



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:46 am BST

PDB ID : 2UU7  
Title : Crystal structure of apo glutamine synthetase from dog (*Canis familiaris*)  
Authors : Krajewski, W.W.; Jones, T.A.; Mowbray, S.L.  
Deposited on : 2007-02-28  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

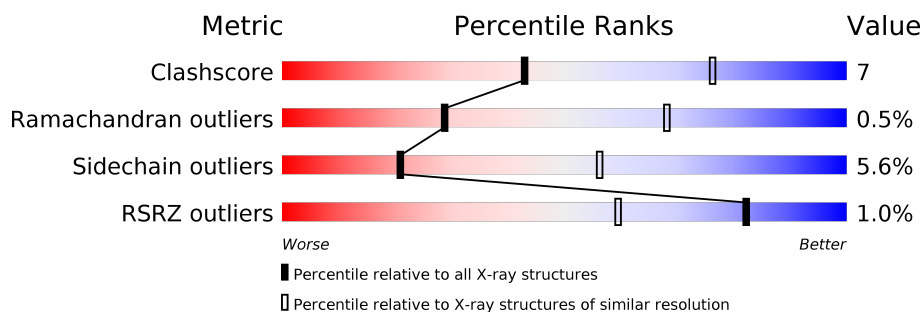
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	381	<div> <div></div> <div>80%16% . .</div> </div>
1	B	381	<div> <div>%</div> <div>81%14% . .</div> </div>
1	C	381	<div> <div>2%</div> <div>80%15% . .</div> </div>
1	D	381	<div> <div></div> <div>78%18% . .</div> </div>
1	E	381	<div> <div>%</div> <div>79%17% . .</div> </div>
1	F	381	<div> <div>2%</div> <div>78%17% . .</div> </div>
1	G	381	<div> <div>%</div> <div>78%17% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	381	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>79%</div><div>17%</div><div><div></div><div></div></div></div></div>
1	I	381	<div><div><div></div><div></div><div></div></div><div>78%</div><div>16%</div><div><div></div><div></div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 44025 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	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	B	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	C	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	D	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	E	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	F	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	G	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	H	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	I	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	J	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	K	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	L	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	M	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	N	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			
1	O	370	Total	C	N	O	S	0	0	0
			2933	1846	517	549	21			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	N	1	Total Mg 1 1	0	0
2	O	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	M	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0

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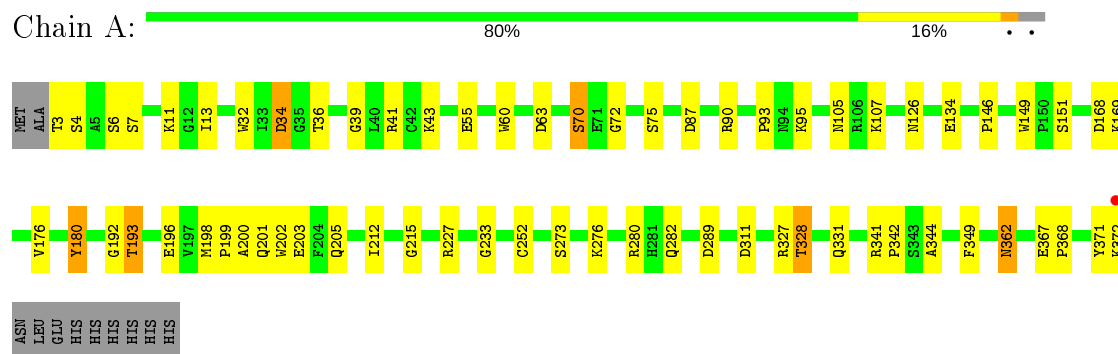
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0
3	N	1	Total 1	Cl 1	0	0
3	O	1	Total 1	Cl 1	0	0
3	L	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0
3	M	1	Total 1	Cl 1	0	0

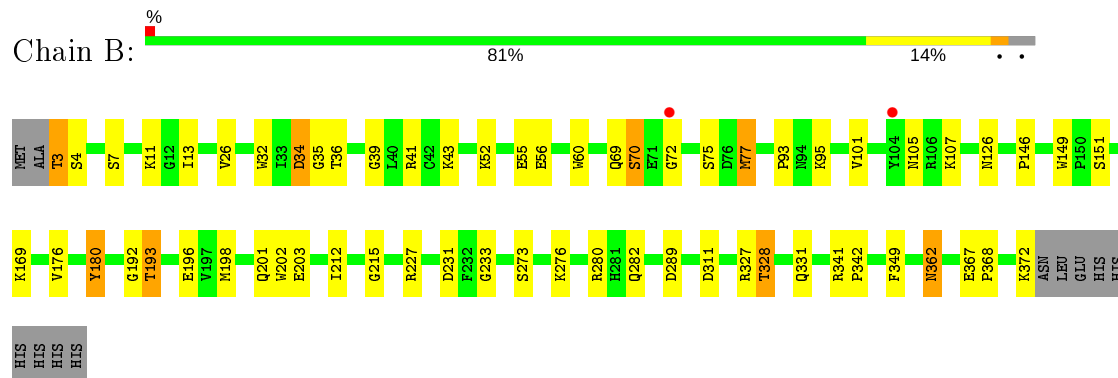
### 3 Residue-property plots [i](#)

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

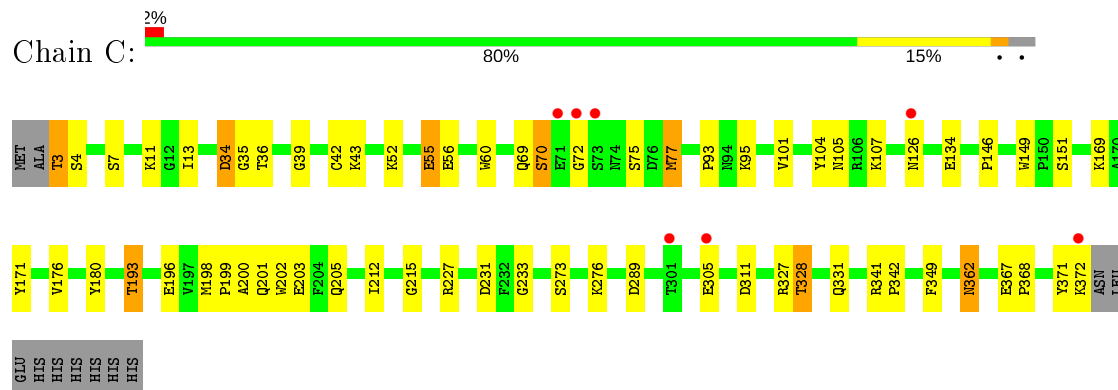
#### • Molecule 1: GLUTAMINE SYNTHETASE



#### • Molecule 1: GLUTAMINE SYNTHETASE

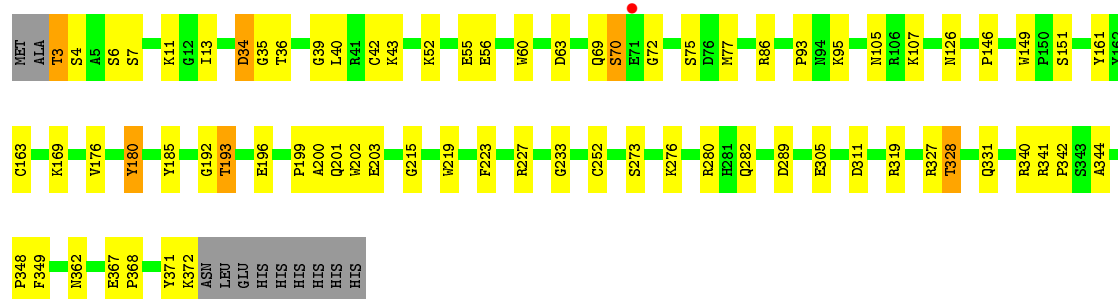


#### • Molecule 1: GLUTAMINE SYNTHETASE

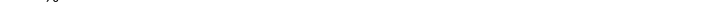


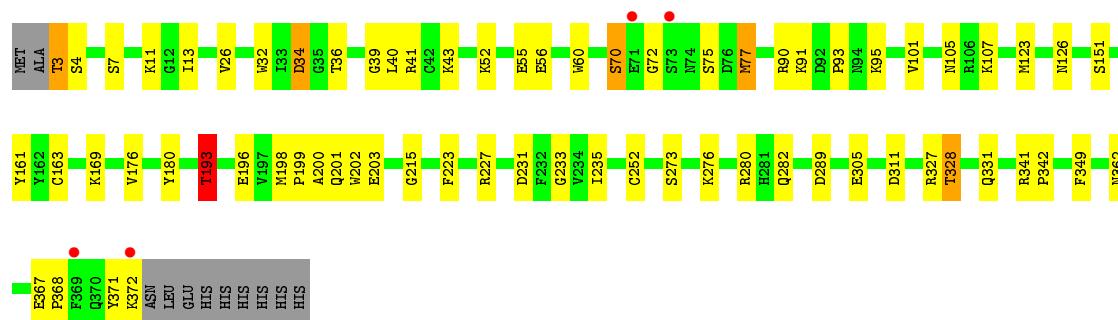
- Molecule 1: GLUTAMINE SYNTHETASE

Chain D:  78% 18% . .

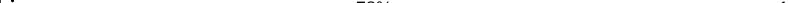


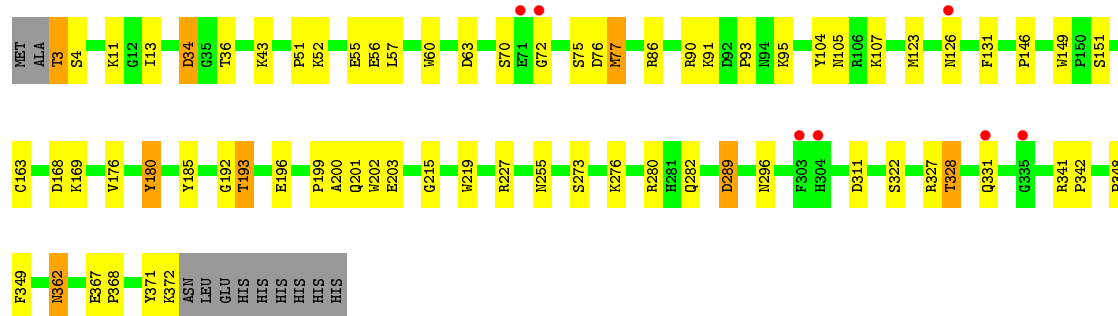
- Molecule 1: GLUTAMINE SYNTHETASE

Chain E:  79% 17% 4%

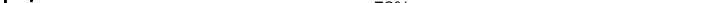


- Molecule 1: GLUTAMINE SYNTHETASE

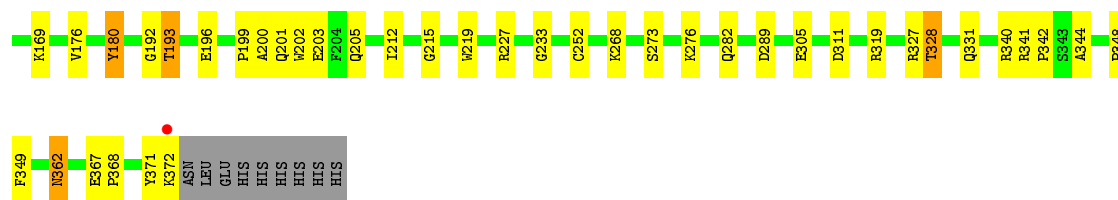
Chain F:  2% 78% 17% ..



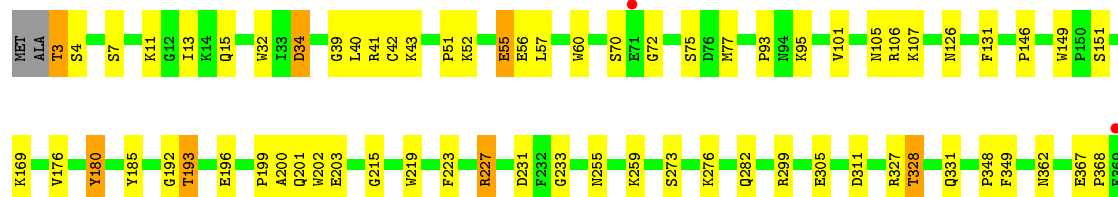
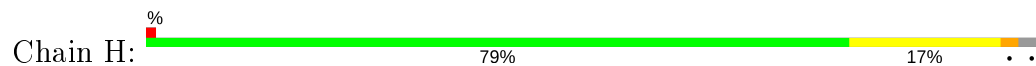
- Molecule 1: GLUTAMINE SYNTHETASE

Chain G:  78% 17% 5%

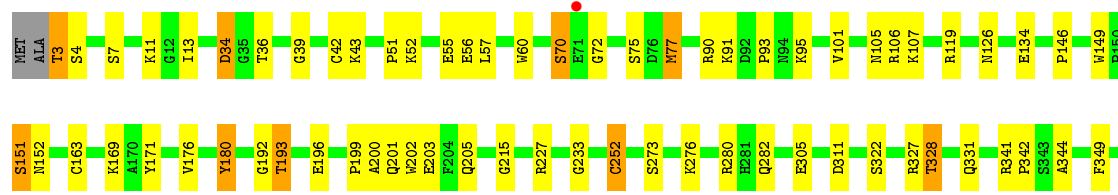




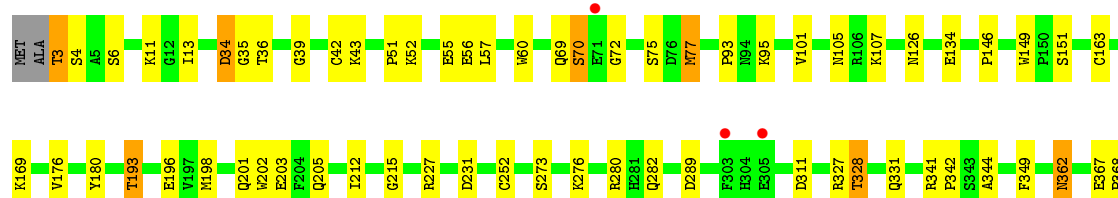
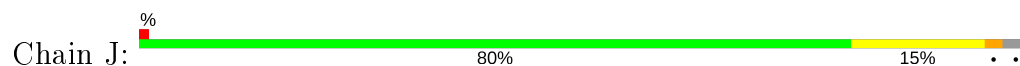
• Molecule 1: GLUTAMINE SYNTHETASE



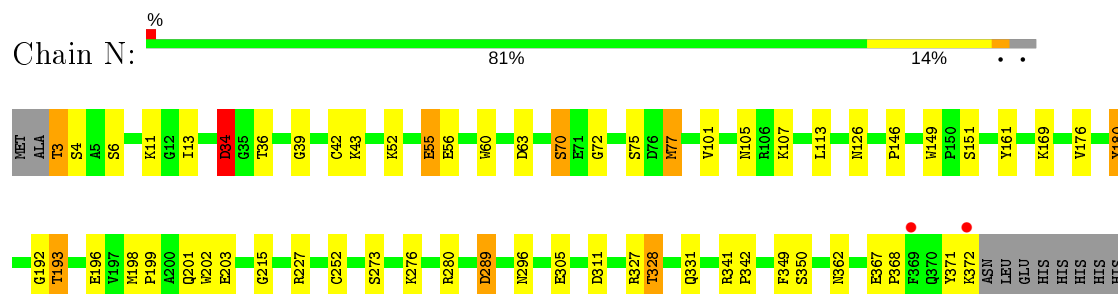
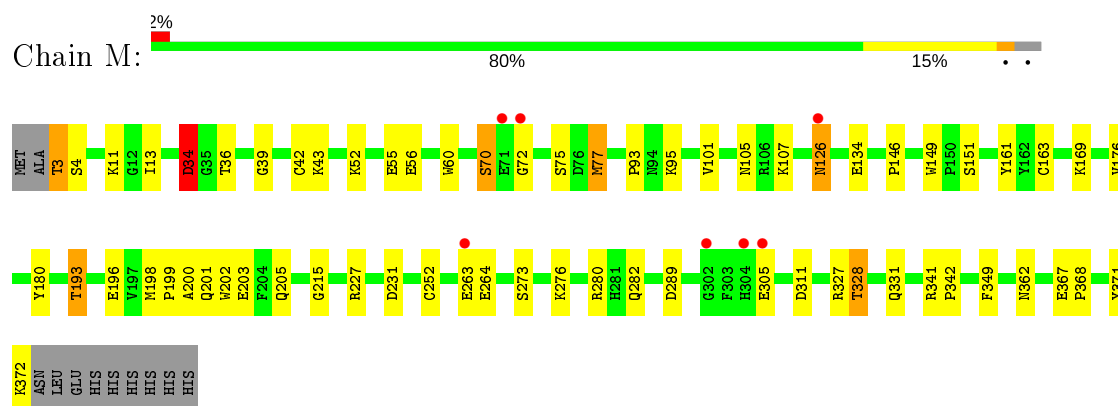
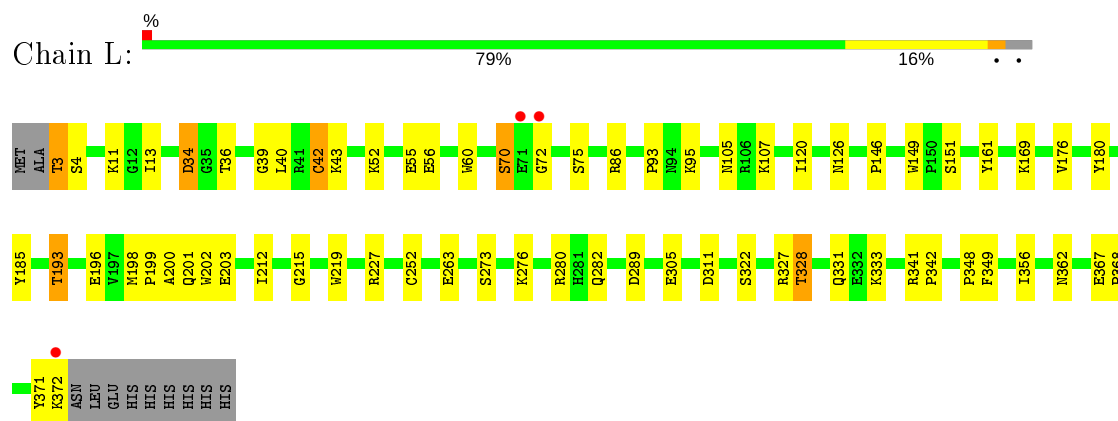
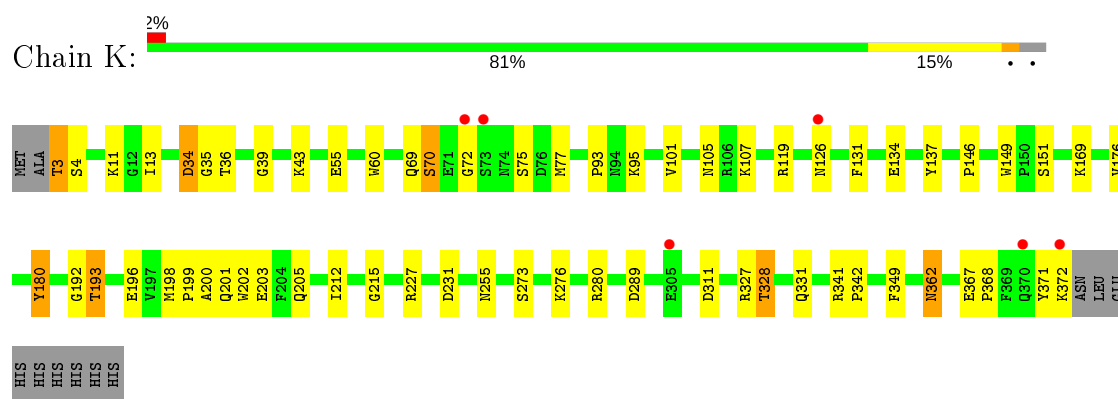
• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE

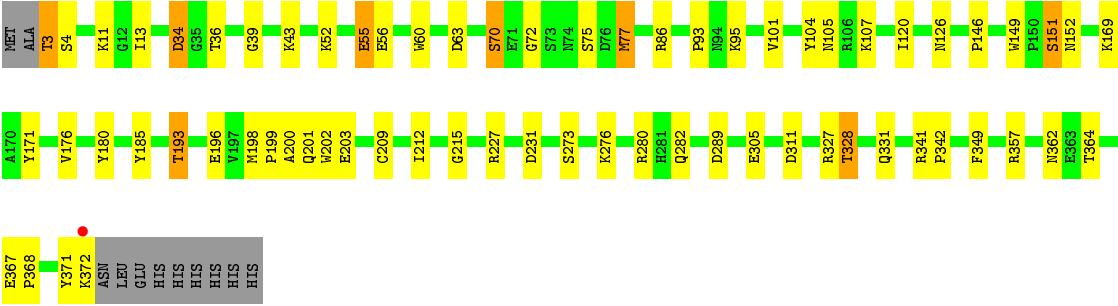
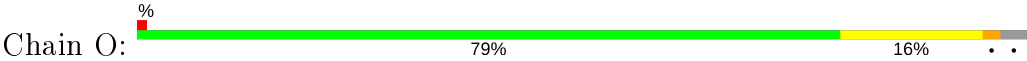


• Molecule 1: GLUTAMINE SYNTHETASE



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● Molecule 1: GLUTAMINE SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.59Å 485.60Å 192.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.00 29.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.99-3.00) 98.9 (29.99-3.00)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.213 , 0.230 0.213 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 27.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	44025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, CL

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	0.66	0/3014	0.67	0/4075
1	B	0.68	1/3014 (0.0%)	0.68	1/4075 (0.0%)
1	C	0.69	1/3014 (0.0%)	0.67	0/4075
1	D	0.65	1/3014 (0.0%)	0.67	1/4075 (0.0%)
1	E	0.66	2/3014 (0.1%)	0.68	1/4075 (0.0%)
1	F	0.71	1/3014 (0.0%)	0.69	0/4075
1	G	0.67	1/3014 (0.0%)	0.69	0/4075
1	H	0.69	1/3014 (0.0%)	0.69	1/4075 (0.0%)
1	I	0.70	2/3014 (0.1%)	0.69	0/4075
1	J	0.68	1/3014 (0.0%)	0.68	1/4075 (0.0%)
1	K	0.67	1/3014 (0.0%)	0.68	1/4075 (0.0%)
1	L	0.69	3/3014 (0.1%)	0.69	1/4075 (0.0%)
1	M	0.66	3/3014 (0.1%)	0.67	0/4075
1	N	0.70	3/3014 (0.1%)	0.67	0/4075
1	O	0.68	2/3014 (0.1%)	0.67	0/4075
All	All	0.68	23/45210 (0.1%)	0.68	7/61125 (0.0%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	3	THR	CA-CB	7.35	1.72	1.53
1	K	3	THR	CA-CB	7.34	1.72	1.53
1	D	3	THR	CA-CB	7.21	1.72	1.53
1	G	3	THR	CA-CB	6.95	1.71	1.53
1	B	3	THR	CA-CB	6.85	1.71	1.53
1	E	252	CYS	CB-SG	-6.79	1.70	1.82
1	E	3	THR	CA-CB	6.41	1.70	1.53
1	L	42	CYS	CB-SG	-6.37	1.71	1.82
1	N	252	CYS	CB-SG	-6.36	1.71	1.82
1	M	3	THR	CA-CB	6.19	1.69	1.53
1	M	42	CYS	CB-SG	-6.17	1.71	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	3	THR	CA-CB	6.09	1.69	1.53
1	H	3	THR	CA-CB	6.08	1.69	1.53
1	C	3	THR	CA-CB	5.99	1.69	1.53
1	N	3	THR	CA-CB	5.97	1.68	1.53
1	N	42	CYS	CB-SG	-5.70	1.72	1.81
1	J	3	THR	CA-CB	5.54	1.67	1.53
1	F	3	THR	CA-CB	5.47	1.67	1.53
1	I	252	CYS	CB-SG	-5.43	1.73	1.81
1	L	252	CYS	CB-SG	-5.36	1.73	1.81
1	I	3	THR	CA-CB	5.31	1.67	1.53
1	M	252	CYS	CB-SG	-5.19	1.73	1.81
1	O	209	CYS	CB-SG	-5.18	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	3	THR	N-CA-CB	5.53	120.81	110.30
1	H	299	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	K	3	THR	N-CA-CB	5.17	120.12	110.30
1	D	3	THR	N-CA-CB	5.13	120.05	110.30
1	E	193	THR	CB-CA-C	-5.07	97.90	111.60
1	B	3	THR	N-CA-CB	5.07	119.93	110.30
1	J	3	THR	N-CA-CB	5.00	119.80	110.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2796	40	0
1	B	2933	0	2796	38	0
1	C	2933	0	2796	44	0
1	D	2933	0	2796	47	0
1	E	2933	0	2796	39	0
1	F	2933	0	2796	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2933	0	2796	47	0
1	H	2933	0	2796	44	8
1	I	2933	0	2796	45	2
1	J	2933	0	2796	41	2
1	K	2933	0	2796	42	2
1	L	2933	0	2796	44	6
1	M	2933	0	2796	38	4
1	N	2933	0	2796	40	0
1	O	2933	0	2796	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
All	All	44025	0	41940	585	12

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 (585) 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:L:276:LYS:NZ	1:L:362:ASN:HD21	1.82	0.78
1:H:193:THR:HG22	1:H:203:GLU:O	1.90	0.72
1:D:215:GLY:HA3	1:D:349:PHE:CE2	2.25	0.72
1:C:193:THR:HG22	1:C:203:GLU:O	1.93	0.69
1:A:193:THR:HG22	1:A:203:GLU:O	1.92	0.69
1:H:371:TYR:O	1:H:372:LYS:HE2	1.94	0.68
1:G:176:VAL:HG21	1:G:202:TRP:CE3	2.29	0.68
1:K:13:ILE:HD11	1:L:11:LYS:HG3	1.76	0.67
1:M:215:GLY:HA3	1:M:349:PHE:CE2	2.30	0.67
1:F:176:VAL:HG21	1:F:202:TRP:CE3	2.30	0.67
1:K:276:LYS:NZ	1:K:362:ASN:HD21	1.92	0.67
1:G:215:GLY:HA3	1:G:349:PHE:CE2	2.29	0.67
1:N:193:THR:HG22	1:N:203:GLU:O	1.94	0.67
1:A:276:LYS:NZ	1:A:362:ASN:HD21	1.94	0.66
1:N:276:LYS:NZ	1:N:362:ASN:HD21	1.93	0.66
1:H:13:ILE:HD11	1:I:11:LYS:HG3	1.77	0.66
1:G:276:LYS:NZ	1:G:362:ASN:HD21	1.94	0.66
1:C:176:VAL:HG21	1:C:202:TRP:CE3	2.30	0.66
1:C:276:LYS:NZ	1:C:362:ASN:HD21	1.93	0.66
1:E:105:ASN:OD1	1:E:107:LYS:HB2	1.96	0.65
1:L:176:VAL:HG21	1:L:202:TRP:CE3	2.31	0.65
1:D:276:LYS:NZ	1:D:362:ASN:HD21	1.93	0.65
1:H:215:GLY:HA3	1:H:349:PHE:CE2	2.32	0.65
1:M:276:LYS:NZ	1:M:362:ASN:HD21	1.95	0.65
1:F:193:THR:HG22	1:F:203:GLU:O	1.98	0.64
1:E:193:THR:HG22	1:E:203:GLU:O	1.98	0.64
1:J:193:THR:HG22	1:J:203:GLU:O	1.98	0.64
1:L:276:LYS:HZ3	1:L:362:ASN:HD21	1.44	0.64
1:G:193:THR:HG22	1:G:203:GLU:O	1.99	0.63
1:J:276:LYS:NZ	1:J:362:ASN:HD21	1.96	0.63
1:B:193:THR:HG22	1:B:203:GLU:O	1.98	0.63
1:F:93:PRO:O	1:F:95:LYS:HE2	1.99	0.63
1:I:193:THR:HG22	1:I:203:GLU:O	1.99	0.63
1:B:105:ASN:OD1	1:B:107:LYS:HB2	1.99	0.62
1:I:105:ASN:OD1	1:I:107:LYS:HB2	1.98	0.62
1:H:276:LYS:NZ	1:H:362:ASN:HD21	1.99	0.61
1:F:11:LYS:HG3	1:J:13:ILE:HD11	1.80	0.61
1:F:70:SER:OG	1:F:75:SER:HA	1.99	0.61
1:M:193:THR:HG22	1:M:203:GLU:O	1.99	0.61
1:K:215:GLY:HA3	1:K:349:PHE:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:193:THR:HG22	1:O:203:GLU:O	2.00	0.61
1:B:176:VAL:HG21	1:B:202:TRP:CE3	2.36	0.60
1:B:276:LYS:NZ	1:B:362:ASN:HD21	1.97	0.60
1:M:105:ASN:OD1	1:M:107:LYS:HB2	2.01	0.60
1:F:13:ILE:HD11	1:G:11:LYS:HG3	1.82	0.60
1:C:70:SER:OG	1:C:75:SER:HA	2.02	0.60
1:F:105:ASN:OD1	1:F:107:LYS:HB2	2.02	0.60
1:K:70:SER:OG	1:K:75:SER:HA	2.02	0.60
1:J:176:VAL:HG21	1:J:202:TRP:CE3	2.37	0.60
1:A:176:VAL:HG21	1:A:202:TRP:CE3	2.37	0.60
1:H:176:VAL:HG21	1:H:202:TRP:CE3	2.37	0.60
1:O:215:GLY:HA3	1:O:349:PHE:CE2	2.37	0.60
1:I:196:GLU:HB3	1:I:201:GLN:HE21	1.67	0.59
1:J:70:SER:OG	1:J:75:SER:HA	2.01	0.59
1:N:13:ILE:HD11	1:O:11:LYS:HG3	1.84	0.59
1:O:276:LYS:NZ	1:O:362:ASN:HD21	2.01	0.59
1:I:215:GLY:HA3	1:I:349:PHE:CE2	2.37	0.59
1:O:70:SER:OG	1:O:75:SER:HA	2.03	0.59
1:E:276:LYS:NZ	1:E:362:ASN:HD21	2.00	0.59
1:D:70:SER:OG	1:D:75:SER:HA	2.02	0.59
1:H:34:ASP:HB2	1:H:39:GLY:O	2.03	0.59
1:F:11:LYS:HE3	1:J:13:ILE:HD11	1.85	0.59
1:L:105:ASN:OD1	1:L:107:LYS:HB2	2.02	0.59
1:M:176:VAL:HG21	1:M:202:TRP:CE3	2.38	0.59
1:B:70:SER:OG	1:B:75:SER:HA	2.03	0.58
1:O:105:ASN:OD1	1:O:107:LYS:HB2	2.03	0.58
1:K:105:ASN:OD1	1:K:107:LYS:HB2	2.03	0.58
1:K:176:VAL:HG21	1:K:202:TRP:CE3	2.38	0.58
1:D:193:THR:HG22	1:D:203:GLU:O	2.02	0.58
1:E:34:ASP:HB3	1:E:36:THR:H	1.68	0.58
1:F:176:VAL:HG21	1:F:202:TRP:CD2	2.38	0.58
1:F:215:GLY:HA3	1:F:349:PHE:CE2	2.39	0.58
1:K:193:THR:HG22	1:K:203:GLU:O	2.04	0.58
1:A:11:LYS:HE3	1:E:13:ILE:HD11	1.85	0.58
1:A:11:LYS:HG3	1:E:13:ILE:HD11	1.84	0.58
1:A:70:SER:OG	1:A:75:SER:HA	2.03	0.58
1:C:13:ILE:HD11	1:D:11:LYS:HG3	1.84	0.58
1:G:13:ILE:HD13	1:H:231:ASP:HB3	1.86	0.58
1:H:105:ASN:OD1	1:H:107:LYS:HB2	2.03	0.58
1:E:176:VAL:HG21	1:E:202:TRP:CE3	2.38	0.58
1:G:34:ASP:HB2	1:G:39:GLY:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:176:VAL:HG21	1:N:202:TRP:CE3	2.39	0.57
1:A:105:ASN:OD1	1:A:107:LYS:HB2	2.03	0.57
1:I:93:PRO:O	1:I:95:LYS:HE2	2.04	0.57
1:N:70:SER:OG	1:N:75:SER:HA	2.05	0.57
1:A:215:GLY:HA3	1:A:349:PHE:CE2	2.39	0.57
1:E:70:SER:OG	1:E:75:SER:HA	2.04	0.57
1:D:176:VAL:HG21	1:D:202:TRP:CE3	2.40	0.57
1:O:43:LYS:HE3	1:O:60:TRP:CZ2	2.40	0.57
1:G:105:ASN:OD1	1:G:107:LYS:HB2	2.05	0.57
1:I:176:VAL:HG21	1:I:202:TRP:CE3	2.39	0.57
1:M:70:SER:OG	1:M:75:SER:HA	2.05	0.57
1:J:105:ASN:OD1	1:J:107:LYS:HB2	2.04	0.57
1:N:105:ASN:OD1	1:N:107:LYS:HB2	2.04	0.57
1:N:215:GLY:HA3	1:N:349:PHE:CE2	2.40	0.57
1:L:276:LYS:HD3	1:L:362:ASN:HD22	1.70	0.56
1:D:105:ASN:OD1	1:D:107:LYS:HB2	2.05	0.56
1:G:70:SER:OG	1:G:75:SER:HA	2.05	0.56
1:F:276:LYS:NZ	1:F:362:ASN:HD21	2.03	0.56
1:H:196:GLU:HB3	1:H:201:GLN:HE21	1.70	0.56
1:K:11:LYS:HE3	1:O:13:ILE:HD11	1.87	0.56
1:L:93:PRO:O	1:L:95:LYS:HE2	2.05	0.56
1:D:276:LYS:HD3	1:D:362:ASN:HD22	1.70	0.56
1:K:93:PRO:O	1:K:95:LYS:HE2	2.05	0.56
1:A:371:TYR:O	1:A:372:LYS:HE2	2.04	0.56
1:D:34:ASP:HB2	1:D:39:GLY:O	2.06	0.56
1:G:176:VAL:HG21	1:G:202:TRP:CD2	2.40	0.56
1:I:276:LYS:NZ	1:I:362:ASN:HD21	2.04	0.56
1:L:70:SER:OG	1:L:75:SER:HA	2.06	0.56
1:O:196:GLU:HB3	1:O:201:GLN:HE21	1.71	0.56
1:G:327:ARG:HH11	1:G:327:ARG:HG3	1.71	0.55
1:H:70:SER:OG	1:H:75:SER:HA	2.06	0.55
1:J:34:ASP:HB3	1:J:36:THR:H	1.71	0.55
1:K:276:LYS:HZ2	1:K:362:ASN:HD21	1.55	0.55
1:C:105:ASN:OD1	1:C:107:LYS:HB2	2.06	0.55
1:L:34:ASP:HB3	1:L:36:THR:H	1.71	0.55
1:A:276:LYS:HZ2	1:A:362:ASN:HD21	1.55	0.54
1:K:371:TYR:O	1:K:372:LYS:HE2	2.06	0.54
1:L:34:ASP:HB2	1:L:39:GLY:O	2.07	0.54
1:O:176:VAL:HG21	1:O:202:TRP:CE3	2.41	0.54
1:K:13:ILE:CD1	1:L:11:LYS:HG3	2.38	0.54
1:C:34:ASP:HB3	1:C:36:THR:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:LYS:HE3	1:H:60:TRP:CZ2	2.43	0.54
1:I:13:ILE:HD13	1:J:231:ASP:HB3	1.90	0.54
1:L:193:THR:HG22	1:L:203:GLU:O	2.08	0.54
1:L:176:VAL:HG21	1:L:202:TRP:CD2	2.42	0.53
1:N:276:LYS:HD3	1:N:362:ASN:HD22	1.71	0.53
1:B:93:PRO:O	1:B:95:LYS:HE2	2.08	0.53
1:C:176:VAL:HG21	1:C:202:TRP:CD2	2.42	0.53
1:K:176:VAL:HG21	1:K:202:TRP:CD2	2.44	0.53
1:M:371:TYR:O	1:M:372:LYS:HE2	2.09	0.53
1:C:43:LYS:HE3	1:C:60:TRP:CZ2	2.43	0.53
1:N:43:LYS:HE3	1:N:60:TRP:CZ2	2.43	0.53
1:G:276:LYS:HZ3	1:G:362:ASN:HD21	1.56	0.53
1:I:176:VAL:HG21	1:I:202:TRP:CD2	2.44	0.53
1:L:371:TYR:O	1:L:372:LYS:HE2	2.09	0.52
1:C:146:PRO:HB2	1:C:149:TRP:CD1	2.45	0.52
1:C:215:GLY:HA3	1:C:349:PHE:CE2	2.44	0.52
1:E:43:LYS:HE3	1:E:60:TRP:CZ2	2.44	0.52
1:B:215:GLY:HA3	1:B:349:PHE:CE2	2.45	0.52
1:F:13:ILE:CD1	1:G:11:LYS:HG3	2.39	0.52
1:M:13:ILE:HD11	1:N:11:LYS:HG3	1.91	0.52
1:O:34:ASP:HB3	1:O:36:THR:H	1.75	0.52
1:E:215:GLY:HA3	1:E:349:PHE:CE2	2.44	0.52
1:I:43:LYS:HE3	1:I:60:TRP:CZ2	2.44	0.52
1:M:176:VAL:HG21	1:M:202:TRP:CD2	2.45	0.52
1:C:328:THR:HA	1:C:331:GLN:HG2	1.92	0.52
1:H:276:LYS:HZ3	1:H:362:ASN:HD21	1.58	0.52
1:K:34:ASP:HB3	1:K:36:THR:H	1.75	0.52
1:H:328:THR:HA	1:H:331:GLN:HG2	1.92	0.52
1:L:13:ILE:HD11	1:M:11:LYS:HG3	1.91	0.52
1:A:34:ASP:HB3	1:A:36:THR:H	1.75	0.52
1:D:327:ARG:HH11	1:D:327:ARG:HG3	1.75	0.52
1:E:196:GLU:HB3	1:E:201:GLN:HE21	1.76	0.51
1:J:146:PRO:HB2	1:J:149:TRP:CD1	2.46	0.51
1:L:146:PRO:HB2	1:L:149:TRP:CD1	2.46	0.51
1:M:43:LYS:HE3	1:M:60:TRP:CZ2	2.45	0.51
1:N:196:GLU:HB3	1:N:201:GLN:HE21	1.75	0.51
1:F:34:ASP:HB3	1:F:36:THR:H	1.76	0.51
1:M:34:ASP:HB2	1:M:39:GLY:O	2.10	0.51
1:L:341:ARG:N	1:L:342:PRO:CD	2.74	0.51
1:L:43:LYS:HE3	1:L:60:TRP:CZ2	2.45	0.51
1:A:93:PRO:O	1:A:95:LYS:HE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ILE:HD11	1:C:11:LYS:HG3	1.93	0.51
1:F:43:LYS:HE3	1:F:60:TRP:CZ2	2.46	0.51
1:H:176:VAL:HG21	1:H:202:TRP:CD2	2.46	0.51
1:I:13:ILE:HD11	1:J:11:LYS:HE3	1.93	0.51
1:M:341:ARG:N	1:M:342:PRO:CD	2.74	0.51
1:K:196:GLU:HB3	1:K:201:GLN:HE21	1.75	0.51
1:N:34:ASP:HB2	1:N:39:GLY:O	2.11	0.51
1:N:276:LYS:HZ2	1:N:362:ASN:HD21	1.56	0.50
1:F:196:GLU:HB3	1:F:201:GLN:HE21	1.76	0.50
1:C:93:PRO:O	1:C:95:LYS:HE2	2.12	0.50
1:F:146:PRO:HB2	1:F:149:TRP:CD1	2.47	0.50
1:K:276:LYS:HD3	1:K:362:ASN:HD22	1.76	0.50
1:A:13:ILE:HD13	1:B:231:ASP:HB3	1.94	0.50
1:I:70:SER:OG	1:I:75:SER:HA	2.11	0.50
1:J:276:LYS:HZ3	1:J:362:ASN:HD21	1.59	0.50
1:D:13:ILE:HD11	1:E:11:LYS:HG3	1.94	0.50
1:K:327:ARG:HH11	1:K:327:ARG:HG3	1.77	0.50
1:B:176:VAL:HG21	1:B:202:TRP:CD2	2.47	0.50
1:F:199:PRO:O	1:F:200:ALA:HB3	2.12	0.50
1:K:199:PRO:O	1:K:200:ALA:HB3	2.11	0.50
1:K:328:THR:HA	1:K:331:GLN:HG2	1.94	0.50
1:B:34:ASP:HB3	1:B:36:THR:H	1.75	0.49
1:D:367:GLU:CG	1:D:368:PRO:HD2	2.42	0.49
1:I:367:GLU:CG	1:I:368:PRO:HD2	2.42	0.49
1:M:13:ILE:HD11	1:N:11:LYS:HE3	1.93	0.49
1:A:43:LYS:HE3	1:A:60:TRP:CZ2	2.46	0.49
1:B:146:PRO:HB2	1:B:149:TRP:CD1	2.47	0.49
1:C:196:GLU:HB3	1:C:201:GLN:HE21	1.76	0.49
1:E:367:GLU:CG	1:E:368:PRO:HD2	2.42	0.49
1:C:367:GLU:CG	1:C:368:PRO:HD2	2.42	0.49
1:F:90:ARG:O	1:F:91:LYS:HB2	2.11	0.49
1:E:176:VAL:HG21	1:E:202:TRP:CD2	2.47	0.49
1:F:367:GLU:CG	1:F:368:PRO:HD2	2.42	0.49
1:G:93:PRO:O	1:G:95:LYS:HE2	2.12	0.49
1:H:7:SER:HB3	1:H:233:GLY:HA3	1.93	0.49
1:K:367:GLU:CG	1:K:368:PRO:HD2	2.43	0.49
1:L:276:LYS:NZ	1:L:362:ASN:ND2	2.56	0.49
1:A:367:GLU:CG	1:A:368:PRO:HD2	2.43	0.49
1:C:13:ILE:CD1	1:D:11:LYS:HG3	2.41	0.49
1:H:13:ILE:HD11	1:I:11:LYS:HE3	1.94	0.49
1:G:43:LYS:HE3	1:G:60:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:196:GLU:HB3	1:J:201:GLN:HE21	1.76	0.49
1:J:43:LYS:HE3	1:J:60:TRP:CZ2	2.46	0.49
1:M:276:LYS:HZ3	1:M:362:ASN:HD21	1.61	0.49
1:N:328:THR:HA	1:N:331:GLN:HG2	1.94	0.49
1:B:13:ILE:HD11	1:C:11:LYS:HE3	1.94	0.49
1:G:327:ARG:HG3	1:G:327:ARG:NH1	2.26	0.49
1:J:176:VAL:HG21	1:J:202:TRP:CD2	2.47	0.49
1:K:146:PRO:HB2	1:K:149:TRP:CD1	2.47	0.49
1:M:327:ARG:HG3	1:M:327:ARG:HH11	1.76	0.49
1:C:146:PRO:HB2	1:C:149:TRP:CG	2.48	0.49
1:O:199:PRO:O	1:O:200:ALA:HB3	2.12	0.49
1:E:77:MET:HE2	1:E:101:VAL:HG12	1.95	0.49
1:E:93:PRO:O	1:E:95:LYS:HE2	2.12	0.49
1:O:327:ARG:HG3	1:O:327:ARG:HH11	1.76	0.49
1:D:341:ARG:N	1:D:342:PRO:CD	2.76	0.49
1:J:215:GLY:HA3	1:J:349:PHE:CE2	2.48	0.49
1:E:161:TYR:CD1	1:E:199:PRO:HD3	2.47	0.48
1:J:327:ARG:HH11	1:J:327:ARG:HG3	1.78	0.48
1:N:34:ASP:HB3	1:N:36:THR:H	1.77	0.48
1:D:176:VAL:HG21	1:D:202:TRP:CD2	2.47	0.48
1:D:371:TYR:O	1:D:372:LYS:HE2	2.12	0.48
1:N:367:GLU:CG	1:N:368:PRO:HD2	2.43	0.48
1:A:34:ASP:HB2	1:A:39:GLY:O	2.14	0.48
1:B:43:LYS:HE3	1:B:60:TRP:CZ2	2.48	0.48
1:N:176:VAL:HG21	1:N:202:TRP:CD2	2.49	0.48
1:I:34:ASP:HB2	1:I:39:GLY:O	2.13	0.48
1:M:93:PRO:O	1:M:95:LYS:HE2	2.14	0.48
1:K:341:ARG:N	1:K:342:PRO:CD	2.76	0.48
1:H:146:PRO:HB2	1:H:149:TRP:CG	2.49	0.48
1:J:252:CYS:HB2	1:J:344:ALA:HA	1.96	0.48
1:A:176:VAL:HG21	1:A:202:TRP:CD2	2.48	0.48
1:B:196:GLU:HB3	1:B:201:GLN:HE21	1.77	0.48
1:M:276:LYS:HD3	1:M:362:ASN:HD22	1.79	0.48
1:B:367:GLU:CG	1:B:368:PRO:HD2	2.44	0.48
1:E:198:MET:O	1:E:201:GLN:HB3	2.14	0.48
1:G:34:ASP:HB3	1:G:36:THR:H	1.79	0.48
1:H:93:PRO:O	1:H:95:LYS:HE2	2.14	0.48
1:J:367:GLU:CG	1:J:368:PRO:HD2	2.43	0.48
1:M:161:TYR:CD1	1:M:199:PRO:HD3	2.49	0.48
1:G:196:GLU:HB3	1:G:201:GLN:HE21	1.79	0.48
1:I:34:ASP:HB3	1:I:36:THR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:328:THR:HA	1:L:331:GLN:HG2	1.96	0.48
1:O:146:PRO:HB2	1:O:149:TRP:CG	2.49	0.48
1:C:134:GLU:HG2	1:C:205:GLN:HG3	1.96	0.47
1:N:371:TYR:O	1:N:372:LYS:HE2	2.14	0.47
1:A:196:GLU:HB3	1:A:201:GLN:HE21	1.78	0.47
1:M:328:THR:HA	1:M:331:GLN:HG2	1.97	0.47
1:O:367:GLU:CG	1:O:368:PRO:HD2	2.44	0.47
1:C:77:MET:HE2	1:C:101:VAL:HG12	1.96	0.47
1:E:276:LYS:HZ3	1:E:362:ASN:HD21	1.60	0.47
1:H:199:PRO:O	1:H:200:ALA:HB3	2.13	0.47
1:J:371:TYR:O	1:J:372:LYS:HE2	2.14	0.47
1:C:276:LYS:HZ3	1:C:362:ASN:HD21	1.61	0.47
1:H:77:MET:HE2	1:H:101:VAL:HG12	1.95	0.47
1:J:51:PRO:HG3	1:J:57:LEU:HD21	1.97	0.47
1:M:34:ASP:HB3	1:M:36:THR:H	1.79	0.47
1:D:276:LYS:HZ2	1:D:362:ASN:HD21	1.60	0.47
1:G:276:LYS:HD3	1:G:362:ASN:HD22	1.79	0.47
1:K:77:MET:HE2	1:K:101:VAL:HG12	1.97	0.47
1:E:327:ARG:HG3	1:E:327:ARG:HH11	1.79	0.47
1:I:134:GLU:HG2	1:I:205:GLN:HG3	1.96	0.47
1:I:180:TYR:OH	1:I:192:GLY:HA2	2.14	0.47
1:L:215:GLY:HA3	1:L:349:PHE:CE2	2.49	0.47
1:B:327:ARG:HG2	1:B:331:GLN:HE21	1.79	0.47
1:B:328:THR:HA	1:B:331:GLN:HG2	1.96	0.47
1:G:146:PRO:HB2	1:G:149:TRP:CD1	2.50	0.47
1:G:371:TYR:O	1:G:372:LYS:HE2	2.15	0.47
1:H:13:ILE:CD1	1:I:11:LYS:HG3	2.43	0.47
1:I:199:PRO:O	1:I:200:ALA:HB3	2.15	0.47
1:O:176:VAL:HG21	1:O:202:TRP:CD2	2.50	0.47
1:I:341:ARG:N	1:I:342:PRO:CD	2.77	0.47
1:O:198:MET:O	1:O:201:GLN:HB3	2.14	0.47
1:A:372:LYS:HA	1:A:372:LYS:HD3	1.66	0.47
1:G:367:GLU:CG	1:G:368:PRO:HD2	2.45	0.47
1:L:161:TYR:CD1	1:L:199:PRO:HD3	2.50	0.47
1:H:52:LYS:HB3	1:H:56:GLU:OE2	2.15	0.47
1:L:367:GLU:CG	1:L:368:PRO:HD2	2.45	0.47
1:O:327:ARG:HG2	1:O:331:GLN:HE21	1.80	0.47
1:B:77:MET:HE2	1:B:101:VAL:HG12	1.96	0.47
1:D:328:THR:HA	1:D:331:GLN:HG2	1.96	0.47
1:G:7:SER:HB3	1:G:233:GLY:HA3	1.97	0.47
1:I:42:CYS:O	1:J:163:CYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:328:THR:HA	1:O:331:GLN:HG2	1.97	0.47
1:O:34:ASP:HB2	1:O:39:GLY:O	2.15	0.47
1:C:34:ASP:HB2	1:C:39:GLY:O	2.14	0.46
1:F:371:TYR:O	1:F:372:LYS:HE2	2.16	0.46
1:A:13:ILE:HD11	1:B:11:LYS:HG3	1.97	0.46
1:B:13:ILE:HD13	1:C:231:ASP:HB3	1.97	0.46
1:E:199:PRO:O	1:E:200:ALA:HB3	2.15	0.46
1:O:63:ASP:C	1:O:63:ASP:OD1	2.53	0.46
1:B:198:MET:O	1:B:201:GLN:HB3	2.16	0.46
1:C:371:TYR:O	1:C:372:LYS:HE2	2.15	0.46
1:F:327:ARG:HG3	1:F:327:ARG:HH11	1.79	0.46
1:F:104:TYR:HB2	1:G:327:ARG:HE	1.80	0.46
1:I:146:PRO:HB2	1:I:149:TRP:CD1	2.51	0.46
1:J:146:PRO:HB2	1:J:149:TRP:CG	2.51	0.46
1:K:34:ASP:HB2	1:K:39:GLY:O	2.15	0.46
1:M:199:PRO:O	1:M:200:ALA:HB3	2.14	0.46
1:A:341:ARG:N	1:A:342:PRO:CD	2.78	0.46
1:E:34:ASP:HB2	1:E:39:GLY:O	2.16	0.46
1:O:52:LYS:HB3	1:O:56:GLU:OE2	2.16	0.46
1:A:328:THR:HA	1:A:331:GLN:HG2	1.98	0.46
1:B:372:LYS:HD3	1:B:372:LYS:HA	1.75	0.46
1:B:52:LYS:HB3	1:B:56:GLU:OE2	2.16	0.46
1:B:282:GLN:HA	1:B:282:GLN:OE1	2.16	0.46
1:H:367:GLU:CG	1:H:368:PRO:HD2	2.46	0.46
1:I:371:TYR:O	1:I:372:LYS:HE2	2.16	0.46
1:O:146:PRO:HB2	1:O:149:TRP:CD1	2.51	0.46
1:B:276:LYS:HD3	1:B:362:ASN:HD22	1.82	0.46
1:G:13:ILE:HD11	1:H:11:LYS:HG3	1.98	0.46
1:I:327:ARG:HG2	1:I:331:GLN:HE21	1.81	0.46
1:C:341:ARG:N	1:C:342:PRO:CD	2.79	0.45
1:F:328:THR:HA	1:F:331:GLN:HG2	1.97	0.45
1:A:327:ARG:HH11	1:A:327:ARG:HG3	1.82	0.45
1:C:199:PRO:O	1:C:200:ALA:HB3	2.17	0.45
1:F:13:ILE:HD11	1:G:11:LYS:HE3	1.98	0.45
1:H:42:CYS:O	1:I:163:CYS:HB3	2.16	0.45
1:J:328:THR:HA	1:J:331:GLN:HG2	1.98	0.45
1:K:327:ARG:HG2	1:K:331:GLN:HE21	1.81	0.45
1:K:43:LYS:HE3	1:K:60:TRP:CZ2	2.51	0.45
1:M:77:MET:HE2	1:M:101:VAL:HG12	1.97	0.45
1:D:196:GLU:HB3	1:D:201:GLN:HE21	1.80	0.45
1:F:341:ARG:N	1:F:342:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:SER:HB3	1:G:233:GLY:CA	2.47	0.45
1:G:341:ARG:N	1:G:342:PRO:CD	2.78	0.45
1:J:93:PRO:O	1:J:95:LYS:HE2	2.17	0.45
1:M:367:GLU:CG	1:M:368:PRO:HD2	2.46	0.45
1:H:327:ARG:HH11	1:H:327:ARG:HG3	1.81	0.45
1:L:199:PRO:O	1:L:200:ALA:HB3	2.17	0.45
1:M:146:PRO:HB2	1:M:149:TRP:CD1	2.51	0.45
1:A:11:LYS:HG3	1:E:13:ILE:CD1	2.46	0.45
1:F:219:TRP:NE1	1:F:348:PRO:HD2	2.31	0.45
1:H:327:ARG:HG2	1:H:331:GLN:HE21	1.81	0.45
1:L:341:ARG:N	1:L:342:PRO:HD3	2.31	0.45
1:B:7:SER:HB3	1:B:233:GLY:HA3	1.99	0.45
1:E:372:LYS:HD3	1:E:372:LYS:HA	1.74	0.45
1:F:11:LYS:HG3	1:J:13:ILE:CD1	2.45	0.45
1:M:146:PRO:HB2	1:M:149:TRP:CG	2.52	0.45
1:D:372:LYS:HD3	1:D:372:LYS:HA	1.72	0.45
1:E:328:THR:HA	1:E:331:GLN:HG2	1.98	0.45
1:F:51:PRO:HG3	1:F:57:LEU:HD21	1.99	0.45
1:G:328:THR:HA	1:G:331:GLN:HG2	1.98	0.45
1:H:372:LYS:HA	1:H:372:LYS:HD3	1.52	0.45
1:J:77:MET:HE2	1:J:101:VAL:HG12	1.99	0.45
1:L:276:LYS:HZ2	1:L:362:ASN:HD21	1.59	0.45
1:B:341:ARG:N	1:B:342:PRO:CD	2.79	0.45
1:D:252:CYS:HB2	1:D:344:ALA:HA	1.99	0.45
1:N:52:LYS:HB3	1:N:56:GLU:OE2	2.17	0.45
1:D:86:ARG:HD3	1:D:185:TYR:O	2.17	0.44
1:E:341:ARG:N	1:E:342:PRO:CD	2.80	0.44
1:F:372:LYS:HD3	1:F:372:LYS:HA	1.77	0.44
1:K:146:PRO:HB2	1:K:149:TRP:CG	2.52	0.44
1:L:13:ILE:CD1	1:M:11:LYS:HG3	2.48	0.44
1:O:212:ILE:HA	1:O:212:ILE:HD12	1.88	0.44
1:F:180:TYR:OH	1:F:192:GLY:HA2	2.17	0.44
1:G:252:CYS:HB2	1:G:344:ALA:HA	2.00	0.44
1:A:282:GLN:HA	1:A:282:GLN:OE1	2.16	0.44
1:B:276:LYS:HZ2	1:B:362:ASN:HD21	1.63	0.44
1:J:35:GLY:CA	1:J:69:GLN:HG3	2.48	0.44
1:L:13:ILE:HD13	1:M:231:ASP:HB3	1.97	0.44
1:N:327:ARG:HG2	1:N:331:GLN:HE21	1.82	0.44
1:N:13:ILE:CD1	1:O:11:LYS:HG3	2.48	0.44
1:J:34:ASP:HB2	1:J:39:GLY:O	2.17	0.44
1:M:198:MET:O	1:M:201:GLN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:276:LYS:NZ	1:N:362:ASN:ND2	2.65	0.44
1:N:276:LYS:HZ3	1:N:362:ASN:HD21	1.66	0.44
1:E:52:LYS:HB3	1:E:56:GLU:OE2	2.18	0.44
1:G:219:TRP:NE1	1:G:348:PRO:HD2	2.32	0.44
1:I:276:LYS:HD3	1:I:362:ASN:HD22	1.83	0.44
1:F:146:PRO:HB2	1:F:149:TRP:CG	2.52	0.44
1:L:52:LYS:HB3	1:L:56:GLU:OE2	2.18	0.44
1:I:7:SER:HB3	1:I:233:GLY:HA3	2.00	0.43
1:I:328:THR:HA	1:I:331:GLN:HG2	1.99	0.43
1:L:219:TRP:NE1	1:L:348:PRO:HD2	2.33	0.43
1:O:341:ARG:N	1:O:342:PRO:CD	2.81	0.43
1:D:219:TRP:NE1	1:D:348:PRO:HD2	2.33	0.43
1:I:151:SER:O	1:I:152:ASN:HB2	2.18	0.43
1:I:341:ARG:N	1:I:342:PRO:HD3	2.33	0.43
1:K:198:MET:O	1:K:201:GLN:HB3	2.19	0.43
1:K:372:LYS:HD3	1:K:372:LYS:HA	1.83	0.43
1:M:134:GLU:HG2	1:M:205:GLN:HG3	2.00	0.43
1:K:212:ILE:HA	1:K:212:ILE:HD12	1.87	0.43
1:K:341:ARG:N	1:K:342:PRO:HD3	2.33	0.43
1:O:77:MET:HE2	1:O:101:VAL:HG12	2.00	0.43
1:B:34:ASP:HB2	1:B:39:GLY:O	2.19	0.43
1:G:35:GLY:CA	1:G:69:GLN:HG3	2.49	0.43
1:J:212:ILE:HA	1:J:212:ILE:HD12	1.89	0.43
1:L:327:ARG:HG3	1:L:327:ARG:HH11	1.82	0.43
1:N:328:THR:HA	1:N:331:GLN:CG	2.48	0.43
1:N:341:ARG:N	1:N:342:PRO:CD	2.81	0.43
1:E:327:ARG:HG3	1:E:327:ARG:NH1	2.34	0.43
1:H:328:THR:HA	1:H:331:GLN:CG	2.48	0.43
1:I:77:MET:HE2	1:I:101:VAL:HG12	2.01	0.43
1:J:341:ARG:N	1:J:342:PRO:CD	2.82	0.43
1:K:371:TYR:HB3	1:K:372:LYS:H	1.64	0.43
1:M:327:ARG:HG2	1:M:331:GLN:HE21	1.82	0.43
1:M:52:LYS:HB3	1:M:56:GLU:OE2	2.18	0.43
1:N:13:ILE:HD13	1:O:231:ASP:HB3	2.01	0.43
1:B:35:GLY:CA	1:B:69:GLN:HG3	2.49	0.43
1:L:196:GLU:HB3	1:L:201:GLN:HE21	1.82	0.43
1:N:161:TYR:CD1	1:N:199:PRO:HD3	2.53	0.43
1:G:13:ILE:HD11	1:H:11:LYS:HE3	2.01	0.43
1:G:199:PRO:O	1:G:200:ALA:HB3	2.18	0.43
1:I:322:SER:HB3	1:I:341:ARG:HD3	2.01	0.43
1:C:276:LYS:HZ2	1:C:362:ASN:HD21	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:LYS:HD3	1:C:362:ASN:HD22	1.83	0.43
1:D:13:ILE:HD13	1:E:231:ASP:HB3	2.00	0.43
1:F:63:ASP:C	1:F:63:ASP:OD1	2.57	0.43
1:K:11:LYS:HG3	1:O:13:ILE:HD11	1.99	0.43
1:L:322:SER:HB3	1:L:341:ARG:HD3	2.01	0.43
1:M:196:GLU:HB3	1:M:201:GLN:HE21	1.83	0.43
1:D:161:TYR:CD1	1:D:199:PRO:HD3	2.54	0.43
1:H:40:LEU:HD13	1:H:223:PHE:HB2	2.01	0.43
1:I:372:LYS:HA	1:I:372:LYS:HD3	1.81	0.43
1:I:52:LYS:HB3	1:I:56:GLU:OE2	2.19	0.43
1:I:13:ILE:HD11	1:J:11:LYS:HG3	2.00	0.43
1:K:328:THR:HA	1:K:331:GLN:CG	2.48	0.43
1:E:26:VAL:HG22	1:E:93:PRO:HG2	2.01	0.43
1:L:212:ILE:HA	1:L:212:ILE:HD12	1.90	0.43
1:B:7:SER:HB3	1:B:233:GLY:CA	2.49	0.42
1:C:198:MET:O	1:C:201:GLN:HB3	2.18	0.42
1:D:7:SER:HB3	1:D:233:GLY:HA3	2.01	0.42
1:G:372:LYS:HA	1:G:372:LYS:HD3	1.83	0.42
1:A:146:PRO:HB2	1:A:149:TRP:CD1	2.55	0.42
1:D:52:LYS:HB3	1:D:56:GLU:OE2	2.19	0.42
1:I:282:GLN:OE1	1:I:282:GLN:HA	2.19	0.42
1:L:86:ARG:HD3	1:L:185:TYR:O	2.19	0.42
1:C:212:ILE:HA	1:C:212:ILE:HD12	1.88	0.42
1:D:319:ARG:O	1:D:340:ARG:NH1	2.52	0.42
1:D:93:PRO:O	1:D:95:LYS:HE2	2.19	0.42
1:F:163:CYS:HB3	1:J:42:CYS:O	2.19	0.42
1:F:52:LYS:HB3	1:F:56:GLU:OE2	2.19	0.42
1:G:137:TYR:CZ	1:G:202:TRP:HB2	2.54	0.42
1:I:252:CYS:HB2	1:I:344:ALA:HA	2.02	0.42
1:J:52:LYS:HB3	1:J:56:GLU:OE2	2.19	0.42
1:M:341:ARG:N	1:M:342:PRO:HD3	2.35	0.42
1:N:63:ASP:OD1	1:N:63:ASP:C	2.58	0.42
1:D:146:PRO:HB2	1:D:149:TRP:CG	2.54	0.42
1:D:35:GLY:CA	1:D:69:GLN:HG3	2.50	0.42
1:F:282:GLN:HA	1:F:282:GLN:OE1	2.19	0.42
1:G:212:ILE:HA	1:G:212:ILE:HD12	1.90	0.42
1:G:282:GLN:OE1	1:G:282:GLN:HA	2.20	0.42
1:I:90:ARG:O	1:I:91:LYS:HB2	2.19	0.42
1:M:276:LYS:HZ2	1:M:362:ASN:HD21	1.66	0.42
1:N:289:ASP:OD2	1:N:296:ASN:HB2	2.20	0.42
1:A:199:PRO:O	1:A:200:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:THR:HA	1:C:331:GLN:CG	2.48	0.42
1:D:327:ARG:NH1	1:D:327:ARG:HG3	2.32	0.42
1:E:40:LEU:HD13	1:E:223:PHE:HB2	2.01	0.42
1:E:7:SER:HB3	1:E:233:GLY:HA3	2.02	0.42
1:F:168:ASP:N	1:F:168:ASP:OD1	2.50	0.42
1:H:219:TRP:NE1	1:H:348:PRO:HD2	2.34	0.42
1:N:55:GLU:CD	1:N:55:GLU:H	2.23	0.42
1:C:7:SER:HB3	1:C:233:GLY:CA	2.50	0.42
1:D:40:LEU:HD13	1:D:223:PHE:HB2	2.02	0.42
1:H:7:SER:HB3	1:H:233:GLY:CA	2.49	0.42
1:L:341:ARG:H	1:L:342:PRO:HD3	1.84	0.42
1:A:212:ILE:HD12	1:A:212:ILE:HA	1.88	0.42
1:D:276:LYS:HD3	1:D:362:ASN:ND2	2.35	0.42
1:D:371:TYR:HB3	1:D:372:LYS:H	1.65	0.42
1:L:327:ARG:HG2	1:L:331:GLN:HE21	1.85	0.42
1:O:371:TYR:HB3	1:O:372:LYS:H	1.62	0.42
1:A:327:ARG:HG2	1:A:331:GLN:HE21	1.85	0.42
1:D:199:PRO:O	1:D:200:ALA:HB3	2.20	0.42
1:E:32:TRP:CE2	1:E:41:ARG:HB2	2.54	0.42
1:H:146:PRO:HB2	1:H:149:TRP:CD1	2.55	0.42
1:I:146:PRO:HB2	1:I:149:TRP:CG	2.54	0.42
1:K:327:ARG:NH1	1:K:327:ARG:HG3	2.35	0.42
1:N:13:ILE:HD11	1:O:11:LYS:HE3	2.01	0.42
1:O:151:SER:O	1:O:152:ASN:HB2	2.20	0.42
1:C:327:ARG:HG3	1:C:327:ARG:HH11	1.85	0.42
1:C:55:GLU:H	1:C:55:GLU:CD	2.22	0.42
1:D:43:LYS:HE3	1:D:60:TRP:CZ2	2.54	0.42
1:F:276:LYS:HD3	1:F:362:ASN:HD22	1.85	0.42
1:J:134:GLU:HG2	1:J:205:GLN:HG3	2.02	0.42
1:O:86:ARG:HD3	1:O:185:TYR:O	2.20	0.42
1:O:282:GLN:HA	1:O:282:GLN:OE1	2.19	0.42
1:O:371:TYR:O	1:O:372:LYS:HE2	2.20	0.42
1:A:7:SER:HB3	1:A:233:GLY:HA3	2.02	0.41
1:D:42:CYS:O	1:E:163:CYS:HB3	2.20	0.41
1:J:282:GLN:OE1	1:J:282:GLN:HA	2.19	0.41
1:J:327:ARG:NH1	1:J:327:ARG:HG3	2.35	0.41
1:B:13:ILE:CD1	1:C:11:LYS:HG3	2.49	0.41
1:E:123:MET:HE1	1:E:371:TYR:CE2	2.55	0.41
1:E:282:GLN:OE1	1:E:282:GLN:HA	2.20	0.41
1:F:86:ARG:HD3	1:F:185:TYR:O	2.20	0.41
1:I:371:TYR:HB3	1:I:372:LYS:H	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:276:LYS:HD3	1:L:362:ASN:ND2	2.35	0.41
1:L:282:GLN:OE1	1:L:282:GLN:HA	2.21	0.41
1:M:282:GLN:OE1	1:M:282:GLN:HA	2.20	0.41
1:O:93:PRO:O	1:O:95:LYS:HE2	2.20	0.41
1:A:180:TYR:OH	1:A:192:GLY:HA2	2.20	0.41
1:A:252:CYS:HB2	1:A:344:ALA:HA	2.03	0.41
1:A:327:ARG:NH1	1:A:327:ARG:HG3	2.35	0.41
1:A:63:ASP:OD1	1:A:63:ASP:C	2.59	0.41
1:A:87:ASP:OD2	1:A:90:ARG:HD2	2.21	0.41
1:B:327:ARG:HG3	1:B:327:ARG:HH11	1.84	0.41
1:C:52:LYS:HB3	1:C:56:GLU:OE2	2.19	0.41
1:G:161:TYR:CD1	1:G:199:PRO:HD3	2.55	0.41
1:L:42:CYS:O	1:M:163:CYS:HB3	2.21	0.41
1:N:146:PRO:HB2	1:N:149:TRP:CG	2.55	0.41
1:N:367:GLU:HG3	1:N:368:PRO:HD2	2.02	0.41
1:C:42:CYS:O	1:D:163:CYS:HB3	2.21	0.41
1:F:76:ASP:O	1:F:77:MET:HG2	2.20	0.41
1:G:52:LYS:HB3	1:G:56:GLU:OE2	2.20	0.41
1:H:32:TRP:CE2	1:H:41:ARG:HB2	2.56	0.41
1:I:327:ARG:HH11	1:I:327:ARG:HG3	1.86	0.41
1:K:137:TYR:CZ	1:K:202:TRP:HB2	2.56	0.41
1:K:35:GLY:CA	1:K:69:GLN:HG3	2.49	0.41
1:L:371:TYR:HB3	1:L:372:LYS:H	1.67	0.41
1:N:372:LYS:HA	1:N:372:LYS:HD3	1.77	0.41
1:B:32:TRP:CE2	1:B:41:ARG:HB2	2.55	0.41
1:C:372:LYS:HD3	1:C:372:LYS:HA	1.81	0.41
1:D:63:ASP:OD1	1:D:63:ASP:C	2.59	0.41
1:H:180:TYR:OH	1:H:192:GLY:HA2	2.21	0.41
1:K:134:GLU:HG2	1:K:205:GLN:HG3	2.01	0.41
1:N:198:MET:O	1:N:201:GLN:HB3	2.21	0.41
1:O:171:TYR:N	1:O:171:TYR:CD2	2.88	0.41
1:F:322:SER:HB3	1:F:341:ARG:HD3	2.03	0.41
1:G:146:PRO:HB2	1:G:149:TRP:CG	2.55	0.41
1:K:131:PHE:HA	1:K:255:ASN:O	2.21	0.41
1:C:327:ARG:HG2	1:C:331:GLN:HE21	1.85	0.41
1:F:367:GLU:HG3	1:F:368:PRO:HD2	2.03	0.41
1:G:77:MET:HE2	1:G:101:VAL:HG12	2.02	0.41
1:H:276:LYS:HD3	1:H:362:ASN:HD22	1.85	0.41
1:H:51:PRO:HG3	1:H:57:LEU:HD21	2.03	0.41
1:C:104:TYR:HB2	1:D:327:ARG:HE	1.85	0.41
1:E:90:ARG:O	1:E:91:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:231:ASP:HB3	1:O:13:ILE:HD13	2.02	0.41
1:O:327:ARG:NH1	1:O:327:ARG:HG3	2.35	0.41
1:B:180:TYR:OH	1:B:192:GLY:HA2	2.21	0.41
1:D:146:PRO:HB2	1:D:149:TRP:CD1	2.56	0.41
1:D:367:GLU:HG3	1:D:368:PRO:HD2	2.02	0.41
1:J:327:ARG:HG2	1:J:331:GLN:HE21	1.85	0.41
1:N:180:TYR:OH	1:N:192:GLY:HA2	2.21	0.41
1:N:77:MET:HE2	1:N:101:VAL:HG12	2.02	0.41
1:O:372:LYS:HA	1:O:372:LYS:HD3	1.86	0.41
1:A:134:GLU:HG2	1:A:205:GLN:HG3	2.03	0.41
1:C:341:ARG:N	1:C:342:PRO:HD3	2.36	0.41
1:A:168:ASP:HB3	1:E:235:ILE:HD11	2.03	0.41
1:F:123:MET:HE1	1:F:371:TYR:CE2	2.55	0.41
1:G:134:GLU:HG2	1:G:205:GLN:HG3	2.03	0.41
1:G:21:PRO:HD2	1:H:185:TYR:CE1	2.56	0.41
1:N:113:LEU:HD12	1:N:350:SER:HB2	2.03	0.41
1:C:171:TYR:N	1:C:171:TYR:CD2	2.87	0.41
1:C:35:GLY:CA	1:C:69:GLN:HG3	2.51	0.41
1:D:327:ARG:HG2	1:D:331:GLN:HE21	1.85	0.41
1:G:319:ARG:O	1:G:340:ARG:NH1	2.54	0.41
1:H:15:GLN:OE1	1:H:15:GLN:HA	2.21	0.41
1:H:227:ARG:HA	1:H:227:ARG:HD2	1.89	0.41
1:N:276:LYS:HD3	1:N:362:ASN:ND2	2.36	0.41
1:A:276:LYS:NZ	1:A:362:ASN:ND2	2.66	0.40
1:A:32:TRP:CE2	1:A:41:ARG:HB2	2.56	0.40
1:B:212:ILE:HA	1:B:212:ILE:HD12	1.93	0.40
1:F:43:LYS:HG3	1:F:60:TRP:CZ3	2.56	0.40
1:G:268:LYS:NZ	1:O:52:LYS:HE3	2.36	0.40
1:K:327:ARG:HE	1:O:104:TYR:HB2	1.86	0.40
1:M:327:ARG:HG3	1:M:327:ARG:NH1	2.35	0.40
1:D:180:TYR:OH	1:D:192:GLY:HA2	2.21	0.40
1:F:131:PHE:HA	1:F:255:ASN:O	2.21	0.40
1:F:289:ASP:OD2	1:F:296:ASN:HB2	2.21	0.40
1:G:180:TYR:OH	1:G:192:GLY:HA2	2.21	0.40
1:H:131:PHE:HA	1:H:255:ASN:O	2.22	0.40
1:L:120:ILE:HG22	1:L:356:ILE:HG21	2.03	0.40
1:D:34:ASP:HB3	1:D:36:THR:H	1.86	0.40
1:E:327:ARG:HG2	1:E:331:GLN:HE21	1.86	0.40
1:F:327:ARG:HG2	1:F:331:GLN:HE21	1.86	0.40
1:H:282:GLN:HA	1:H:282:GLN:OE1	2.21	0.40
1:J:276:LYS:HD3	1:J:362:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:180:TYR:OH	1:K:192:GLY:HA2	2.22	0.40
1:L:40:LEU:HD21	1:L:219:TRP:CE3	2.56	0.40
1:A:198:MET:O	1:A:201:GLN:HB3	2.21	0.40
1:B:26:VAL:HG22	1:B:93:PRO:HG2	2.02	0.40
1:I:171:TYR:N	1:I:171:TYR:CD2	2.90	0.40
1:J:198:MET:O	1:J:201:GLN:HB3	2.20	0.40
1:J:52:LYS:HD2	1:J:52:LYS:HA	1.91	0.40
1:L:198:MET:O	1:L:201:GLN:HB3	2.21	0.40
1:O:55:GLU:H	1:O:55:GLU:CD	2.24	0.40
1:D:282:GLN:HA	1:D:282:GLN:OE1	2.20	0.40
1:I:51:PRO:HG3	1:I:57:LEU:HD21	2.04	0.40
1:O:120:ILE:HD11	1:O:357:ARG:NH2	2.37	0.40

All (12) 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:I:119:ARG:NH2	1:M:264:GLU:OE2[1_554]	1.49	0.71
1:H:106:ARG:CZ	1:L:263:GLU:OE1[3_555]	1.66	0.54
1:H:106:ARG:NH2	1:L:263:GLU:CB[3_555]	1.80	0.40
1:J:331:GLN:O	1:M:126:ASN:ND2[1_554]	1.85	0.35
1:H:106:ARG:NE	1:L:263:GLU:OE1[3_555]	1.86	0.34
1:H:106:ARG:NH1	1:L:263:GLU:OE1[3_555]	1.86	0.34
1:H:55:GLU:CB	1:L:333:LYS:NZ[3_555]	1.91	0.29
1:H:259:LYS:CE	1:K:119:ARG:NH2[3_555]	1.91	0.29
1:H:259:LYS:NZ	1:K:119:ARG:NH2[3_555]	1.96	0.24
1:I:106:ARG:CZ	1:M:263:GLU:OE1[1_554]	1.98	0.22
1:J:331:GLN:O	1:M:126:ASN:CG[1_554]	1.99	0.21
1:H:55:GLU:CG	1:L:333:LYS:NZ[3_555]	2.08	0.12

## 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	368/381 (97%)	354 (96%)	12 (3%)	2 (0%)	29	68
1	B	368/381 (97%)	350 (95%)	16 (4%)	2 (0%)	29	68
1	C	368/381 (97%)	348 (95%)	18 (5%)	2 (0%)	29	68
1	D	368/381 (97%)	352 (96%)	15 (4%)	1 (0%)	41	76
1	E	368/381 (97%)	350 (95%)	17 (5%)	1 (0%)	41	76
1	F	368/381 (97%)	350 (95%)	16 (4%)	2 (0%)	29	68
1	G	368/381 (97%)	348 (95%)	18 (5%)	2 (0%)	29	68
1	H	368/381 (97%)	350 (95%)	17 (5%)	1 (0%)	41	76
1	I	368/381 (97%)	347 (94%)	19 (5%)	2 (0%)	29	68
1	J	368/381 (97%)	350 (95%)	16 (4%)	2 (0%)	29	68
1	K	368/381 (97%)	352 (96%)	14 (4%)	2 (0%)	29	68
1	L	368/381 (97%)	351 (95%)	16 (4%)	1 (0%)	41	76
1	M	368/381 (97%)	350 (95%)	16 (4%)	2 (0%)	29	68
1	N	368/381 (97%)	351 (95%)	15 (4%)	2 (0%)	29	68
1	O	368/381 (97%)	352 (96%)	15 (4%)	1 (0%)	41	76
All	All	5520/5715 (97%)	5255 (95%)	240 (4%)	25 (0%)	29	68

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	GLY
1	B	72	GLY
1	C	72	GLY
1	D	72	GLY
1	E	72	GLY
1	F	72	GLY
1	G	72	GLY
1	H	72	GLY
1	I	72	GLY
1	J	72	GLY
1	K	72	GLY
1	K	362	ASN
1	L	72	GLY
1	M	72	GLY
1	N	72	GLY
1	O	72	GLY
1	A	362	ASN
1	B	362	ASN

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Mol	Chain	Res	Type
1	C	362	ASN
1	I	362	ASN
1	J	362	ASN
1	F	362	ASN
1	G	362	ASN
1	M	34	ASP
1	N	34	ASP

### 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	310/320 (97%)	293 (94%)	17 (6%)	21	57
1	B	310/320 (97%)	293 (94%)	17 (6%)	21	57
1	C	310/320 (97%)	293 (94%)	17 (6%)	21	57
1	D	310/320 (97%)	291 (94%)	19 (6%)	18	53
1	E	310/320 (97%)	292 (94%)	18 (6%)	20	55
1	F	310/320 (97%)	294 (95%)	16 (5%)	23	59
1	G	310/320 (97%)	294 (95%)	16 (5%)	23	59
1	H	310/320 (97%)	296 (96%)	14 (4%)	27	64
1	I	310/320 (97%)	292 (94%)	18 (6%)	20	55
1	J	310/320 (97%)	292 (94%)	18 (6%)	20	55
1	K	310/320 (97%)	294 (95%)	16 (5%)	23	59
1	L	310/320 (97%)	293 (94%)	17 (6%)	21	57
1	M	310/320 (97%)	292 (94%)	18 (6%)	20	55
1	N	310/320 (97%)	291 (94%)	19 (6%)	18	53
1	O	310/320 (97%)	291 (94%)	19 (6%)	18	53
All	All	4650/4800 (97%)	4391 (94%)	259 (6%)	21	56

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	SER
1	A	6	SER
1	A	34	ASP
1	A	55	GLU
1	A	70	SER
1	A	126	ASN
1	A	151	SER
1	A	169	LYS
1	A	180	TYR
1	A	193	THR
1	A	227	ARG
1	A	273	SER
1	A	280	ARG
1	A	289	ASP
1	A	311	ASP
1	A	328	THR
1	B	3	THR
1	B	4	SER
1	B	34	ASP
1	B	55	GLU
1	B	70	SER
1	B	77	MET
1	B	126	ASN
1	B	151	SER
1	B	169	LYS
1	B	180	TYR
1	B	193	THR
1	B	227	ARG
1	B	273	SER
1	B	280	ARG
1	B	289	ASP
1	B	311	ASP
1	B	328	THR
1	C	3	THR
1	C	4	SER
1	C	34	ASP
1	C	55	GLU
1	C	70	SER
1	C	77	MET
1	C	126	ASN
1	C	151	SER
1	C	169	LYS

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Mol	Chain	Res	Type
1	C	180	TYR
1	C	193	THR
1	C	227	ARG
1	C	273	SER
1	C	289	ASP
1	C	305	GLU
1	C	311	ASP
1	C	328	THR
1	D	3	THR
1	D	4	SER
1	D	6	SER
1	D	34	ASP
1	D	55	GLU
1	D	70	SER
1	D	77	MET
1	D	126	ASN
1	D	151	SER
1	D	169	LYS
1	D	180	TYR
1	D	193	THR
1	D	227	ARG
1	D	273	SER
1	D	280	ARG
1	D	289	ASP
1	D	305	GLU
1	D	311	ASP
1	D	328	THR
1	E	3	THR
1	E	4	SER
1	E	34	ASP
1	E	55	GLU
1	E	70	SER
1	E	77	MET
1	E	126	ASN
1	E	151	SER
1	E	169	LYS
1	E	180	TYR
1	E	193	THR
1	E	227	ARG
1	E	273	SER
1	E	280	ARG
1	E	289	ASP

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Mol	Chain	Res	Type
1	E	305	GLU
1	E	311	ASP
1	E	328	THR
1	F	3	THR
1	F	4	SER
1	F	34	ASP
1	F	55	GLU
1	F	77	MET
1	F	126	ASN
1	F	151	SER
1	F	169	LYS
1	F	180	TYR
1	F	193	THR
1	F	227	ARG
1	F	273	SER
1	F	280	ARG
1	F	289	ASP
1	F	311	ASP
1	F	328	THR
1	G	3	THR
1	G	4	SER
1	G	34	ASP
1	G	55	GLU
1	G	77	MET
1	G	126	ASN
1	G	151	SER
1	G	169	LYS
1	G	180	TYR
1	G	193	THR
1	G	227	ARG
1	G	273	SER
1	G	289	ASP
1	G	305	GLU
1	G	311	ASP
1	G	328	THR
1	H	3	THR
1	H	4	SER
1	H	34	ASP
1	H	55	GLU
1	H	126	ASN
1	H	151	SER
1	H	169	LYS

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Mol	Chain	Res	Type
1	H	180	TYR
1	H	193	THR
1	H	227	ARG
1	H	273	SER
1	H	305	GLU
1	H	311	ASP
1	H	328	THR
1	I	3	THR
1	I	4	SER
1	I	34	ASP
1	I	55	GLU
1	I	70	SER
1	I	77	MET
1	I	126	ASN
1	I	151	SER
1	I	169	LYS
1	I	180	TYR
1	I	193	THR
1	I	227	ARG
1	I	273	SER
1	I	280	ARG
1	I	305	GLU
1	I	311	ASP
1	I	328	THR
1	I	367	GLU
1	J	3	THR
1	J	4	SER
1	J	6	SER
1	J	34	ASP
1	J	55	GLU
1	J	70	SER
1	J	77	MET
1	J	126	ASN
1	J	151	SER
1	J	169	LYS
1	J	180	TYR
1	J	193	THR
1	J	227	ARG
1	J	273	SER
1	J	280	ARG
1	J	289	ASP
1	J	311	ASP

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Mol	Chain	Res	Type
1	J	328	THR
1	K	3	THR
1	K	4	SER
1	K	34	ASP
1	K	55	GLU
1	K	70	SER
1	K	126	ASN
1	K	151	SER
1	K	169	LYS
1	K	180	TYR
1	K	193	THR
1	K	227	ARG
1	K	273	SER
1	K	280	ARG
1	K	289	ASP
1	K	311	ASP
1	K	328	THR
1	L	3	THR
1	L	4	SER
1	L	34	ASP
1	L	55	GLU
1	L	70	SER
1	L	126	ASN
1	L	151	SER
1	L	169	LYS
1	L	180	TYR
1	L	193	THR
1	L	227	ARG
1	L	273	SER
1	L	280	ARG
1	L	289	ASP
1	L	305	GLU
1	L	311	ASP
1	L	328	THR
1	M	3	THR
1	M	4	SER
1	M	34	ASP
1	M	55	GLU
1	M	70	SER
1	M	77	MET
1	M	126	ASN
1	M	151	SER

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Mol	Chain	Res	Type
1	M	169	LYS
1	M	180	TYR
1	M	193	THR
1	M	227	ARG
1	M	273	SER
1	M	280	ARG
1	M	289	ASP
1	M	305	GLU
1	M	311	ASP
1	M	328	THR
1	N	3	THR
1	N	4	SER
1	N	6	SER
1	N	34	ASP
1	N	55	GLU
1	N	70	SER
1	N	77	MET
1	N	126	ASN
1	N	151	SER
1	N	169	LYS
1	N	180	TYR
1	N	193	THR
1	N	227	ARG
1	N	273	SER
1	N	280	ARG
1	N	289	ASP
1	N	305	GLU
1	N	311	ASP
1	N	328	THR
1	O	3	THR
1	O	4	SER
1	O	34	ASP
1	O	55	GLU
1	O	70	SER
1	O	77	MET
1	O	126	ASN
1	O	151	SER
1	O	169	LYS
1	O	180	TYR
1	O	193	THR
1	O	227	ARG
1	O	273	SER

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Mol	Chain	Res	Type
1	O	280	ARG
1	O	289	ASP
1	O	305	GLU
1	O	311	ASP
1	O	328	THR
1	O	364	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	201	GLN
1	A	304	HIS
1	A	331	GLN
1	A	362	ASN
1	B	201	GLN
1	B	304	HIS
1	B	331	GLN
1	B	362	ASN
1	C	201	GLN
1	C	304	HIS
1	C	331	GLN
1	C	362	ASN
1	D	201	GLN
1	D	304	HIS
1	D	331	GLN
1	D	362	ASN
1	E	201	GLN
1	E	304	HIS
1	E	331	GLN
1	E	362	ASN
1	F	201	GLN
1	F	304	HIS
1	F	331	GLN
1	F	362	ASN
1	G	201	GLN
1	G	304	HIS
1	G	362	ASN
1	H	201	GLN
1	H	304	HIS
1	H	331	GLN
1	H	362	ASN

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Mol	Chain	Res	Type
1	I	201	GLN
1	I	304	HIS
1	I	331	GLN
1	I	362	ASN
1	J	201	GLN
1	J	304	HIS
1	J	331	GLN
1	J	362	ASN
1	K	201	GLN
1	K	304	HIS
1	K	331	GLN
1	K	362	ASN
1	L	8	HIS
1	L	201	GLN
1	L	304	HIS
1	L	331	GLN
1	L	362	ASN
1	M	201	GLN
1	M	304	HIS
1	M	331	GLN
1	M	362	ASN
1	N	201	GLN
1	N	304	HIS
1	N	331	GLN
1	N	362	ASN
1	O	201	GLN
1	O	304	HIS
1	O	331	GLN
1	O	362	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	370/381 (97%)	-0.41	1 (0%) 94 84	14, 38, 80, 121	0
1	B	370/381 (97%)	-0.39	2 (0%) 91 75	14, 38, 80, 121	0
1	C	370/381 (97%)	-0.35	7 (1%) 66 37	14, 39, 80, 121	0
1	D	370/381 (97%)	-0.40	1 (0%) 94 84	14, 38, 80, 121	0
1	E	370/381 (97%)	-0.41	4 (1%) 80 56	14, 38, 80, 121	0
1	F	370/381 (97%)	-0.28	7 (1%) 66 37	14, 39, 80, 121	0
1	G	370/381 (97%)	-0.35	2 (0%) 91 75	14, 39, 80, 121	0
1	H	370/381 (97%)	-0.41	3 (0%) 86 65	14, 39, 80, 121	0
1	I	370/381 (97%)	-0.39	1 (0%) 94 84	14, 39, 80, 121	0
1	J	370/381 (97%)	-0.39	5 (1%) 75 49	14, 39, 80, 121	0
1	K	370/381 (97%)	-0.39	6 (1%) 72 44	14, 39, 80, 121	0
1	L	370/381 (97%)	-0.30	3 (0%) 86 65	14, 39, 80, 121	0
1	M	370/381 (97%)	-0.39	7 (1%) 66 37	14, 39, 80, 121	0
1	N	370/381 (97%)	-0.41	2 (0%) 91 75	14, 38, 80, 121	0
1	O	370/381 (97%)	-0.37	3 (0%) 86 65	13, 38, 80, 121	0
All	All	5550/5715 (97%)	-0.38	54 (0%) 82 59	13, 39, 80, 121	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	GLU	3.4
1	F	72	GLY	3.3
1	G	71	GLU	3.1
1	M	72	GLY	3.1
1	C	372	LYS	3.0
1	E	372	LYS	3.0
1	O	372	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	73	SER	3.0
1	C	73	SER	2.9
1	B	72	GLY	2.9
1	E	73	SER	2.7
1	M	304	HIS	2.7
1	H	71	GLU	2.7
1	F	331	GLN	2.6
1	M	305	GLU	2.6
1	H	372	LYS	2.6
1	D	71	GLU	2.6
1	B	104	TYR	2.6
1	E	369	PHE	2.6
1	M	263	GLU	2.5
1	K	370	GLN	2.5
1	F	335	GLY	2.5
1	F	303	PHE	2.5
1	K	372	LYS	2.4
1	J	370	GLN	2.4
1	M	71	GLU	2.4
1	F	126	ASN	2.4
1	F	304	HIS	2.4
1	G	372	LYS	2.4
1	N	372	LYS	2.4
1	J	305	GLU	2.4
1	L	71	GLU	2.3
1	J	372	LYS	2.3
1	C	72	GLY	2.3
1	K	72	GLY	2.3
1	L	372	LYS	2.3
1	J	303	PHE	2.3
1	N	369	PHE	2.3
1	O	72	GLY	2.2
1	H	369	PHE	2.2
1	I	71	GLU	2.2
1	J	71	GLU	2.2
1	A	372	LYS	2.2
1	M	126	ASN	2.2
1	C	126	ASN	2.1
1	C	305	GLU	2.1
1	K	305	GLU	2.1
1	O	73	SER	2.1
1	L	72	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	71	GLU	2.1
1	M	302	GLY	2.0
1	K	126	ASN	2.0
1	C	301	THR	2.0
1	E	71	GLU	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	I	401	1/1	0.70	0.14	30,30,30,30	0
3	CL	C	1373	1/1	0.83	0.27	62,62,62,62	0
3	CL	J	1373	1/1	0.84	0.31	66,66,66,66	0
2	MG	F	401	1/1	0.85	0.18	29,29,29,29	0
2	MG	M	401	1/1	0.85	0.23	29,29,29,29	0
3	CL	E	1373	1/1	0.87	0.16	33,33,33,33	0
3	CL	O	1373	1/1	0.88	0.15	38,38,38,38	0
2	MG	C	401	1/1	0.90	0.34	30,30,30,30	0
2	MG	K	401	1/1	0.91	0.34	29,29,29,29	0
2	MG	N	401	1/1	0.92	0.42	29,29,29,29	0
3	CL	A	1373	1/1	0.92	0.16	50,50,50,50	0
3	CL	L	1373	1/1	0.92	0.19	45,45,45,45	0
3	CL	M	1373	1/1	0.93	0.18	42,42,42,42	0
3	CL	H	1373	1/1	0.93	0.19	55,55,55,55	0
2	MG	H	401	1/1	0.94	0.36	29,29,29,29	0
3	CL	F	1373	1/1	0.95	0.18	64,64,64,64	0
3	CL	K	1373	1/1	0.95	0.16	45,45,45,45	0
2	MG	E	401	1/1	0.95	0.39	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	D	1373	1/1	0.95	0.11	38,38,38,38	0
2	MG	J	401	1/1	0.96	0.43	29,29,29,29	0
2	MG	G	401	1/1	0.96	0.39	29,29,29,29	0
2	MG	B	401	1/1	0.96	0.40	29,29,29,29	0
2	MG	A	401	1/1	0.96	0.41	29,29,29,29	0
2	MG	L	401	1/1	0.96	0.33	29,29,29,29	0
3	CL	G	1373	1/1	0.96	0.13	59,59,59,59	0
2	MG	D	401	1/1	0.96	0.33	29,29,29,29	0
2	MG	O	401	1/1	0.97	0.29	29,29,29,29	0
3	CL	B	1373	1/1	0.98	0.10	51,51,51,51	0
3	CL	I	1373	1/1	0.98	0.13	33,33,33,33	0
3	CL	N	1373	1/1	0.98	0.09	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.