



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:18 AM GMT

PDB ID : 2WGS
Title : CRYSTAL STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS GLUTAMINE SYNTHETASE IN COMPLEX WITH A PURINE ANALOGUE INHIBITOR.
Authors : Nilsson, M.T.; Krajewski, W.W.; Jones, T.A.; Mowbray, S.L.
Deposited on : 2009-04-27
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

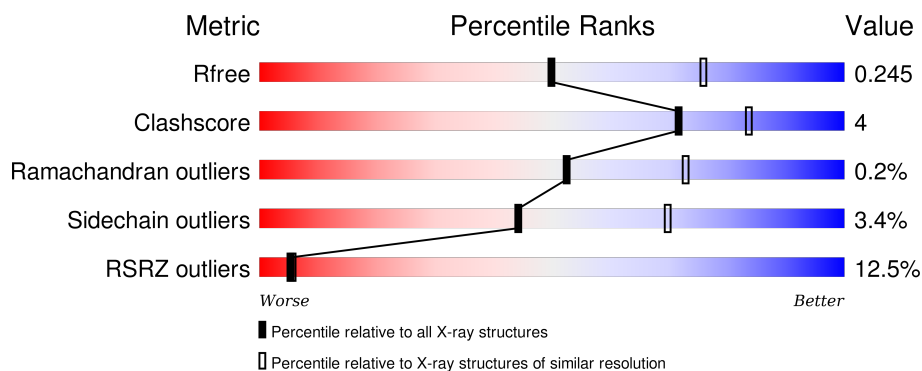
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	486	<div> <div>10%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
1	B	486	<div> <div>11%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
1	C	486	<div> <div>15%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
1	D	486	<div> <div>10%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
1	E	486	<div> <div>10%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	486	<div><div></div><div>10%</div><div>84%</div><div>11%</div><div>5%</div></div>
1	G	486	<div><div></div><div>11%</div><div>84%</div><div>10%</div><div>5%</div></div>
1	H	486	<div><div></div><div>12%</div><div>85%</div><div>9%</div><div>5%</div></div>
1	I	486	<div><div></div><div>13%</div><div>85%</div><div>9%</div><div>5%</div></div>
1	J	486	<div><div></div><div>19%</div><div>83%</div><div>11%</div><div>5%</div></div>
1	K	486	<div><div></div><div>12%</div><div>85%</div><div>10%</div><div>5%</div></div>
1	L	486	<div><div></div><div>11%</div><div>86%</div><div>8%</div><div>5%</div></div>

2 Entry composition

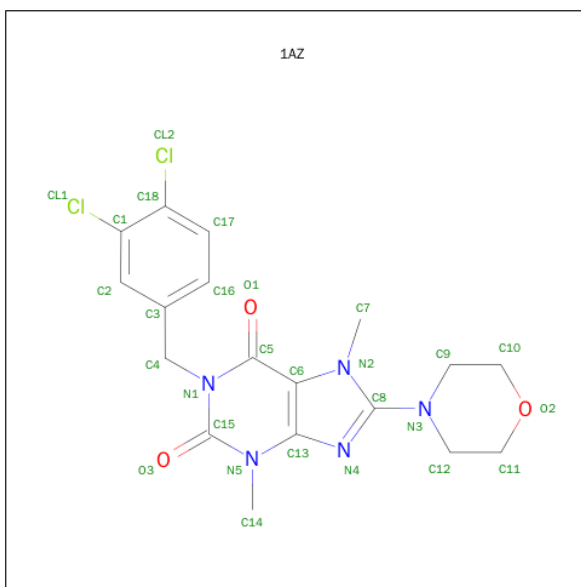
There are 4 unique types of molecules in this entry. The entry contains 45804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	B	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	C	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	D	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	E	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	F	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	G	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	H	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	I	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	J	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	K	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	L	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			

- Molecule 2 is 1-(3,4-DICHLOROBENZYL)-3,7-DIMETHYL-8-MORPHOLIN-4-YL-3,7-DIHYDRO-1H-PURINE-2,6-DIONE (three-letter code: 1AZ) (formula: C₁₈H₁₉Cl₂N₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	B	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	C	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	D	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	E	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	F	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	G	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	H	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	I	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	J	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	K	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	L	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		

- 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
3	H	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	126	Total O 126 126	0	0
4	B	129	Total O 129 129	0	0
4	C	130	Total O 130 130	0	0
4	D	127	Total O 127 127	0	0
4	E	130	Total O 130 130	0	0
4	F	127	Total O 127 127	0	0
4	G	126	Total O 126 126	0	0
4	H	129	Total O 129 129	0	0

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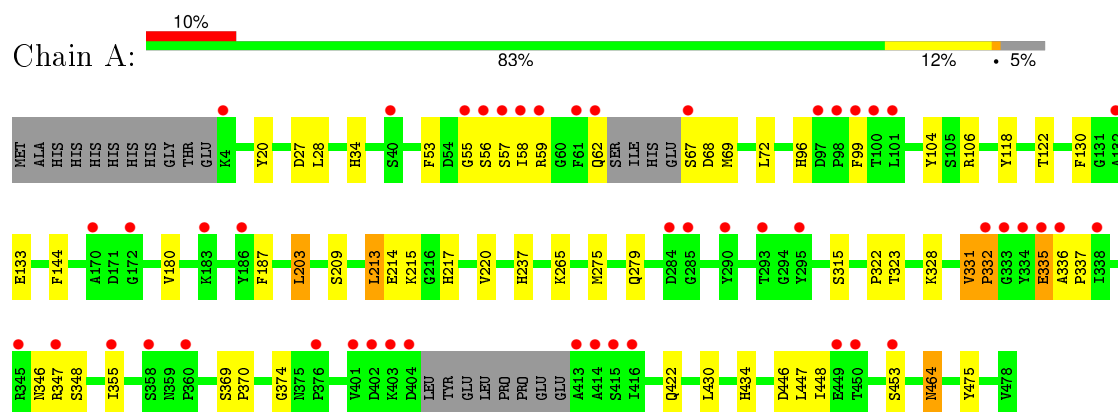
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	126	Total 126	O 126	0	0
4	J	126	Total 126	O 126	0	0
4	K	131	Total 131	O 131	0	0
4	L	129	Total 129	O 129	0	0

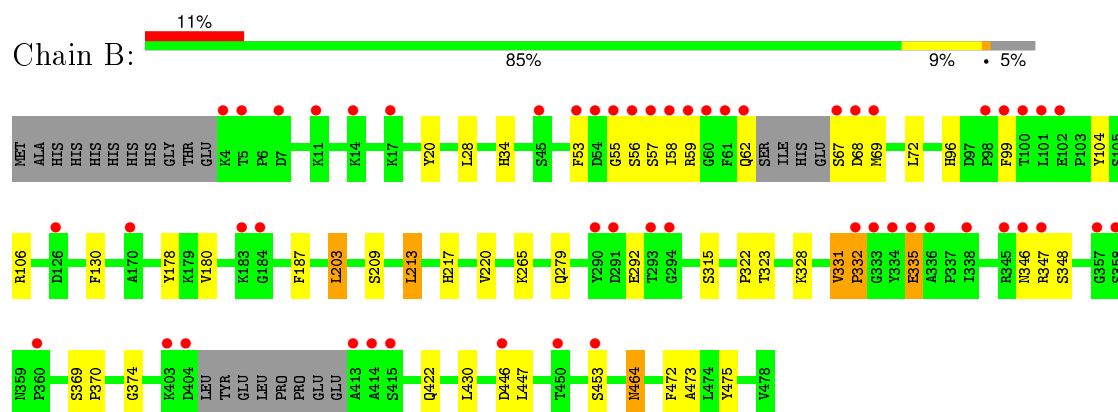
3 Residue-property plots [i](#)

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

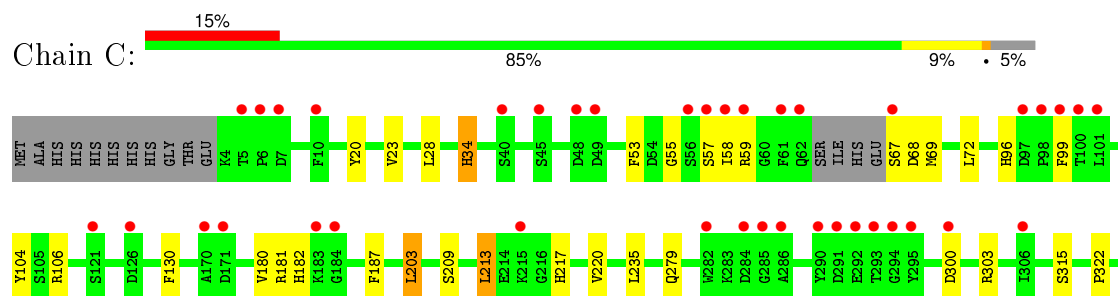
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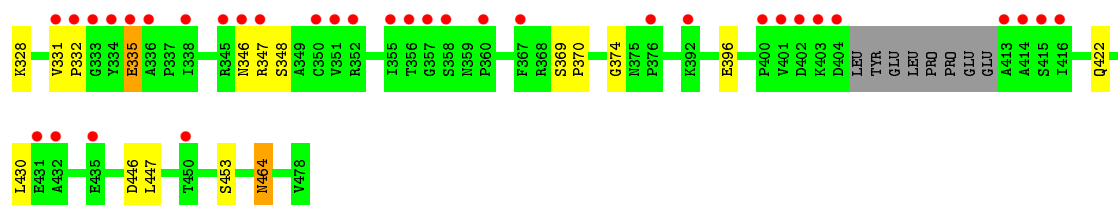


• Molecule 1: GLUTAMINE SYNTHETASE 1

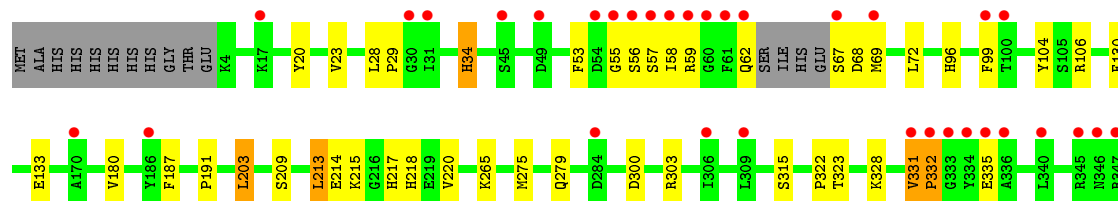
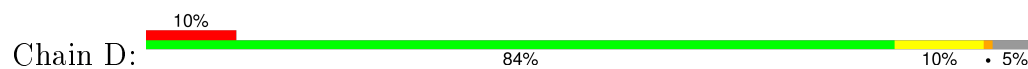


• Molecule 1: GLUTAMINE SYNTHETASE 1

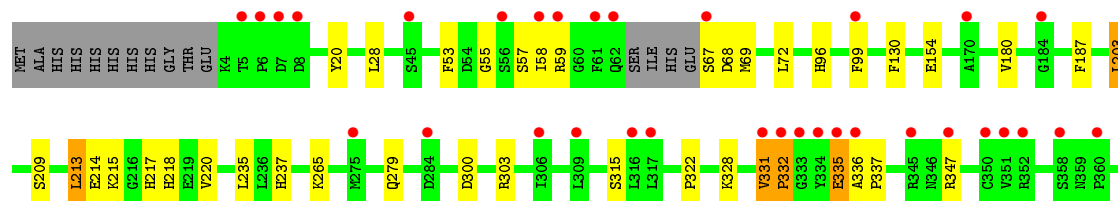
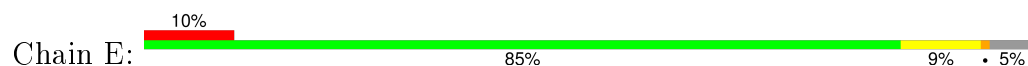




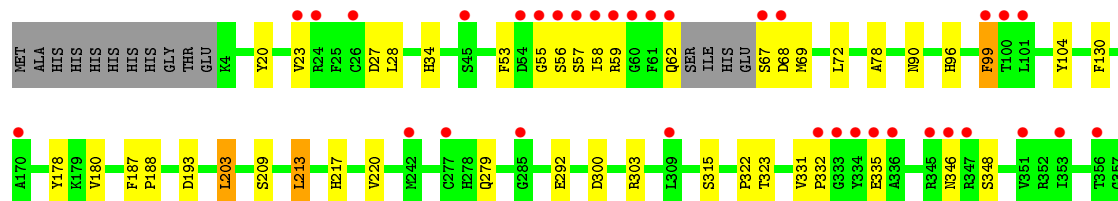
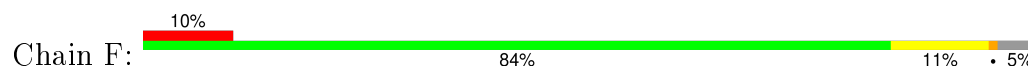
• Molecule 1: GLUTAMINE SYNTHETASE 1



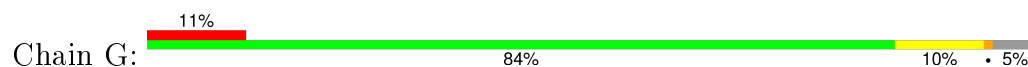
• Molecule 1: GLUTAMINE SYNTHETASE 1

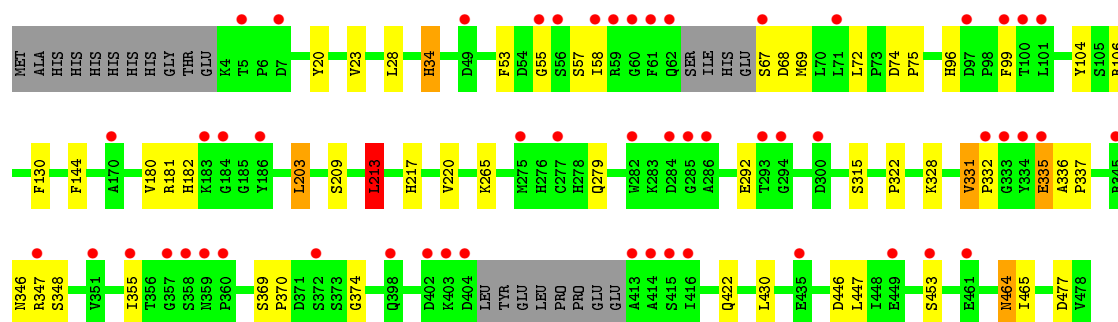


• Molecule 1: GLUTAMINE SYNTHETASE 1

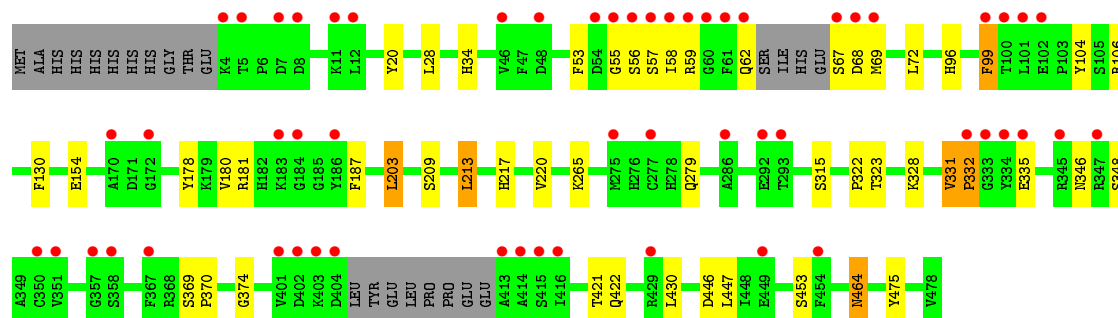
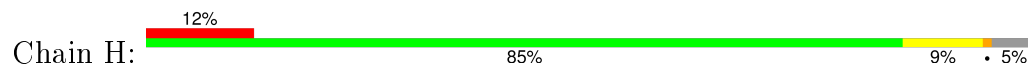


• Molecule 1: GLUTAMINE SYNTHETASE 1

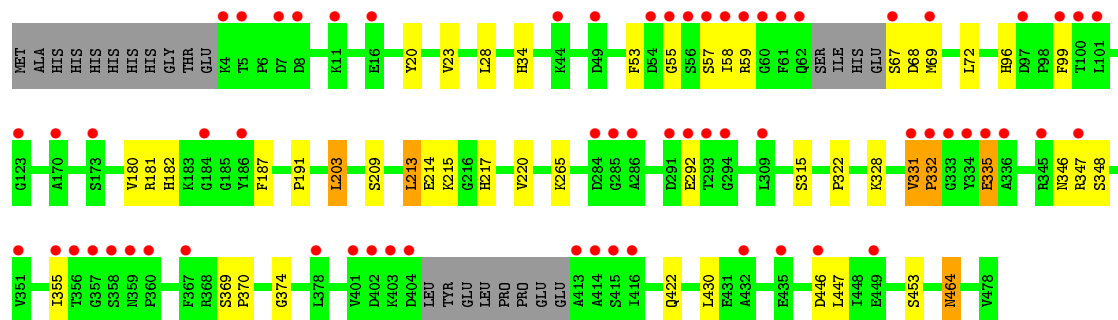
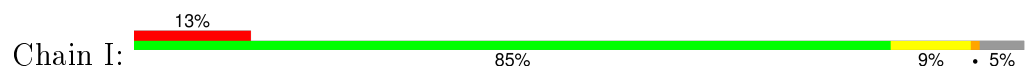




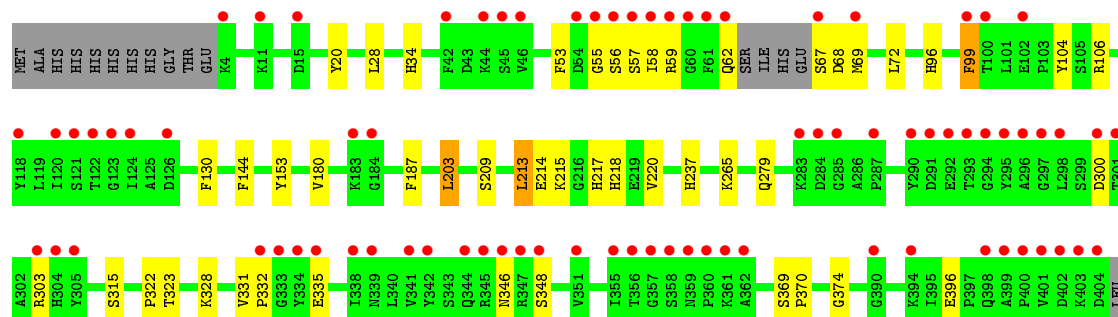
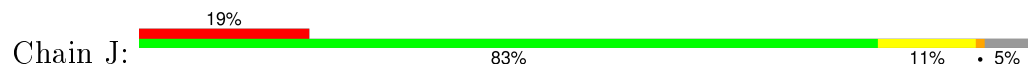
• Molecule 1: GLUTAMINE SYNTHETASE 1

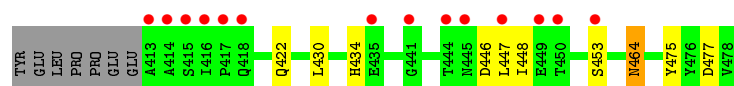


• Molecule 1: GLUTAMINE SYNTHETASE 1

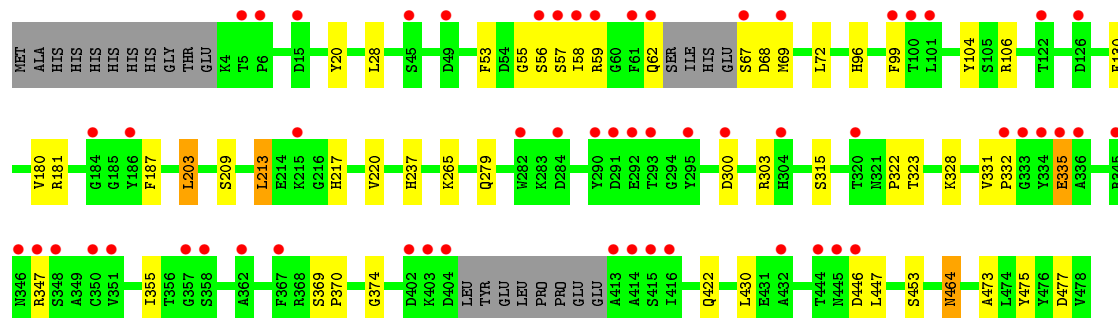
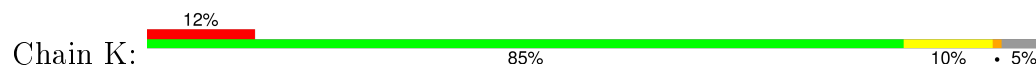


• Molecule 1: GLUTAMINE SYNTHETASE 1

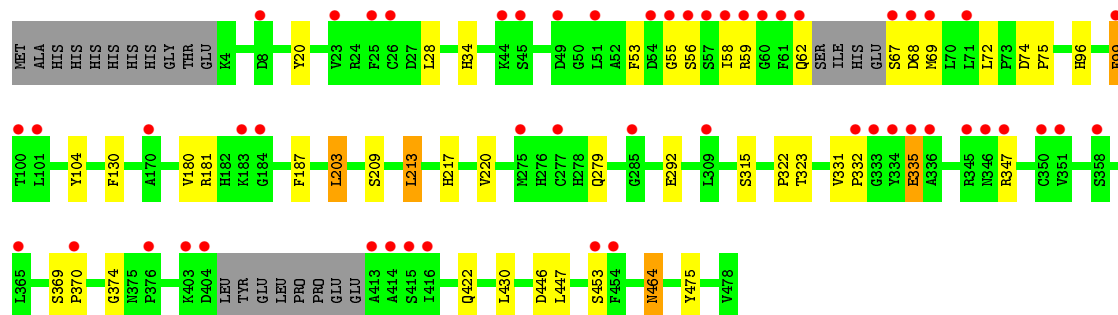
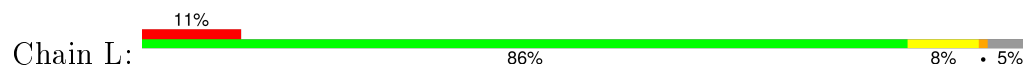




● Molecule 1: GLUTAMINE SYNTHETASE 1



● Molecule 1: GLUTAMINE SYNTHETASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.95Å 203.18Å 230.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 2.55 29.94 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.95-2.55) 99.8 (29.94-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.246 0.229 , 0.245	Depositor DCC
R_{free} test set	10318 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 204985 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	45804	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.94 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0653e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 1AZ

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	0.52	0/3760	0.60	1/5105 (0.0%)
1	B	0.53	0/3760	0.60	0/5105
1	C	0.54	0/3760	0.59	0/5105
1	D	0.52	0/3760	0.60	0/5105
1	E	0.52	0/3760	0.60	0/5105
1	F	0.51	0/3760	0.60	1/5105 (0.0%)
1	G	0.53	0/3760	0.60	1/5105 (0.0%)
1	H	0.53	0/3760	0.60	0/5105
1	I	0.53	0/3760	0.60	0/5105
1	J	0.59	0/3760	0.60	0/5105
1	K	0.55	0/3760	0.59	0/5105
1	L	0.52	0/3760	0.59	0/5105
All	All	0.53	0/45120	0.60	3/61260 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	27	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	27	ASP	CB-CG-OD1	5.14	122.93	118.30
1	G	213	LEU	CA-CB-CG	5.09	127.02	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3660	0	3497	47	0
1	B	3660	0	3497	41	0
1	C	3660	0	3497	39	0
1	D	3660	0	3497	40	0
1	E	3660	0	3497	43	0
1	F	3660	0	3497	41	0
1	G	3660	0	3497	41	0
1	H	3660	0	3497	42	0
1	I	3660	0	3497	39	0
1	J	3660	0	3497	43	0
1	K	3660	0	3497	42	0
1	L	3660	0	3497	35	0
2	A	28	0	19	0	0
2	B	28	0	19	0	0
2	C	28	0	19	0	0
2	D	28	0	19	0	0
2	E	28	0	19	0	0
2	F	28	0	19	0	0
2	G	28	0	19	0	0
2	H	28	0	19	0	0
2	I	28	0	19	0	0
2	J	28	0	19	0	0
2	K	28	0	19	0	0
2	L	28	0	19	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
4	A	126	0	0	1	0
4	B	129	0	0	0	0
4	C	130	0	0	0	0
4	D	127	0	0	1	0
4	E	130	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	127	0	0	0	0
4	G	126	0	0	0	0
4	H	129	0	0	0	0
4	I	126	0	0	0	0
4	J	126	0	0	2	0
4	K	131	0	0	1	0
4	L	129	0	0	0	0
All	All	45804	0	42192	372	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (372) 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:55:GLY:HA3	1:L:67:SER:O	1.35	1.26
1:B:55:GLY:HA3	1:B:67:SER:O	1.36	1.23
1:C:55:GLY:HA3	1:C:67:SER:O	1.39	1.22
1:H:55:GLY:HA3	1:H:67:SER:O	1.37	1.22
1:I:55:GLY:HA3	1:I:67:SER:O	1.41	1.20
1:J:55:GLY:HA3	1:J:67:SER:O	1.39	1.19
1:G:55:GLY:HA3	1:G:67:SER:O	1.41	1.19
1:A:55:GLY:HA3	1:A:67:SER:O	1.37	1.18
1:D:55:GLY:HA3	1:D:67:SER:O	1.39	1.18
1:F:55:GLY:HA3	1:F:67:SER:O	1.39	1.18
1:K:55:GLY:HA3	1:K:67:SER:O	1.42	1.17
1:E:55:GLY:HA3	1:E:67:SER:O	1.40	1.16
1:C:464:ASN:HD21	1:I:422:GLN:HE22	1.09	0.99
1:E:422:GLN:HE22	1:G:464:ASN:HD21	1.11	0.98
1:L:55:GLY:CA	1:L:67:SER:O	2.17	0.93
1:A:55:GLY:CA	1:A:67:SER:O	2.18	0.92
1:B:55:GLY:CA	1:B:67:SER:O	2.17	0.91
1:C:422:GLN:HE22	1:I:464:ASN:HD21	1.13	0.91
1:H:55:GLY:CA	1:H:67:SER:O	2.18	0.90
1:J:55:GLY:CA	1:J:67:SER:O	2.20	0.90
1:F:55:GLY:CA	1:F:67:SER:O	2.19	0.90
1:D:55:GLY:CA	1:D:67:SER:O	2.20	0.89
1:G:335:GLU:OE1	1:L:62:GLN:HB3	1.73	0.89
1:E:464:ASN:HD21	1:G:422:GLN:HE22	1.19	0.89
1:C:55:GLY:CA	1:C:67:SER:O	2.20	0.89
1:E:55:GLY:CA	1:E:67:SER:O	2.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:55:GLY:CA	1:K:67:SER:O	2.21	0.88
1:I:55:GLY:CA	1:I:67:SER:O	2.21	0.87
1:G:55:GLY:CA	1:G:67:SER:O	2.22	0.87
1:H:62:GLN:HB3	1:I:335:GLU:OE1	1.77	0.85
1:A:335:GLU:OE1	1:F:62:GLN:HB3	1.78	0.82
1:A:464:ASN:HD21	1:K:422:GLN:HE22	1.30	0.79
1:I:57:SER:HB3	1:J:187:PHE:HE2	1.46	0.78
1:D:464:ASN:HD21	1:H:422:GLN:HE22	1.29	0.78
1:G:57:SER:HB3	1:H:187:PHE:HE2	1.50	0.77
1:B:422:GLN:HE22	1:J:464:ASN:HD21	1.33	0.76
1:E:57:SER:HB3	1:F:187:PHE:HE2	1.51	0.76
1:E:422:GLN:NE2	1:G:464:ASN:HD21	1.81	0.75
1:C:20:TYR:CE1	1:D:203:LEU:HD13	2.21	0.75
1:C:464:ASN:HD21	1:I:422:GLN:NE2	1.85	0.75
1:G:347:ARG:HH11	1:L:56:SER:HB3	1.50	0.75
1:H:56:SER:HB3	1:I:347:ARG:HH11	1.52	0.73
1:E:20:TYR:CE1	1:F:203:LEU:HD13	2.22	0.72
1:K:20:TYR:CE1	1:L:203:LEU:HD13	2.23	0.72
1:A:347:ARG:HH11	1:F:56:SER:HB3	1.54	0.72
1:I:57:SER:HB3	1:J:187:PHE:CE2	2.24	0.71
1:B:20:TYR:CE1	1:C:203:LEU:HD13	2.25	0.71
1:G:355:ILE:HG21	1:L:99:PHE:HE1	1.56	0.71
1:B:62:GLN:HB3	1:C:335:GLU:OE1	1.90	0.71
1:E:422:GLN:HE22	1:G:464:ASN:ND2	1.87	0.70
1:G:203:LEU:HD13	1:L:20:TYR:CE1	2.27	0.69
1:A:422:GLN:HE22	1:K:464:ASN:HD21	1.40	0.69
1:C:422:GLN:NE2	1:I:464:ASN:HD21	1.89	0.69
1:A:203:LEU:HD13	1:F:20:TYR:CE1	2.28	0.69
1:A:20:TYR:CE1	1:B:203:LEU:HD13	2.27	0.69
1:G:57:SER:HB3	1:H:187:PHE:CE2	2.28	0.69
1:E:57:SER:HB3	1:F:187:PHE:CE2	2.28	0.69
1:H:20:TYR:CE1	1:I:203:LEU:HD13	2.28	0.68
1:E:464:ASN:HD21	1:G:422:GLN:NE2	1.93	0.67
1:F:422:GLN:HE22	1:L:464:ASN:HD21	1.41	0.67
1:D:422:GLN:HE22	1:H:464:ASN:HD21	1.42	0.67
1:J:62:GLN:HB3	1:K:335:GLU:OE1	1.95	0.66
1:J:20:TYR:CE1	1:K:203:LEU:HD13	2.31	0.66
1:G:20:TYR:CE1	1:H:203:LEU:HD13	2.30	0.65
1:F:464:ASN:HD21	1:L:422:GLN:HE22	1.45	0.63
1:I:20:TYR:CE1	1:J:203:LEU:HD13	2.33	0.63
1:E:464:ASN:O	1:G:328:LYS:HE3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:57:SER:HB3	1:K:187:PHE:CE2	2.34	0.62
1:D:58:ILE:HD12	1:D:69:MET:HB2	1.80	0.61
1:L:58:ILE:HD12	1:L:69:MET:HB2	1.81	0.61
1:E:464:ASN:ND2	1:G:422:GLN:HE22	1.95	0.61
1:H:58:ILE:HD12	1:H:69:MET:HB2	1.83	0.61
1:C:57:SER:HB3	1:D:187:PHE:HE2	1.65	0.61
1:J:56:SER:HB3	1:K:347:ARG:HH11	1.66	0.61
1:B:56:SER:HB3	1:C:347:ARG:HH11	1.66	0.60
1:B:475:TYR:CZ	1:J:323:THR:HB	2.36	0.60
1:K:62:GLN:HB3	1:L:335:GLU:OE1	2.02	0.60
1:B:58:ILE:HD12	1:B:69:MET:HB2	1.84	0.60
1:E:477:ASP:HB2	1:H:178:TYR:CE1	2.36	0.60
1:C:464:ASN:ND2	1:I:422:GLN:HE22	1.91	0.59
1:K:28:LEU:HD11	1:K:447:LEU:HD11	1.84	0.59
1:F:28:LEU:HD11	1:F:447:LEU:HD11	1.84	0.59
1:I:58:ILE:HD12	1:I:69:MET:HB2	1.84	0.59
1:K:58:ILE:HD12	1:K:69:MET:HB2	1.84	0.59
1:H:28:LEU:HD11	1:H:447:LEU:HD11	1.84	0.58
1:F:58:ILE:HD12	1:F:69:MET:HB2	1.83	0.58
1:D:218:HIS:ND1	4:D:2080:HOH:O	2.32	0.58
1:L:28:LEU:HD11	1:L:447:LEU:HD11	1.84	0.58
1:B:464:ASN:HD21	1:J:422:GLN:HE22	1.50	0.58
1:B:422:GLN:NE2	1:J:464:ASN:HD21	2.00	0.58
1:E:58:ILE:HD12	1:E:69:MET:HB2	1.86	0.58
1:D:57:SER:HB3	1:E:187:PHE:HE2	1.69	0.58
1:E:328:LYS:HE3	1:G:464:ASN:O	2.03	0.57
1:C:58:ILE:HD12	1:C:69:MET:HB2	1.86	0.57
1:A:28:LEU:HD11	1:A:447:LEU:HD11	1.87	0.57
1:J:315:SER:HB2	1:J:430:LEU:HA	1.85	0.57
1:J:58:ILE:HD12	1:J:69:MET:HB2	1.86	0.57
1:D:57:SER:HB3	1:E:187:PHE:CE2	2.39	0.57
1:H:99:PHE:HE1	1:I:355:ILE:HG21	1.70	0.57
1:K:57:SER:HB3	1:L:187:PHE:CE2	2.39	0.56
1:A:57:SER:HB3	1:B:187:PHE:CE2	2.40	0.56
1:G:58:ILE:HD12	1:G:69:MET:HB2	1.88	0.56
1:K:57:SER:HB3	1:L:187:PHE:HE2	1.70	0.56
1:D:20:TYR:CE1	1:E:203:LEU:HD13	2.41	0.56
1:B:315:SER:HB2	1:B:430:LEU:HA	1.88	0.56
1:A:464:ASN:HD21	1:K:422:GLN:NE2	1.99	0.56
1:J:57:SER:HB3	1:K:187:PHE:HE2	1.70	0.56
1:C:57:SER:HB3	1:D:187:PHE:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:59:ARG:HE	1:L:69:MET:HE2	1.71	0.56
1:A:57:SER:HB3	1:B:187:PHE:HE2	1.71	0.56
1:H:59:ARG:HE	1:H:69:MET:HE2	1.71	0.55
1:A:58:ILE:HD12	1:A:69:MET:HB2	1.88	0.55
1:C:315:SER:HB2	1:C:430:LEU:HA	1.88	0.55
1:A:464:ASN:O	1:K:328:LYS:HE3	2.07	0.55
1:C:28:LEU:HD11	1:C:447:LEU:HD11	1.88	0.55
1:D:464:ASN:HD21	1:H:422:GLN:NE2	2.01	0.55
1:B:59:ARG:HE	1:B:69:MET:HE2	1.71	0.55
1:F:323:THR:HB	1:L:475:TYR:CZ	2.42	0.54
1:B:28:LEU:HD11	1:B:447:LEU:HD11	1.88	0.54
1:D:62:GLN:HB3	1:E:335:GLU:OE1	2.08	0.54
1:C:464:ASN:O	1:I:328:LYS:HE3	2.08	0.54
1:K:315:SER:HB2	1:K:430:LEU:HA	1.89	0.54
1:E:28:LEU:HD11	1:E:447:LEU:HD11	1.89	0.54
1:J:53:PHE:HB3	1:J:58:ILE:HD11	1.89	0.54
1:F:53:PHE:HB3	1:F:58:ILE:HD11	1.90	0.53
1:F:315:SER:HB2	1:F:430:LEU:HA	1.91	0.53
1:H:56:SER:HB3	1:I:347:ARG:NH1	2.21	0.53
1:I:315:SER:HB2	1:I:430:LEU:HA	1.90	0.53
1:B:53:PHE:HB3	1:B:58:ILE:HD11	1.90	0.53
1:A:53:PHE:HB3	1:A:58:ILE:HD11	1.89	0.53
1:D:323:THR:HB	1:H:475:TYR:CZ	2.43	0.53
1:A:59:ARG:HE	1:A:69:MET:HE2	1.72	0.53
1:A:62:GLN:HB3	1:B:335:GLU:OE1	2.08	0.53
1:K:56:SER:HB3	1:L:347:ARG:HH11	1.73	0.53
1:H:315:SER:HB2	1:H:430:LEU:HA	1.90	0.53
1:L:72:LEU:HD12	1:L:96:HIS:CD2	2.43	0.53
1:G:28:LEU:HD11	1:G:447:LEU:HD11	1.90	0.53
1:F:72:LEU:HD12	1:F:96:HIS:CD2	2.44	0.52
1:K:130:PHE:CE1	1:K:279:GLN:HG2	2.44	0.52
1:C:213:LEU:HD13	1:C:217:HIS:HB3	1.91	0.52
1:D:464:ASN:O	1:H:328:LYS:HE3	2.10	0.52
1:J:56:SER:HB3	1:K:347:ARG:NH1	2.25	0.52
1:I:28:LEU:HD11	1:I:447:LEU:HD11	1.91	0.52
1:J:28:LEU:HD11	1:J:447:LEU:HD11	1.92	0.52
1:G:347:ARG:NH1	1:L:56:SER:HB3	2.21	0.52
1:D:315:SER:HB2	1:D:430:LEU:HA	1.92	0.52
1:D:28:LEU:HD11	1:D:447:LEU:HD11	1.92	0.52
1:A:187:PHE:CE2	1:F:57:SER:HB3	2.45	0.52
1:E:315:SER:HB2	1:E:430:LEU:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:237:HIS:ND1	4:J:2083:HOH:O	2.34	0.51
1:H:213:LEU:HD13	1:H:217:HIS:HB3	1.92	0.51
1:E:53:PHE:HB3	1:E:58:ILE:HD11	1.92	0.51
1:A:213:LEU:HD13	1:A:217:HIS:HB3	1.93	0.51
1:J:130:PHE:CE1	1:J:279:GLN:HG2	2.45	0.51
1:L:53:PHE:HB3	1:L:58:ILE:HD11	1.92	0.51
1:D:477:ASP:OD1	1:I:182:HIS:NE2	2.44	0.51
1:E:331:VAL:HG11	1:G:465:ILE:HG22	1.91	0.51
1:E:465:ILE:HG22	1:G:331:VAL:HG11	1.92	0.51
1:A:347:ARG:NH1	1:F:56:SER:HB3	2.22	0.51
1:G:53:PHE:HB3	1:G:58:ILE:HD11	1.93	0.51
1:E:265:LYS:HG2	1:E:328:LYS:HB3	1.93	0.51
1:A:315:SER:HB2	1:A:430:LEU:HA	1.93	0.51
1:K:53:PHE:HB3	1:K:58:ILE:HD11	1.92	0.50
1:F:475:TYR:CZ	1:L:323:THR:HB	2.46	0.50
1:A:355:ILE:HG21	1:F:99:PHE:HE1	1.75	0.50
1:H:53:PHE:HB3	1:H:58:ILE:HD11	1.93	0.50
1:F:59:ARG:HE	1:F:69:MET:HE2	1.76	0.50
1:E:72:LEU:HD12	1:E:96:HIS:CD2	2.47	0.50
1:E:473:ALA:HA	1:G:144:PHE:CE1	2.46	0.50
1:D:213:LEU:HD13	1:D:217:HIS:HB3	1.93	0.50
1:J:99:PHE:HE1	1:K:355:ILE:HG21	1.76	0.50
1:B:213:LEU:HD13	1:B:217:HIS:HB3	1.94	0.50
1:G:72:LEU:HD12	1:G:96:HIS:CD2	2.47	0.50
1:K:72:LEU:HD12	1:K:96:HIS:CD2	2.47	0.49
1:A:323:THR:HB	1:K:475:TYR:CZ	2.47	0.49
1:A:237:HIS:ND1	4:A:2086:HOH:O	2.34	0.49
1:D:475:TYR:CZ	1:H:323:THR:HB	2.46	0.49
1:J:59:ARG:HE	1:J:69:MET:HE2	1.78	0.49
1:A:53:PHE:HD2	1:A:58:ILE:HG13	1.78	0.49
1:F:130:PHE:CE1	1:F:279:GLN:HG2	2.47	0.49
1:D:328:LYS:HE3	1:H:464:ASN:O	2.13	0.49
1:H:130:PHE:CE1	1:H:279:GLN:HG2	2.47	0.49
1:B:57:SER:HB3	1:C:187:PHE:CE2	2.47	0.49
1:C:53:PHE:HB3	1:C:58:ILE:HD11	1.94	0.49
1:D:53:PHE:HB3	1:D:58:ILE:HD11	1.95	0.49
1:E:130:PHE:CE1	1:E:279:GLN:HG2	2.48	0.49
1:B:130:PHE:CE1	1:B:279:GLN:HG2	2.47	0.49
1:A:328:LYS:HE3	1:K:464:ASN:O	2.13	0.49
1:H:57:SER:HB3	1:I:187:PHE:CE2	2.48	0.48
1:E:237:HIS:ND1	4:E:2085:HOH:O	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:LEU:HD12	1:I:96:HIS:CD2	2.48	0.48
1:H:265:LYS:HG2	1:H:328:LYS:HB3	1.96	0.48
1:C:328:LYS:HE3	1:I:464:ASN:O	2.14	0.48
1:A:56:SER:HB3	1:B:347:ARG:HH11	1.78	0.48
1:H:322:PRO:HG3	1:H:374:GLY:HA3	1.95	0.48
1:F:213:LEU:HD13	1:F:217:HIS:HB3	1.96	0.48
1:J:218:HIS:ND1	4:J:2078:HOH:O	2.34	0.48
1:J:53:PHE:HD2	1:J:58:ILE:HG13	1.79	0.48
1:I:213:LEU:HD13	1:I:217:HIS:HB3	1.95	0.48
1:E:59:ARG:HE	1:E:69:MET:HE2	1.79	0.48
1:D:130:PHE:CE1	1:D:279:GLN:HG2	2.49	0.48
1:L:315:SER:HB2	1:L:430:LEU:HA	1.96	0.48
1:G:315:SER:HB2	1:G:430:LEU:HA	1.96	0.48
1:B:57:SER:HB3	1:C:187:PHE:HE2	1.79	0.47
1:A:422:GLN:NE2	1:K:464:ASN:HD21	2.10	0.47
1:L:53:PHE:HD2	1:L:58:ILE:HG13	1.80	0.47
1:J:369:SER:N	1:J:370:PRO:CD	2.77	0.47
1:B:72:LEU:HD12	1:B:96:HIS:CD2	2.49	0.47
1:C:72:LEU:HD12	1:C:96:HIS:CD2	2.50	0.47
1:J:300:ASP:OD1	1:J:303:ARG:NH2	2.47	0.47
1:I:369:SER:N	1:I:370:PRO:CD	2.77	0.47
1:H:72:LEU:HD12	1:H:96:HIS:CD2	2.49	0.47
1:I:53:PHE:HB3	1:I:58:ILE:HD11	1.95	0.47
1:H:104:TYR:CZ	1:H:106:ARG:HB2	2.50	0.47
1:K:213:LEU:HD13	1:K:217:HIS:HB3	1.97	0.47
1:D:72:LEU:HD12	1:D:96:HIS:CD2	2.50	0.47
1:B:472:PHE:CZ	1:J:153:TYR:CE1	3.03	0.47
1:K:59:ARG:HE	1:K:69:MET:HE2	1.80	0.47
1:J:72:LEU:HD12	1:J:96:HIS:CD2	2.49	0.47
1:C:369:SER:N	1:C:370:PRO:CD	2.78	0.46
1:K:322:PRO:HG3	1:K:374:GLY:HA3	1.97	0.46
1:G:130:PHE:CE1	1:G:279:GLN:HG2	2.51	0.46
1:K:369:SER:N	1:K:370:PRO:CD	2.78	0.46
1:J:104:TYR:CZ	1:J:106:ARG:HB2	2.50	0.46
1:H:53:PHE:HD2	1:H:58:ILE:HG13	1.80	0.46
1:I:59:ARG:HE	1:I:69:MET:HE2	1.81	0.46
1:J:265:LYS:HG2	1:J:328:LYS:HB3	1.97	0.46
1:F:53:PHE:HD2	1:F:58:ILE:HG13	1.80	0.46
1:E:213:LEU:HD13	1:E:217:HIS:HB3	1.98	0.46
1:F:322:PRO:HG3	1:F:374:GLY:HA3	1.98	0.46
1:D:331:VAL:HA	1:D:332:PRO:HD3	1.85	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLU:CD	1:F:62:GLN:HB3	2.36	0.46
1:A:133:GLU:O	1:A:275:MET:HA	2.16	0.46
1:B:323:THR:HB	1:J:475:TYR:CZ	2.51	0.46
1:C:53:PHE:HD2	1:C:58:ILE:HG13	1.81	0.46
1:C:59:ARG:HE	1:C:69:MET:HE2	1.80	0.46
1:D:56:SER:HB3	1:E:347:ARG:HH11	1.80	0.46
1:K:53:PHE:HD2	1:K:58:ILE:HG13	1.81	0.45
1:F:477:ASP:OD1	1:G:182:HIS:NE2	2.50	0.45
1:A:130:PHE:CE1	1:A:279:GLN:HG2	2.51	0.45
1:A:475:TYR:CZ	1:K:323:THR:HB	2.50	0.45
1:G:322:PRO:HG3	1:G:374:GLY:HA3	1.99	0.45
1:L:213:LEU:HD13	1:L:217:HIS:HB3	1.98	0.45
1:I:181:ARG:HE	1:I:181:ARG:HB2	1.58	0.45
1:I:265:LYS:HG2	1:I:328:LYS:HB3	1.99	0.45
1:I:53:PHE:HD2	1:I:58:ILE:HG13	1.81	0.45
1:D:53:PHE:HD2	1:D:58:ILE:HG13	1.81	0.45
1:I:23:VAL:O	1:I:34:HIS:HA	2.17	0.45
1:D:369:SER:N	1:D:370:PRO:CD	2.79	0.45
1:J:213:LEU:HD13	1:J:217:HIS:HB3	1.98	0.45
1:A:322:PRO:HG3	1:A:374:GLY:HA3	1.99	0.45
1:B:53:PHE:HD2	1:B:58:ILE:HG13	1.82	0.45
1:B:464:ASN:O	1:J:328:LYS:HE3	2.16	0.45
1:G:213:LEU:HD13	1:G:217:HIS:HB3	1.98	0.45
1:L:322:PRO:HG3	1:L:374:GLY:HA3	1.99	0.45
1:E:369:SER:N	1:E:370:PRO:CD	2.80	0.45
1:E:331:VAL:HA	1:E:332:PRO:HD3	1.83	0.45
1:C:235:LEU:C	1:C:235:LEU:HD23	2.37	0.45
1:E:53:PHE:HD2	1:E:58:ILE:HG13	1.82	0.44
1:B:322:PRO:HG3	1:B:374:GLY:HA3	1.99	0.44
1:C:181:ARG:HB2	1:C:181:ARG:HE	1.55	0.44
1:A:144:PHE:CE1	1:K:473:ALA:HA	2.52	0.44
1:C:20:TYR:CZ	1:D:203:LEU:HD13	2.51	0.44
1:G:53:PHE:HD2	1:G:58:ILE:HG13	1.81	0.44
1:B:265:LYS:HG2	1:B:328:LYS:HB3	1.99	0.44
1:E:300:ASP:OD1	1:E:303:ARG:NH2	2.51	0.44
1:G:181:ARG:HB2	1:G:181:ARG:HE	1.59	0.44
1:B:104:TYR:CZ	1:B:106:ARG:HB2	2.53	0.44
1:E:322:PRO:HG3	1:E:374:GLY:HA3	1.99	0.44
1:B:328:LYS:HE3	1:J:464:ASN:O	2.18	0.44
1:D:300:ASP:OD1	1:D:303:ARG:NH2	2.50	0.44
1:A:72:LEU:HD12	1:A:96:HIS:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PRO:HG3	1:C:374:GLY:HA3	1.99	0.44
1:L:130:PHE:CE1	1:L:279:GLN:HG2	2.52	0.44
1:K:69:MET:HE3	1:K:104:TYR:CG	2.53	0.44
1:A:346:ASN:OD1	1:A:348:SER:HB3	2.18	0.44
1:H:346:ASN:OD1	1:H:348:SER:HB3	2.17	0.44
1:A:331:VAL:HA	1:A:332:PRO:HD3	1.84	0.44
1:G:265:LYS:HG2	1:G:328:LYS:HB3	2.00	0.43
1:C:130:PHE:CE1	1:C:279:GLN:HG2	2.53	0.43
1:K:181:ARG:HB2	1:K:181:ARG:HE	1.58	0.43
1:E:477:ASP:HB2	1:H:178:TYR:CD1	2.53	0.43
1:B:59:ARG:NE	1:B:69:MET:HE2	2.33	0.43
1:A:104:TYR:CZ	1:A:106:ARG:HB2	2.53	0.43
1:F:323:THR:HB	1:L:475:TYR:CE1	2.53	0.43
1:E:336:ALA:HA	1:E:337:PRO:HD2	1.94	0.43
1:A:187:PHE:HE2	1:F:57:SER:HB3	1.83	0.43
1:J:303:ARG:NH1	1:J:396:GLU:OE2	2.52	0.43
1:C:346:ASN:OD1	1:C:348:SER:HB3	2.19	0.43
1:H:331:VAL:HA	1:H:332:PRO:HD3	1.86	0.43
1:G:346:ASN:OD1	1:G:348:SER:HB3	2.18	0.43
1:I:322:PRO:HG3	1:I:374:GLY:HA3	1.99	0.43
1:I:331:VAL:HA	1:I:332:PRO:HD3	1.81	0.43
1:J:346:ASN:OD1	1:J:348:SER:HB3	2.18	0.43
1:L:292:GLU:H	1:L:292:GLU:HG3	1.65	0.43
1:D:104:TYR:CZ	1:D:106:ARG:HB2	2.54	0.42
1:B:346:ASN:OD1	1:B:348:SER:HB3	2.19	0.42
1:D:59:ARG:HE	1:D:69:MET:HE2	1.85	0.42
1:H:369:SER:N	1:H:370:PRO:CD	2.82	0.42
1:C:422:GLN:HE22	1:I:464:ASN:ND2	1.96	0.42
1:E:218:HIS:ND1	4:E:2079:HOH:O	2.37	0.42
1:E:235:LEU:C	1:E:235:LEU:HD23	2.40	0.42
1:K:300:ASP:OD1	1:K:303:ARG:NH2	2.52	0.42
1:B:369:SER:N	1:B:370:PRO:CD	2.82	0.42
1:F:292:GLU:H	1:F:292:GLU:HG3	1.69	0.42
1:B:292:GLU:HG3	1:B:292:GLU:H	1.68	0.42
1:L:369:SER:N	1:L:370:PRO:CD	2.82	0.42
1:J:322:PRO:HG3	1:J:374:GLY:HA3	2.02	0.42
1:E:214:GLU:HB3	1:E:215:LYS:H	1.74	0.42
1:C:182:HIS:NE2	1:J:477:ASP:OD1	2.53	0.42
1:K:265:LYS:HG2	1:K:328:LYS:HB3	2.02	0.42
1:H:57:SER:HB3	1:I:187:PHE:HE2	1.83	0.42
1:G:104:TYR:CZ	1:G:106:ARG:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:PRO:HG3	1:D:374:GLY:HA3	2.02	0.42
1:L:74:ASP:HA	1:L:75:PRO:HD2	1.95	0.42
1:D:214:GLU:HB3	1:D:215:LYS:H	1.74	0.41
1:D:28:LEU:HB3	1:D:29:PRO:HD3	2.02	0.41
1:H:181:ARG:HB2	1:H:181:ARG:HE	1.64	0.41
1:D:23:VAL:O	1:D:34:HIS:HA	2.20	0.41
1:B:69:MET:HE3	1:B:104:TYR:CG	2.56	0.41
1:A:336:ALA:HA	1:A:337:PRO:HD2	1.96	0.41
1:H:62:GLN:HB3	1:I:335:GLU:CD	2.39	0.41
1:H:69:MET:HE3	1:H:104:TYR:CG	2.55	0.41
1:H:332:PRO:HG3	1:H:421:THR:HG21	2.02	0.41
1:F:188:PRO:O	1:F:193:ASP:HB2	2.20	0.41
1:C:23:VAL:O	1:C:34:HIS:HA	2.20	0.41
1:G:292:GLU:HG3	1:G:292:GLU:H	1.66	0.41
1:L:58:ILE:CD1	1:L:69:MET:HB2	2.48	0.41
1:G:369:SER:N	1:G:370:PRO:CD	2.84	0.41
1:C:104:TYR:CZ	1:C:106:ARG:HB2	2.56	0.41
1:G:336:ALA:HA	1:G:337:PRO:HD2	1.96	0.41
1:I:214:GLU:HB3	1:I:215:LYS:H	1.74	0.41
1:C:303:ARG:NH1	1:C:396:GLU:OE2	2.53	0.41
1:L:181:ARG:HE	1:L:181:ARG:HB2	1.60	0.41
1:F:346:ASN:OD1	1:F:348:SER:HB3	2.20	0.41
1:K:20:TYR:CZ	1:L:203:LEU:HD13	2.54	0.41
1:A:265:LYS:HG2	1:A:328:LYS:HB3	2.02	0.41
1:H:59:ARG:NE	1:H:69:MET:HE2	2.35	0.41
1:I:292:GLU:HG3	1:I:292:GLU:H	1.68	0.41
1:B:56:SER:HB3	1:C:347:ARG:NH1	2.34	0.41
1:F:178:TYR:CE1	1:G:477:ASP:HB2	2.56	0.41
1:D:265:LYS:HG2	1:D:328:LYS:HB3	2.03	0.41
1:H:58:ILE:CD1	1:H:69:MET:HB2	2.49	0.41
1:A:434:HIS:HB2	1:A:448:ILE:HD13	2.03	0.41
1:J:369:SER:N	1:J:370:PRO:HD3	2.36	0.41
1:B:331:VAL:HA	1:B:332:PRO:HD3	1.86	0.41
1:J:214:GLU:HB3	1:J:215:LYS:H	1.72	0.41
1:B:473:ALA:HA	1:J:144:PHE:CE1	2.56	0.41
1:I:346:ASN:OD1	1:I:348:SER:HB3	2.20	0.41
1:F:78:ALA:HA	1:F:90:ASN:O	2.21	0.41
1:F:69:MET:HE3	1:F:104:TYR:CG	2.56	0.40
1:F:369:SER:N	1:F:370:PRO:CD	2.84	0.40
1:A:369:SER:N	1:A:370:PRO:CD	2.84	0.40
1:K:237:HIS:ND1	4:K:2087:HOH:O	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:MET:HE3	1:D:104:TYR:CG	2.56	0.40
1:G:23:VAL:O	1:G:34:HIS:HA	2.22	0.40
1:B:178:TYR:CE1	1:K:477:ASP:HB2	2.56	0.40
1:F:434:HIS:HB2	1:F:448:ILE:HD13	2.03	0.40
1:F:23:VAL:O	1:F:34:HIS:HA	2.22	0.40
1:A:335:GLU:OE2	1:F:62:GLN:CB	2.70	0.40
1:L:59:ARG:NE	1:L:69:MET:HE2	2.36	0.40
1:D:133:GLU:O	1:D:275:MET:HA	2.21	0.40
1:F:300:ASP:OD1	1:F:303:ARG:NH2	2.54	0.40
1:E:20:TYR:CZ	1:F:203:LEU:HD13	2.57	0.40
1:L:69:MET:HE3	1:L:104:TYR:CG	2.57	0.40
1:A:214:GLU:HB3	1:A:215:LYS:H	1.70	0.40
1:G:74:ASP:HA	1:G:75:PRO:HD2	1.98	0.40
1:K:104:TYR:CZ	1:K:106:ARG:HB2	2.56	0.40
1:A:69:MET:HE3	1:A:104:TYR:CG	2.56	0.40
1:C:300:ASP:OD1	1:C:303:ARG:NH2	2.54	0.40
1:A:118:TYR:O	1:A:122:THR:HG23	2.22	0.40
1:J:434:HIS:HB2	1:J:448:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/486 (94%)	442 (97%)	14 (3%)	1 (0%)	52	73
1	B	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	52	73
1	C	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	52	73
1	D	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	52	73
1	E	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	52	73
1	F	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	52	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	52	73
1	H	457/486 (94%)	441 (96%)	15 (3%)	1 (0%)	52	73
1	I	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	52	73
1	J	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	52	73
1	K	457/486 (94%)	441 (96%)	15 (3%)	1 (0%)	52	73
1	L	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	52	73
All	All	5484/5832 (94%)	5279 (96%)	193 (4%)	12 (0%)	52	73

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	PRO
1	B	332	PRO
1	C	332	PRO
1	D	332	PRO
1	E	332	PRO
1	F	332	PRO
1	G	332	PRO
1	H	332	PRO
1	I	332	PRO
1	J	332	PRO
1	K	332	PRO
1	L	332	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	390/411 (95%)	377 (97%)	13 (3%)	45	71
1	B	390/411 (95%)	377 (97%)	13 (3%)	45	71
1	C	390/411 (95%)	377 (97%)	13 (3%)	45	71
1	D	390/411 (95%)	375 (96%)	15 (4%)	40	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	390/411 (95%)	377 (97%)	13 (3%)	45	71
1	F	390/411 (95%)	378 (97%)	12 (3%)	47	73
1	G	390/411 (95%)	377 (97%)	13 (3%)	45	71
1	H	390/411 (95%)	376 (96%)	14 (4%)	42	67
1	I	390/411 (95%)	377 (97%)	13 (3%)	45	71
1	J	390/411 (95%)	377 (97%)	13 (3%)	45	71
1	K	390/411 (95%)	378 (97%)	12 (3%)	47	73
1	L	390/411 (95%)	377 (97%)	13 (3%)	45	71
All	All	4680/4932 (95%)	4523 (97%)	157 (3%)	44	70

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	68	ASP
1	A	99	PHE
1	A	180	VAL
1	A	203	LEU
1	A	209	SER
1	A	213	LEU
1	A	220	VAL
1	A	331	VAL
1	A	335	GLU
1	A	446	ASP
1	A	453	SER
1	A	464	ASN
1	B	34	HIS
1	B	68	ASP
1	B	99	PHE
1	B	180	VAL
1	B	203	LEU
1	B	209	SER
1	B	213	LEU
1	B	220	VAL
1	B	331	VAL
1	B	335	GLU
1	B	446	ASP
1	B	453	SER
1	B	464	ASN

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Mol	Chain	Res	Type
1	C	34	HIS
1	C	68	ASP
1	C	99	PHE
1	C	180	VAL
1	C	203	LEU
1	C	209	SER
1	C	213	LEU
1	C	220	VAL
1	C	331	VAL
1	C	335	GLU
1	C	446	ASP
1	C	453	SER
1	C	464	ASN
1	D	34	HIS
1	D	68	ASP
1	D	99	PHE
1	D	180	VAL
1	D	191	PRO
1	D	203	LEU
1	D	209	SER
1	D	213	LEU
1	D	220	VAL
1	D	331	VAL
1	D	335	GLU
1	D	426	VAL
1	D	446	ASP
1	D	453	SER
1	D	464	ASN
1	E	68	ASP
1	E	99	PHE
1	E	154	GLU
1	E	180	VAL
1	E	203	LEU
1	E	209	SER
1	E	213	LEU
1	E	220	VAL
1	E	331	VAL
1	E	335	GLU
1	E	446	ASP
1	E	453	SER
1	E	464	ASN
1	F	68	ASP

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Mol	Chain	Res	Type
1	F	99	PHE
1	F	180	VAL
1	F	203	LEU
1	F	209	SER
1	F	213	LEU
1	F	220	VAL
1	F	331	VAL
1	F	335	GLU
1	F	446	ASP
1	F	453	SER
1	F	464	ASN
1	G	34	HIS
1	G	68	ASP
1	G	99	PHE
1	G	180	VAL
1	G	203	LEU
1	G	209	SER
1	G	213	LEU
1	G	220	VAL
1	G	331	VAL
1	G	335	GLU
1	G	446	ASP
1	G	453	SER
1	G	464	ASN
1	H	34	HIS
1	H	68	ASP
1	H	99	PHE
1	H	154	GLU
1	H	180	VAL
1	H	203	LEU
1	H	209	SER
1	H	213	LEU
1	H	220	VAL
1	H	331	VAL
1	H	335	GLU
1	H	446	ASP
1	H	453	SER
1	H	464	ASN
1	I	68	ASP
1	I	99	PHE
1	I	180	VAL
1	I	191	PRO

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Mol	Chain	Res	Type
1	I	203	LEU
1	I	209	SER
1	I	213	LEU
1	I	220	VAL
1	I	331	VAL
1	I	335	GLU
1	I	446	ASP
1	I	453	SER
1	I	464	ASN
1	J	34	HIS
1	J	68	ASP
1	J	99	PHE
1	J	180	VAL
1	J	203	LEU
1	J	209	SER
1	J	213	LEU
1	J	220	VAL
1	J	331	VAL
1	J	335	GLU
1	J	446	ASP
1	J	453	SER
1	J	464	ASN
1	K	68	ASP
1	K	99	PHE
1	K	180	VAL
1	K	203	LEU
1	K	209	SER
1	K	213	LEU
1	K	220	VAL
1	K	331	VAL
1	K	335	GLU
1	K	446	ASP
1	K	453	SER
1	K	464	ASN
1	L	34	HIS
1	L	68	ASP
1	L	99	PHE
1	L	180	VAL
1	L	203	LEU
1	L	209	SER
1	L	213	LEU
1	L	220	VAL

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Mol	Chain	Res	Type
1	L	331	VAL
1	L	335	GLU
1	L	446	ASP
1	L	453	SER
1	L	464	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	GLN
1	A	458	ASN
1	B	398	GLN
1	B	422	GLN
1	B	458	ASN
1	B	464	ASN
1	C	398	GLN
1	C	422	GLN
1	C	458	ASN
1	D	398	GLN
1	D	458	ASN
1	E	398	GLN
1	E	422	GLN
1	E	458	ASN
1	F	398	GLN
1	F	458	ASN
1	F	464	ASN
1	G	398	GLN
1	G	422	GLN
1	G	458	ASN
1	H	398	GLN
1	H	422	GLN
1	H	458	ASN
1	H	464	ASN
1	I	398	GLN
1	I	422	GLN
1	I	458	ASN
1	J	398	GLN
1	J	458	ASN
1	K	398	GLN
1	K	422	GLN
1	K	458	ASN
1	K	464	ASN

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Mol	Chain	Res	Type
1	L	398	GLN
1	L	458	ASN
1	L	464	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 24 ligands modelled in this entry, 12 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
2	1AZ	A	501	-	24,31,31	1.22	3 (12%)	25,46,46	1.61	5 (20%)
2	1AZ	B	501	-	24,31,31	1.20	3 (12%)	25,46,46	1.81	5 (20%)
2	1AZ	C	501	-	24,31,31	1.19	2 (8%)	25,46,46	1.68	7 (28%)
2	1AZ	D	501	-	24,31,31	1.29	3 (12%)	25,46,46	1.67	5 (20%)
2	1AZ	E	501	-	24,31,31	1.12	2 (8%)	25,46,46	1.74	4 (16%)
2	1AZ	F	501	-	24,31,31	1.14	4 (16%)	25,46,46	1.59	3 (12%)
2	1AZ	G	501	-	24,31,31	1.26	4 (16%)	25,46,46	1.65	5 (20%)
2	1AZ	H	501	-	24,31,31	1.20	4 (16%)	25,46,46	1.59	5 (20%)
2	1AZ	I	501	-	24,31,31	1.24	2 (8%)	25,46,46	1.68	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1AZ	J	501	-	24,31,31	1.48	4 (16%)	25,46,46	1.75	5 (20%)
2	1AZ	K	501	-	24,31,31	1.23	2 (8%)	25,46,46	1.63	5 (20%)
2	1AZ	L	501	-	24,31,31	1.23	4 (16%)	25,46,46	1.85	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1AZ	A	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	B	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	C	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	D	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	E	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	F	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	G	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	H	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	I	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	J	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	K	501	-	-	0/4/16/16	0/4/4/4
2	1AZ	L	501	-	-	0/4/16/16	0/4/4/4

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	501	1AZ	C13-N5	-3.91	1.34	1.39
2	K	501	1AZ	C13-N5	-3.91	1.34	1.39
2	B	501	1AZ	C13-N5	-3.55	1.35	1.39
2	G	501	1AZ	C13-N5	-3.51	1.35	1.39
2	E	501	1AZ	C13-N5	-3.44	1.35	1.39
2	D	501	1AZ	C13-N5	-3.37	1.35	1.39
2	I	501	1AZ	C13-N5	-3.30	1.35	1.39
2	A	501	1AZ	C13-N5	-3.23	1.35	1.39
2	L	501	1AZ	C13-N5	-3.12	1.35	1.39
2	C	501	1AZ	C13-N5	-2.96	1.35	1.39
2	F	501	1AZ	C13-N5	-2.90	1.35	1.39
2	H	501	1AZ	C13-N5	-2.56	1.36	1.39
2	J	501	1AZ	C5-N1	-2.49	1.34	1.38
2	F	501	1AZ	C5-N1	-2.42	1.34	1.38
2	B	501	1AZ	C5-N1	-2.23	1.35	1.38
2	L	501	1AZ	C5-N1	-2.04	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	1AZ	C5-N1	-2.00	1.35	1.38
2	G	501	1AZ	C18-CL2	2.04	1.78	1.73
2	L	501	1AZ	C13-N4	2.07	1.35	1.33
2	A	501	1AZ	C18-CL2	2.09	1.78	1.73
2	F	501	1AZ	C1-CL1	2.11	1.78	1.73
2	F	501	1AZ	C18-CL2	2.20	1.79	1.73
2	E	501	1AZ	C1-CL1	2.24	1.79	1.73
2	B	501	1AZ	C1-CL1	2.27	1.79	1.73
2	H	501	1AZ	C13-N4	2.34	1.35	1.33
2	H	501	1AZ	C1-CL1	2.36	1.79	1.73
2	C	501	1AZ	C1-CL1	2.40	1.79	1.73
2	D	501	1AZ	C18-CL2	2.44	1.79	1.73
2	G	501	1AZ	C1-CL1	2.51	1.79	1.73
2	K	501	1AZ	C1-CL1	2.57	1.79	1.73
2	J	501	1AZ	C1-CL1	2.59	1.80	1.73
2	I	501	1AZ	C18-CL2	2.69	1.80	1.73
2	D	501	1AZ	C1-CL1	2.76	1.80	1.73
2	H	501	1AZ	C18-CL2	2.76	1.80	1.73
2	A	501	1AZ	C1-CL1	2.90	1.80	1.73
2	L	501	1AZ	C18-CL2	2.95	1.80	1.73
2	J	501	1AZ	C18-CL2	3.48	1.82	1.73

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	1AZ	C1-C2-C3	-4.97	117.15	120.36
2	L	501	1AZ	C1-C2-C3	-4.49	117.46	120.36
2	J	501	1AZ	C10-C9-N3	-4.47	102.15	110.02
2	E	501	1AZ	C1-C2-C3	-4.41	117.51	120.36
2	L	501	1AZ	C10-C9-N3	-4.36	102.34	110.02
2	H	501	1AZ	C10-C9-N3	-4.20	102.61	110.02
2	C	501	1AZ	C10-C9-N3	-4.20	102.62	110.02
2	D	501	1AZ	C10-C9-N3	-4.19	102.63	110.02
2	A	501	1AZ	C10-C9-N3	-4.12	102.76	110.02
2	G	501	1AZ	C10-C9-N3	-3.96	103.05	110.02
2	F	501	1AZ	C10-C9-N3	-3.91	103.12	110.02
2	B	501	1AZ	C10-C9-N3	-3.90	103.16	110.02
2	I	501	1AZ	C10-C9-N3	-3.77	103.38	110.02
2	K	501	1AZ	C1-C2-C3	-3.77	117.93	120.36
2	I	501	1AZ	C1-C2-C3	-3.64	118.01	120.36
2	K	501	1AZ	C10-C9-N3	-3.61	103.66	110.02
2	G	501	1AZ	C1-C2-C3	-3.56	118.06	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	501	1AZ	C6-C5-N1	-3.55	118.43	120.52
2	E	501	1AZ	C10-C9-N3	-3.50	103.86	110.02
2	C	501	1AZ	C1-C2-C3	-3.46	118.12	120.36
2	F	501	1AZ	C1-C2-C3	-3.44	118.14	120.36
2	J	501	1AZ	C1-C2-C3	-3.29	118.24	120.36
2	H	501	1AZ	C1-C2-C3	-3.22	118.28	120.36
2	H	501	1AZ	C11-C12-N3	-3.22	104.35	110.02
2	D	501	1AZ	C1-C2-C3	-3.15	118.33	120.36
2	L	501	1AZ	C11-C12-N3	-2.94	104.84	110.02
2	K	501	1AZ	C11-C12-N3	-2.91	104.89	110.02
2	J	501	1AZ	C11-C12-N3	-2.91	104.90	110.02
2	J	501	1AZ	C6-C5-N1	-2.88	118.82	120.52
2	I	501	1AZ	C11-C12-N3	-2.86	104.97	110.02
2	C	501	1AZ	C6-C5-N1	-2.83	118.85	120.52
2	A	501	1AZ	C1-C2-C3	-2.76	118.58	120.36
2	F	501	1AZ	C11-C12-N3	-2.76	105.16	110.02
2	D	501	1AZ	C6-C5-N1	-2.73	118.91	120.52
2	B	501	1AZ	C11-C12-N3	-2.58	105.48	110.02
2	A	501	1AZ	C6-C5-N1	-2.50	119.05	120.52
2	D	501	1AZ	C6-C13-N4	-2.44	106.11	110.83
2	A	501	1AZ	C6-C13-N4	-2.36	106.27	110.83
2	K	501	1AZ	C6-C5-N1	-2.30	119.16	120.52
2	G	501	1AZ	C11-C12-N3	-2.30	105.97	110.02
2	E	501	1AZ	C6-C13-N4	-2.28	106.41	110.83
2	I	501	1AZ	C6-C5-N1	-2.28	119.17	120.52
2	J	501	1AZ	C6-C13-N4	-2.20	106.58	110.83
2	C	501	1AZ	C11-C12-N3	-2.18	106.18	110.02
2	H	501	1AZ	C6-C13-N4	-2.16	106.64	110.83
2	D	501	1AZ	C11-C12-N3	-2.15	106.23	110.02
2	B	501	1AZ	C6-C13-N4	-2.14	106.70	110.83
2	K	501	1AZ	C6-C13-N4	-2.13	106.70	110.83
2	C	501	1AZ	C6-C13-N4	-2.12	106.73	110.83
2	E	501	1AZ	C11-C12-N3	-2.11	106.30	110.02
2	G	501	1AZ	C6-C13-N4	-2.09	106.79	110.83
2	B	501	1AZ	C6-C5-N1	-2.06	119.31	120.52
2	I	501	1AZ	C6-C13-N4	-2.04	106.88	110.83
2	L	501	1AZ	C6-C13-N4	-2.03	106.90	110.83
2	H	501	1AZ	C5-C6-C13	-2.03	118.48	119.93
2	G	501	1AZ	C2-C1-CL1	2.01	121.59	118.50
2	C	501	1AZ	C14-N5-C13	2.07	121.49	118.39
2	C	501	1AZ	C16-C3-C2	2.07	121.62	118.55
2	A	501	1AZ	C14-N5-C13	2.19	121.67	118.39

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	463/486 (95%)	0.67	48 (10%) 8 9	22, 38, 70, 99	0
1	B	463/486 (95%)	0.67	53 (11%) 7 7	22, 39, 70, 99	0
1	C	463/486 (95%)	0.77	73 (15%) 3 3	22, 39, 70, 99	0
1	D	463/486 (95%)	0.69	47 (10%) 9 10	22, 39, 70, 99	0
1	E	463/486 (95%)	0.70	48 (10%) 8 9	22, 38, 70, 99	0
1	F	463/486 (95%)	0.81	48 (10%) 8 9	22, 38, 70, 99	0
1	G	463/486 (95%)	0.69	54 (11%) 6 6	22, 38, 70, 99	0
1	H	463/486 (95%)	0.76	56 (12%) 6 6	22, 38, 70, 99	0
1	I	463/486 (95%)	0.73	65 (14%) 4 4	22, 39, 70, 99	0
1	J	463/486 (95%)	1.14	93 (20%) 1 1	22, 39, 70, 99	0
1	K	463/486 (95%)	0.72	57 (12%) 5 6	22, 39, 70, 99	0
1	L	463/486 (95%)	0.79	53 (11%) 7 7	22, 38, 70, 99	0
All	All	5556/5832 (95%)	0.76	695 (12%) 5 6	22, 39, 71, 99	0

All (695) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	333	GLY	13.3
1	I	334	TYR	11.4
1	L	61	PHE	10.0
1	J	296	ALA	10.0
1	C	414	ALA	9.6
1	J	347	ARG	9.4
1	I	61	PHE	9.3
1	L	413	ALA	9.3
1	J	334	TYR	9.3
1	H	58	ILE	9.2
1	G	414	ALA	9.1

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Mol	Chain	Res	Type	RSRZ
1	J	414	ALA	9.0
1	H	59	ARG	8.8
1	H	413	ALA	8.8
1	I	333	GLY	8.8
1	A	58	ILE	8.6
1	L	99	PHE	8.6
1	J	403	LYS	8.5
1	J	60	GLY	8.4
1	A	413	ALA	8.4
1	J	413	ALA	8.4
1	J	59	ARG	8.3
1	I	414	ALA	8.2
1	L	60	GLY	8.1
1	H	56	SER	8.0
1	L	334	TYR	8.0
1	E	414	ALA	8.0
1	A	414	ALA	7.9
1	F	99	PHE	7.9
1	K	414	ALA	7.8
1	H	57	SER	7.7
1	K	332	PRO	7.6
1	J	57	SER	7.6
1	C	99	PHE	7.5
1	H	61	PHE	7.5
1	A	404	ASP	7.5
1	J	401	VAL	7.5
1	F	404	ASP	7.5
1	K	333	GLY	7.4
1	B	58	ILE	7.4
1	J	61	PHE	7.3
1	B	413	ALA	7.2
1	G	99	PHE	7.2
1	E	415	SER	7.1
1	D	334	TYR	7.0
1	G	67	SER	7.0
1	A	403	LYS	7.0
1	F	413	ALA	6.9
1	A	334	TYR	6.9
1	E	334	TYR	6.9
1	J	58	ILE	6.9
1	D	413	ALA	6.9
1	L	58	ILE	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	56	SER	6.8
1	D	333	GLY	6.8
1	F	61	PHE	6.8
1	L	403	LYS	6.7
1	C	347	ARG	6.6
1	C	332	PRO	6.6
1	D	99	PHE	6.6
1	J	402	ASP	6.6
1	B	414	ALA	6.5
1	H	347	ARG	6.5
1	H	67	SER	6.4
1	J	404	ASP	6.4
1	B	61	PHE	6.4
1	D	403	LYS	6.4
1	A	61	PHE	6.3
1	C	355	ILE	6.3
1	A	347	ARG	6.2
1	F	56	SER	6.2
1	H	404	ASP	6.2
1	G	61	PHE	6.1
1	C	403	LYS	6.1
1	F	334	TYR	6.1
1	F	58	ILE	6.1
1	F	335	GLU	6.1
1	C	357	GLY	6.0
1	J	415	SER	6.0
1	E	67	SER	6.0
1	F	403	LYS	6.0
1	B	404	ASP	6.0
1	F	414	ALA	6.0
1	I	413	ALA	6.0
1	H	332	PRO	5.9
1	G	413	ALA	5.9
1	J	56	SER	5.9
1	C	334	TYR	5.9
1	H	55	GLY	5.8
1	B	59	ARG	5.8
1	I	67	SER	5.8
1	H	333	GLY	5.8
1	B	347	ARG	5.7
1	H	334	TYR	5.7
1	I	355	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	J	184	GLY	5.7
1	E	333	GLY	5.7
1	C	413	ALA	5.7
1	H	414	ALA	5.7
1	L	56	SER	5.7
1	D	347	ARG	5.7
1	A	99	PHE	5.7
1	J	292	GLU	5.6
1	K	62	GLN	5.6
1	F	62	GLN	5.6
1	H	403	LYS	5.6
1	D	58	ILE	5.6
1	F	401	VAL	5.6
1	J	293	THR	5.6
1	D	404	ASP	5.6
1	H	335	GLU	5.5
1	I	56	SER	5.5
1	D	60	GLY	5.5
1	C	404	ASP	5.5
1	J	356	THR	5.5
1	J	416	ILE	5.5
1	F	333	GLY	5.5
1	B	99	PHE	5.5
1	E	403	LYS	5.5
1	C	358	SER	5.4
1	L	404	ASP	5.4
1	B	62	GLN	5.4
1	D	415	SER	5.4
1	D	332	PRO	5.4
1	H	184	GLY	5.4
1	J	358	SER	5.4
1	B	336	ALA	5.4
1	J	346	ASN	5.3
1	L	57	SER	5.3
1	D	61	PHE	5.3
1	L	45	SER	5.3
1	C	335	GLU	5.3
1	L	59	ARG	5.3
1	B	335	GLU	5.3
1	J	295	TYR	5.3
1	G	347	ARG	5.3
1	J	355	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	68	ASP	5.2
1	J	332	PRO	5.2
1	C	333	GLY	5.2
1	K	334	TYR	5.2
1	L	335	GLU	5.1
1	J	357	GLY	5.1
1	B	403	LYS	5.1
1	D	414	ALA	5.1
1	G	334	TYR	5.1
1	L	414	ALA	5.1
1	K	58	ILE	5.1
1	K	293	THR	5.1
1	D	335	GLU	5.1
1	A	335	GLU	5.0
1	K	345	ARG	5.0
1	L	68	ASP	5.0
1	I	403	LYS	5.0
1	J	122	THR	5.0
1	B	334	TYR	5.0
1	A	333	GLY	4.9
1	H	62	GLN	4.9
1	J	345	ARG	4.9
1	B	332	PRO	4.9
1	I	99	PHE	4.8
1	G	335	GLU	4.8
1	D	55	GLY	4.8
1	I	332	PRO	4.8
1	G	403	LYS	4.8
1	D	345	ARG	4.8
1	A	67	SER	4.8
1	G	293	THR	4.8
1	I	402	ASP	4.8
1	H	99	PHE	4.7
1	C	331	VAL	4.7
1	G	404	ASP	4.7
1	B	333	GLY	4.7
1	I	358	SER	4.7
1	J	398	GLN	4.7
1	C	401	VAL	4.7
1	F	57	SER	4.6
1	G	415	SER	4.6
1	H	415	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	416	ILE	4.6
1	E	332	PRO	4.6
1	J	341	VAL	4.6
1	D	67	SER	4.6
1	E	58	ILE	4.6
1	H	60	GLY	4.6
1	K	347	ARG	4.6
1	C	61	PHE	4.6
1	K	358	SER	4.6
1	B	57	SER	4.5
1	E	5	THR	4.5
1	J	399	ALA	4.5
1	F	415	SER	4.5
1	L	358	SER	4.5
1	K	335	GLU	4.5
1	A	401	VAL	4.5
1	D	59	ARG	4.5
1	K	415	SER	4.4
1	A	57	SER	4.4
1	A	345	ARG	4.4
1	C	62	GLN	4.4
1	D	170	ALA	4.4
1	C	415	SER	4.4
1	A	62	GLN	4.3
1	C	45	SER	4.3
1	H	401	VAL	4.3
1	J	362	ALA	4.3
1	J	335	GLU	4.3
1	L	62	GLN	4.3
1	I	184	GLY	4.3
1	D	62	GLN	4.3
1	I	62	GLN	4.3
1	E	345	ARG	4.3
1	I	335	GLU	4.3
1	J	99	PHE	4.3
1	B	5	THR	4.3
1	E	336	ALA	4.3
1	H	345	ARG	4.3
1	E	335	GLU	4.2
1	J	120	ILE	4.2
1	J	45	SER	4.2
1	D	57	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	62	GLN	4.1
1	B	55	GLY	4.1
1	B	101	LEU	4.1
1	I	69	MET	4.1
1	C	67	SER	4.1
1	E	309	LEU	4.1
1	A	336	ALA	4.1
1	J	62	GLN	4.1
1	E	404	ASP	4.1
1	B	415	SER	4.0
1	B	293	THR	4.0
1	G	56	SER	4.0
1	J	449	GLU	4.0
1	B	68	ASP	4.0
1	I	404	ASP	4.0
1	K	57	SER	4.0
1	A	358	SER	3.9
1	F	59	ARG	3.9
1	K	300	ASP	3.9
1	C	346	ASN	3.9
1	K	362	ALA	3.9
1	J	342	TYR	3.9
1	C	56	SER	3.9
1	I	170	ALA	3.9
1	A	402	ASP	3.9
1	J	55	GLY	3.9
1	I	59	ARG	3.9
1	E	61	PHE	3.9
1	K	67	SER	3.8
1	C	360	PRO	3.8
1	E	413	ALA	3.8
1	J	284	ASP	3.8
1	C	183	LYS	3.8
1	G	449	GLU	3.8
1	C	336	ALA	3.7
1	J	291	ASP	3.7
1	K	404	ASP	3.7
1	C	293	THR	3.7
1	D	56	SER	3.7
1	H	293	THR	3.7
1	J	344	GLN	3.7
1	D	100	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	100	THR	3.7
1	J	348	SER	3.7
1	K	403	LYS	3.7
1	A	415	SER	3.6
1	F	60	GLY	3.6
1	I	415	SER	3.6
1	C	416	ILE	3.6
1	C	402	ASP	3.6
1	E	347	ARG	3.6
1	C	59	ARG	3.6
1	B	346	ASN	3.6
1	E	45	SER	3.6
1	I	293	THR	3.6
1	L	415	SER	3.6
1	D	402	ASP	3.6
1	F	332	PRO	3.6
1	F	347	ARG	3.6
1	B	345	ARG	3.6
1	C	285	GLY	3.6
1	K	336	ALA	3.5
1	K	367	PHE	3.5
1	I	347	ARG	3.5
1	H	358	SER	3.5
1	K	59	ARG	3.5
1	L	100	THR	3.5
1	A	101	LEU	3.5
1	L	55	GLY	3.5
1	K	184	GLY	3.5
1	E	351	VAL	3.5
1	G	355	ILE	3.5
1	F	277	CYS	3.5
1	L	54	ASP	3.5
1	H	100	THR	3.4
1	I	5	THR	3.4
1	F	346	ASN	3.4
1	G	285	GLY	3.4
1	J	67	SER	3.4
1	G	333	GLY	3.4
1	I	58	ILE	3.4
1	F	101	LEU	3.4
1	C	48	ASP	3.4
1	J	360	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	56	SER	3.4
1	L	332	PRO	3.4
1	A	416	ILE	3.4
1	D	401	VAL	3.3
1	J	418	GLN	3.3
1	J	118	TYR	3.3
1	J	400	PRO	3.3
1	G	416	ILE	3.3
1	I	292	GLU	3.3
1	F	402	ASP	3.3
1	H	416	ILE	3.3
1	H	5	THR	3.3
1	I	55	GLY	3.2
1	G	59	ARG	3.2
1	J	417	PRO	3.2
1	A	170	ALA	3.2
1	E	383	MET	3.2
1	K	61	PHE	3.2
1	J	450	THR	3.2
1	B	54	ASP	3.2
1	I	435	GLU	3.2
1	C	286	ALA	3.2
1	C	291	ASP	3.2
1	C	345	ARG	3.2
1	H	170	ALA	3.2
1	D	186	TYR	3.2
1	L	454	PHE	3.2
1	B	183	LYS	3.2
1	A	295	TYR	3.2
1	F	45	SER	3.2
1	L	101	LEU	3.1
1	C	6	PRO	3.1
1	K	99	PHE	3.1
1	H	101	LEU	3.1
1	L	416	ILE	3.1
1	A	59	ARG	3.1
1	I	97	ASP	3.1
1	D	45	SER	3.1
1	C	7	ASP	3.1
1	C	290	TYR	3.1
1	E	99	PHE	3.1
1	B	67	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	449	GLU	3.1
1	G	101	LEU	3.1
1	J	283	LYS	3.1
1	B	17	LYS	3.0
1	I	284	ASP	3.0
1	J	102	GLU	3.0
1	B	60	GLY	3.0
1	E	449	GLU	3.0
1	K	445	ASN	3.0
1	B	450	THR	3.0
1	C	5	THR	3.0
1	C	338	ILE	3.0
1	H	69	MET	3.0
1	K	416	ILE	3.0
1	L	347	ARG	3.0
1	J	44	LYS	3.0
1	F	454	PHE	3.0
1	K	291	ASP	3.0
1	F	67	SER	3.0
1	K	350	CYS	3.0
1	K	444	THR	3.0
1	B	357	GLY	3.0
1	L	333	GLY	3.0
1	G	300	ASP	3.0
1	J	290	TYR	3.0
1	F	358	SER	2.9
1	F	54	ASP	2.9
1	I	100	THR	2.9
1	K	5	THR	2.9
1	C	170	ALA	2.9
1	J	304	HIS	2.9
1	K	304	HIS	2.9
1	A	332	PRO	2.9
1	C	98	PRO	2.9
1	J	42	PHE	2.9
1	B	100	THR	2.9
1	D	30	GLY	2.9
1	I	101	LEU	2.9
1	L	67	SER	2.9
1	B	98	PRO	2.9
1	H	48	ASP	2.9
1	J	183	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	293	THR	2.9
1	E	352	ARG	2.9
1	G	332	PRO	2.9
1	E	7	ASP	2.9
1	J	300	ASP	2.9
1	G	358	SER	2.9
1	K	101	LEU	2.9
1	L	365	LEU	2.9
1	L	170	ALA	2.9
1	J	11	LYS	2.9
1	B	291	ASP	2.8
1	A	285	GLY	2.8
1	C	294	GLY	2.8
1	B	338	ILE	2.8
1	L	351	VAL	2.8
1	B	290	TYR	2.8
1	F	351	VAL	2.8
1	G	55	GLY	2.8
1	J	297	GLY	2.8
1	G	170	ALA	2.8
1	A	186	TYR	2.8
1	C	49	ASP	2.8
1	J	351	VAL	2.8
1	C	356	THR	2.8
1	C	450	THR	2.8
1	I	44	LYS	2.8
1	E	358	SER	2.8
1	H	68	ASP	2.8
1	I	8	ASP	2.8
1	L	277	CYS	2.8
1	F	100	THR	2.8
1	G	184	GLY	2.8
1	J	441	GLY	2.8
1	D	336	ALA	2.8
1	J	121	SER	2.8
1	C	97	ASP	2.8
1	G	58	ILE	2.8
1	A	450	THR	2.8
1	L	346	ASN	2.8
1	G	345	ARG	2.8
1	G	284	ASP	2.8
1	K	15	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	351	VAL	2.7
1	K	413	ALA	2.7
1	G	5	THR	2.7
1	A	98	PRO	2.7
1	H	8	ASP	2.7
1	F	336	ALA	2.7
1	L	285	GLY	2.7
1	D	309	LEU	2.7
1	C	184	GLY	2.7
1	K	126	ASP	2.7
1	C	392	LYS	2.7
1	I	416	ILE	2.7
1	A	360	PRO	2.7
1	C	435	GLU	2.7
1	E	380	PHE	2.7
1	J	435	GLU	2.7
1	C	300	ASP	2.7
1	F	367	PHE	2.7
1	L	350	CYS	2.7
1	J	285	GLY	2.6
1	J	294	GLY	2.6
1	J	46	VAL	2.6
1	C	126	ASP	2.6
1	G	402	ASP	2.6
1	K	100	THR	2.6
1	F	399	ALA	2.6
1	G	286	ALA	2.6
1	L	345	ARG	2.6
1	C	282	TRP	2.6
1	F	55	GLY	2.6
1	B	126	ASP	2.6
1	G	97	ASP	2.6
1	G	183	LYS	2.6
1	A	355	ILE	2.6
1	C	58	ILE	2.6
1	C	292	GLU	2.6
1	I	173	SER	2.6
1	D	360	PRO	2.6
1	K	357	GLY	2.6
1	A	100	THR	2.6
1	E	62	GLN	2.6
1	B	184	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	376	PRO	2.6
1	K	6	PRO	2.6
1	J	445	ASN	2.6
1	D	284	ASP	2.6
1	I	309	LEU	2.6
1	D	346	ASN	2.5
1	C	101	LEU	2.5
1	H	4	LYS	2.5
1	I	432	ALA	2.5
1	A	40	SER	2.5
1	B	102	GLU	2.5
1	H	183	LYS	2.5
1	A	284	ASP	2.5
1	F	170	ALA	2.5
1	H	367	PHE	2.5
1	J	298	LEU	2.5
1	C	295	TYR	2.5
1	H	449	GLU	2.5
1	K	69	MET	2.5
1	K	402	ASP	2.5
1	I	294	GLY	2.5
1	I	345	ARG	2.5
1	I	360	PRO	2.5
1	B	4	LYS	2.5
1	H	292	GLU	2.5
1	I	16	GLU	2.5
1	F	309	LEU	2.5
1	D	49	ASP	2.5
1	J	54	ASP	2.5
1	J	126	ASP	2.5
1	I	357	GLY	2.5
1	J	69	MET	2.5
1	E	379	ALA	2.5
1	C	57	SER	2.5
1	B	360	PRO	2.5
1	L	376	PRO	2.5
1	H	11	LYS	2.5
1	H	54	ASP	2.5
1	J	303	ARG	2.5
1	K	295	TYR	2.5
1	A	453	SER	2.5
1	B	170	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	57	SER	2.5
1	F	26	CYS	2.4
1	A	132	ALA	2.4
1	J	361	LYS	2.4
1	K	45	SER	2.4
1	E	376	PRO	2.4
1	A	55	GLY	2.4
1	G	294	GLY	2.4
1	H	402	ASP	2.4
1	I	49	ASP	2.4
1	E	417	PRO	2.4
1	G	282	TRP	2.4
1	K	122	THR	2.4
1	A	338	ILE	2.4
1	E	284	ASP	2.4
1	G	7	ASP	2.4
1	G	398	GLN	2.4
1	E	360	PRO	2.4
1	D	331	VAL	2.4
1	D	31	ILE	2.4
1	H	7	ASP	2.4
1	I	7	ASP	2.4
1	D	17	LYS	2.4
1	E	170	ALA	2.4
1	I	286	ALA	2.4
1	J	390	GLY	2.4
1	G	351	VAL	2.4
1	F	24	ARG	2.4
1	J	338	ILE	2.4
1	E	367	PHE	2.4
1	K	292	GLU	2.4
1	C	171	ASP	2.4
1	C	100	THR	2.4
1	I	356	THR	2.4
1	A	449	GLU	2.4
1	D	398	GLN	2.3
1	G	71	LEU	2.3
1	I	449	GLU	2.3
1	G	275	MET	2.3
1	B	7	ASP	2.3
1	H	186	TYR	2.3
1	G	277	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	351	VAL	2.3
1	C	215	LYS	2.3
1	K	346	ASN	2.3
1	F	242	MET	2.3
1	G	360	PRO	2.3
1	L	8	ASP	2.3
1	K	282	TRP	2.3
1	G	372	SER	2.3
1	J	453	SER	2.3
1	H	350	CYS	2.3
1	C	400	PRO	2.3
1	H	286	ALA	2.3
1	K	284	ASP	2.3
1	L	44	LYS	2.3
1	K	186	TYR	2.3
1	K	290	TYR	2.3
1	K	348	SER	2.3
1	L	309	LEU	2.3
1	B	294	GLY	2.3
1	F	374	GLY	2.3
1	L	184	GLY	2.3
1	L	25	PHE	2.3
1	C	284	ASP	2.3
1	E	184	GLY	2.3
1	I	401	VAL	2.3
1	I	54	ASP	2.3
1	L	183	LYS	2.3
1	A	376	PRO	2.3
1	F	416	ILE	2.3
1	E	59	ARG	2.3
1	B	358	SER	2.3
1	B	453	SER	2.3
1	K	56	SER	2.3
1	A	4	LYS	2.3
1	D	340	LEU	2.3
1	J	359	ASN	2.3
1	G	186	TYR	2.3
1	D	351	VAL	2.3
1	B	53	PHE	2.2
1	I	367	PHE	2.2
1	J	287	PRO	2.2
1	D	358	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	49	ASP	2.2
1	K	215	LYS	2.2
1	C	376	PRO	2.2
1	C	432	ALA	2.2
1	D	399	ALA	2.2
1	L	69	MET	2.2
1	A	97	ASP	2.2
1	L	51	LEU	2.2
1	E	416	ILE	2.2
1	I	285	GLY	2.2
1	L	71	LEU	2.2
1	K	320	THR	2.2
1	E	331	VAL	2.2
1	E	306	ILE	2.2
1	G	435	GLU	2.2
1	B	11	LYS	2.2
1	I	446	ASP	2.2
1	B	45	SER	2.2
1	H	277	CYS	2.2
1	L	370	PRO	2.2
1	H	46	VAL	2.1
1	I	123	GLY	2.1
1	I	186	TYR	2.1
1	L	336	ALA	2.1
1	E	350	CYS	2.1
1	E	8	ASP	2.1
1	J	15	ASP	2.1
1	G	461	GLU	2.1
1	F	353	ILE	2.1
1	E	443	PHE	2.1
1	H	172	GLY	2.1
1	A	290	TYR	2.1
1	D	69	MET	2.1
1	C	431	GLU	2.1
1	I	11	LYS	2.1
1	F	356	THR	2.1
1	G	60	GLY	2.1
1	L	453	SER	2.1
1	D	54	ASP	2.1
1	G	49	ASP	2.1
1	K	446	ASP	2.1
1	L	275	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	10	PHE	2.1
1	E	317	LEU	2.1
1	H	429	ARG	2.1
1	G	453	SER	2.1
1	H	102	GLU	2.1
1	B	14	LYS	2.1
1	B	446	ASP	2.1
1	C	350	CYS	2.1
1	J	4	LYS	2.1
1	C	306	ILE	2.1
1	H	454	PHE	2.1
1	K	351	VAL	2.1
1	C	352	ARG	2.1
1	F	345	ARG	2.1
1	I	60	GLY	2.1
1	J	305	TYR	2.1
1	H	12	LEU	2.1
1	J	394	LYS	2.1
1	I	291	ASP	2.1
1	K	49	ASP	2.1
1	I	359	ASN	2.0
1	A	172	GLY	2.0
1	A	183	LYS	2.0
1	G	357	GLY	2.0
1	J	123	GLY	2.0
1	J	124	ILE	2.0
1	C	367	PHE	2.0
1	E	316	LEU	2.0
1	E	453	SER	2.0
1	J	100	THR	2.0
1	J	339	ASN	2.0
1	I	336	ALA	2.0
1	K	432	ALA	2.0
1	I	4	LYS	2.0
1	E	275	MET	2.0
1	I	331	VAL	2.0
1	I	351	VAL	2.0
1	F	285	GLY	2.0
1	H	357	GLY	2.0
1	D	306	ILE	2.0
1	I	378	LEU	2.0
1	C	121	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	301	THR	2.0
1	J	444	THR	2.0
1	L	26	CYS	2.0
1	G	359	ASN	2.0
1	B	69	MET	2.0
1	F	23	VAL	2.0
1	H	275	MET	2.0
1	L	23	VAL	2.0
1	E	6	PRO	2.0
1	C	40	SER	2.0
1	E	56	SER	2.0
1	J	447	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	1AZ	C	501	28/28	0.88	0.25	1.95	46,47,49,50	0
2	1AZ	A	501	28/28	0.88	0.25	1.40	46,47,49,49	0
2	1AZ	I	501	28/28	0.92	0.23	1.13	46,47,49,50	0
2	1AZ	J	501	28/28	0.87	0.28	0.83	46,47,49,50	0
2	1AZ	G	501	28/28	0.89	0.23	0.71	46,47,48,50	0
2	1AZ	H	501	28/28	0.86	0.21	0.68	46,47,48,50	0
2	1AZ	K	501	28/28	0.86	0.22	0.24	46,47,49,50	0
2	1AZ	D	501	28/28	0.87	0.19	0.01	46,47,48,49	0
2	1AZ	B	501	28/28	0.89	0.17	-0.09	46,47,48,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	1AZ	E	501	28/28	0.87	0.18	-0.20	46,47,48,49	0
2	1AZ	L	501	28/28	0.88	0.16	-0.81	46,47,48,49	0
2	1AZ	F	501	28/28	0.90	0.17	-0.85	46,47,48,49	0
3	CL	G	502	1/1	0.89	0.14	-	57,57,57,57	0
3	CL	C	502	1/1	0.89	0.14	-	57,57,57,57	0
3	CL	A	502	1/1	0.89	0.11	-	57,57,57,57	0
3	CL	L	502	1/1	0.98	0.30	-	57,57,57,57	0
3	CL	H	502	1/1	0.95	0.16	-	57,57,57,57	0
3	CL	K	502	1/1	0.98	0.37	-	58,58,58,58	0
3	CL	D	502	1/1	0.98	0.14	-	57,57,57,57	0
3	CL	E	502	1/1	0.97	0.18	-	57,57,57,57	0
3	CL	I	502	1/1	0.95	0.13	-	57,57,57,57	0
3	CL	J	502	1/1	0.85	0.21	-	57,57,57,57	0
3	CL	F	502	1/1	0.94	0.22	-	57,57,57,57	0
3	CL	B	502	1/1	0.92	0.22	-	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.