.53
2	F	601	P3S	CB-CG	-2.11	1.50	1.52
3	L	502	ADP	PB-O2B	-2.08	1.46	1.54
3	H	602	ADP	O4'-C4'	-2.01	1.40	1.45
2	H	601	P3S	CB-CG	-2.00	1.50	1.52
2	B	501	P3S	PA-NE	2.08	1.67	1.59
2	K	501	P3S	PA-NE	2.11	1.67	1.59
3	E	502	ADP	C5-C4	2.15	1.45	1.40
2	H	601	P3S	PA-O1A	2.24	1.50	1.46
3	F	602	ADP	O4'-C1'	2.27	1.44	1.41
2	C	501	P3S	PA-NE	2.31	1.68	1.59
2	E	501	P3S	CB-CG	2.32	1.55	1.52
2	F	601	P3S	PA-NE	2.38	1.68	1.59
3	C	502	ADP	C5-C4	2.43	1.46	1.40
3	A	502	ADP	C5-C4	2.47	1.46	1.40
3	B	502	ADP	C5-C4	2.49	1.46	1.40
2	H	601	P3S	PA-NE	2.52	1.68	1.59
2	L	501	P3S	PA-NE	2.54	1.69	1.59
3	I	502	ADP	C2-N3	2.55	1.36	1.32
3	H	602	ADP	C5-C4	2.58	1.46	1.40
3	J	502	ADP	C5-C4	2.62	1.46	1.40
2	D	501	P3S	PA-NE	2.64	1.69	1.59
2	G	601	P3S	PA-O1A	2.72	1.51	1.46
3	K	502	ADP	C5-C4	2.73	1.46	1.40
3	I	502	ADP	C5-C4	2.89	1.47	1.40
3	G	602	ADP	C5-C4	3.21	1.47	1.40
3	L	502	ADP	C5-C4	3.38	1.48	1.40
2	F	601	P3S	OE-SD	3.55	1.66	1.45
2	J	501	P3S	OE-SD	3.63	1.67	1.45
2	C	501	P3S	OE-SD	3.68	1.67	1.45
2	D	501	P3S	OE-SD	3.76	1.67	1.45
2	A	501	P3S	OE-SD	3.82	1.68	1.45
2	E	501	P3S	OE-SD	3.82	1.68	1.45
2	H	601	P3S	OE-SD	3.85	1.68	1.45
2	L	501	P3S	OE-SD	3.87	1.68	1.45
2	K	501	P3S	OE-SD	3.93	1.68	1.45
2	B	501	P3S	OE-SD	4.03	1.69	1.45
2	G	601	P3S	OE-SD	4.04	1.69	1.45
2	I	501	P3S	CE-SD	4.29	1.98	1.74
2	I	501	P3S	OE-SD	4.43	1.71	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	P3S	CE-SD	4.46	1.99	1.74
2	E	501	P3S	CE-SD	4.49	1.99	1.74
2	A	501	P3S	CE-SD	4.61	1.99	1.74
2	K	501	P3S	CE-SD	4.67	2.00	1.74
2	B	501	P3S	CE-SD	4.73	2.00	1.74
2	L	501	P3S	CE-SD	4.88	2.01	1.74
2	J	501	P3S	CE-SD	4.89	2.01	1.74
2	G	601	P3S	CE-SD	4.97	2.01	1.74
2	H	601	P3S	CE-SD	4.98	2.01	1.74
2	F	601	P3S	CE-SD	5.11	2.02	1.74
2	D	501	P3S	CE-SD	5.33	2.03	1.74
2	F	601	P3S	CG-SD	13.18	1.93	1.79
2	I	501	P3S	CG-SD	13.42	1.93	1.79
2	J	501	P3S	CG-SD	13.60	1.94	1.79
2	A	501	P3S	CG-SD	14.11	1.94	1.79
2	K	501	P3S	CG-SD	14.44	1.95	1.79
2	D	501	P3S	CG-SD	14.46	1.95	1.79
2	H	601	P3S	CG-SD	14.89	1.95	1.79
2	L	501	P3S	CG-SD	15.05	1.95	1.79
2	B	501	P3S	CG-SD	15.45	1.96	1.79
2	G	601	P3S	CG-SD	15.84	1.96	1.79
2	C	501	P3S	CG-SD	16.32	1.97	1.79
2	E	501	P3S	CG-SD	16.37	1.97	1.79

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	ADP	N3-C2-N1	-13.18	117.38	128.86
3	C	502	ADP	N3-C2-N1	-11.11	119.18	128.86
3	K	502	ADP	N3-C2-N1	-11.05	119.23	128.86
3	F	602	ADP	N3-C2-N1	-10.05	120.10	128.86
2	C	501	P3S	CE-SD-CG	-9.86	68.35	105.21
2	G	601	P3S	CE-SD-CG	-9.80	68.60	105.21
3	H	602	ADP	N3-C2-N1	-9.42	120.65	128.86
3	D	502	ADP	N3-C2-N1	-9.21	120.83	128.86
3	B	502	ADP	N3-C2-N1	-8.87	121.13	128.86
2	E	501	P3S	CE-SD-CG	-8.87	72.08	105.21
2	F	601	P3S	CE-SD-CG	-8.76	72.47	105.21
3	A	502	ADP	N3-C2-N1	-8.70	121.28	128.86
2	J	501	P3S	CE-SD-CG	-8.60	73.05	105.21
2	L	501	P3S	CE-SD-CG	-8.58	73.16	105.21
2	B	501	P3S	CE-SD-CG	-8.40	73.80	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	501	P3S	CE-SD-CG	-8.12	74.86	105.21
2	A	501	P3S	CE-SD-CG	-7.95	75.51	105.21
3	J	502	ADP	N3-C2-N1	-7.95	121.94	128.86
2	D	501	P3S	CE-SD-CG	-7.90	75.70	105.21
3	I	502	ADP	N3-C2-N1	-7.54	122.29	128.86
2	K	501	P3S	CE-SD-CG	-7.42	77.50	105.21
2	H	601	P3S	CE-SD-CG	-7.24	78.16	105.21
3	L	502	ADP	N3-C2-N1	-6.83	122.91	128.86
3	G	602	ADP	N3-C2-N1	-5.15	124.37	128.86
3	F	602	ADP	C1'-N9-C4	-4.98	118.02	126.64
3	I	502	ADP	C4-C5-N7	-4.42	105.14	109.41
3	J	502	ADP	C1'-N9-C4	-4.04	119.65	126.64
3	G	602	ADP	C4'-O4'-C1'	-3.88	105.64	109.77
3	K	502	ADP	C1'-N9-C4	-3.86	119.96	126.64
3	D	502	ADP	C1'-N9-C4	-3.60	120.42	126.64
3	C	502	ADP	O3A-PB-O1B	-3.43	90.32	111.44
3	E	502	ADP	C4'-O4'-C1'	-3.41	106.14	109.77
3	H	602	ADP	C1'-N9-C4	-3.30	120.93	126.64
3	B	502	ADP	C4-C5-N7	-3.25	106.27	109.41
2	E	501	P3S	OE-SD-CG	-3.21	105.90	108.34
3	I	502	ADP	C1'-N9-C4	-3.12	121.24	126.64
3	I	502	ADP	C4'-O4'-C1'	-3.11	106.46	109.77
3	C	502	ADP	C1'-N9-C4	-3.10	121.27	126.64
3	E	502	ADP	C1'-N9-C4	-2.94	121.55	126.64
3	F	602	ADP	O3A-PB-O1B	-2.94	93.38	111.44
2	I	501	P3S	OE-SD-CG	-2.93	106.12	108.34
3	D	502	ADP	C4'-O4'-C1'	-2.90	106.68	109.77
3	A	502	ADP	C1'-N9-C4	-2.87	121.67	126.64
3	L	502	ADP	C4-C5-N7	-2.80	106.71	109.41
3	L	502	ADP	C1'-N9-C4	-2.73	121.91	126.64
3	F	602	ADP	O2B-PB-O1B	-2.70	99.92	110.50
3	B	502	ADP	O3'-C3'-C2'	-2.68	103.25	111.83
3	L	502	ADP	C4'-O4'-C1'	-2.61	106.99	109.77
3	B	502	ADP	O5'-PA-O1A	-2.56	98.94	109.25
3	B	502	ADP	C1'-N9-C4	-2.52	122.29	126.64
3	G	602	ADP	C1'-N9-C4	-2.45	122.40	126.64
3	G	602	ADP	C4-C5-N7	-2.28	107.20	109.41
3	J	502	ADP	C4-C5-N7	-2.28	107.21	109.41
3	K	502	ADP	C4-C5-N7	-2.09	107.39	109.41
3	F	602	ADP	O3'-C3'-C4'	-2.04	105.13	111.09
3	D	502	ADP	N6-C6-N1	2.00	122.73	118.77
3	K	502	ADP	C5-C6-N6	2.00	124.55	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	ADP	O3B-PB-O1B	2.01	118.36	110.50
3	C	502	ADP	O3B-PB-O2B	2.01	115.72	107.61
3	E	502	ADP	O3B-PB-O1B	2.03	118.43	110.50
3	G	602	ADP	N6-C6-N1	2.03	122.79	118.77
2	B	501	P3S	O2A-PA-O3A	2.04	114.66	106.64
3	J	502	ADP	O3B-PB-O1B	2.05	118.54	110.50
3	E	502	ADP	O2A-PA-O1A	2.06	122.92	112.28
3	J	502	ADP	O2A-PA-O1A	2.07	122.97	112.28
3	H	602	ADP	O2A-PA-O1A	2.08	123.06	112.28
2	B	501	P3S	CE-SD-NE	2.10	114.83	107.48
3	G	602	ADP	O4'-C4'-C3'	2.17	109.49	105.17
3	G	602	ADP	O3B-PB-O2B	2.18	116.42	107.61
3	L	502	ADP	C2-N1-C6	2.22	122.65	118.77
3	G	602	ADP	O2A-PA-O1A	2.22	123.75	112.28
3	K	502	ADP	O2A-PA-O1A	2.24	123.86	112.28
3	H	602	ADP	C2-N1-C6	2.27	122.74	118.77
3	I	502	ADP	O2A-PA-O1A	2.28	124.08	112.28
3	A	502	ADP	O3B-PB-O2B	2.29	116.85	107.61
3	K	502	ADP	O3B-PB-O1B	2.37	119.77	110.50
3	I	502	ADP	C2-N1-C6	2.37	122.92	118.77
3	E	502	ADP	O4'-C4'-C3'	2.45	110.04	105.17
2	E	501	P3S	O2A-PA-O1A	2.46	119.61	112.31
3	F	602	ADP	O3B-PB-O1B	2.46	120.11	110.50
3	D	502	ADP	O3B-PB-O2B	2.52	117.76	107.61
3	A	502	ADP	O2A-PA-O1A	2.56	125.53	112.28
3	B	502	ADP	C2-N1-C6	2.63	123.37	118.77
3	F	602	ADP	C2-N1-C6	2.64	123.39	118.77
3	G	602	ADP	O3B-PB-O1B	2.82	121.54	110.50
2	I	501	P3S	CE-SD-NE	2.85	117.43	107.48
3	I	502	ADP	O3B-PB-O1B	3.09	122.60	110.50
3	B	502	ADP	O3B-PB-O2B	3.12	120.21	107.61
3	F	602	ADP	O3B-PB-O2B	3.17	120.38	107.61
2	G	601	P3S	CE-SD-NE	3.18	118.61	107.48
3	D	502	ADP	C2-N1-C6	3.25	124.45	118.77
3	F	602	ADP	O2A-PA-O1A	3.27	129.21	112.28
3	C	502	ADP	O2A-PA-O1A	3.38	129.77	112.28
2	C	501	P3S	CE-SD-NE	3.43	119.46	107.48
3	K	502	ADP	O3B-PB-O2B	3.48	121.67	107.61
3	C	502	ADP	C2-N1-C6	3.55	124.98	118.77
3	E	502	ADP	C2-N1-C6	3.57	125.01	118.77
3	C	502	ADP	O3B-PB-O1B	3.73	125.08	110.50
2	B	501	P3S	OE-SD-CG	4.24	111.57	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	502	ADP	C2-N1-C6	4.29	126.28	118.77
2	A	501	P3S	OE-SD-CG	8.74	114.99	108.34
2	C	501	P3S	OE-SD-CE	8.92	123.53	109.18
2	L	501	P3S	OE-SD-CE	9.05	123.73	109.18
2	F	601	P3S	OE-SD-CE	9.72	124.81	109.18
2	K	501	P3S	OE-SD-CG	9.75	115.76	108.34
2	K	501	P3S	OE-SD-CE	10.75	126.47	109.18
2	D	501	P3S	OE-SD-CE	10.80	126.54	109.18
2	J	501	P3S	OE-SD-CG	11.21	116.87	108.34
2	H	601	P3S	OE-SD-CG	11.36	116.99	108.34
2	I	501	P3S	OE-SD-CE	11.52	127.71	109.18
2	H	601	P3S	OE-SD-CE	11.64	127.89	109.18
2	G	601	P3S	OE-SD-CE	12.10	128.63	109.18
2	G	601	P3S	OE-SD-CG	13.16	118.36	108.34
2	J	501	P3S	OE-SD-CE	13.18	130.37	109.18
2	B	501	P3S	OE-SD-CE	13.99	131.68	109.18
2	E	501	P3S	OE-SD-CE	14.89	133.12	109.18
2	A	501	P3S	OE-SD-CE	15.46	134.05	109.18
2	L	501	P3S	OE-SD-CG	16.68	121.03	108.34
2	F	601	P3S	OE-SD-CG	21.04	124.35	108.34
2	D	501	P3S	OE-SD-CG	21.27	124.53	108.34
2	C	501	P3S	OE-SD-CG	23.96	126.57	108.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	P3S	4	0
2	B	501	P3S	1	0
2	C	501	P3S	4	0
2	D	501	P3S	6	0
2	E	501	P3S	1	0
3	E	502	ADP	1	0
2	F	601	P3S	6	0
3	F	602	ADP	1	0
2	G	601	P3S	8	0
2	H	601	P3S	5	0
2	I	501	P3S	2	0
2	J	501	P3S	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	501	P3S	2	0
2	L	501	P3S	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	443/443 (100%)	-0.21	2 (0%) 90 90	8, 19, 44, 77	0
1	B	443/443 (100%)	-0.20	1 (0%) 94 95	9, 19, 45, 79	0
1	C	443/443 (100%)	-0.25	0 100 100	8, 19, 45, 61	0
1	D	443/443 (100%)	-0.21	2 (0%) 90 90	9, 19, 42, 67	0
1	E	443/443 (100%)	-0.22	1 (0%) 94 95	7, 19, 42, 72	0
1	F	443/443 (100%)	-0.21	2 (0%) 90 90	9, 20, 45, 74	0
1	G	443/443 (100%)	-0.21	3 (0%) 87 86	8, 19, 45, 73	0
1	H	443/443 (100%)	-0.18	1 (0%) 94 95	7, 19, 44, 74	0
1	I	443/443 (100%)	-0.25	1 (0%) 94 95	7, 19, 43, 70	0
1	J	441/443 (99%)	-0.21	0 100 100	7, 19, 42, 65	0
1	K	443/443 (100%)	-0.22	2 (0%) 90 90	7, 19, 44, 67	0
1	L	443/443 (100%)	-0.22	2 (0%) 90 90	9, 21, 45, 72	0
All	All	5314/5316 (99%)	-0.22	17 (0%) 93 93	7, 19, 44, 79	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	8.2
1	E	2	ALA	6.9
1	B	2	ALA	6.1
1	K	2	ALA	4.9
1	F	2	ALA	4.2
1	K	17	ASN	3.3
1	H	2	ALA	3.1
1	G	2	ALA	2.7
1	I	2	ALA	2.6
1	L	2	ALA	2.5
1	A	269	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	264	ASP	2.4
1	D	2	ALA	2.4
1	G	3	LYS	2.2
1	F	384	GLY	2.1
1	L	264	ASP	2.0
1	D	377	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	MG	B	503	1/1	0.99	0.23	9.39	0,0,0,0	0
4	MG	D	503	1/1	0.97	0.19	8.98	5,5,5,5	0
4	MG	E	503	1/1	0.99	0.22	4.59	1,1,1,1	0
4	MG	C	503	1/1	0.99	0.20	3.91	0,0,0,0	0
4	MG	I	503	1/1	0.99	0.19	2.86	0,0,0,0	0
2	P3S	D	501	15/15	0.99	0.17	2.81	8,18,34,41	0
4	MG	K	503	1/1	1.00	0.16	2.64	0,0,0,0	0
4	MG	L	503	1/1	0.99	0.16	2.53	2,2,2,2	0
2	P3S	K	501	15/15	0.98	0.17	2.33	10,15,21,23	0
4	MG	A	503	1/1	0.99	0.17	2.32	4,4,4,4	0
2	P3S	F	601	15/15	0.98	0.18	2.32	12,21,32,45	0
4	MG	B	504	1/1	0.97	0.17	2.23	4,4,4,4	0
4	MG	C	505	1/1	0.98	0.16	2.20	5,5,5,5	0
2	P3S	A	501	15/15	0.98	0.18	2.20	8,16,28,34	0
4	MG	D	505	1/1	0.97	0.17	2.06	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	H	603	1/1	0.99	0.17	2.05	1,1,1,1	0
4	MG	J	503	1/1	0.99	0.18	1.67	5,5,5,5	0
2	P3S	C	501	15/15	0.98	0.16	1.48	4,13,27,40	0
2	P3S	I	501	15/15	0.98	0.17	1.38	9,13,27,28	0
2	P3S	G	601	15/15	0.98	0.16	1.31	13,24,38,39	0
2	P3S	J	501	15/15	0.99	0.16	1.13	8,16,22,24	0
2	P3S	E	501	15/15	0.98	0.16	0.93	7,15,26,33	0
2	P3S	L	501	15/15	0.98	0.15	0.86	13,18,26,32	0
2	P3S	B	501	15/15	0.99	0.15	0.83	7,15,22,31	0
4	MG	F	603	1/1	0.99	0.15	0.78	5,5,5,5	0
4	MG	G	603	1/1	0.98	0.15	0.54	4,4,4,4	0
2	P3S	H	601	15/15	0.98	0.15	0.36	9,13,21,26	0
4	MG	A	504	1/1	1.00	0.15	0.28	4,4,4,4	0
3	ADP	J	502	27/27	0.99	0.14	0.25	13,18,24,33	0
3	ADP	C	502	27/27	0.99	0.14	0.21	11,18,21,23	0
3	ADP	A	502	27/27	0.98	0.14	0.02	14,18,24,25	0
4	MG	F	604	1/1	0.98	0.14	-0.21	6,6,6,6	0
4	MG	F	605	1/1	0.99	0.14	-0.21	5,5,5,5	0
3	ADP	L	502	27/27	0.99	0.14	-0.25	16,24,35,37	0
3	ADP	D	502	27/27	0.98	0.14	-0.25	11,19,28,32	0
3	ADP	K	502	27/27	0.98	0.13	-0.25	8,15,22,25	0
3	ADP	F	602	27/27	0.99	0.14	-0.36	10,20,27,30	0
3	ADP	I	502	27/27	0.98	0.14	-0.39	13,18,25,26	0
3	ADP	H	602	27/27	0.99	0.13	-0.48	11,18,23,25	0
4	MG	I	504	1/1	0.98	0.14	-0.55	5,5,5,5	0
4	MG	H	604	1/1	0.99	0.14	-0.57	5,5,5,5	0
4	MG	E	504	1/1	0.96	0.14	-0.62	3,3,3,3	0
3	ADP	B	502	27/27	0.98	0.13	-0.67	11,19,23,28	0
3	ADP	G	602	27/27	0.98	0.12	-0.75	16,22,31,32	0
3	ADP	E	502	27/27	0.99	0.11	-1.23	8,15,23,31	0
4	MG	G	604	1/1	0.99	0.13	-1.37	10,10,10,10	0
4	MG	J	504	1/1	0.99	0.12	-1.48	4,4,4,4	0
4	MG	C	504	1/1	0.99	0.11	-1.62	6,6,6,6	0
4	MG	K	504	1/1	0.98	0.11	-1.94	5,5,5,5	0
4	MG	D	504	1/1	0.98	0.09	-3.18	2,2,2,2	0
4	MG	L	504	1/1	0.99	0.12	-3.92	7,7,7,7	0
4	MG	I	505	1/1	0.97	0.17	-	6,6,6,6	0
4	MG	L	505	1/1	0.99	0.15	-	0,0,0,0	0
4	MG	A	505	1/1	0.99	0.17	-	6,6,6,6	0
4	MG	J	505	1/1	0.98	0.17	-	0,0,0,0	0
4	MG	B	505	1/1	0.96	0.17	-	7,7,7,7	0
4	MG	E	505	1/1	0.99	0.16	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	H	605	1/1	0.99	0.17	-	1,1,1,1	0
4	MG	G	605	1/1	0.93	0.12	-	7,7,7,7	0
4	MG	K	505	1/1	0.98	0.20	-	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.