Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 09:47 AM EST

PDB ID	:	2LGS
Title	:	FEEDBACK INHIBITION OF FULLY UNADENYLYLATED GLUTAMINE SYNTHETASE FROM SALMONELLA TYPHIMURIUM BY GLYCINE, ALANINE, AND SERINE
Authors	:	Liaw, S.-H.; Eisenberg, D.
Deposited on	:	1994-08-05
Resolution	:	2.80 Å(reported)

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

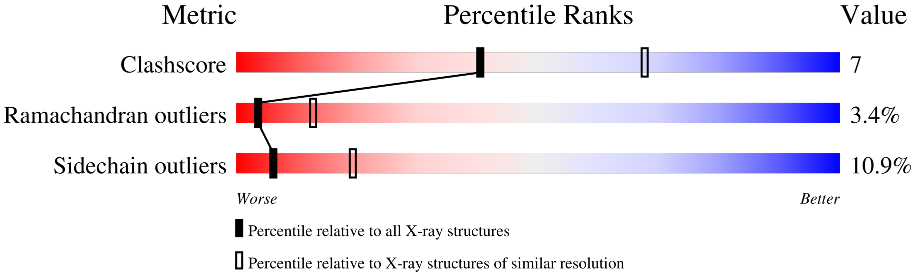
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	468	
1	B	468	
1	C	468	
1	D	468	
1	E	468	
1	F	468	
1	G	468	
1	H	468	

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Mol	Chain	Length	Quality of chain
1	I	468	
1	J	468	
1	K	468	
1	L	468	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41604 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	B	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	C	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	D	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	E	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	F	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	G	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	H	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	I	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	J	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	K	445	Total C N O S 3455 2187 596 652 20	0	0	0
1	L	445	Total C N O S 3455 2187 596 652 20	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0

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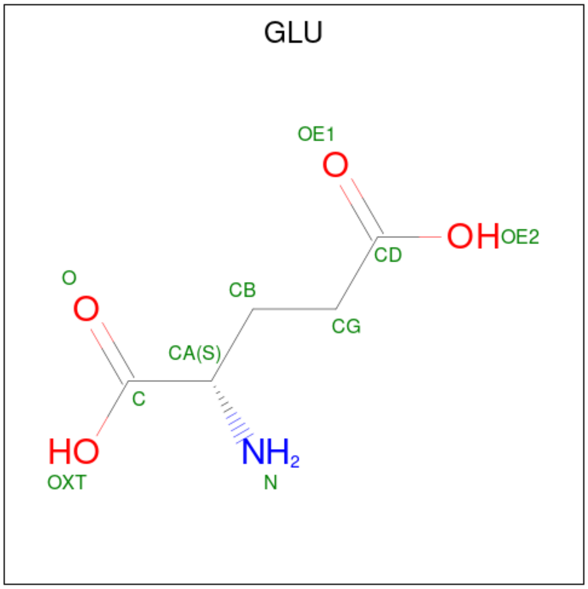
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	E	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0
2	G	2	Total Mn 2 2	0	0
2	H	2	Total Mn 2 2	0	0
2	I	2	Total Mn 2 2	0	0
2	J	2	Total Mn 2 2	0	0
2	K	2	Total Mn 2 2	0	0
2	L	2	Total Mn 2 2	0	0

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 5 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 10 5 1 4	0	0
3	C	1	Total C N O 10 5 1 4	0	0
3	D	1	Total C N O 10 5 1 4	0	0
3	E	1	Total C N O 10 5 1 4	0	0
3	F	1	Total C N O 10 5 1 4	0	0
3	G	1	Total C N O 10 5 1 4	0	0
3	H	1	Total C N O 10 5 1 4	0	0
3	I	1	Total C N O 10 5 1 4	0	0
3	J	1	Total C N O 10 5 1 4	0	0
3	K	1	Total C N O 10 5 1 4	0	0
3	L	1	Total C N O 10 5 1 4	0	0

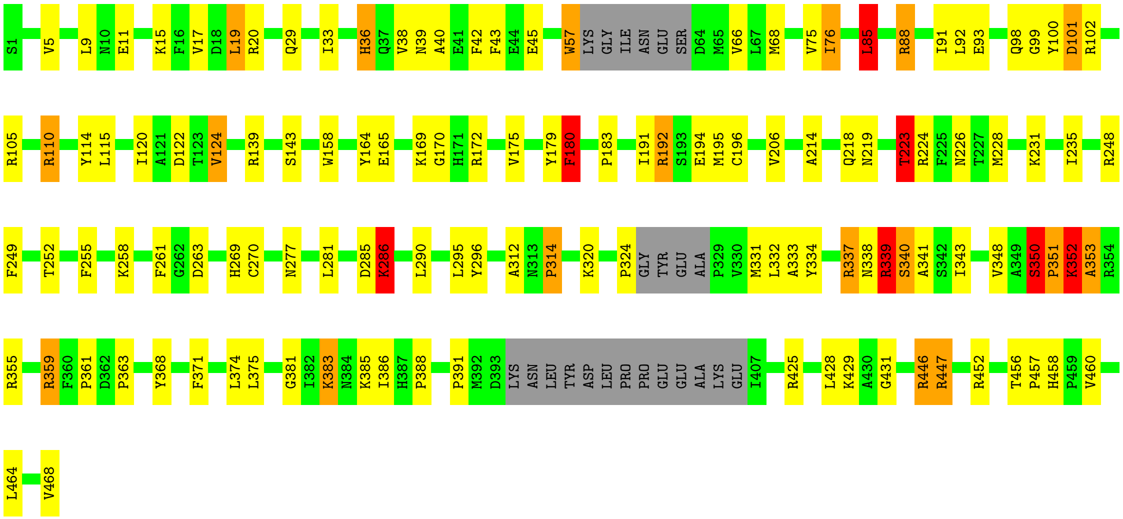
3 Residue-property plots ⓘ

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

Note EDS was not executed.

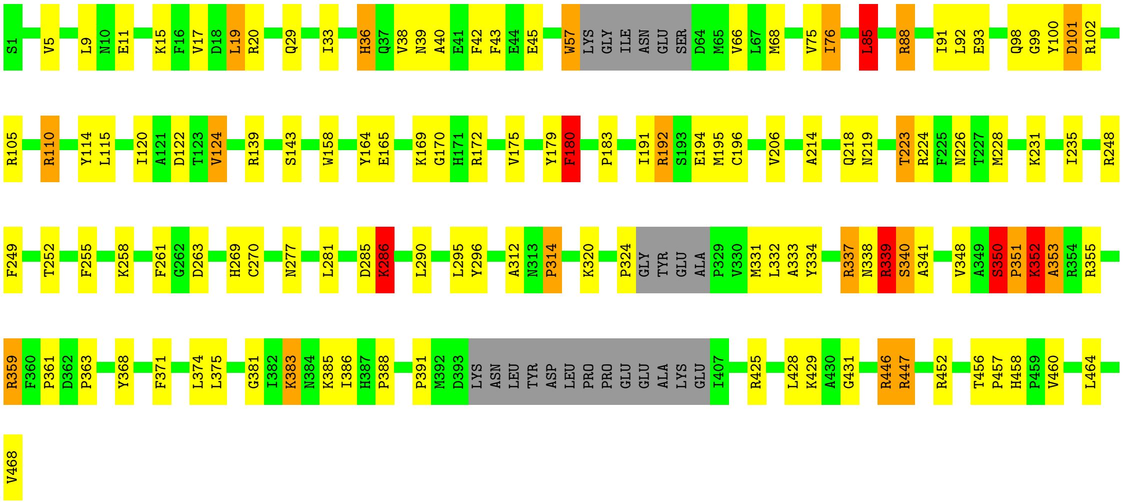
- Molecule 1: GLUTAMINE SYNTHETASE

Chain A:

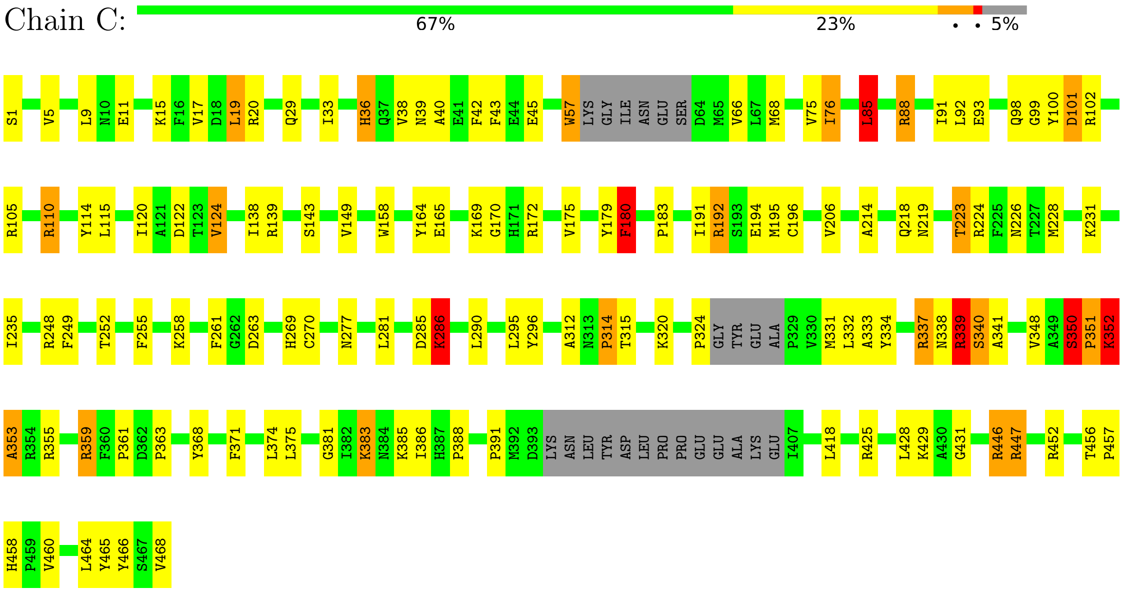


- Molecule 1: GLUTAMINE SYNTHETASE

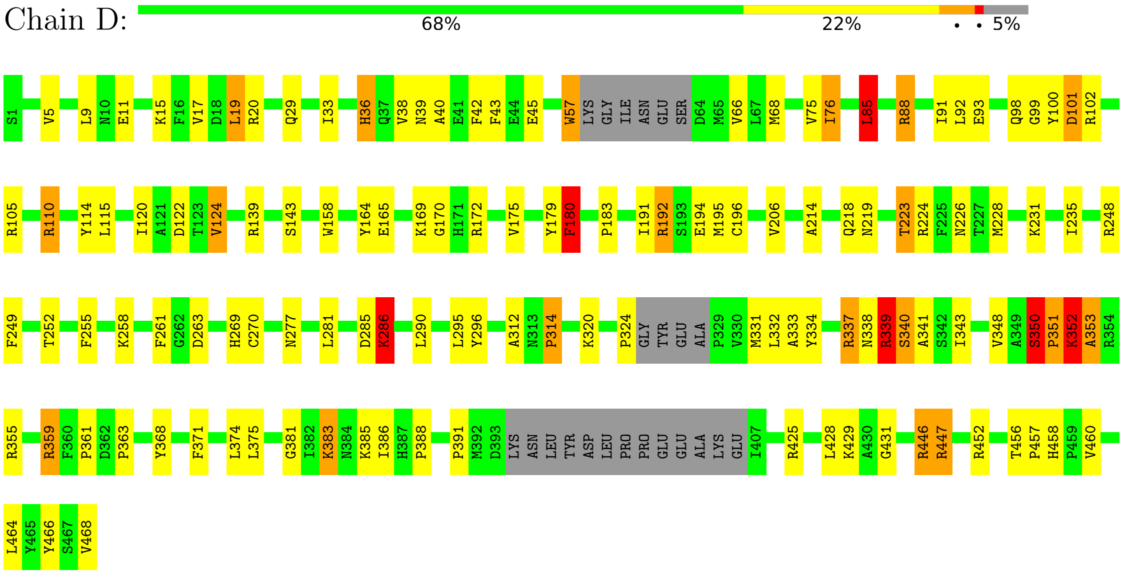
Chain B:



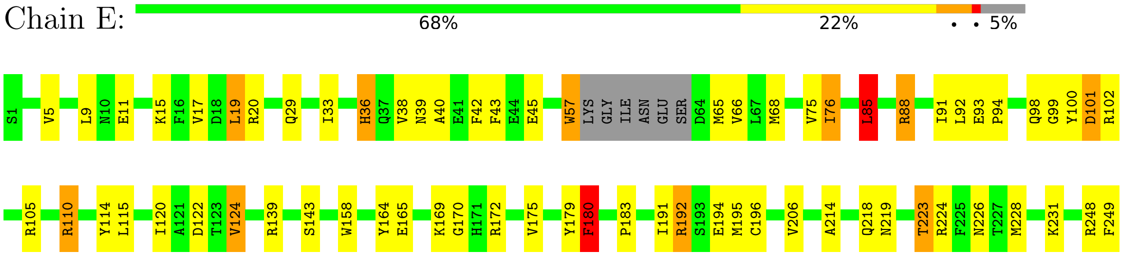
- Molecule 1: GLUTAMINE SYNTHETASE

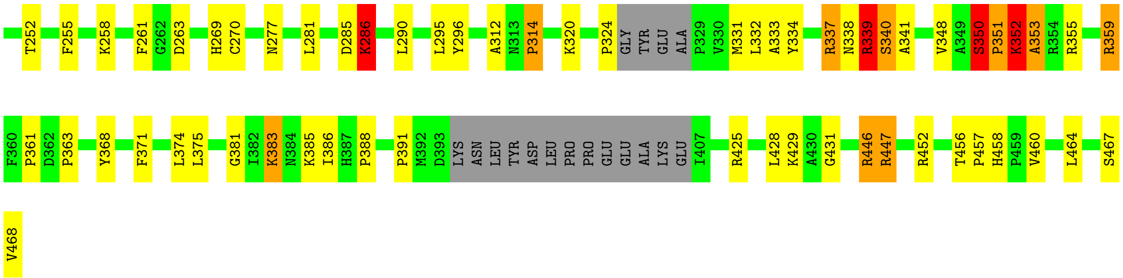


- Molecule 1: GLUTAMINE SYNTHETASE



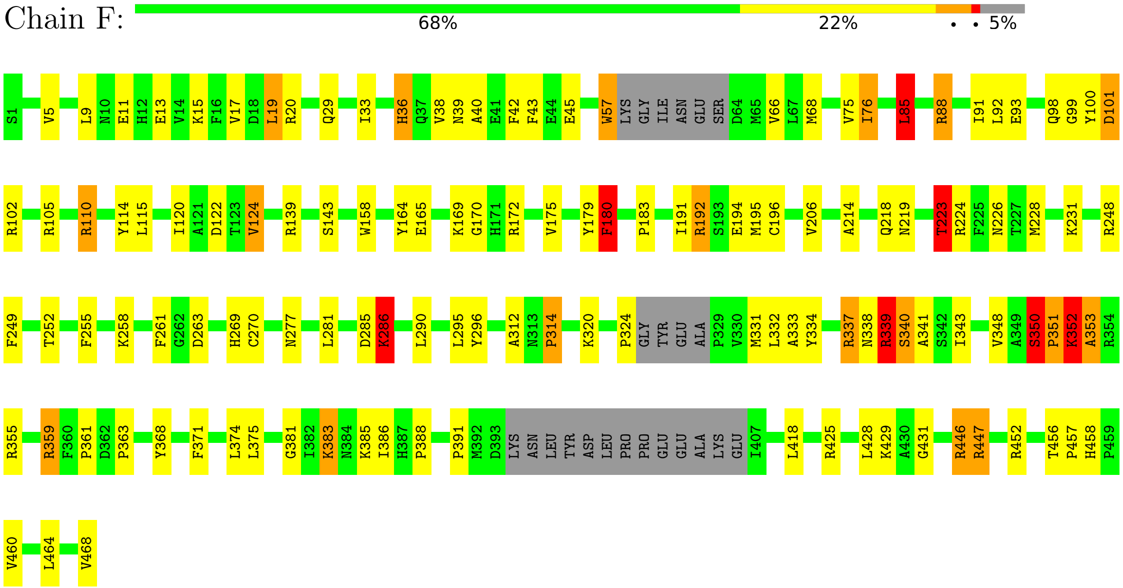
- Molecule 1: GLUTAMINE SYNTHETASE





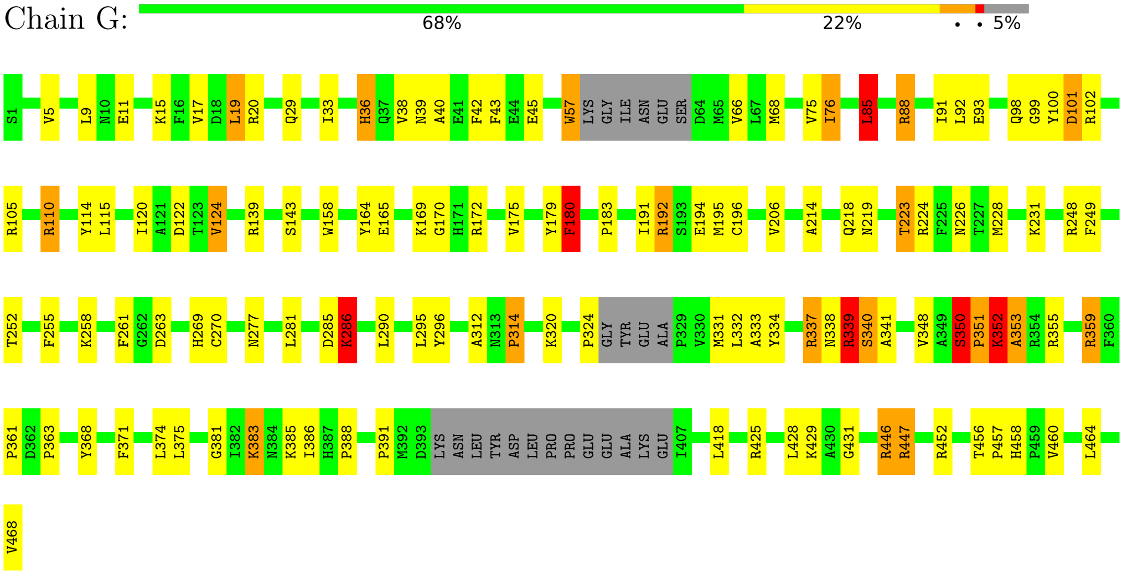
- Molecule 1: GLUTAMINE SYNTHETASE

Chain F:



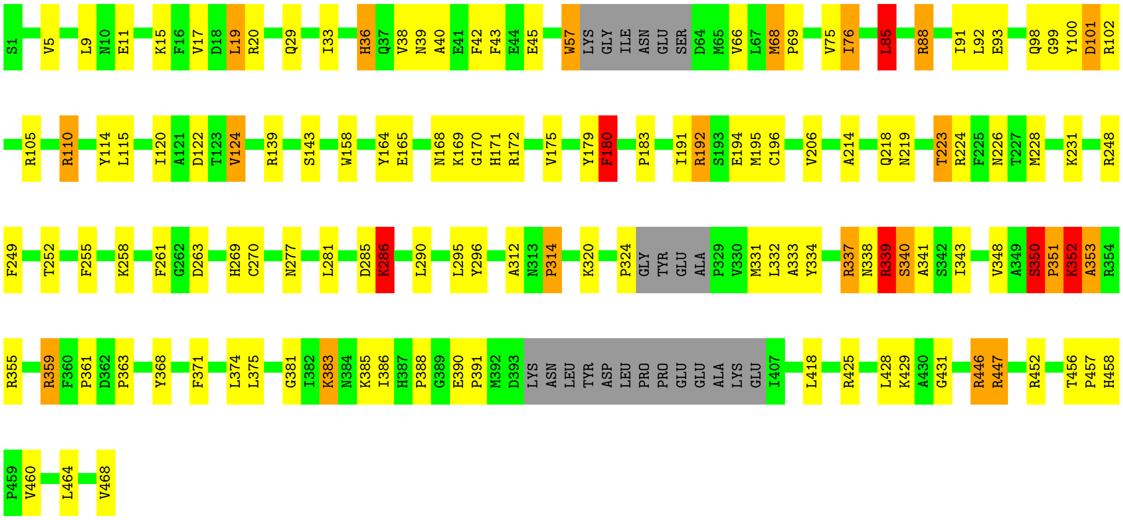
- Molecule 1: GLUTAMINE SYNTHETASE

Chain G:



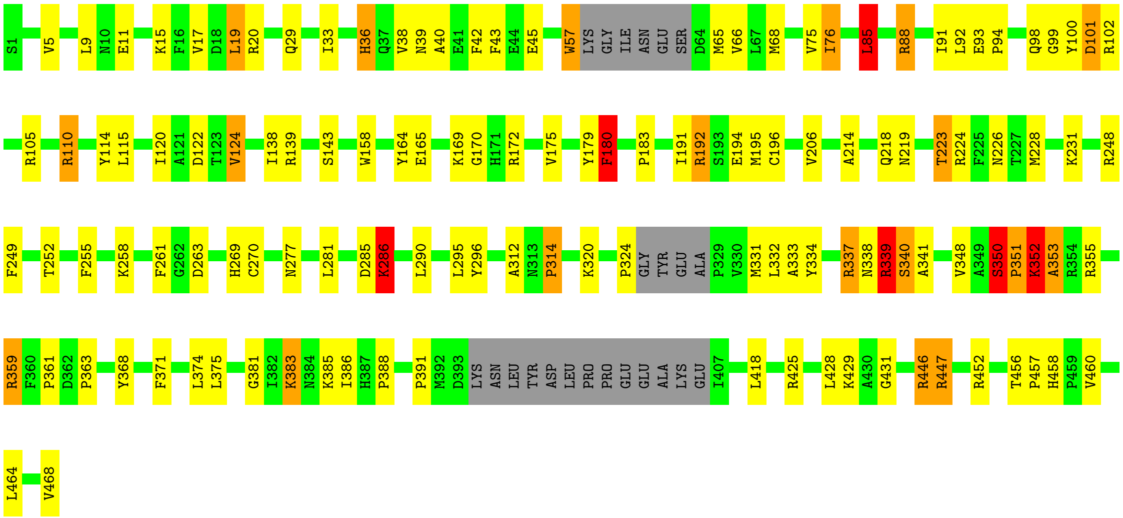
- Molecule 1: GLUTAMINE SYNTHETASE

Chain H:



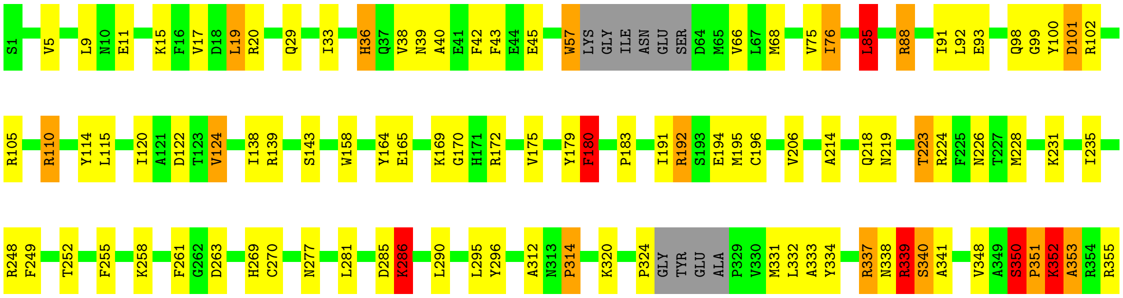
- Molecule 1: GLUTAMINE SYNTHETASE

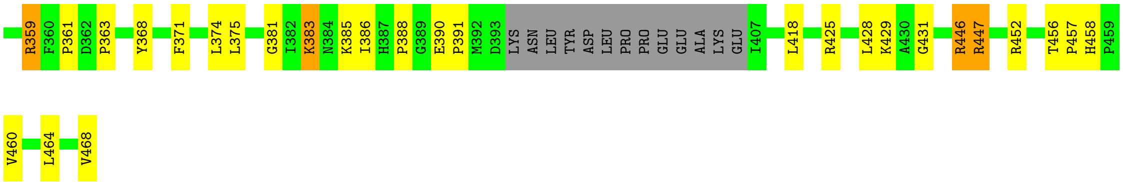
Chain I:



- Molecule 1: GLUTAMINE SYNTHETASE

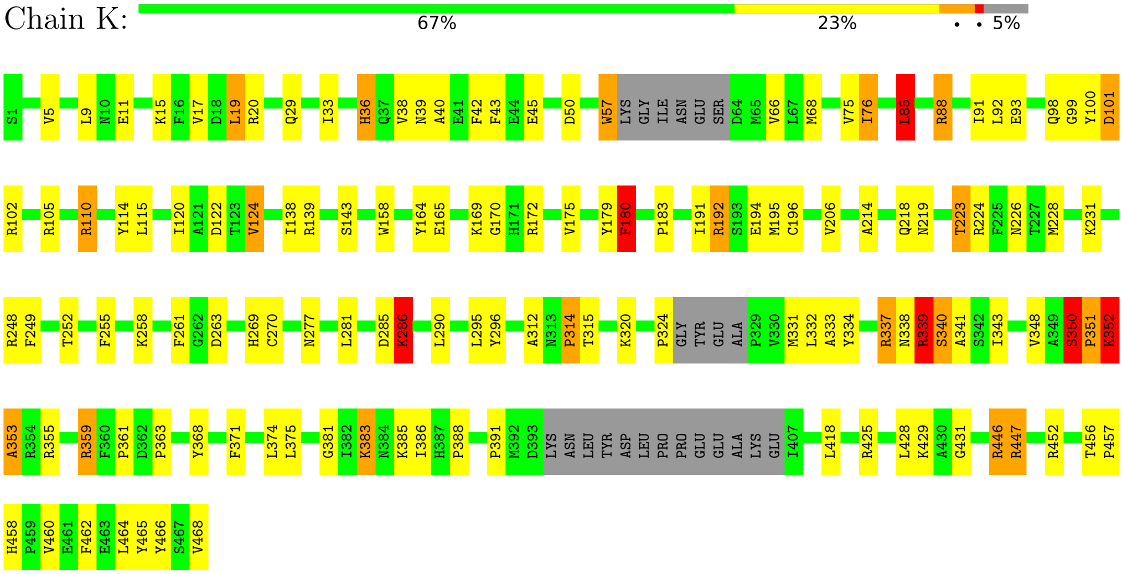
Chain J:





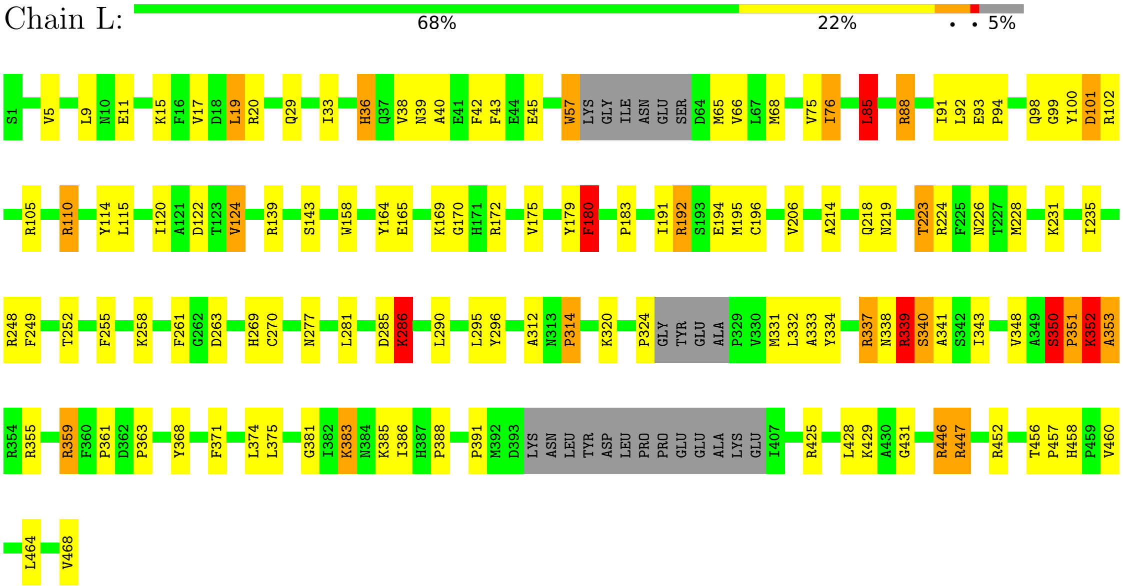
- Molecule 1: GLUTAMINE SYNTHETASE

Chain K:



- Molecule 1: GLUTAMINE SYNTHETASE

Chain L:



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.50Å 134.50Å 200.10Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.235 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41604	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.72	0/3535	1.51	34/4782 (0.7%)
1	B	0.72	0/3535	1.51	34/4782 (0.7%)
1	C	0.72	0/3535	1.51	34/4782 (0.7%)
1	D	0.72	0/3535	1.51	34/4782 (0.7%)
1	E	0.72	0/3535	1.51	34/4782 (0.7%)
1	F	0.72	0/3535	1.50	34/4782 (0.7%)
1	G	0.72	0/3535	1.51	34/4782 (0.7%)
1	H	0.72	0/3535	1.51	34/4782 (0.7%)
1	I	0.72	0/3535	1.51	34/4782 (0.7%)
1	J	0.72	0/3535	1.51	34/4782 (0.7%)
1	K	0.72	0/3535	1.51	34/4782 (0.7%)
1	L	0.72	0/3535	1.51	34/4782 (0.7%)
All	All	0.72	0/42420	1.51	408/57384 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	24

There are no bond length outliers.

All (408) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	359	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	G	359	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	B	359	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	I	88	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	H	88	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	J	88	ARG	NE-CZ-NH1	10.69	125.64	120.30
1	I	359	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	D	359	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	E	359	ARG	NE-CZ-NH1	10.67	125.63	120.30
1	H	359	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	G	88	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	K	359	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	A	88	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	A	359	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	L	88	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	J	359	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	C	88	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	D	88	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	E	88	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	K	88	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	F	359	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	B	88	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	C	359	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	F	88	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	J	452	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	G	452	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	D	452	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	K	452	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	L	452	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	I	452	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	A	452	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	C	452	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	H	452	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	E	452	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	B	452	ARG	NE-CZ-NH1	9.56	125.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	452	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	G	248	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	D	248	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	I	248	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	H	248	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	248	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	L	248	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	B	248	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	K	248	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	J	248	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	E	248	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	C	248	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	F	248	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	E	88	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	I	88	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	H	88	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	G	179	TYR	CA-C-N	-7.92	99.77	117.20
1	D	179	TYR	CA-C-N	-7.91	99.80	117.20
1	J	88	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	F	179	TYR	CA-C-N	-7.91	99.81	117.20
1	J	179	TYR	CA-C-N	-7.90	99.81	117.20
1	K	179	TYR	CA-C-N	-7.90	99.81	117.20
1	A	179	TYR	CA-C-N	-7.90	99.82	117.20
1	B	179	TYR	CA-C-N	-7.90	99.82	117.20
1	C	88	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	E	179	TYR	CA-C-N	-7.90	99.82	117.20
1	H	179	TYR	CA-C-N	-7.90	99.82	117.20
1	C	179	TYR	CA-C-N	-7.90	99.83	117.20
1	I	179	TYR	CA-C-N	-7.90	99.83	117.20
1	K	88	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	A	88	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	L	179	TYR	CA-C-N	-7.88	99.86	117.20
1	G	88	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	D	88	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	L	88	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	F	88	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	88	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	K	158	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	D	158	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	L	158	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	C	158	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	I	158	TRP	CD1-CG-CD2	7.74	112.49	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TRP	CD1-CG-CD2	7.73	112.49	106.30
1	E	158	TRP	CD1-CG-CD2	7.73	112.49	106.30
1	F	158	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	G	158	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	J	158	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	H	158	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	B	158	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	F	57	TRP	CD1-CG-CD2	7.23	112.08	106.30
1	H	57	TRP	CD1-CG-CD2	7.22	112.08	106.30
1	C	57	TRP	CD1-CG-CD2	7.22	112.07	106.30
1	G	57	TRP	CD1-CG-CD2	7.20	112.06	106.30
1	B	57	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	E	57	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	A	57	TRP	CD1-CG-CD2	7.18	112.04	106.30
1	L	57	TRP	CD1-CG-CD2	7.18	112.04	106.30
1	K	57	TRP	CD1-CG-CD2	7.17	112.04	106.30
1	D	57	TRP	CD1-CG-CD2	7.17	112.04	106.30
1	I	57	TRP	CD1-CG-CD2	7.14	112.02	106.30
1	J	57	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	G	110	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	110	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	J	110	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	I	110	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	K	110	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	D	110	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	110	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	110	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	L	110	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	E	110	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	H	110	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	F	110	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	H	57	TRP	CE2-CD2-CG	-6.76	101.89	107.30
1	C	57	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	E	57	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	G	57	TRP	CE2-CD2-CG	-6.75	101.90	107.30
1	J	180	PHE	N-CA-C	6.74	129.20	111.00
1	L	180	PHE	N-CA-C	6.74	129.20	111.00
1	B	180	PHE	N-CA-C	6.74	129.19	111.00
1	K	180	PHE	N-CA-C	6.74	129.19	111.00
1	C	180	PHE	N-CA-C	6.73	129.18	111.00
1	A	180	PHE	N-CA-C	6.73	129.18	111.00
1	D	180	PHE	N-CA-C	6.73	129.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	57	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	F	180	PHE	N-CA-C	6.73	129.17	111.00
1	I	180	PHE	N-CA-C	6.73	129.18	111.00
1	E	180	PHE	N-CA-C	6.73	129.16	111.00
1	L	57	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	B	57	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	G	180	PHE	N-CA-C	6.72	129.15	111.00
1	H	180	PHE	N-CA-C	6.72	129.14	111.00
1	D	57	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	A	57	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	I	57	TRP	CE2-CD2-CG	-6.71	101.94	107.30
1	K	57	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	J	57	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	I	248	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	L	339	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	D	339	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	339	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	I	339	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	339	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	C	339	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	K	339	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	J	339	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	368	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	H	248	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	B	248	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	355	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	H	339	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	J	248	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	D	248	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	G	368	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	E	248	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	G	248	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	248	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	G	339	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	248	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	E	339	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	F	248	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	F	339	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	368	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	K	368	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	C	368	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	F	368	TYR	CB-CG-CD2	-6.42	117.15	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	355	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	F	355	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	J	368	TYR	CB-CG-CD2	-6.40	117.16	121.00
1	K	248	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	L	248	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	H	368	TYR	CB-CG-CD2	-6.40	117.16	121.00
1	E	337	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	J	337	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	E	355	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	L	368	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	L	355	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	355	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	G	355	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	D	368	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	B	355	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	C	355	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	E	368	TYR	CB-CG-CD2	-6.36	117.18	121.00
1	K	355	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	I	368	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	I	355	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	G	337	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	I	337	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	J	355	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	337	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	337	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	K	158	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	F	337	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	L	158	TRP	CE2-CD2-CG	-6.27	102.28	107.30
1	D	158	TRP	CE2-CD2-CG	-6.27	102.28	107.30
1	D	337	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	C	158	TRP	CE2-CD2-CG	-6.26	102.30	107.30
1	L	337	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	G	158	TRP	CE2-CD2-CG	-6.25	102.30	107.30
1	H	337	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	E	158	TRP	CE2-CD2-CG	-6.25	102.30	107.30
1	I	158	TRP	CE2-CD2-CG	-6.24	102.31	107.30
1	C	337	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	F	158	TRP	CE2-CD2-CG	-6.24	102.31	107.30
1	A	158	TRP	CE2-CD2-CG	-6.24	102.31	107.30
1	K	337	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	158	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	J	158	TRP	CE2-CD2-CG	-6.20	102.34	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	158	TRP	CE2-CD2-CG	-6.19	102.34	107.30
1	F	124	VAL	CB-CA-C	-6.16	99.69	111.40
1	H	124	VAL	CB-CA-C	-6.16	99.69	111.40
1	D	124	VAL	CB-CA-C	-6.16	99.70	111.40
1	E	124	VAL	CB-CA-C	-6.16	99.70	111.40
1	J	124	VAL	CB-CA-C	-6.15	99.72	111.40
1	G	124	VAL	CB-CA-C	-6.14	99.73	111.40
1	A	124	VAL	CB-CA-C	-6.14	99.73	111.40
1	L	124	VAL	CB-CA-C	-6.14	99.74	111.40
1	K	124	VAL	CB-CA-C	-6.14	99.74	111.40
1	C	124	VAL	CB-CA-C	-6.13	99.75	111.40
1	B	124	VAL	CB-CA-C	-6.13	99.75	111.40
1	I	124	VAL	CB-CA-C	-6.13	99.76	111.40
1	G	223	THR	N-CA-CB	-5.93	99.04	110.30
1	E	223	THR	N-CA-CB	-5.92	99.06	110.30
1	A	223	THR	N-CA-CB	-5.92	99.06	110.30
1	I	223	THR	N-CA-CB	-5.92	99.06	110.30
1	C	223	THR	N-CA-CB	-5.91	99.07	110.30
1	F	223	THR	N-CA-CB	-5.91	99.08	110.30
1	K	223	THR	N-CA-CB	-5.90	99.08	110.30
1	H	223	THR	N-CA-CB	-5.90	99.09	110.30
1	L	223	THR	N-CA-CB	-5.90	99.09	110.30
1	B	223	THR	N-CA-CB	-5.89	99.10	110.30
1	D	223	THR	N-CA-CB	-5.89	99.10	110.30
1	J	223	THR	N-CA-CB	-5.89	99.11	110.30
1	F	192	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	192	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	G	192	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	I	192	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	J	192	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	L	192	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	H	192	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	192	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	K	85	LEU	CA-CB-CG	5.74	128.50	115.30
1	F	85	LEU	CA-CB-CG	5.74	128.50	115.30
1	D	192	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	85	LEU	CA-CB-CG	5.73	128.48	115.30
1	D	85	LEU	CA-CB-CG	5.73	128.48	115.30
1	J	85	LEU	CA-CB-CG	5.73	128.47	115.30
1	B	85	LEU	CA-CB-CG	5.73	128.47	115.30
1	K	192	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	85	LEU	CA-CB-CG	5.72	128.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	85	LEU	CA-CB-CG	5.72	128.47	115.30
1	B	192	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	E	192	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	G	85	LEU	CA-CB-CG	5.72	128.46	115.30
1	L	85	LEU	CA-CB-CG	5.72	128.45	115.30
1	I	85	LEU	CA-CB-CG	5.72	128.45	115.30
1	E	85	LEU	CA-CB-CG	5.71	128.43	115.30
1	F	139	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	J	139	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	E	139	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	H	139	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	I	350	SER	N-CA-CB	-5.55	102.17	110.50
1	G	350	SER	N-CA-CB	-5.55	102.18	110.50
1	C	350	SER	N-CA-CB	-5.54	102.20	110.50
1	J	350	SER	N-CA-CB	-5.53	102.20	110.50
1	F	350	SER	N-CA-CB	-5.53	102.20	110.50
1	A	139	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	D	350	SER	N-CA-CB	-5.53	102.21	110.50
1	A	350	SER	N-CA-CB	-5.52	102.22	110.50
1	B	139	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	350	SER	N-CA-CB	-5.52	102.22	110.50
1	C	179	TYR	O-C-N	5.52	131.53	122.70
1	J	179	TYR	O-C-N	5.52	131.53	122.70
1	K	139	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	G	179	TYR	O-C-N	5.51	131.52	122.70
1	K	350	SER	N-CA-CB	-5.51	102.23	110.50
1	H	350	SER	N-CA-CB	-5.50	102.25	110.50
1	L	350	SER	N-CA-CB	-5.50	102.25	110.50
1	E	350	SER	N-CA-CB	-5.50	102.25	110.50
1	F	179	TYR	O-C-N	5.50	131.49	122.70
1	J	452	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	K	179	TYR	O-C-N	5.49	131.48	122.70
1	K	452	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	179	TYR	O-C-N	5.49	131.48	122.70
1	L	139	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	D	139	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	H	179	TYR	O-C-N	5.48	131.46	122.70
1	E	179	TYR	O-C-N	5.48	131.46	122.70
1	D	179	TYR	O-C-N	5.47	131.46	122.70
1	C	139	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	I	179	TYR	O-C-N	5.47	131.45	122.70
1	B	179	TYR	O-C-N	5.46	131.44	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	452	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	L	179	TYR	O-C-N	5.45	131.42	122.70
1	E	68	MET	CG-SD-CE	-5.45	91.49	100.20
1	H	452	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	68	MET	CG-SD-CE	-5.44	91.49	100.20
1	I	139	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	J	68	MET	CG-SD-CE	-5.44	91.49	100.20
1	L	68	MET	CG-SD-CE	-5.44	91.50	100.20
1	A	68	MET	CG-SD-CE	-5.44	91.50	100.20
1	B	68	MET	CG-SD-CE	-5.44	91.50	100.20
1	H	68	MET	CG-SD-CE	-5.44	91.50	100.20
1	I	68	MET	CG-SD-CE	-5.43	91.51	100.20
1	G	68	MET	CG-SD-CE	-5.43	91.51	100.20
1	G	139	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	F	68	MET	CG-SD-CE	-5.43	91.51	100.20
1	K	68	MET	CG-SD-CE	-5.43	91.51	100.20
1	L	452	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	452	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	D	68	MET	CG-SD-CE	-5.41	91.55	100.20
1	B	20	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	L	20	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	J	20	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	452	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	D	20	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	452	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	I	452	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	C	20	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	G	20	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	452	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	20	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	20	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	452	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	20	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	452	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	E	20	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	G	20	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	175	VAL	CA-C-N	5.30	128.87	117.20
1	B	175	VAL	CA-C-N	5.30	128.85	117.20
1	E	175	VAL	CA-C-N	5.30	128.85	117.20
1	A	175	VAL	CA-C-N	5.29	128.85	117.20
1	F	20	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	20	ARG	NE-CZ-NH2	-5.29	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	175	VAL	CA-C-N	5.29	128.85	117.20
1	I	175	VAL	CA-C-N	5.29	128.84	117.20
1	K	175	VAL	CA-C-N	5.29	128.83	117.20
1	L	20	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	F	175	VAL	CA-C-N	5.29	128.83	117.20
1	G	175	VAL	CA-C-N	5.29	128.83	117.20
1	J	175	VAL	CA-C-N	5.29	128.83	117.20
1	J	20	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	L	175	VAL	CA-C-N	5.28	128.82	117.20
1	A	20	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	H	175	VAL	CA-C-N	5.27	128.80	117.20
1	I	20	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	H	172	ARG	N-CA-CB	-5.26	101.12	110.60
1	E	172	ARG	N-CA-CB	-5.26	101.13	110.60
1	B	172	ARG	N-CA-CB	-5.26	101.13	110.60
1	D	20	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	J	172	ARG	N-CA-CB	-5.26	101.13	110.60
1	G	164	TYR	O-C-N	-5.26	114.29	122.70
1	H	20	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	K	172	ARG	N-CA-CB	-5.25	101.14	110.60
1	F	20	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	I	20	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	172	ARG	N-CA-CB	-5.25	101.15	110.60
1	H	164	TYR	O-C-N	-5.25	114.30	122.70
1	K	263	ASP	CB-CG-OD1	5.25	123.02	118.30
1	L	164	TYR	O-C-N	-5.25	114.30	122.70
1	A	172	ARG	N-CA-CB	-5.24	101.16	110.60
1	B	447	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	172	ARG	N-CA-CB	-5.24	101.16	110.60
1	D	263	ASP	CB-CG-OD1	5.24	123.02	118.30
1	F	172	ARG	N-CA-CB	-5.24	101.16	110.60
1	J	164	TYR	O-C-N	-5.24	114.31	122.70
1	K	20	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	164	TYR	O-C-N	-5.24	114.32	122.70
1	B	164	TYR	O-C-N	-5.24	114.32	122.70
1	E	263	ASP	CB-CG-OD1	5.23	123.01	118.30
1	G	263	ASP	CB-CG-OD1	5.23	123.01	118.30
1	I	263	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	164	TYR	O-C-N	-5.23	114.33	122.70
1	D	164	TYR	O-C-N	-5.23	114.33	122.70
1	K	164	TYR	O-C-N	-5.23	114.34	122.70
1	L	172	ARG	N-CA-CB	-5.23	101.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	172	ARG	N-CA-CB	-5.22	101.19	110.60
1	I	172	ARG	N-CA-CB	-5.22	101.20	110.60
1	C	263	ASP	CB-CG-OD1	5.22	123.00	118.30
1	G	447	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	J	263	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	447	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	F	164	TYR	O-C-N	-5.21	114.36	122.70
1	K	20	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	164	TYR	O-C-N	-5.21	114.36	122.70
1	F	263	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	263	ASP	CB-CG-OD1	5.21	122.98	118.30
1	K	447	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	263	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	447	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	L	263	ASP	CB-CG-OD1	5.19	122.97	118.30
1	I	164	TYR	O-C-N	-5.19	114.39	122.70
1	C	447	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	447	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	L	447	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	H	263	ASP	CB-CG-OD1	5.17	122.95	118.30
1	H	20	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	I	447	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	H	447	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	J	447	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	F	447	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	I	15	LYS	CA-CB-CG	-5.05	102.29	113.40
1	D	15	LYS	CA-CB-CG	-5.04	102.32	113.40
1	G	15	LYS	CA-CB-CG	-5.04	102.32	113.40
1	B	15	LYS	CA-CB-CG	-5.03	102.33	113.40
1	L	15	LYS	CA-CB-CG	-5.03	102.33	113.40
1	C	15	LYS	CA-CB-CG	-5.03	102.34	113.40
1	K	15	LYS	CA-CB-CG	-5.03	102.34	113.40
1	A	15	LYS	CA-CB-CG	-5.03	102.34	113.40
1	E	15	LYS	CA-CB-CG	-5.02	102.35	113.40
1	F	15	LYS	CA-CB-CG	-5.02	102.35	113.40
1	J	15	LYS	CA-CB-CG	-5.02	102.36	113.40
1	H	15	LYS	CA-CB-CG	-5.01	102.38	113.40

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	352	LYS	Peptide
1	B	224	ARG	Sidechain
1	B	352	LYS	Peptide
1	C	224	ARG	Sidechain
1	C	352	LYS	Peptide
1	D	224	ARG	Sidechain
1	D	352	LYS	Peptide
1	E	224	ARG	Sidechain
1	E	352	LYS	Peptide
1	F	224	ARG	Sidechain
1	F	352	LYS	Peptide
1	G	224	ARG	Sidechain
1	G	352	LYS	Peptide
1	H	224	ARG	Sidechain
1	H	352	LYS	Peptide
1	I	224	ARG	Sidechain
1	I	352	LYS	Peptide
1	J	224	ARG	Sidechain
1	J	352	LYS	Peptide
1	K	224	ARG	Sidechain
1	K	352	LYS	Peptide
1	L	224	ARG	Sidechain
1	L	352	LYS	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	3455	0	3371	53	0
1	B	3455	0	3371	51	0
1	C	3455	0	3371	57	2
1	D	3455	0	3371	54	0
1	E	3455	0	3371	52	0
1	F	3455	0	3371	53	2
1	G	3455	0	3371	51	0
1	H	3455	0	3371	56	0
1	I	3455	0	3371	54	0
1	J	3455	0	3371	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3455	0	3371	59	0
1	L	3455	0	3371	54	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	10	0	5	1	0
3	B	10	0	5	1	0
3	C	10	0	5	1	0
3	D	10	0	5	1	0
3	E	10	0	5	1	0
3	F	10	0	5	1	0
3	G	10	0	5	1	0
3	H	10	0	5	1	0
3	I	10	0	5	1	0
3	J	10	0	5	1	0
3	K	10	0	5	1	0
3	L	10	0	5	1	0
All	All	41604	0	40512	592	2

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 7.

All (592) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:258:LYS:HG2	1:K:320:LYS:HB3	1.79	0.65
1:C:258:LYS:HG2	1:C:320:LYS:HB3	1.79	0.65
1:E:258:LYS:HG2	1:E:320:LYS:HB3	1.79	0.65
1:G:258:LYS:HG2	1:G:320:LYS:HB3	1.79	0.65
1:F:258:LYS:HG2	1:F:320:LYS:HB3	1.79	0.65
1:I:258:LYS:HG2	1:I:320:LYS:HB3	1.79	0.65
1:B:258:LYS:HG2	1:B:320:LYS:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:258:LYS:HG2	1:L:320:LYS:HB3	1.79	0.64
1:A:258:LYS:HG2	1:A:320:LYS:HB3	1.79	0.63
1:J:258:LYS:HG2	1:J:320:LYS:HB3	1.79	0.63
1:H:258:LYS:HG2	1:H:320:LYS:HB3	1.79	0.63
1:D:258:LYS:HG2	1:D:320:LYS:HB3	1.79	0.63
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.64	0.63
1:C:261:PHE:HB2	1:K:457:PRO:HD2	1.79	0.63
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.64	0.63
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.64	0.62
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.64	0.62
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.64	0.62
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.64	0.62
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.64	0.62
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.64	0.62
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.64	0.62
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.64	0.61
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.64	0.61
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.64	0.61
1:C:92:LEU:HA	1:C:99:GLY:HA2	1.83	0.61
1:A:92:LEU:HA	1:A:99:GLY:HA2	1.83	0.61
1:D:456:THR:O	1:J:458:HIS:HE1	1.84	0.61
1:E:92:LEU:HA	1:E:99:GLY:HA2	1.83	0.61
1:C:383:LYS:NZ	1:C:383:LYS:HB3	2.16	0.61
1:I:92:LEU:HA	1:I:99:GLY:HA2	1.83	0.61
1:A:383:LYS:NZ	1:A:383:LYS:HB3	2.16	0.61
1:J:92:LEU:HA	1:J:99:GLY:HA2	1.83	0.60
1:L:92:LEU:HA	1:L:99:GLY:HA2	1.83	0.60
1:D:383:LYS:NZ	1:D:383:LYS:HB3	2.16	0.60
1:G:92:LEU:HA	1:G:99:GLY:HA2	1.83	0.60
1:H:92:LEU:HA	1:H:99:GLY:HA2	1.83	0.60
1:H:383:LYS:NZ	1:H:383:LYS:HB3	2.16	0.60
1:K:92:LEU:HA	1:K:99:GLY:HA2	1.83	0.60
1:L:383:LYS:NZ	1:L:383:LYS:HB3	2.16	0.60
1:D:92:LEU:HA	1:D:99:GLY:HA2	1.83	0.60
1:J:383:LYS:HB3	1:J:383:LYS:NZ	2.16	0.60
1:E:383:LYS:NZ	1:E:383:LYS:HB3	2.16	0.60
1:H:214:ALA:HB3	1:H:218:GLN:HB2	1.84	0.60
1:F:214:ALA:HB3	1:F:218:GLN:HB2	1.84	0.60
1:F:92:LEU:HA	1:F:99:GLY:HA2	1.83	0.60
1:C:214:ALA:HB3	1:C:218:GLN:HB2	1.84	0.59
1:B:92:LEU:HA	1:B:99:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LYS:HB3	1:B:383:LYS:NZ	2.16	0.59
1:F:383:LYS:NZ	1:F:383:LYS:HB3	2.16	0.59
1:I:383:LYS:NZ	1:I:383:LYS:HB3	2.16	0.59
1:J:214:ALA:HB3	1:J:218:GLN:HB2	1.84	0.59
1:K:383:LYS:NZ	1:K:383:LYS:HB3	2.16	0.59
1:A:214:ALA:HB3	1:A:218:GLN:HB2	1.84	0.59
1:C:457:PRO:HD2	1:K:261:PHE:HB2	1.84	0.59
1:D:214:ALA:HB3	1:D:218:GLN:HB2	1.84	0.59
1:I:214:ALA:HB3	1:I:218:GLN:HB2	1.84	0.59
1:K:214:ALA:HB3	1:K:218:GLN:HB2	1.84	0.59
1:B:457:PRO:HD2	1:L:261:PHE:HB2	1.84	0.59
1:L:214:ALA:HB3	1:L:218:GLN:HB2	1.84	0.59
1:E:214:ALA:HB3	1:E:218:GLN:HB2	1.84	0.59
1:A:269:HIS:HE1	1:A:359:ARG:NH1	2.01	0.59
1:G:383:LYS:NZ	1:G:383:LYS:HB3	2.16	0.59
1:F:269:HIS:HE1	1:F:359:ARG:NH1	2.01	0.59
1:B:214:ALA:HB3	1:B:218:GLN:HB2	1.84	0.59
1:G:214:ALA:HB3	1:G:218:GLN:HB2	1.84	0.59
1:G:269:HIS:HE1	1:G:359:ARG:NH1	2.01	0.59
1:H:425:ARG:HG2	1:H:429:LYS:HD2	1.85	0.59
1:J:180:PHE:HB3	1:K:29:GLN:HB3	1.82	0.59
1:J:269:HIS:HE1	1:J:359:ARG:NH1	2.01	0.59
1:C:269:HIS:HE1	1:C:359:ARG:NH1	2.01	0.58
1:A:425:ARG:HG2	1:A:429:LYS:HD2	1.85	0.58
1:D:269:HIS:HE1	1:D:359:ARG:NH1	2.01	0.58
1:D:180:PHE:HB3	1:E:29:GLN:HB3	1.84	0.58
1:E:457:PRO:HD2	1:I:261:PHE:HB2	1.86	0.58
1:B:76:ILE:HD12	1:B:85:LEU:HD23	1.86	0.58
1:D:458:HIS:HE1	1:J:456:THR:O	1.86	0.58
1:E:425:ARG:HG2	1:E:429:LYS:HD2	1.85	0.58
1:G:76:ILE:HD12	1:G:85:LEU:HD23	1.86	0.58
1:G:425:ARG:HG2	1:G:429:LYS:HD2	1.85	0.58
1:I:269:HIS:HE1	1:I:359:ARG:NH1	2.01	0.58
1:K:425:ARG:HG2	1:K:429:LYS:HD2	1.85	0.58
1:D:425:ARG:HG2	1:D:429:LYS:HD2	1.85	0.58
1:E:76:ILE:HD12	1:E:85:LEU:HD23	1.86	0.58
1:J:76:ILE:HD12	1:J:85:LEU:HD23	1.86	0.58
1:D:76:ILE:HD12	1:D:85:LEU:HD23	1.86	0.58
1:E:269:HIS:HE1	1:E:359:ARG:NH1	2.01	0.58
1:F:76:ILE:HD12	1:F:85:LEU:HD23	1.86	0.58
1:B:19:LEU:HD11	1:B:42:PHE:HZ	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:76:ILE:HD12	1:I:85:LEU:HD23	1.86	0.58
1:J:425:ARG:HG2	1:J:429:LYS:HD2	1.84	0.58
1:L:76:ILE:HD12	1:L:85:LEU:HD23	1.86	0.58
1:F:456:THR:O	1:H:458:HIS:HE1	1.85	0.58
1:H:19:LEU:HD11	1:H:42:PHE:HZ	1.69	0.58
1:B:425:ARG:HG2	1:B:429:LYS:HD2	1.85	0.58
1:F:19:LEU:HD11	1:F:42:PHE:HZ	1.69	0.58
1:F:458:HIS:HE1	1:H:456:THR:O	1.86	0.58
1:J:19:LEU:HD11	1:J:42:PHE:HZ	1.69	0.58
1:L:269:HIS:HE1	1:L:359:ARG:NH1	2.01	0.58
1:L:425:ARG:HG2	1:L:429:LYS:HD2	1.85	0.58
1:A:76:ILE:HD12	1:A:85:LEU:HD23	1.86	0.57
1:C:76:ILE:HD12	1:C:85:LEU:HD23	1.86	0.57
1:K:269:HIS:HE1	1:K:359:ARG:NH1	2.01	0.57
1:H:269:HIS:HE1	1:H:359:ARG:NH1	2.01	0.57
1:F:425:ARG:HG2	1:F:429:LYS:HD2	1.85	0.57
1:I:425:ARG:HG2	1:I:429:LYS:HD2	1.85	0.57
1:C:425:ARG:HG2	1:C:429:LYS:HD2	1.85	0.57
1:E:456:THR:O	1:I:458:HIS:HE1	1.87	0.57
1:G:19:LEU:HD11	1:G:42:PHE:HZ	1.69	0.57
1:L:314:PRO:HB2	1:L:446:ARG:NH1	2.20	0.57
1:E:19:LEU:HD11	1:E:42:PHE:HZ	1.69	0.57
1:E:314:PRO:HB2	1:E:446:ARG:NH1	2.20	0.57
1:K:19:LEU:HD11	1:K:42:PHE:HZ	1.69	0.57
1:H:66:VAL:HG13	1:H:92:LEU:HB2	1.87	0.57
1:K:66:VAL:HG13	1:K:92:LEU:HB2	1.87	0.57
1:B:269:HIS:HE1	1:B:359:ARG:NH1	2.01	0.57
1:E:66:VAL:HG13	1:E:92:LEU:HB2	1.87	0.57
1:L:19:LEU:HD11	1:L:42:PHE:HZ	1.69	0.57
1:L:66:VAL:HG13	1:L:92:LEU:HB2	1.87	0.57
1:B:261:PHE:HB2	1:L:457:PRO:HD2	1.86	0.57
1:H:76:ILE:HD12	1:H:85:LEU:HD23	1.86	0.57
1:I:66:VAL:HG13	1:I:92:LEU:HB2	1.87	0.57
1:K:76:ILE:HD12	1:K:85:LEU:HD23	1.86	0.57
1:B:66:VAL:HG13	1:B:92:LEU:HB2	1.87	0.57
1:A:456:THR:O	1:G:458:HIS:HE1	1.88	0.56
1:D:19:LEU:HD11	1:D:42:PHE:HZ	1.69	0.56
1:A:66:VAL:HG13	1:A:92:LEU:HB2	1.87	0.56
1:A:314:PRO:HB2	1:A:446:ARG:NH1	2.20	0.56
1:A:457:PRO:HD2	1:G:261:PHE:HB2	1.87	0.56
1:C:19:LEU:HD11	1:C:42:PHE:HZ	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:VAL:HG13	1:D:92:LEU:HB2	1.87	0.56
1:D:314:PRO:HB2	1:D:446:ARG:NH1	2.20	0.56
1:H:314:PRO:HB2	1:H:446:ARG:NH1	2.20	0.56
1:I:314:PRO:HB2	1:I:446:ARG:NH1	2.20	0.56
1:J:314:PRO:HB2	1:J:446:ARG:NH1	2.20	0.56
1:A:19:LEU:HD11	1:A:42:PHE:HZ	1.69	0.56
1:B:351:PRO:HB2	1:B:352:LYS:HG3	1.88	0.56
1:C:66:VAL:HG13	1:C:92:LEU:HB2	1.87	0.56
1:I:19:LEU:HD11	1:I:42:PHE:HZ	1.69	0.56
1:J:351:PRO:HB2	1:J:352:LYS:HG3	1.88	0.56
1:K:314:PRO:HB2	1:K:446:ARG:NH1	2.20	0.56
1:A:261:PHE:HB2	1:G:457:PRO:HD2	1.88	0.56
1:C:314:PRO:HB2	1:C:446:ARG:NH1	2.20	0.56
1:F:66:VAL:HG13	1:F:92:LEU:HB2	1.87	0.56
1:G:314:PRO:HB2	1:G:446:ARG:NH1	2.20	0.56
1:L:351:PRO:HB2	1:L:352:LYS:HG3	1.88	0.56
1:C:351:PRO:HB2	1:C:352:LYS:HG3	1.88	0.56
1:E:351:PRO:HB2	1:E:352:LYS:HG3	1.88	0.56
1:B:314:PRO:HB2	1:B:446:ARG:NH1	2.20	0.56
1:E:261:PHE:HB2	1:I:457:PRO:HD2	1.88	0.56
1:G:66:VAL:HG13	1:G:92:LEU:HB2	1.87	0.56
1:K:351:PRO:HB2	1:K:352:LYS:HG3	1.88	0.56
1:F:314:PRO:HB2	1:F:446:ARG:NH1	2.20	0.55
1:J:66:VAL:HG13	1:J:92:LEU:HB2	1.87	0.55
1:F:351:PRO:HB2	1:F:352:LYS:HG3	1.88	0.55
1:G:351:PRO:HB2	1:G:352:LYS:HG3	1.88	0.55
1:A:93:GLU:HB3	1:A:98:GLN:OE1	2.07	0.55
1:A:458:HIS:HE1	1:G:456:THR:O	1.89	0.55
1:C:93:GLU:HB3	1:C:98:GLN:OE1	2.07	0.55
1:I:351:PRO:HB2	1:I:352:LYS:HG3	1.88	0.55
1:D:93:GLU:HB3	1:D:98:GLN:OE1	2.07	0.55
1:H:351:PRO:HB2	1:H:352:LYS:HG3	1.88	0.55
1:K:93:GLU:HB3	1:K:98:GLN:OE1	2.07	0.55
1:L:458:HIS:HD2	1:L:460:VAL:H	1.55	0.55
1:A:458:HIS:HD2	1:A:460:VAL:H	1.55	0.55
1:B:93:GLU:HB3	1:B:98:GLN:OE1	2.07	0.54
1:D:351:PRO:HB2	1:D:352:LYS:HG3	1.88	0.54
1:H:93:GLU:HB3	1:H:98:GLN:OE1	2.07	0.54
1:J:93:GLU:HB3	1:J:98:GLN:OE1	2.07	0.54
1:A:351:PRO:HB2	1:A:352:LYS:HG3	1.88	0.54
1:I:93:GLU:HB3	1:I:98:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:HIS:HE1	1:I:456:THR:O	1.89	0.54
1:G:93:GLU:HB3	1:G:98:GLN:OE1	2.07	0.54
1:I:458:HIS:HD2	1:I:460:VAL:H	1.55	0.54
1:E:458:HIS:HD2	1:E:460:VAL:H	1.55	0.54
1:F:93:GLU:HB3	1:F:98:GLN:OE1	2.07	0.54
1:H:458:HIS:HD2	1:H:460:VAL:H	1.55	0.54
1:C:180:PHE:HB3	1:D:29:GLN:HB3	1.90	0.54
1:G:458:HIS:HD2	1:G:460:VAL:H	1.55	0.54
1:H:180:PHE:HB3	1:I:29:GLN:HB3	1.89	0.54
1:J:458:HIS:HD2	1:J:460:VAL:H	1.55	0.54
1:L:93:GLU:HB3	1:L:98:GLN:OE1	2.07	0.54
1:F:458:HIS:HD2	1:F:460:VAL:H	1.55	0.54
1:C:192:ARG:HD3	1:C:219:ASN:ND2	2.23	0.53
1:C:458:HIS:HD2	1:C:460:VAL:H	1.55	0.53
1:D:458:HIS:HD2	1:D:460:VAL:H	1.55	0.53
1:I:192:ARG:HD3	1:I:219:ASN:ND2	2.23	0.53
1:B:458:HIS:HE1	1:L:456:THR:O	1.91	0.53
1:E:93:GLU:HB3	1:E:98:GLN:OE1	2.07	0.53
1:G:192:ARG:HD3	1:G:219:ASN:ND2	2.23	0.53
1:A:192:ARG:HD3	1:A:219:ASN:ND2	2.23	0.53
1:B:456:THR:O	1:L:458:HIS:HE1	1.90	0.53
1:D:457:PRO:HD2	1:J:261:PHE:HB2	1.89	0.53
1:H:286:LYS:HB2	1:H:290:LEU:O	2.09	0.53
1:L:286:LYS:HB2	1:L:290:LEU:O	2.09	0.53
1:K:192:ARG:HD3	1:K:219:ASN:ND2	2.23	0.53
1:F:286:LYS:HB2	1:F:290:LEU:O	2.09	0.53
1:D:261:PHE:HB2	1:J:457:PRO:HD2	1.89	0.53
1:D:286:LYS:HB2	1:D:290:LEU:O	2.09	0.53
1:F:192:ARG:HD3	1:F:219:ASN:ND2	2.23	0.53
1:G:286:LYS:HB2	1:G:290:LEU:O	2.09	0.53
1:J:192:ARG:HD3	1:J:219:ASN:ND2	2.24	0.53
1:B:458:HIS:HD2	1:B:460:VAL:H	1.55	0.53
1:F:457:PRO:HD2	1:H:261:PHE:HB2	1.90	0.53
1:H:192:ARG:HD3	1:H:219:ASN:ND2	2.23	0.53
1:E:286:LYS:HB2	1:E:290:LEU:O	2.09	0.53
1:B:180:PHE:HB3	1:C:29:GLN:HB3	1.91	0.53
1:D:192:ARG:HD3	1:D:219:ASN:ND2	2.23	0.53
1:J:286:LYS:HB2	1:J:290:LEU:O	2.09	0.53
1:B:286:LYS:HB2	1:B:290:LEU:O	2.09	0.52
1:C:286:LYS:HB2	1:C:290:LEU:O	2.09	0.52
1:K:458:HIS:HD2	1:K:460:VAL:H	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:ARG:HD3	1:E:219:ASN:ND2	2.23	0.52
1:I:286:LYS:HB2	1:I:290:LEU:O	2.09	0.52
1:D:348:VAL:HG21	1:D:353:ALA:HB3	1.92	0.52
1:G:348:VAL:HG21	1:G:353:ALA:HB3	1.92	0.52
1:L:192:ARG:HD3	1:L:219:ASN:ND2	2.23	0.52
1:A:29:GLN:HB3	1:F:180:PHE:HB3	1.90	0.52
1:A:286:LYS:HB2	1:A:290:LEU:O	2.09	0.52
1:B:192:ARG:HD3	1:B:219:ASN:ND2	2.23	0.52
1:G:5:VAL:HG11	1:G:43:PHE:HZ	1.75	0.52
1:K:348:VAL:HG21	1:K:353:ALA:HB3	1.92	0.52
1:I:348:VAL:HG21	1:I:353:ALA:HB3	1.92	0.52
1:A:348:VAL:HG21	1:A:353:ALA:HB3	1.92	0.52
1:D:5:VAL:HG11	1:D:43:PHE:HZ	1.75	0.52
1:F:348:VAL:HG21	1:F:353:ALA:HB3	1.92	0.52
1:K:286:LYS:HB2	1:K:290:LEU:O	2.09	0.52
1:A:180:PHE:HB3	1:B:29:GLN:HB3	1.90	0.52
1:C:5:VAL:HG11	1:C:43:PHE:HZ	1.75	0.52
1:C:348:VAL:HG21	1:C:353:ALA:HB3	1.92	0.52
1:K:5:VAL:HG11	1:K:43:PHE:HZ	1.75	0.51
1:E:5:VAL:HG11	1:E:43:PHE:HZ	1.75	0.51
1:K:180:PHE:HB3	1:L:29:GLN:HB3	1.92	0.51
1:L:348:VAL:HG21	1:L:353:ALA:HB3	1.92	0.51
1:B:5:VAL:HG11	1:B:43:PHE:HZ	1.75	0.51
1:I:5:VAL:HG11	1:I:43:PHE:HZ	1.75	0.51
1:K:169:LYS:HA	1:L:252:THR:HB	1.91	0.51
1:H:5:VAL:HG11	1:H:43:PHE:HZ	1.75	0.51
1:I:180:PHE:HB3	1:J:29:GLN:HB3	1.93	0.51
1:B:348:VAL:HG21	1:B:353:ALA:HB3	1.92	0.51
1:F:5:VAL:HG11	1:F:43:PHE:HZ	1.75	0.51
1:E:348:VAL:HG21	1:E:353:ALA:HB3	1.92	0.51
1:E:467:SER:OG	1:H:171:HIS:ND1	2.35	0.51
1:F:261:PHE:HB2	1:H:457:PRO:HD2	1.92	0.51
1:B:169:LYS:HA	1:C:252:THR:HB	1.92	0.50
1:J:348:VAL:HG21	1:J:353:ALA:HB3	1.92	0.50
1:D:169:LYS:HA	1:E:252:THR:HB	1.92	0.50
1:E:333:ALA:O	1:E:341:ALA:HB1	2.12	0.50
1:G:29:GLN:HB3	1:L:180:PHE:HB3	1.93	0.50
1:K:101:ASP:HB3	1:K:110:ARG:HH22	1.76	0.50
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.47	0.50
1:C:458:HIS:HE1	1:K:456:THR:O	1.93	0.50
1:J:5:VAL:HG11	1:J:43:PHE:HZ	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:333:ALA:O	1:K:341:ALA:HB1	2.12	0.50
1:L:5:VAL:HG11	1:L:43:PHE:HZ	1.75	0.50
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.47	0.50
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.47	0.50
1:B:333:ALA:O	1:B:341:ALA:HB1	2.12	0.50
1:C:101:ASP:HB3	1:C:110:ARG:HH22	1.77	0.50
1:G:333:ALA:O	1:G:341:ALA:HB1	2.12	0.50
1:H:348:VAL:HG21	1:H:353:ALA:HB3	1.92	0.50
1:D:101:ASP:HB3	1:D:110:ARG:HH22	1.77	0.50
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.47	0.50
1:E:101:ASP:HB3	1:E:110:ARG:HH22	1.76	0.50
1:G:296:TYR:CZ	1:G:385:LYS:HG2	2.47	0.50
1:H:333:ALA:O	1:H:341:ALA:HB1	2.12	0.50
1:H:359:ARG:NH1	3:H:471:GLU:OE1	2.44	0.50
1:E:296:TYR:CZ	1:E:385:LYS:HG2	2.47	0.49
1:F:101:ASP:HB3	1:F:110:ARG:HH22	1.77	0.49
1:F:333:ALA:O	1:F:341:ALA:HB1	2.12	0.49
1:H:101:ASP:HB3	1:H:110:ARG:HH22	1.77	0.49
1:B:296:TYR:CZ	1:B:385:LYS:HG2	2.47	0.49
1:I:296:TYR:CZ	1:I:385:LYS:HG2	2.47	0.49
1:I:333:ALA:O	1:I:341:ALA:HB1	2.12	0.49
1:K:296:TYR:CZ	1:K:385:LYS:HG2	2.47	0.49
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.47	0.49
1:F:296:TYR:CZ	1:F:385:LYS:HG2	2.47	0.49
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.47	0.49
1:A:5:VAL:HG11	1:A:43:PHE:HZ	1.75	0.49
1:D:296:TYR:CZ	1:D:385:LYS:HG2	2.47	0.49
1:C:333:ALA:O	1:C:341:ALA:HB1	2.12	0.49
1:I:101:ASP:HB3	1:I:110:ARG:HH22	1.77	0.49
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.47	0.49
1:J:101:ASP:HB3	1:J:110:ARG:HH22	1.77	0.49
1:J:296:TYR:CZ	1:J:385:LYS:HG2	2.47	0.49
1:J:333:ALA:O	1:J:341:ALA:HB1	2.12	0.49
1:K:359:ARG:NH1	3:K:471:GLU:OE1	2.45	0.49
1:B:101:ASP:HB3	1:B:110:ARG:HH22	1.76	0.49
1:D:333:ALA:O	1:D:341:ALA:HB1	2.12	0.49
1:E:359:ARG:NH1	3:E:471:GLU:OE1	2.45	0.49
1:F:334:TYR:CE1	1:F:388:PRO:HB2	2.48	0.49
1:G:334:TYR:CE1	1:G:388:PRO:HB2	2.48	0.49
1:L:333:ALA:O	1:L:341:ALA:HB1	2.12	0.49
1:A:17:VAL:HG21	1:A:38:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:HB3	1:A:110:ARG:HH22	1.76	0.49
1:H:334:TYR:CE1	1:H:388:PRO:HB2	2.48	0.49
1:I:334:TYR:CE1	1:I:388:PRO:HB2	2.48	0.49
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.47	0.49
1:L:296:TYR:CZ	1:L:385:LYS:HG2	2.47	0.49
1:C:296:TYR:CZ	1:C:385:LYS:HG2	2.47	0.49
1:C:359:ARG:NH1	3:C:471:GLU:OE1	2.45	0.49
1:G:101:ASP:HB3	1:G:110:ARG:HH22	1.76	0.49
1:A:296:TYR:CZ	1:A:385:LYS:HG2	2.47	0.48
1:B:334:TYR:CE1	1:B:388:PRO:HB2	2.48	0.48
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.47	0.48
1:J:334:TYR:CE1	1:J:388:PRO:HB2	2.48	0.48
1:D:334:TYR:CE1	1:D:388:PRO:HB2	2.48	0.48
1:G:180:PHE:HB3	1:H:29:GLN:HB3	1.94	0.48
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.47	0.48
1:K:334:TYR:CE1	1:K:388:PRO:HB2	2.48	0.48
1:L:101:ASP:HB3	1:L:110:ARG:HH22	1.76	0.48
1:A:169:LYS:HA	1:B:252:THR:HB	1.96	0.48
1:I:17:VAL:HG21	1:I:38:VAL:HG21	1.95	0.48
1:L:17:VAL:HG21	1:L:38:VAL:HG21	1.95	0.48
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.47	0.48
1:C:334:TYR:CE1	1:C:388:PRO:HB2	2.48	0.48
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.47	0.48
1:C:17:VAL:HG21	1:C:38:VAL:HG21	1.95	0.48
1:C:456:THR:O	1:K:458:HIS:HE1	1.95	0.48
1:E:334:TYR:CE1	1:E:388:PRO:HB2	2.48	0.48
1:L:231:LYS:HA	1:L:231:LYS:HD2	1.66	0.48
1:L:334:TYR:CE1	1:L:388:PRO:HB2	2.48	0.48
1:E:17:VAL:HG21	1:E:38:VAL:HG21	1.95	0.48
1:H:17:VAL:HG21	1:H:38:VAL:HG21	1.95	0.48
1:H:296:TYR:CZ	1:H:385:LYS:HG2	2.47	0.48
1:J:17:VAL:HG21	1:J:38:VAL:HG21	1.95	0.48
1:A:334:TYR:CE1	1:A:388:PRO:HB2	2.48	0.48
1:D:17:VAL:HG21	1:D:38:VAL:HG21	1.95	0.48
1:D:120:ILE:O	1:D:281:LEU:HD21	2.14	0.48
1:E:270:CYS:HG	1:E:371:PHE:HE1	1.62	0.48
1:A:333:ALA:O	1:A:341:ALA:HB1	2.12	0.48
1:B:17:VAL:HG21	1:B:38:VAL:HG21	1.95	0.48
1:G:120:ILE:O	1:G:281:LEU:HD21	2.14	0.48
1:H:120:ILE:O	1:H:281:LEU:HD21	2.14	0.48
1:B:458:HIS:CD2	1:B:460:VAL:H	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:O	1:C:281:LEU:HD21	2.14	0.48
1:F:120:ILE:O	1:F:281:LEU:HD21	2.14	0.48
1:J:270:CYS:HG	1:J:371:PHE:HE1	1.62	0.48
1:K:120:ILE:O	1:K:281:LEU:HD21	2.14	0.48
1:A:120:ILE:O	1:A:281:LEU:HD21	2.14	0.47
1:B:120:ILE:O	1:B:281:LEU:HD21	2.14	0.47
1:B:359:ARG:NH1	3:B:473:GLU:OE1	2.45	0.47
1:G:231:LYS:HD2	1:G:231:LYS:HA	1.66	0.47
1:J:120:ILE:O	1:J:281:LEU:HD21	2.14	0.47
1:C:169:LYS:HA	1:D:252:THR:HB	1.96	0.47
1:C:270:CYS:HG	1:C:371:PHE:HE1	1.62	0.47
1:E:458:HIS:CD2	1:E:460:VAL:H	2.32	0.47
1:G:17:VAL:HG21	1:G:38:VAL:HG21	1.95	0.47
1:H:169:LYS:HA	1:I:252:THR:HB	1.96	0.47
1:K:458:HIS:CD2	1:K:460:VAL:H	2.32	0.47
1:L:65:MET:HE2	1:L:94:PRO:HD3	1.96	0.47
1:F:339:ARG:CZ	1:F:359:ARG:NH2	2.78	0.47
1:J:458:HIS:CD2	1:J:460:VAL:H	2.32	0.47
1:K:17:VAL:HG21	1:K:38:VAL:HG21	1.95	0.47
1:D:339:ARG:CZ	1:D:359:ARG:NH2	2.78	0.47
1:G:339:ARG:CZ	1:G:359:ARG:NH2	2.78	0.47
1:L:120:ILE:O	1:L:281:LEU:HD21	2.14	0.47
1:A:339:ARG:CZ	1:A:359:ARG:NH2	2.78	0.47
1:B:339:ARG:CZ	1:B:359:ARG:NH2	2.78	0.47
1:D:359:ARG:NH1	3:D:471:GLU:OE1	2.45	0.47
1:E:120:ILE:O	1:E:281:LEU:HD21	2.14	0.47
1:F:17:VAL:HG21	1:F:38:VAL:HG21	1.95	0.47
1:G:458:HIS:CD2	1:G:460:VAL:H	2.32	0.47
1:H:339:ARG:CZ	1:H:359:ARG:NH2	2.78	0.47
1:H:458:HIS:CD2	1:H:460:VAL:H	2.32	0.47
1:I:359:ARG:NH1	3:I:471:GLU:OE1	2.45	0.47
1:E:231:LYS:HD2	1:E:231:LYS:HA	1.66	0.47
1:E:339:ARG:CZ	1:E:359:ARG:NH2	2.78	0.47
1:E:180:PHE:HB3	1:F:29:GLN:HB3	1.96	0.47
1:F:359:ARG:NH1	3:F:471:GLU:OE1	2.44	0.47
1:G:252:THR:HB	1:L:169:LYS:HA	1.96	0.47
1:L:339:ARG:CZ	1:L:359:ARG:NH2	2.78	0.47
1:I:65:MET:HE2	1:I:94:PRO:HD3	1.98	0.47
1:I:169:LYS:HA	1:J:252:THR:HB	1.96	0.47
1:K:339:ARG:CZ	1:K:359:ARG:NH2	2.78	0.46
1:A:458:HIS:CD2	1:A:460:VAL:H	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:PHE:HB3	1:F:363:PRO:HB2	1.98	0.46
1:I:383:LYS:HB3	1:I:383:LYS:HZ3	1.79	0.46
1:I:458:HIS:CD2	1:I:460:VAL:H	2.32	0.46
1:I:339:ARG:CZ	1:I:359:ARG:NH2	2.78	0.46
1:J:339:ARG:CZ	1:J:359:ARG:NH2	2.78	0.46
1:B:255:PHE:HB3	1:B:363:PRO:HB2	1.98	0.46
1:L:458:HIS:CD2	1:L:460:VAL:H	2.32	0.46
1:A:270:CYS:HG	1:A:371:PHE:HE1	1.64	0.46
1:D:270:CYS:HG	1:D:371:PHE:HE1	1.63	0.46
1:G:255:PHE:HB3	1:G:363:PRO:HB2	1.98	0.46
1:L:359:ARG:NH1	3:L:471:GLU:OE1	2.45	0.46
1:D:458:HIS:CD2	1:D:460:VAL:H	2.32	0.46
1:H:270:CYS:HG	1:H:371:PHE:HE1	1.63	0.46
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.98	0.46
1:L:255:PHE:HB3	1:L:363:PRO:HB2	1.98	0.46
1:A:359:ARG:NH1	3:A:471:GLU:OE1	2.45	0.46
1:C:339:ARG:CZ	1:C:359:ARG:NH2	2.78	0.46
1:B:270:CYS:HG	1:B:371:PHE:HE1	1.64	0.46
1:D:255:PHE:HB3	1:D:363:PRO:HB2	1.98	0.46
1:E:169:LYS:HA	1:F:252:THR:HB	1.98	0.46
1:H:255:PHE:HB3	1:H:363:PRO:HB2	1.98	0.46
1:C:458:HIS:CD2	1:C:460:VAL:H	2.32	0.46
1:B:231:LYS:HA	1:B:231:LYS:HD2	1.66	0.45
1:H:168:ASN:HB3	1:I:138:ILE:O	2.16	0.45
1:I:255:PHE:HB3	1:I:363:PRO:HB2	1.98	0.45
1:J:359:ARG:NH1	3:J:471:GLU:OE1	2.45	0.45
1:F:458:HIS:CD2	1:F:460:VAL:H	2.32	0.45
1:I:196:CYS:SG	1:I:206:VAL:HG11	2.57	0.45
1:J:169:LYS:HA	1:K:252:THR:HB	1.98	0.45
1:B:196:CYS:SG	1:B:206:VAL:HG11	2.57	0.45
1:F:270:CYS:HG	1:F:371:PHE:HE1	1.62	0.45
1:I:120:ILE:O	1:I:281:LEU:HD21	2.14	0.45
1:J:339:ARG:NH2	1:K:50:ASP:CG	2.69	0.45
1:A:196:CYS:SG	1:A:206:VAL:HG11	2.57	0.45
1:A:255:PHE:HB3	1:A:363:PRO:HB2	1.98	0.45
1:C:255:PHE:HB3	1:C:363:PRO:HB2	1.98	0.45
1:K:255:PHE:HB3	1:K:363:PRO:HB2	1.98	0.45
1:C:196:CYS:SG	1:C:206:VAL:HG11	2.57	0.45
1:E:255:PHE:HB3	1:E:363:PRO:HB2	1.98	0.45
1:D:196:CYS:SG	1:D:206:VAL:HG11	2.57	0.45
1:I:270:CYS:HG	1:I:371:PHE:HE1	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:270:CYS:HG	1:L:371:PHE:HE1	1.63	0.45
1:A:231:LYS:HD2	1:A:231:LYS:HA	1.66	0.45
1:G:196:CYS:SG	1:G:206:VAL:HG11	2.57	0.45
1:G:359:ARG:NH1	3:G:471:GLU:OE1	2.45	0.45
1:J:196:CYS:SG	1:J:206:VAL:HG11	2.57	0.45
1:J:231:LYS:HD2	1:J:231:LYS:HA	1.66	0.45
1:G:269:HIS:HE1	1:G:359:ARG:CZ	2.31	0.45
1:H:196:CYS:SG	1:H:206:VAL:HG11	2.57	0.45
1:E:196:CYS:SG	1:E:206:VAL:HG11	2.57	0.44
1:E:269:HIS:HE1	1:E:359:ARG:CZ	2.31	0.44
1:K:191:ILE:HG12	1:K:249:PHE:CD2	2.53	0.44
1:K:270:CYS:HG	1:K:371:PHE:HE1	1.63	0.44
1:B:191:ILE:HG12	1:B:249:PHE:CD2	2.53	0.44
1:C:269:HIS:HE1	1:C:359:ARG:CZ	2.31	0.44
1:E:191:ILE:HG12	1:E:249:PHE:CD2	2.53	0.44
1:G:270:CYS:HG	1:G:371:PHE:HE1	1.64	0.44
1:L:191:ILE:HG12	1:L:249:PHE:CD2	2.53	0.44
1:D:191:ILE:HG12	1:D:249:PHE:CD2	2.53	0.44
1:J:269:HIS:HE1	1:J:359:ARG:CZ	2.31	0.44
1:K:196:CYS:SG	1:K:206:VAL:HG11	2.57	0.44
1:A:191:ILE:HG12	1:A:249:PHE:CD2	2.53	0.44
1:K:383:LYS:HB3	1:K:383:LYS:HZ3	1.81	0.44
1:F:196:CYS:SG	1:F:206:VAL:HG11	2.57	0.44
1:I:191:ILE:HG12	1:I:249:PHE:CD2	2.53	0.44
1:L:269:HIS:HE1	1:L:359:ARG:CZ	2.31	0.44
1:B:269:HIS:HE1	1:B:359:ARG:CZ	2.31	0.44
1:C:191:ILE:HG12	1:C:249:PHE:CD2	2.53	0.44
1:C:114:TYR:CD1	1:C:431:GLY:HA3	2.53	0.44
1:C:295:LEU:O	1:C:388:PRO:HD3	2.18	0.44
1:H:191:ILE:HG12	1:H:249:PHE:CD2	2.53	0.44
1:I:269:HIS:HE1	1:I:359:ARG:CZ	2.31	0.44
1:J:114:TYR:CD1	1:J:431:GLY:HA3	2.53	0.44
1:L:196:CYS:SG	1:L:206:VAL:HG11	2.57	0.44
1:A:114:TYR:CD1	1:A:431:GLY:HA3	2.53	0.43
1:A:295:LEU:O	1:A:388:PRO:HD3	2.18	0.43
1:D:192:ARG:HH11	1:D:219:ASN:ND2	2.16	0.43
1:G:114:TYR:CD1	1:G:431:GLY:HA3	2.53	0.43
1:E:65:MET:HE1	1:E:94:PRO:HD3	2.00	0.43
1:E:114:TYR:CD1	1:E:431:GLY:HA3	2.53	0.43
1:F:114:TYR:CD1	1:F:431:GLY:HA3	2.53	0.43
1:F:192:ARG:HH11	1:F:219:ASN:ND2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:HIS:HE1	1:F:359:ARG:CZ	2.31	0.43
1:H:114:TYR:CD1	1:H:431:GLY:HA3	2.53	0.43
1:J:191:ILE:HG12	1:J:249:PHE:CD2	2.53	0.43
1:A:192:ARG:HH11	1:A:219:ASN:ND2	2.17	0.43
1:D:269:HIS:HE1	1:D:359:ARG:CZ	2.31	0.43
1:E:192:ARG:HH11	1:E:219:ASN:ND2	2.17	0.43
1:G:191:ILE:HG12	1:G:249:PHE:CD2	2.53	0.43
1:I:231:LYS:HD2	1:I:231:LYS:HA	1.66	0.43
1:K:231:LYS:HA	1:K:231:LYS:HD2	1.66	0.43
1:B:295:LEU:O	1:B:388:PRO:HD3	2.18	0.43
1:H:269:HIS:HE1	1:H:359:ARG:CZ	2.31	0.43
1:I:114:TYR:CD1	1:I:431:GLY:HA3	2.53	0.43
1:J:295:LEU:O	1:J:388:PRO:HD3	2.18	0.43
1:L:295:LEU:O	1:L:388:PRO:HD3	2.18	0.43
1:B:192:ARG:HH11	1:B:219:ASN:ND2	2.17	0.43
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.86	0.43
1:D:114:TYR:CD1	1:D:431:GLY:HA3	2.53	0.43
1:K:269:HIS:HE1	1:K:359:ARG:CZ	2.31	0.43
1:A:269:HIS:HE1	1:A:359:ARG:CZ	2.31	0.43
1:G:100:TYR:CE2	1:G:102:ARG:HB3	2.54	0.43
1:H:295:LEU:O	1:H:388:PRO:HD3	2.18	0.43
1:L:192:ARG:HH11	1:L:219:ASN:ND2	2.17	0.43
1:A:100:TYR:CE2	1:A:102:ARG:HB3	2.54	0.43
1:B:114:TYR:CD1	1:B:431:GLY:HA3	2.53	0.43
1:L:114:TYR:CD1	1:L:431:GLY:HA3	2.53	0.43
1:C:231:LYS:HD2	1:C:231:LYS:HA	1.66	0.43
1:D:100:TYR:CE2	1:D:102:ARG:HB3	2.54	0.43
1:F:191:ILE:HG12	1:F:249:PHE:CD2	2.53	0.43
1:F:295:LEU:O	1:F:388:PRO:HD3	2.18	0.43
1:I:295:LEU:O	1:I:388:PRO:HD3	2.18	0.43
1:C:100:TYR:CE2	1:C:102:ARG:HB3	2.54	0.43
1:D:231:LYS:HA	1:D:231:LYS:HD2	1.66	0.43
1:J:100:TYR:CE2	1:J:102:ARG:HB3	2.54	0.43
1:K:100:TYR:CE2	1:K:102:ARG:HB3	2.54	0.43
1:K:114:TYR:CD1	1:K:431:GLY:HA3	2.53	0.43
1:L:100:TYR:CE2	1:L:102:ARG:HB3	2.54	0.43
1:G:295:LEU:O	1:G:388:PRO:HD3	2.18	0.42
1:B:100:TYR:CE2	1:B:102:ARG:HB3	2.54	0.42
1:B:191:ILE:O	1:B:195:MET:HG3	2.19	0.42
1:C:149:VAL:HG21	1:K:462:PHE:CD1	2.54	0.42
1:E:100:TYR:CE2	1:E:102:ARG:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:ARG:HH11	1:G:219:ASN:ND2	2.17	0.42
1:I:100:TYR:CE2	1:I:102:ARG:HB3	2.54	0.42
1:C:192:ARG:HH11	1:C:219:ASN:ND2	2.17	0.42
1:D:295:LEU:O	1:D:388:PRO:HD3	2.18	0.42
1:E:191:ILE:O	1:E:195:MET:HG3	2.20	0.42
1:E:295:LEU:O	1:E:388:PRO:HD3	2.18	0.42
1:H:191:ILE:O	1:H:195:MET:HG3	2.20	0.42
1:H:192:ARG:HH11	1:H:219:ASN:ND2	2.17	0.42
1:K:191:ILE:O	1:K:195:MET:HG3	2.20	0.42
1:C:191:ILE:O	1:C:195:MET:HG3	2.20	0.42
1:C:315:THR:HB	1:K:465:TYR:CE2	2.53	0.42
1:J:191:ILE:O	1:J:195:MET:HG3	2.20	0.42
1:K:192:ARG:HH11	1:K:219:ASN:ND2	2.17	0.42
1:K:295:LEU:O	1:K:388:PRO:HD3	2.18	0.42
1:D:383:LYS:HB3	1:D:383:LYS:HZ2	1.84	0.42
1:G:191:ILE:O	1:G:195:MET:HG3	2.19	0.42
1:I:192:ARG:HH11	1:I:219:ASN:ND2	2.17	0.42
1:J:235:ILE:HD13	1:J:235:ILE:HA	1.86	0.42
1:A:252:THR:HB	1:F:169:LYS:HA	2.01	0.42
1:F:100:TYR:CE2	1:F:102:ARG:HB3	2.54	0.42
1:L:191:ILE:O	1:L:195:MET:HG3	2.20	0.42
1:F:191:ILE:O	1:F:195:MET:HG3	2.20	0.42
1:G:169:LYS:HA	1:H:252:THR:HB	2.02	0.42
1:H:100:TYR:CE2	1:H:102:ARG:HB3	2.54	0.42
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.66	0.42
1:J:192:ARG:HH11	1:J:219:ASN:ND2	2.17	0.42
1:D:466:TYR:CZ	1:J:138:ILE:HG21	2.55	0.42
1:F:296:TYR:O	1:F:381:GLY:HA3	2.20	0.42
1:G:296:TYR:O	1:G:381:GLY:HA3	2.20	0.42
1:H:296:TYR:O	1:H:381:GLY:HA3	2.20	0.42
1:L:383:LYS:HB3	1:L:383:LYS:HZ3	1.84	0.42
1:E:296:TYR:O	1:E:381:GLY:HA3	2.20	0.42
1:F:57:TRP:CH2	1:F:91:ILE:HG13	2.55	0.42
1:I:312:ALA:HB1	1:I:361:PRO:HB3	2.02	0.42
1:J:296:TYR:O	1:J:381:GLY:HA3	2.20	0.42
1:L:57:TRP:CH2	1:L:91:ILE:HG13	2.55	0.42
1:C:138:ILE:HG21	1:K:466:TYR:CZ	2.55	0.41
1:C:312:ALA:HB1	1:C:361:PRO:HB3	2.02	0.41
1:D:296:TYR:O	1:D:381:GLY:HA3	2.20	0.41
1:K:296:TYR:O	1:K:381:GLY:HA3	2.20	0.41
1:E:57:TRP:CH2	1:E:91:ILE:HG13	2.55	0.41

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:G:312:ALA:HB1	1:G:361:PRO:HB3	2.02	0.41
1:B:296:TYR:O	1:B:381:GLY:HA3	2.20	0.41
1:C:296:TYR:O	1:C:381:GLY:HA3	2.20	0.41
1:G:57:TRP:CH2	1:G:91:ILE:HG13	2.55	0.41
1:I:191:ILE:O	1:I:195:MET:HG3	2.20	0.41
1:K:312:ALA:HB1	1:K:361:PRO:HB3	2.02	0.41
1:L:235:ILE:HD13	1:L:235:ILE:HA	1.86	0.41
1:D:57:TRP:CH2	1:D:91:ILE:HG13	2.55	0.41
1:F:418:LEU:HD11	1:F:446:ARG:HB3	2.02	0.41
1:I:57:TRP:CH2	1:I:91:ILE:HG13	2.55	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.86	0.41
1:A:296:TYR:O	1:A:381:GLY:HA3	2.20	0.41
1:A:312:ALA:HB1	1:A:361:PRO:HB3	2.02	0.41
1:C:57:TRP:CH2	1:C:91:ILE:HG13	2.55	0.41
1:C:418:LEU:HD11	1:C:446:ARG:HB3	2.02	0.41
1:H:57:TRP:CH2	1:H:91:ILE:HG13	2.55	0.41
1:E:312:ALA:HB1	1:E:361:PRO:HB3	2.02	0.41
1:G:418:LEU:HD11	1:G:446:ARG:HB3	2.02	0.41
1:J:312:ALA:HB1	1:J:361:PRO:HB3	2.02	0.41
1:K:418:LEU:HD11	1:K:446:ARG:HB3	2.02	0.41
1:A:191:ILE:O	1:A:195:MET:HG3	2.20	0.41
1:B:312:ALA:HB1	1:B:361:PRO:HB3	2.02	0.41
1:F:312:ALA:HB1	1:F:361:PRO:HB3	2.02	0.41
1:D:191:ILE:O	1:D:195:MET:HG3	2.19	0.41
1:F:223:THR:HG23	1:F:231:LYS:HZ1	1.85	0.41
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.66	0.41
1:J:418:LEU:HD11	1:J:446:ARG:HB3	2.02	0.41
1:L:296:TYR:O	1:L:381:GLY:HA3	2.20	0.41
1:L:312:ALA:HB1	1:L:361:PRO:HB3	2.02	0.41
1:B:57:TRP:CH2	1:B:91:ILE:HG13	2.55	0.41
1:D:312:ALA:HB1	1:D:361:PRO:HB3	2.02	0.41
1:F:334:TYR:HA	1:F:343:ILE:HB	2.04	0.41
1:H:334:TYR:HA	1:H:343:ILE:HB	2.04	0.41
1:H:418:LEU:HD11	1:H:446:ARG:HB3	2.02	0.41
1:L:334:TYR:HA	1:L:343:ILE:HB	2.03	0.41
1:C:466:TYR:CZ	1:K:138:ILE:HG21	2.56	0.40
1:H:312:ALA:HB1	1:H:361:PRO:HB3	2.02	0.40
1:J:390:GLU:HA	1:J:391:PRO:HD3	1.92	0.40
1:C:235:ILE:HD13	1:C:235:ILE:HA	1.86	0.40
1:C:465:TYR:CE2	1:K:315:THR:HB	2.56	0.40
1:D:334:TYR:HA	1:D:343:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:418:LEU:HD11	1:I:446:ARG:HB3	2.02	0.40
1:J:57:TRP:CH2	1:J:91:ILE:HG13	2.55	0.40
1:K:57:TRP:CH2	1:K:91:ILE:HG13	2.55	0.40
1:H:68:MET:HA	1:H:69:PRO:HD2	1.94	0.40
1:H:390:GLU:HA	1:H:391:PRO:HD3	1.92	0.40
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.86	0.40
1:A:57:TRP:CH2	1:A:91:ILE:HG13	2.55	0.40
1:A:223:THR:HG23	1:A:231:LYS:HZ1	1.87	0.40
1:A:334:TYR:HA	1:A:343:ILE:HB	2.03	0.40
1:I:296:TYR:O	1:I:381:GLY:HA3	2.20	0.40
1:K:334:TYR:HA	1:K:343:ILE:HB	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:SER:OG	1:F:13:GLU:OE2[4_454]	1.12	1.08
1:C:1:SER:OG	1:F:13:GLU:CD[4_454]	2.07	0.13

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	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	13
1	B	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	13
1	C	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	13
1	D	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	13
1	E	437/468 (93%)	392 (90%)	30 (7%)	15 (3%)	3	13
1	F	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	13
1	G	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	13
1	I	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	13
1	J	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	13
1	K	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	13
1	L	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	13
All	All	5244/5616 (93%)	4723 (90%)	341 (6%)	180 (3%)	3	13

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	B	180	PHE
1	C	180	PHE
1	D	180	PHE
1	E	180	PHE
1	F	180	PHE
1	G	180	PHE
1	H	180	PHE
1	I	180	PHE
1	J	180	PHE
1	K	180	PHE
1	L	180	PHE
1	A	40	ALA
1	A	286	LYS
1	A	338	ASN
1	A	340	SER
1	B	40	ALA
1	B	286	LYS
1	B	338	ASN
1	B	340	SER
1	C	40	ALA
1	C	286	LYS
1	C	338	ASN
1	C	340	SER
1	D	40	ALA
1	D	286	LYS
1	D	338	ASN
1	D	340	SER
1	E	40	ALA
1	E	286	LYS

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Mol	Chain	Res	Type
1	E	338	ASN
1	E	340	SER
1	F	40	ALA
1	F	286	LYS
1	F	338	ASN
1	F	340	SER
1	G	40	ALA
1	G	286	LYS
1	G	338	ASN
1	G	340	SER
1	H	40	ALA
1	H	286	LYS
1	H	338	ASN
1	H	340	SER
1	I	40	ALA
1	I	286	LYS
1	I	338	ASN
1	I	340	SER
1	J	40	ALA
1	J	286	LYS
1	J	338	ASN
1	J	340	SER
1	K	40	ALA
1	K	286	LYS
1	K	338	ASN
1	K	340	SER
1	L	40	ALA
1	L	286	LYS
1	L	338	ASN
1	L	340	SER
1	A	285	ASP
1	A	350	SER
1	B	285	ASP
1	B	350	SER
1	C	285	ASP
1	C	350	SER
1	D	285	ASP
1	D	350	SER
1	E	285	ASP
1	E	350	SER
1	F	285	ASP
1	F	350	SER

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Mol	Chain	Res	Type
1	G	285	ASP
1	G	350	SER
1	H	285	ASP
1	H	350	SER
1	I	285	ASP
1	I	350	SER
1	J	285	ASP
1	J	350	SER
1	K	285	ASP
1	K	350	SER
1	L	285	ASP
1	L	350	SER
1	A	36	HIS
1	A	170	GLY
1	A	351	PRO
1	A	353	ALA
1	B	36	HIS
1	B	170	GLY
1	B	351	PRO
1	B	353	ALA
1	C	36	HIS
1	C	170	GLY
1	C	351	PRO
1	C	353	ALA
1	D	36	HIS
1	D	170	GLY
1	D	351	PRO
1	D	353	ALA
1	E	36	HIS
1	E	170	GLY
1	E	351	PRO
1	E	353	ALA
1	F	36	HIS
1	F	170	GLY
1	F	351	PRO
1	F	353	ALA
1	G	36	HIS
1	G	170	GLY
1	G	351	PRO
1	G	353	ALA
1	H	36	HIS
1	H	170	GLY

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Mol	Chain	Res	Type
1	H	351	PRO
1	H	353	ALA
1	I	36	HIS
1	I	170	GLY
1	I	351	PRO
1	I	353	ALA
1	J	36	HIS
1	J	170	GLY
1	J	351	PRO
1	J	353	ALA
1	K	36	HIS
1	K	170	GLY
1	K	351	PRO
1	K	353	ALA
1	L	36	HIS
1	L	170	GLY
1	L	351	PRO
1	L	353	ALA
1	A	228	MET
1	A	277	ASN
1	A	352	LYS
1	B	228	MET
1	B	277	ASN
1	B	352	LYS
1	C	228	MET
1	C	277	ASN
1	C	352	LYS
1	D	228	MET
1	D	277	ASN
1	D	352	LYS
1	E	228	MET
1	E	277	ASN
1	E	352	LYS
1	F	228	MET
1	F	277	ASN
1	F	352	LYS
1	G	228	MET
1	G	277	ASN
1	G	352	LYS
1	H	228	MET
1	H	277	ASN
1	H	352	LYS

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Mol	Chain	Res	Type
1	I	228	MET
1	I	277	ASN
1	I	352	LYS
1	J	228	MET
1	J	277	ASN
1	J	352	LYS
1	K	228	MET
1	K	277	ASN
1	K	352	LYS
1	L	228	MET
1	L	277	ASN
1	L	352	LYS
1	A	386	ILE
1	B	386	ILE
1	C	386	ILE
1	D	386	ILE
1	E	386	ILE
1	F	386	ILE
1	G	386	ILE
1	H	386	ILE
1	I	386	ILE
1	J	386	ILE
1	K	386	ILE
1	L	386	ILE

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	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	B	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	C	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	D	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	E	365/384 (95%)	325 (89%)	40 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	G	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	H	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	I	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	J	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	K	365/384 (95%)	325 (89%)	40 (11%)	6	19
1	L	365/384 (95%)	325 (89%)	40 (11%)	6	19
All	All	4380/4608 (95%)	3900 (89%)	480 (11%)	6	19

All (480) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	GLU
1	A	19	LEU
1	A	33	ILE
1	A	36	HIS
1	A	39	ASN
1	A	45	GLU
1	A	75	VAL
1	A	76	ILE
1	A	85	LEU
1	A	88	ARG
1	A	101	ASP
1	A	105	ARG
1	A	115	LEU
1	A	122	ASP
1	A	124	VAL
1	A	143	SER
1	A	165	GLU
1	A	183	PRO
1	A	194	GLU
1	A	223	THR
1	A	226	ASN
1	A	286	LYS
1	A	314	PRO
1	A	324	PRO
1	A	331	MET
1	A	332	LEU
1	A	337	ARG

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Mol	Chain	Res	Type
1	A	339	ARG
1	A	340	SER
1	A	350	SER
1	A	352	LYS
1	A	374	LEU
1	A	375	LEU
1	A	383	LYS
1	A	428	LEU
1	A	446	ARG
1	A	447	ARG
1	A	464	LEU
1	A	468	VAL
1	B	9	LEU
1	B	11	GLU
1	B	19	LEU
1	B	33	ILE
1	B	36	HIS
1	B	39	ASN
1	B	45	GLU
1	B	75	VAL
1	B	76	ILE
1	B	85	LEU
1	B	88	ARG
1	B	101	ASP
1	B	105	ARG
1	B	115	LEU
1	B	122	ASP
1	B	124	VAL
1	B	143	SER
1	B	165	GLU
1	B	183	PRO
1	B	194	GLU
1	B	223	THR
1	B	226	ASN
1	B	286	LYS
1	B	314	PRO
1	B	324	PRO
1	B	331	MET
1	B	332	LEU
1	B	337	ARG
1	B	339	ARG
1	B	340	SER

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Mol	Chain	Res	Type
1	B	350	SER
1	B	352	LYS
1	B	374	LEU
1	B	375	LEU
1	B	383	LYS
1	B	428	LEU
1	B	446	ARG
1	B	447	ARG
1	B	464	LEU
1	B	468	VAL
1	C	9	LEU
1	C	11	GLU
1	C	19	LEU
1	C	33	ILE
1	C	36	HIS
1	C	39	ASN
1	C	45	GLU
1	C	75	VAL
1	C	76	ILE
1	C	85	LEU
1	C	88	ARG
1	C	101	ASP
1	C	105	ARG
1	C	115	LEU
1	C	122	ASP
1	C	124	VAL
1	C	143	SER
1	C	165	GLU
1	C	183	PRO
1	C	194	GLU
1	C	223	THR
1	C	226	ASN
1	C	286	LYS
1	C	314	PRO
1	C	324	PRO
1	C	331	MET
1	C	332	LEU
1	C	337	ARG
1	C	339	ARG
1	C	340	SER
1	C	350	SER
1	C	352	LYS

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Mol	Chain	Res	Type
1	C	374	LEU
1	C	375	LEU
1	C	383	LYS
1	C	428	LEU
1	C	446	ARG
1	C	447	ARG
1	C	464	LEU
1	C	468	VAL
1	D	9	LEU
1	D	11	GLU
1	D	19	LEU
1	D	33	ILE
1	D	36	HIS
1	D	39	ASN
1	D	45	GLU
1	D	75	VAL
1	D	76	ILE
1	D	85	LEU
1	D	88	ARG
1	D	101	ASP
1	D	105	ARG
1	D	115	LEU
1	D	122	ASP
1	D	124	VAL
1	D	143	SER
1	D	165	GLU
1	D	183	PRO
1	D	194	GLU
1	D	223	THR
1	D	226	ASN
1	D	286	LYS
1	D	314	PRO
1	D	324	PRO
1	D	331	MET
1	D	332	LEU
1	D	337	ARG
1	D	339	ARG
1	D	340	SER
1	D	350	SER
1	D	352	LYS
1	D	374	LEU
1	D	375	LEU

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Mol	Chain	Res	Type
1	D	383	LYS
1	D	428	LEU
1	D	446	ARG
1	D	447	ARG
1	D	464	LEU
1	D	468	VAL
1	E	9	LEU
1	E	11	GLU
1	E	19	LEU
1	E	33	ILE
1	E	36	HIS
1	E	39	ASN
1	E	45	GLU
1	E	75	VAL
1	E	76	ILE
1	E	85	LEU
1	E	88	ARG
1	E	101	ASP
1	E	105	ARG
1	E	115	LEU
1	E	122	ASP
1	E	124	VAL
1	E	143	SER
1	E	165	GLU
1	E	183	PRO
1	E	194	GLU
1	E	223	THR
1	E	226	ASN
1	E	286	LYS
1	E	314	PRO
1	E	324	PRO
1	E	331	MET
1	E	332	LEU
1	E	337	ARG
1	E	339	ARG
1	E	340	SER
1	E	350	SER
1	E	352	LYS
1	E	374	LEU
1	E	375	LEU
1	E	383	LYS
1	E	428	LEU

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Mol	Chain	Res	Type
1	E	446	ARG
1	E	447	ARG
1	E	464	LEU
1	E	468	VAL
1	F	9	LEU
1	F	11	GLU
1	F	19	LEU
1	F	33	ILE
1	F	36	HIS
1	F	39	ASN
1	F	45	GLU
1	F	75	VAL
1	F	76	ILE
1	F	85	LEU
1	F	88	ARG
1	F	101	ASP
1	F	105	ARG
1	F	115	LEU
1	F	122	ASP
1	F	124	VAL
1	F	143	SER
1	F	165	GLU
1	F	183	PRO
1	F	194	GLU
1	F	223	THR
1	F	226	ASN
1	F	286	LYS
1	F	314	PRO
1	F	324	PRO
1	F	331	MET
1	F	332	LEU
1	F	337	ARG
1	F	339	ARG
1	F	340	SER
1	F	350	SER
1	F	352	LYS
1	F	374	LEU
1	F	375	LEU
1	F	383	LYS
1	F	428	LEU
1	F	446	ARG
1	F	447	ARG

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Mol	Chain	Res	Type
1	F	464	LEU
1	F	468	VAL
1	G	9	LEU
1	G	11	GLU
1	G	19	LEU
1	G	33	ILE
1	G	36	HIS
1	G	39	ASN
1	G	45	GLU
1	G	75	VAL
1	G	76	ILE
1	G	85	LEU
1	G	88	ARG
1	G	101	ASP
1	G	105	ARG
1	G	115	LEU
1	G	122	ASP
1	G	124	VAL
1	G	143	SER
1	G	165	GLU
1	G	183	PRO
1	G	194	GLU
1	G	223	THR
1	G	226	ASN
1	G	286	LYS
1	G	314	PRO
1	G	324	PRO
1	G	331	MET
1	G	332	LEU
1	G	337	ARG
1	G	339	ARG
1	G	340	SER
1	G	350	SER
1	G	352	LYS
1	G	374	LEU
1	G	375	LEU
1	G	383	LYS
1	G	428	LEU
1	G	446	ARG
1	G	447	ARG
1	G	464	LEU
1	G	468	VAL

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Mol	Chain	Res	Type
1	H	9	LEU
1	H	11	GLU
1	H	19	LEU
1	H	33	ILE
1	H	36	HIS
1	H	39	ASN
1	H	45	GLU
1	H	75	VAL
1	H	76	ILE
1	H	85	LEU
1	H	88	ARG
1	H	101	ASP
1	H	105	ARG
1	H	115	LEU
1	H	122	ASP
1	H	124	VAL
1	H	143	SER
1	H	165	GLU
1	H	183	PRO
1	H	194	GLU
1	H	223	THR
1	H	226	ASN
1	H	286	LYS
1	H	314	PRO
1	H	324	PRO
1	H	331	MET
1	H	332	LEU
1	H	337	ARG
1	H	339	ARG
1	H	340	SER
1	H	350	SER
1	H	352	LYS
1	H	374	LEU
1	H	375	LEU
1	H	383	LYS
1	H	428	LEU
1	H	446	ARG
1	H	447	ARG
1	H	464	LEU
1	H	468	VAL
1	I	9	LEU
1	I	11	GLU

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Mol	Chain	Res	Type
1	I	19	LEU
1	I	33	ILE
1	I	36	HIS
1	I	39	ASN
1	I	45	GLU
1	I	75	VAL
1	I	76	ILE
1	I	85	LEU
1	I	88	ARG
1	I	101	ASP
1	I	105	ARG
1	I	115	LEU
1	I	122	ASP
1	I	124	VAL
1	I	143	SER
1	I	165	GLU
1	I	183	PRO
1	I	194	GLU
1	I	223	THR
1	I	226	ASN
1	I	286	LYS
1	I	314	PRO
1	I	324	PRO
1	I	331	MET
1	I	332	LEU
1	I	337	ARG
1	I	339	ARG
1	I	340	SER
1	I	350	SER
1	I	352	LYS
1	I	374	LEU
1	I	375	LEU
1	I	383	LYS
1	I	428	LEU
1	I	446	ARG
1	I	447	ARG
1	I	464	LEU
1	I	468	VAL
1	J	9	LEU
1	J	11	GLU
1	J	19	LEU
1	J	33	ILE

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Mol	Chain	Res	Type
1	J	36	HIS
1	J	39	ASN
1	J	45	GLU
1	J	75	VAL
1	J	76	ILE
1	J	85	LEU
1	J	88	ARG
1	J	101	ASP
1	J	105	ARG
1	J	115	LEU
1	J	122	ASP
1	J	124	VAL
1	J	143	SER
1	J	165	GLU
1	J	183	PRO
1	J	194	GLU
1	J	223	THR
1	J	226	ASN
1	J	286	LYS
1	J	314	PRO
1	J	324	PRO
1	J	331	MET
1	J	332	LEU
1	J	337	ARG
1	J	339	ARG
1	J	340	SER
1	J	350	SER
1	J	352	LYS
1	J	374	LEU
1	J	375	LEU
1	J	383	LYS
1	J	428	LEU
1	J	446	ARG
1	J	447	ARG
1	J	464	LEU
1	J	468	VAL
1	K	9	LEU
1	K	11	GLU
1	K	19	LEU
1	K	33	ILE
1	K	36	HIS
1	K	39	ASN

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Mol	Chain	Res	Type
1	K	45	GLU
1	K	75	VAL
1	K	76	ILE
1	K	85	LEU
1	K	88	ARG
1	K	101	ASP
1	K	105	ARG
1	K	115	LEU
1	K	122	ASP
1	K	124	VAL
1	K	143	SER
1	K	165	GLU
1	K	183	PRO
1	K	194	GLU
1	K	223	THR
1	K	226	ASN
1	K	286	LYS
1	K	314	PRO
1	K	324	PRO
1	K	331	MET
1	K	332	LEU
1	K	337	ARG
1	K	339	ARG
1	K	340	SER
1	K	350	SER
1	K	352	LYS
1	K	374	LEU
1	K	375	LEU
1	K	383	LYS
1	K	428	LEU
1	K	446	ARG
1	K	447	ARG
1	K	464	LEU
1	K	468	VAL
1	L	9	LEU
1	L	11	GLU
1	L	19	LEU
1	L	33	ILE
1	L	36	HIS
1	L	39	ASN
1	L	45	GLU
1	L	75	VAL

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Mol	Chain	Res	Type
1	L	76	ILE
1	L	85	LEU
1	L	88	ARG
1	L	101	ASP
1	L	105	ARG
1	L	115	LEU
1	L	122	ASP
1	L	124	VAL
1	L	143	SER
1	L	165	GLU
1	L	183	PRO
1	L	194	GLU
1	L	223	THR
1	L	226	ASN
1	L	286	LYS
1	L	314	PRO
1	L	324	PRO
1	L	331	MET
1	L	332	LEU
1	L	337	ARG
1	L	339	ARG
1	L	340	SER
1	L	350	SER
1	L	352	LYS
1	L	374	LEU
1	L	375	LEU
1	L	383	LYS
1	L	428	LEU
1	L	446	ARG
1	L	447	ARG
1	L	464	LEU
1	L	468	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	159	ASN
1	A	189	GLN
1	A	219	ASN
1	A	269	HIS
1	A	458	HIS

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Mol	Chain	Res	Type
1	B	30	HIS
1	B	159	ASN
1	B	189	GLN
1	B	219	ASN
1	B	269	HIS
1	B	458	HIS
1	C	30	HIS
1	C	159	ASN
1	C	189	GLN
1	C	219	ASN
1	C	269	HIS
1	C	458	HIS
1	D	30	HIS
1	D	159	ASN
1	D	189	GLN
1	D	219	ASN
1	D	269	HIS
1	D	458	HIS
1	E	30	HIS
1	E	159	ASN
1	E	189	GLN
1	E	219	ASN
1	E	269	HIS
1	E	458	HIS
1	F	30	HIS
1	F	159	ASN
1	F	189	GLN
1	F	219	ASN
1	F	269	HIS
1	F	458	HIS
1	G	30	HIS
1	G	159	ASN
1	G	189	GLN
1	G	219	ASN
1	G	269	HIS
1	G	458	HIS
1	H	30	HIS
1	H	159	ASN
1	H	189	GLN
1	H	219	ASN
1	H	269	HIS
1	H	458	HIS

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Mol	Chain	Res	Type
1	I	30	HIS
1	I	159	ASN
1	I	189	GLN
1	I	219	ASN
1	I	269	HIS
1	I	458	HIS
1	J	30	HIS
1	J	159	ASN
1	J	189	GLN
1	J	219	ASN
1	J	269	HIS
1	J	458	HIS
1	K	30	HIS
1	K	159	ASN
1	K	189	GLN
1	K	219	ASN
1	K	269	HIS
1	K	458	HIS
1	L	30	HIS
1	L	159	ASN
1	L	189	GLN
1	L	219	ASN
1	L	269	HIS
1	L	458	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLU	G	471	-	8,9,9	1.25	1 (12%)	10,11,11	1.27	1 (10%)
3	GLU	I	471	-	8,9,9	1.26	2 (25%)	10,11,11	1.28	1 (10%)
3	GLU	E	471	-	8,9,9	1.26	2 (25%)	10,11,11	1.28	1 (10%)
3	GLU	J	471	-	8,9,9	1.25	1 (12%)	10,11,11	1.28	1 (10%)
3	GLU	A	471	-	8,9,9	1.25	1 (12%)	10,11,11	1.27	1 (10%)
3	GLU	D	471	-	8,9,9	1.25	2 (25%)	10,11,11	1.27	1 (10%)
3	GLU	C	471	-	8,9,9	1.24	1 (12%)	10,11,11	1.28	1 (10%)
3	GLU	K	471	-	8,9,9	1.25	1 (12%)	10,11,11	1.28	1 (10%)
3	GLU	B	473	-	8,9,9	1.25	2 (25%)	10,11,11	1.28	1 (10%)
3	GLU	H	471	-	8,9,9	1.25	1 (12%)	10,11,11	1.27	1 (10%)
3	GLU	L	471	-	8,9,9	1.25	1 (12%)	10,11,11	1.27	1 (10%)
3	GLU	F	471	-	8,9,9	1.25	2 (25%)	10,11,11	1.28	1 (10%)

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

Mol	**Type**	**Chain**	**Res**	**Link**	**Chirals**	**Torsions**	**Rings**
3	GLU	G	471	-	-	6/9/9/9	-
3	GLU	I	471	-	-	6/9/9/9	-
3	GLU	E	471	-	-	6/9/9/9	-
3	GLU	J	471	-	-	6/9/9/9	-
3	GLU	A	471	-	-	6/9/9/9	-
3	GLU	D	471	-	-	6/9/9/9	-
3	GLU	C	471	-	-	6/9/9/9	-
3	GLU	K	471	-	-	6/9/9/9	-
3	GLU	B	473	-	-	6/9/9/9	-
3	GLU	H	471	-	-	6/9/9/9	-
3	GLU	L	471	-	-	6/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	F	471	-	-	6/9/9/9	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	471	GLU	OE2-CD	-2.23	1.23	1.30
3	I	471	GLU	OE2-CD	-2.22	1.23	1.30
3	J	471	GLU	OE2-CD	-2.21	1.23	1.30
3	E	471	GLU	OE2-CD	-2.21	1.23	1.30
3	A	471	GLU	OE2-CD	-2.21	1.23	1.30
3	F	471	GLU	OE2-CD	-2.21	1.23	1.30
3	K	471	GLU	OE2-CD	-2.21	1.23	1.30
3	H	471	GLU	OE2-CD	-2.21	1.23	1.30
3	C	471	GLU	OE2-CD	-2.21	1.23	1.30
3	D	471	GLU	OE2-CD	-2.20	1.23	1.30
3	L	471	GLU	OE2-CD	-2.20	1.23	1.30
3	B	473	GLU	OE2-CD	-2.18	1.23	1.30
3	I	471	GLU	OXT-C	-2.02	1.23	1.30
3	E	471	GLU	OXT-C	-2.02	1.23	1.30
3	B	473	GLU	OXT-C	-2.01	1.24	1.30
3	F	471	GLU	OXT-C	-2.00	1.24	1.30
3	D	471	GLU	OXT-C	-2.00	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	473	GLU	OXT-C-CA	2.07	120.42	113.38
3	J	471	GLU	OXT-C-CA	2.07	120.42	113.38
3	I	471	GLU	OXT-C-CA	2.07	120.42	113.38
3	K	471	GLU	OXT-C-CA	2.06	120.42	113.38
3	E	471	GLU	OXT-C-CA	2.06	120.40	113.38
3	A	471	GLU	OXT-C-CA	2.06	120.39	113.38
3	C	471	GLU	OXT-C-CA	2.06	120.39	113.38
3	D	471	GLU	OXT-C-CA	2.06	120.39	113.38
3	F	471	GLU	OXT-C-CA	2.06	120.38	113.38
3	H	471	GLU	OXT-C-CA	2.05	120.38	113.38
3	G	471	GLU	OXT-C-CA	2.05	120.37	113.38
3	L	471	GLU	OXT-C-CA	2.05	120.35	113.38

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	471	GLU	OXT-C-CA-CB
3	B	473	GLU	OXT-C-CA-CB
3	C	471	GLU	OXT-C-CA-CB
3	D	471	GLU	OXT-C-CA-CB
3	E	471	GLU	OXT-C-CA-CB
3	F	471	GLU	OXT-C-CA-CB
3	G	471	GLU	OXT-C-CA-CB
3	H	471	GLU	OXT-C-CA-CB
3	I	471	GLU	OXT-C-CA-CB
3	J	471	GLU	OXT-C-CA-CB
3	K	471	GLU	OXT-C-CA-CB
3	L	471	GLU	OXT-C-CA-CB
3	A	471	GLU	O-C-CA-CB
3	B	473	GLU	O-C-CA-CB
3	C	471	GLU	O-C-CA-CB
3	D	471	GLU	O-C-CA-CB
3	E	471	GLU	O-C-CA-CB
3	F	471	GLU	O-C-CA-CB
3	G	471	GLU	O-C-CA-CB
3	H	471	GLU	O-C-CA-CB
3	I	471	GLU	O-C-CA-CB
3	J	471	GLU	O-C-CA-CB
3	K	471	GLU	O-C-CA-CB
3	L	471	GLU	O-C-CA-CB
3	A	471	GLU	OXT-C-CA-N
3	B	473	GLU	OXT-C-CA-N
3	C	471	GLU	OXT-C-CA-N
3	D	471	GLU	OXT-C-CA-N
3	E	471	GLU	OXT-C-CA-N
3	F	471	GLU	OXT-C-CA-N
3	G	471	GLU	OXT-C-CA-N
3	H	471	GLU	OXT-C-CA-N
3	I	471	GLU	OXT-C-CA-N
3	J	471	GLU	OXT-C-CA-N
3	K	471	GLU	OXT-C-CA-N
3	L	471	GLU	OXT-C-CA-N
3	A	471	GLU	O-C-CA-N
3	B	473	GLU	O-C-CA-N
3	C	471	GLU	O-C-CA-N
3	D	471	GLU	O-C-CA-N
3	E	471	GLU	O-C-CA-N
3	F	471	GLU	O-C-CA-N
3	G	471	GLU	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	H	471	GLU	O-C-CA-N
3	I	471	GLU	O-C-CA-N
3	J	471	GLU	O-C-CA-N
3	K	471	GLU	O-C-CA-N
3	L	471	GLU	O-C-CA-N
3	C	471	GLU	OE2-CD-CG-CB
3	E	471	GLU	OE2-CD-CG-CB
3	F	471	GLU	OE2-CD-CG-CB
3	G	471	GLU	OE2-CD-CG-CB
3	H	471	GLU	OE2-CD-CG-CB
3	L	471	GLU	OE2-CD-CG-CB
3	A	471	GLU	OE2-CD-CG-CB
3	B	473	GLU	OE2-CD-CG-CB
3	D	471	GLU	OE2-CD-CG-CB
3	I	471	GLU	OE2-CD-CG-CB
3	J	471	GLU	OE2-CD-CG-CB
3	K	471	GLU	OE2-CD-CG-CB
3	J	471	GLU	OE1-CD-CG-CB
3	A	471	GLU	OE1-CD-CG-CB
3	B	473	GLU	OE1-CD-CG-CB
3	C	471	GLU	OE1-CD-CG-CB
3	D	471	GLU	OE1-CD-CG-CB
3	E	471	GLU	OE1-CD-CG-CB
3	F	471	GLU	OE1-CD-CG-CB
3	G	471	GLU	OE1-CD-CG-CB
3	H	471	GLU	OE1-CD-CG-CB
3	I	471	GLU	OE1-CD-CG-CB
3	K	471	GLU	OE1-CD-CG-CB
3	L	471	GLU	OE1-CD-CG-CB

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	471	GLU	1	0
3	I	471	GLU	1	0
3	E	471	GLU	1	0
3	J	471	GLU	1	0
3	A	471	GLU	1	0
3	D	471	GLU	1	0
3	C	471	GLU	1	0
3	K	471	GLU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	473	GLU	1	0
3	H	471	GLU	1	0
3	L	471	GLU	1	0
3	F	471	GLU	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.