



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:12 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

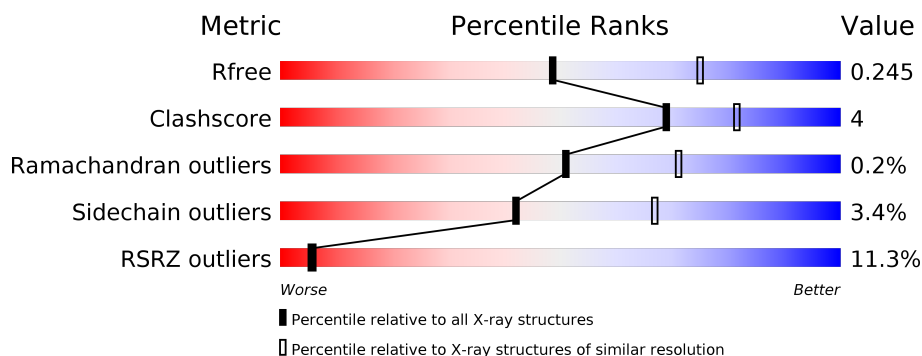
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (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>9%</div> <div>83% 12% • 5%</div> </div>
1	B	486	<div> <div>10%</div> <div>85% 9% • 5%</div> </div>
1	C	486	<div> <div>14%</div> <div>85% 9% • 5%</div> </div>
1	D	486	<div> <div>9%</div> <div>84% 10% • 5%</div> </div>
1	E	486	<div> <div>8%</div> <div>85% 9% • 5%</div> </div>
1	F	486	<div> <div>9%</div> <div>84% 11% • 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	486	<div><div></div><div>10%</div><div>84%</div><div>10%</div><div>5%</div></div>
1	H	486	<div><div></div><div>10%</div><div>85%</div><div>9%</div><div>5%</div></div>
1	I	486	<div><div></div><div>12%</div><div>85%</div><div>9%</div><div>5%</div></div>
1	J	486	<div><div></div><div>17%</div><div>83%</div><div>11%</div><div>5%</div></div>
1	K	486	<div><div></div><div>11%</div><div>85%</div><div>10%</div><div>5%</div></div>
1	L	486	<div><div></div><div>10%</div><div>86%</div><div>8%</div><div>5%</div></div>

2 Entry composition

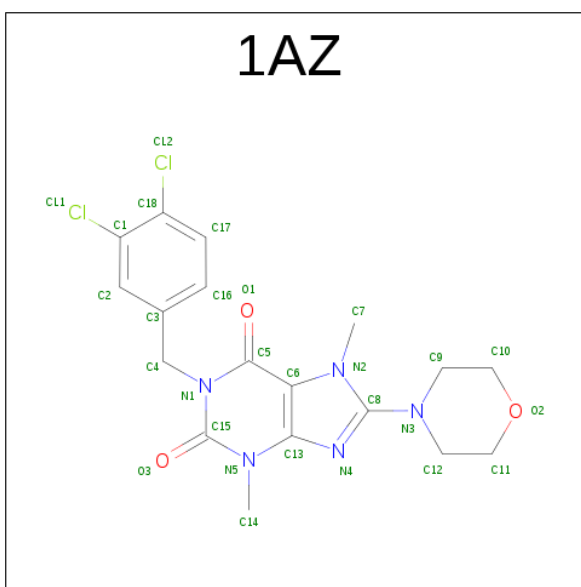
There are 4 unique types of molecules in this entry. The entry contains 45804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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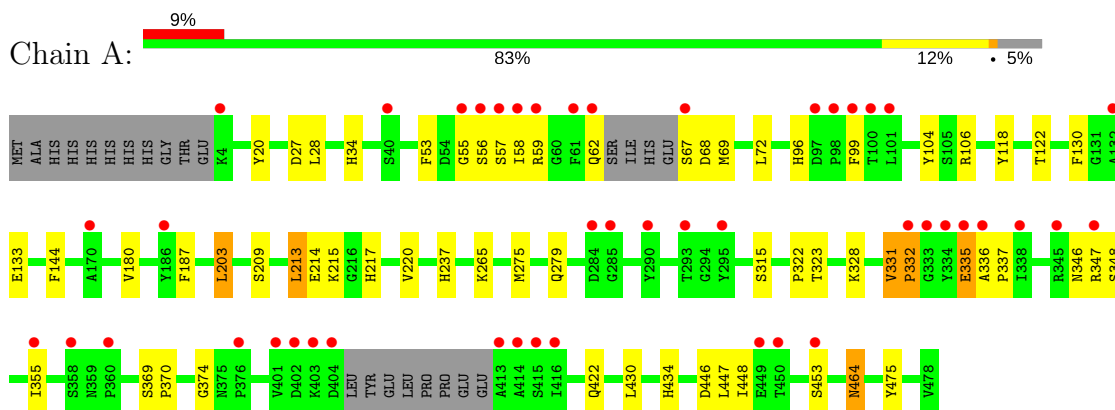
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	126	Total 126	O 126	0	0
4	J	126	Total 126	O 126	0	0
4	K	131	Total 131	O 131	0	0
4	L	129	Total 129	O 129	0	0

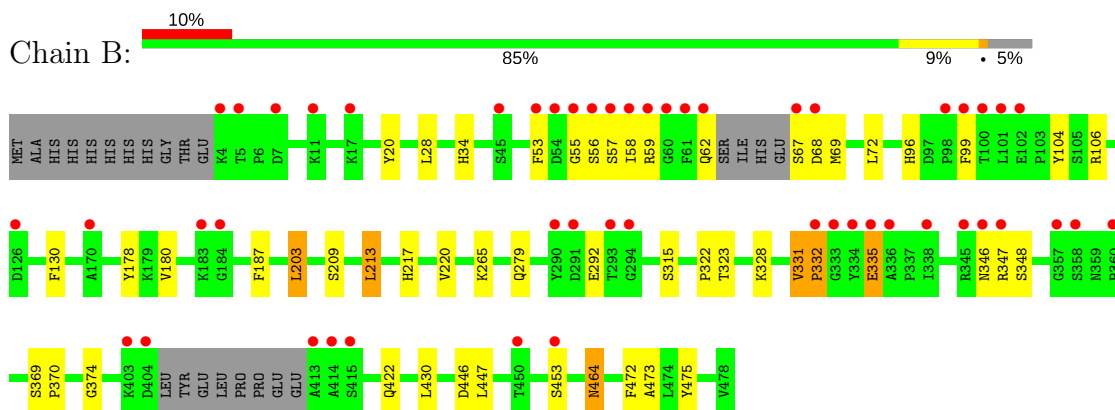
3 Residue-property plots [i](#)

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

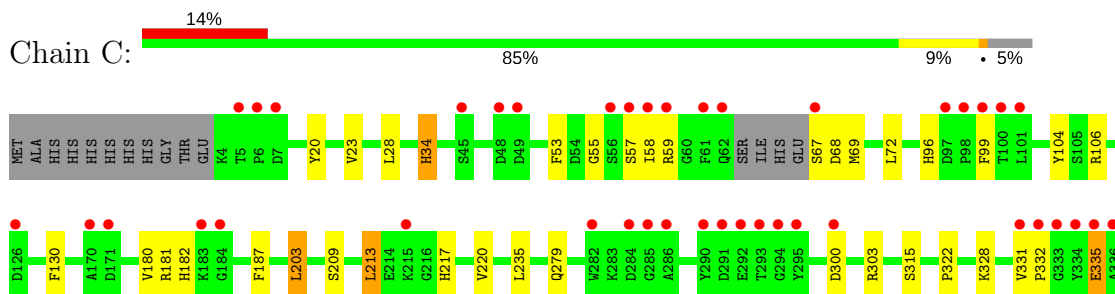
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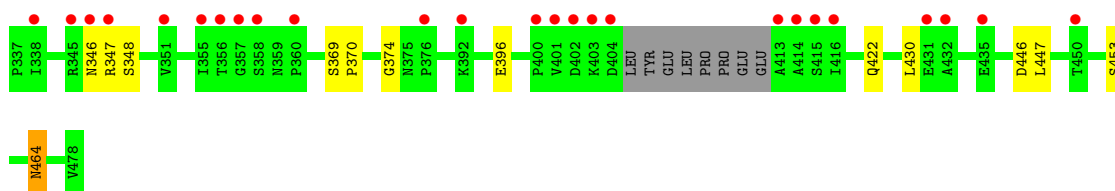


• Molecule 1: GLUTAMINE SYNTHETASE 1

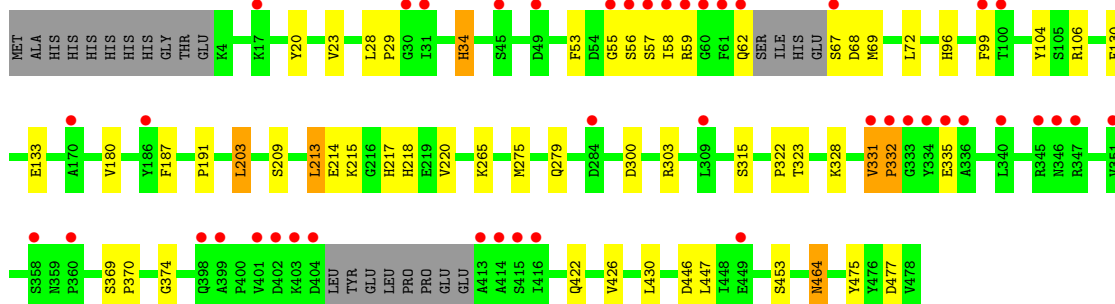
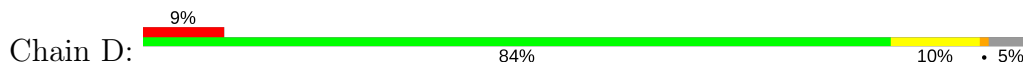


• Molecule 1: GLUTAMINE SYNTHETASE 1

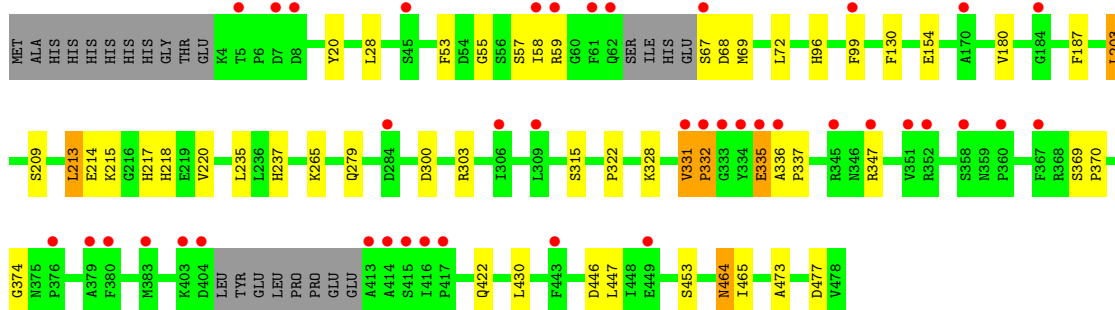
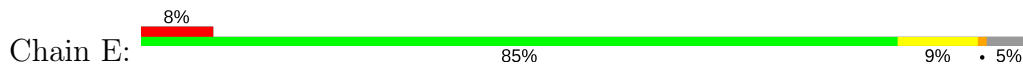




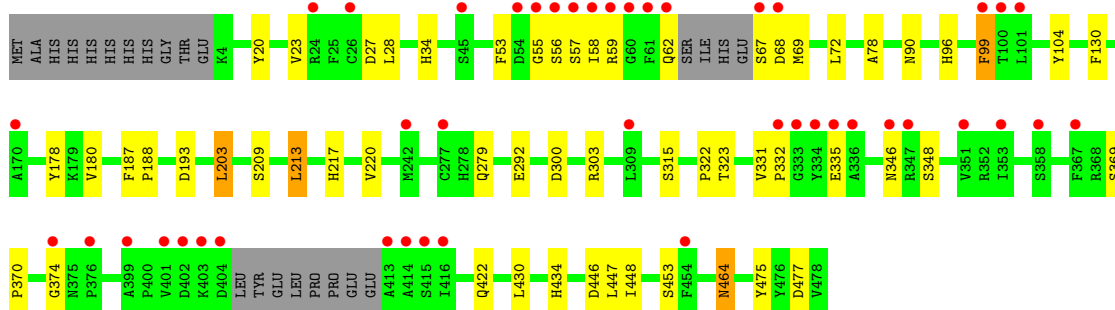
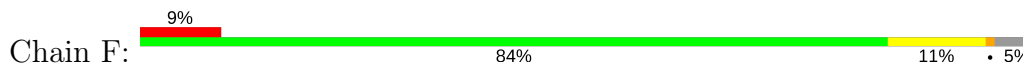
• Molecule 1: GLUTAMINE SYNTHETASE 1



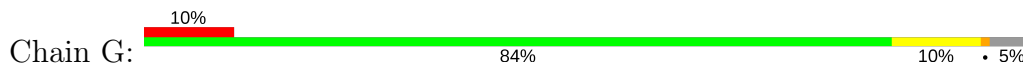
• Molecule 1: GLUTAMINE SYNTHETASE 1

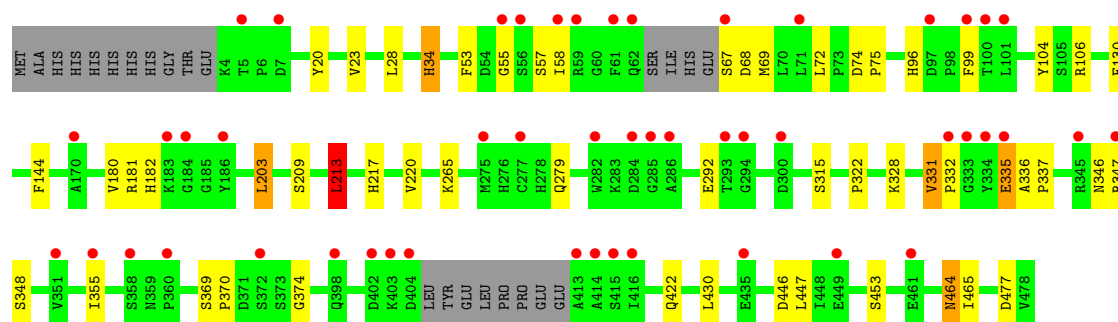


• Molecule 1: GLUTAMINE SYNTHETASE 1

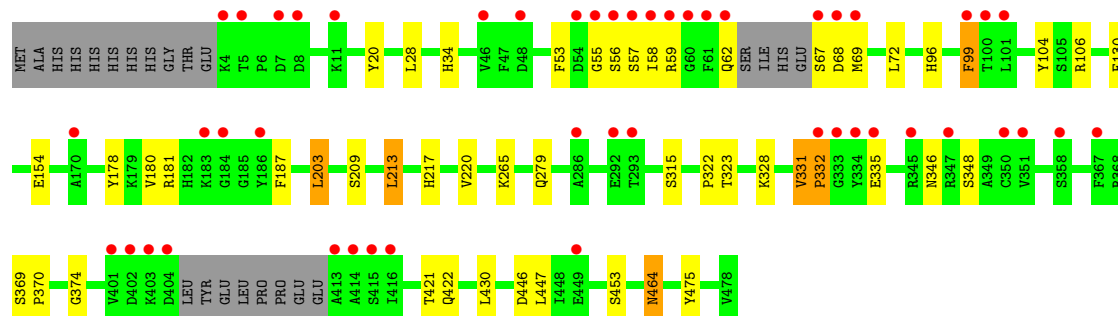
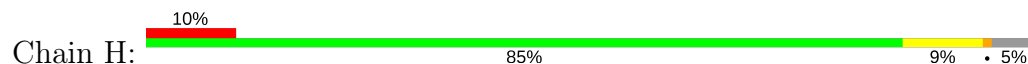


• Molecule 1: GLUTAMINE SYNTHETASE 1

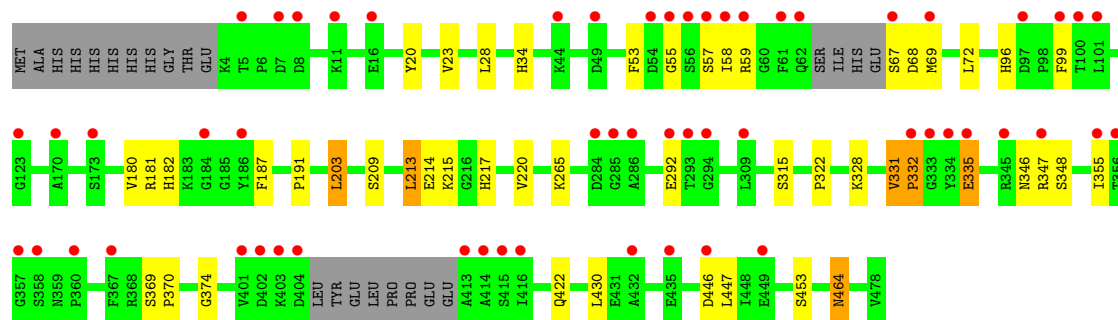
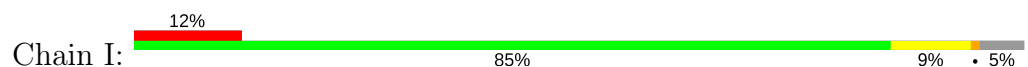




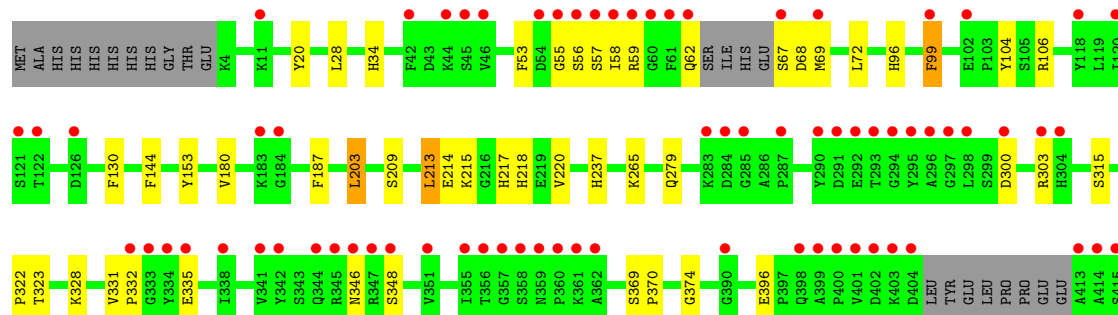
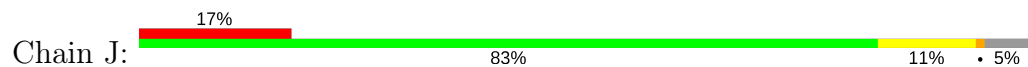
• Molecule 1: GLUTAMINE SYNTHETASE 1

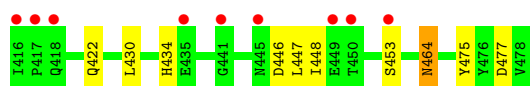


• Molecule 1: GLUTAMINE SYNTHETASE 1

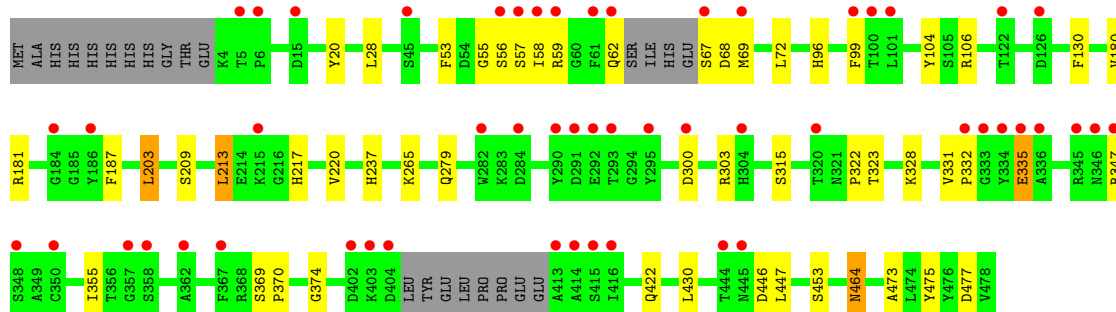
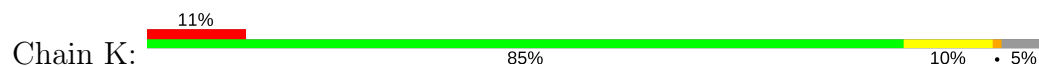


• Molecule 1: GLUTAMINE SYNTHETASE 1

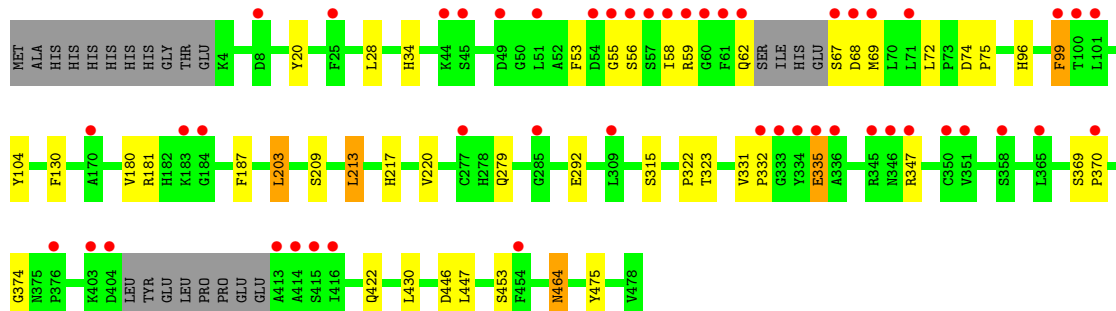
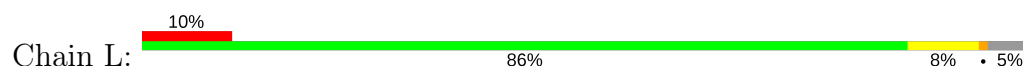




● Molecule 1: GLUTAMINE SYNTHETASE 1



● 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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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:B:62:GLN:HB3	1:C:335:GLU:OE1	1.90	0.71
1:G:355:ILE:HG21	1:L:99:PHE:HE1	1.56	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:C:57:SER:HB3	1:D:187:PHE:HE2	1.65	0.61
1:H:58:ILE:HD12	1:H:69:MET:HB2	1.83	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:D:57:SER:HB3	1:E:187:PHE:HE2	1.69	0.58
1:E:58:ILE:HD12	1:E:69:MET:HB2	1.86	0.58
1:C:58:ILE:HD12	1:C:69:MET:HB2	1.86	0.57
1:E:328:LYS:HE3	1:G:464:ASN:O	2.03	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:C:57:SER:HB3	1:D:187:PHE:CE2	2.41	0.56
1:J:57:SER:HB3	1:K:187:PHE:HE2	1.70	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:B:59:ARG:HE	1:B:69:MET:HE2	1.71	0.55
1:D:464:ASN:HD21	1:H:422:GLN:NE2	2.01	0.55
1:B:28:LEU:HD11	1:B:447:LEU:HD11	1.88	0.54
1:F:323:THR:HB	1:L:475:TYR:CZ	2.42	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:315:SER:HB2	1:F:430:LEU:HA	1.91	0.53
1:F:53:PHE:HB3	1:F:58:ILE:HD11	1.90	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:A:53:PHE:HB3	1:A:58:ILE:HD11	1.89	0.53
1:B:53:PHE:HB3	1:B:58:ILE:HD11	1.90	0.53
1:D:323:THR:HB	1:H:475:TYR:CZ	2.43	0.53
1:A:62:GLN:HB3	1:B:335:GLU:OE1	2.08	0.53
1:A:59:ARG:HE	1:A:69:MET:HE2	1.72	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:C:213:LEU:HD13	1:C:217:HIS:HB3	1.91	0.52
1:K:130:PHE:CE1	1:K:279:GLN:HG2	2.44	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: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:G:347:ARG:NH1	1:L:56:SER:HB3	2.21	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:A:213:LEU:HD13	1:A:217:HIS:HB3	1.93	0.51
1:E:53:PHE:HB3	1:E:58:ILE:HD11	1.92	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:A:315:SER:HB2	1:A:430:LEU:HA	1.93	0.51
1:E:265:LYS:HG2	1:E:328:LYS:HB3	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:E:72:LEU:HD12	1:E:96:HIS:CD2	2.47	0.50
1:F:59:ARG:HE	1:F:69:MET:HE2	1.76	0.50
1:E:473:ALA:HA	1:G:144:PHE:CE1	2.46	0.50
1:H:53:PHE:HB3	1:H:58:ILE:HD11	1.93	0.50
1:B:213:LEU:HD13	1:B:217:HIS:HB3	1.94	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:G:72:LEU:HD12	1:G:96:HIS:CD2	2.47	0.50
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:A:323:THR:HB	1:K:475:TYR:CZ	2.47	0.49
1:K:72:LEU:HD12	1:K:96:HIS:CD2	2.47	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:J:59:ARG:HE	1:J:69:MET:HE2	1.78	0.49
1:B:57:SER:HB3	1:C:187:PHE:CE2	2.47	0.49
1:H:130:PHE:CE1	1:H:279:GLN:HG2	2.47	0.49
1:D:328:LYS:HE3	1:H:464:ASN:O	2.13	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:A:56:SER:HB3	1:B:347:ARG:HH11	1.78	0.48
1:F:213:LEU:HD13	1:F:217:HIS:HB3	1.96	0.48
1:H:322:PRO:HG3	1:H:374:GLY:HA3	1.95	0.48
1:C:328:LYS:HE3	1:I:464:ASN:O	2.14	0.48
1:J:218:HIS:ND1	4:J:2078:HOH:O	2.34	0.48
1:I:213:LEU:HD13	1:I:217:HIS:HB3	1.95	0.48
1:J:53:PHE:HD2	1:J:58:ILE:HG13	1.79	0.48
1:D:130:PHE:CE1	1:D:279:GLN:HG2	2.49	0.48
1:E:59:ARG:HE	1:E:69:MET:HE2	1.79	0.48
1:G:315:SER:HB2	1:G:430:LEU:HA	1.96	0.48
1:L:315:SER:HB2	1:L:430:LEU:HA	1.96	0.48
1:B:57:SER:HB3	1:C:187:PHE:HE2	1.79	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:J:369:SER:N	1:J:370:PRO:CD	2.77	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:H:72:LEU:HD12	1:H:96:HIS:CD2	2.49	0.47
1:I:369:SER:N	1:I:370:PRO:CD	2.77	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:E:213:LEU:HD13	1:E:217:HIS:HB3	1.98	0.46
1:F:53:PHE:HD2	1:F:58:ILE:HG13	1.80	0.46
1:D:331:VAL:HA	1:D:332:PRO:HD3	1.85	0.46
1:F:322:PRO:HG3	1:F:374:GLY:HA3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:335:GLU:CD	1:F:62:GLN:HB3	2.36	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: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:F:477:ASP:OD1	1:G:182:HIS:NE2	2.50	0.45
1:K:53:PHE:HD2	1:K:58:ILE:HG13	1.81	0.45
1:G:322:PRO:HG3	1:G:374:GLY:HA3	1.99	0.45
1:I:181:ARG:HE	1:I:181:ARG:HB2	1.58	0.45
1:L:213:LEU:HD13	1:L:217:HIS:HB3	1.98	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:369:SER:N	1:D:370:PRO:CD	2.79	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:A:322:PRO:HG3	1:A:374:GLY:HA3	1.99	0.45
1:J:213:LEU:HD13	1:J:217:HIS:HB3	1.98	0.45
1:B:53:PHE:HD2	1:B:58:ILE:HG13	1.82	0.45
1:G:213:LEU:HD13	1:G:217:HIS:HB3	1.98	0.45
1:B:464:ASN:O	1:J:328:LYS:HE3	2.16	0.45
1:E:369:SER:N	1:E:370:PRO:CD	2.80	0.45
1:L:322:PRO:HG3	1:L:374:GLY:HA3	1.99	0.45
1:C:235:LEU:C	1:C:235:LEU:HD23	2.37	0.45
1:E:331:VAL:HA	1:E:332:PRO:HD3	1.83	0.45
1:B:322:PRO:HG3	1:B:374:GLY:HA3	1.99	0.44
1:E:53:PHE:HD2	1:E:58:ILE:HG13	1.82	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:A:72:LEU:HD12	1:A:96:HIS:CD2	2.51	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

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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:A:331:VAL:HA	1:A:332:PRO:HD3	1.84	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:K:69:MET:HE3	1:K:104:TYR:CG	2.53	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:A:104:TYR:CZ	1:A:106:ARG:HB2	2.53	0.43
1:B:59:ARG:NE	1:B:69:MET:HE2	2.33	0.43
1:E:336:ALA:HA	1:E:337:PRO:HD2	1.94	0.43
1:F:323:THR:HB	1:L:475:TYR:CE1	2.53	0.43
1:A:187:PHE:HE2	1:F:57:SER:HB3	1.83	0.43
1:C:346:ASN:OD1	1:C:348:SER:HB3	2.19	0.43
1:J:303:ARG:NH1	1:J:396:GLU:OE2	2.52	0.43
1:G:346:ASN:OD1	1:G:348:SER:HB3	2.18	0.43
1:H:331:VAL:HA	1:H:332:PRO:HD3	1.86	0.43
1:I:331:VAL:HA	1:I:332:PRO:HD3	1.81	0.43
1:I:322:PRO:HG3	1:I:374:GLY:HA3	1.99	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:B:346:ASN:OD1	1:B:348:SER:HB3	2.19	0.42
1:D:104:TYR:CZ	1:D:106:ARG:HB2	2.54	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: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:K:300:ASP:OD1	1:K:303:ARG:NH2	2.52	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:C:182:HIS:NE2	1:J:477:ASP:OD1	2.53	0.42
1:E:214:GLU:HB3	1:E:215:LYS:H	1.74	0.42
1:J:322:PRO:HG3	1:J:374:GLY:HA3	2.02	0.42
1:D:322:PRO:HG3	1:D:374:GLY:HA3	2.02	0.42
1:G:104:TYR:CZ	1:G:106:ARG:HB2	2.55	0.42
1:H:57:SER:HB3	1:I:187:PHE:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:265:LYS:HG2	1:K:328:LYS:HB3	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:D:23:VAL:O	1:D:34:HIS:HA	2.20	0.41
1:H:181:ARG:HB2	1:H:181:ARG:HE	1.64	0.41
1:A:336:ALA:HA	1:A:337:PRO:HD2	1.96	0.41
1:B:69:MET:HE3	1:B:104:TYR:CG	2.56	0.41
1:C:23:VAL:O	1:C:34:HIS:HA	2.20	0.41
1:F:188:PRO:O	1:F:193:ASP:HB2	2.20	0.41
1:G:292:GLU:HG3	1:G:292:GLU:H	1.66	0.41
1:H:332:PRO:HG3	1:H:421:THR:HG21	2.02	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:C:104:TYR:CZ	1:C:106:ARG:HB2	2.56	0.41
1:C:303:ARG:NH1	1:C:396:GLU:OE2	2.53	0.41
1:G:336:ALA:HA	1:G:337:PRO:HD2	1.96	0.41
1:G:369:SER:N	1:G:370:PRO:CD	2.84	0.41
1:I:214:GLU:HB3	1:I:215:LYS:H	1.74	0.41
1:L:58:ILE:CD1	1:L:69:MET:HB2	2.48	0.41
1:F:346:ASN:OD1	1:F:348:SER:HB3	2.20	0.41
1:L:181:ARG:HE	1:L:181:ARG:HB2	1.60	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:K:20:TYR:CZ	1:L:203:LEU:HD13	2.54	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:A:434:HIS:HB2	1:A:448:ILE:HD13	2.03	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:B:331:VAL:HA	1:B:332:PRO:HD3	1.86	0.41
1:F:78:ALA:HA	1:F:90:ASN:O	2.21	0.41
1:I:346:ASN:OD1	1:I:348:SER:HB3	2.20	0.41
1:B:473:ALA:HA	1:J:144:PHE:CE1	2.56	0.41
1:J:214:GLU:HB3	1:J:215:LYS:H	1.72	0.41
1:J:369:SER:N	1:J:370:PRO:HD3	2.36	0.41
1:A:369:SER:N	1:A:370:PRO:CD	2.84	0.40
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: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:B:178:TYR:CE1	1:K:477:ASP:HB2	2.56	0.40
1:D:69:MET:HE3	1:D:104:TYR:CG	2.56	0.40
1:F:23:VAL:O	1:F:34:HIS:HA	2.22	0.40
1:F:434:HIS:HB2	1:F:448:ILE:HD13	2.03	0.40
1:G:23:VAL:O	1:G:34:HIS:HA	2.22	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: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:A:214:GLU:HB3	1:A:215:LYS:H	1.70	0.40
1:E:20:TYR:CZ	1:F:203:LEU:HD13	2.57	0.40
1:G:74:ASP:HA	1:G:75:PRO:HD2	1.98	0.40
1:L:69:MET:HE3	1:L:104:TYR:CG	2.57	0.40
1:A:69:MET:HE3	1:A:104:TYR:CG	2.56	0.40
1:A:118:TYR:O	1:A:122:THR:HG23	2.22	0.40
1:C:300:ASP:OD1	1:C:303:ARG:NH2	2.54	0.40
1:J:434:HIS:HB2	1:J:448:ILE:HD13	2.03	0.40
1:K:104:TYR:CZ	1:K:106:ARG:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/486 (94%)	442 (97%)	14 (3%)	1 (0%)	51	71
1	B	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	51	71
1	C	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	51	71
1	D	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	51	71
1	E	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	51	71
1	F	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	51	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	51	71
1	H	457/486 (94%)	441 (96%)	15 (3%)	1 (0%)	51	71
1	I	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	51	71
1	J	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	51	71
1	K	457/486 (94%)	441 (96%)	15 (3%)	1 (0%)	51	71
1	L	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	51	71
All	All	5484/5832 (94%)	5279 (96%)	193 (4%)	12 (0%)	51	71

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%)	43	68
1	B	390/411 (95%)	377 (97%)	13 (3%)	43	68
1	C	390/411 (95%)	377 (97%)	13 (3%)	43	68
1	D	390/411 (95%)	375 (96%)	15 (4%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	390/411 (95%)	377 (97%)	13 (3%)	43	68
1	F	390/411 (95%)	378 (97%)	12 (3%)	45	70
1	G	390/411 (95%)	377 (97%)	13 (3%)	43	68
1	H	390/411 (95%)	376 (96%)	14 (4%)	40	64
1	I	390/411 (95%)	377 (97%)	13 (3%)	43	68
1	J	390/411 (95%)	377 (97%)	13 (3%)	43	68
1	K	390/411 (95%)	378 (97%)	12 (3%)	45	70
1	L	390/411 (95%)	377 (97%)	13 (3%)	43	68
All	All	4680/4932 (95%)	4523 (97%)	157 (3%)	42	67

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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	-	23,31,31	1.06	2 (8%)	28,46,46	1.98	8 (28%)
2	1AZ	B	501	-	23,31,31	0.99	3 (13%)	28,46,46	2.15	7 (25%)
2	1AZ	C	501	-	23,31,31	1.06	2 (8%)	28,46,46	1.99	9 (32%)
2	1AZ	D	501	-	23,31,31	1.13	2 (8%)	28,46,46	2.04	9 (32%)
2	1AZ	E	501	-	23,31,31	0.91	1 (4%)	28,46,46	2.10	7 (25%)
2	1AZ	F	501	-	23,31,31	1.00	3 (13%)	28,46,46	1.99	6 (21%)
2	1AZ	G	501	-	23,31,31	1.07	3 (13%)	28,46,46	1.99	5 (17%)
2	1AZ	H	501	-	23,31,31	1.12	3 (13%)	28,46,46	2.02	9 (32%)
2	1AZ	I	501	-	23,31,31	1.08	2 (8%)	28,46,46	2.03	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1AZ	J	501	-	23,31,31	1.29	3 (13%)	28,46,46	2.10	8 (28%)
2	1AZ	K	501	-	23,31,31	0.97	1 (4%)	28,46,46	2.01	8 (28%)
2	1AZ	L	501	-	23,31,31	1.09	3 (13%)	28,46,46	2.16	6 (21%)

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 (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
2	G	501	1AZ	C5-N1	-2.00	1.35	1.38
2	B	501	1AZ	C18-CL2	2.01	1.78	1.73
2	C	501	1AZ	C18-CL2	2.03	1.78	1.73
2	I	501	1AZ	C1-CL1	2.04	1.78	1.73
2	L	501	1AZ	C13-N4	2.07	1.35	1.33
2	G	501	1AZ	C18-CL2	2.09	1.78	1.73
2	A	501	1AZ	C18-CL2	2.14	1.78	1.73
2	F	501	1AZ	C1-CL1	2.16	1.78	1.73
2	F	501	1AZ	C18-CL2	2.26	1.79	1.73
2	E	501	1AZ	C1-CL1	2.30	1.79	1.73
2	B	501	1AZ	C1-CL1	2.33	1.79	1.73
2	H	501	1AZ	C13-N4	2.34	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	1AZ	C1-CL1	2.42	1.79	1.73
2	C	501	1AZ	C1-CL1	2.46	1.79	1.73
2	D	501	1AZ	C18-CL2	2.50	1.79	1.73
2	G	501	1AZ	C1-CL1	2.57	1.79	1.73
2	K	501	1AZ	C1-CL1	2.63	1.79	1.73
2	J	501	1AZ	C1-CL1	2.65	1.80	1.73
2	I	501	1AZ	C18-CL2	2.75	1.80	1.73
2	D	501	1AZ	C1-CL1	2.83	1.80	1.73
2	H	501	1AZ	C18-CL2	2.83	1.80	1.73
2	A	501	1AZ	C1-CL1	2.97	1.80	1.73
2	L	501	1AZ	C18-CL2	3.03	1.80	1.73
2	J	501	1AZ	C18-CL2	3.56	1.82	1.73

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	1AZ	C12-N3-C8	-5.27	110.32	122.07
2	E	501	1AZ	C12-N3-C8	-5.12	110.67	122.07
2	L	501	1AZ	C12-N3-C8	-5.12	110.67	122.07
2	B	501	1AZ	C12-N3-C8	-5.08	110.76	122.07
2	D	501	1AZ	C12-N3-C8	-5.05	110.81	122.07
2	B	501	1AZ	C1-C2-C3	-4.99	117.15	120.46
2	K	501	1AZ	C12-N3-C8	-4.93	111.08	122.07
2	I	501	1AZ	C12-N3-C8	-4.90	111.16	122.07
2	F	501	1AZ	C12-N3-C8	-4.88	111.20	122.07
2	H	501	1AZ	C12-N3-C8	-4.80	111.37	122.07
2	A	501	1AZ	C12-N3-C8	-4.77	111.43	122.07
2	G	501	1AZ	C12-N3-C8	-4.63	111.76	122.07
2	C	501	1AZ	C12-N3-C8	-4.63	111.76	122.07
2	J	501	1AZ	C9-N3-C8	-4.53	111.99	122.07
2	L	501	1AZ	C1-C2-C3	-4.52	117.46	120.46
2	H	501	1AZ	C9-N3-C8	-4.46	112.12	122.07
2	B	501	1AZ	C9-N3-C8	-4.45	112.16	122.07
2	E	501	1AZ	C1-C2-C3	-4.44	117.51	120.46
2	F	501	1AZ	C9-N3-C8	-4.44	112.18	122.07
2	D	501	1AZ	C9-N3-C8	-4.43	112.19	122.07
2	E	501	1AZ	C9-N3-C8	-4.42	112.22	122.07
2	A	501	1AZ	C9-N3-C8	-4.39	112.29	122.07
2	I	501	1AZ	C9-N3-C8	-4.38	112.32	122.07
2	G	501	1AZ	C9-N3-C8	-4.37	112.34	122.07
2	J	501	1AZ	C10-C9-N3	-4.35	102.15	109.98
2	K	501	1AZ	C9-N3-C8	-4.32	112.44	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	501	1AZ	C9-N3-C8	-4.29	112.50	122.07
2	L	501	1AZ	C10-C9-N3	-4.24	102.34	109.98
2	C	501	1AZ	C9-N3-C8	-4.14	112.86	122.07
2	H	501	1AZ	C10-C9-N3	-4.09	102.61	109.98
2	C	501	1AZ	C10-C9-N3	-4.09	102.62	109.98
2	D	501	1AZ	C10-C9-N3	-4.08	102.63	109.98
2	A	501	1AZ	C10-C9-N3	-4.01	102.76	109.98
2	G	501	1AZ	C10-C9-N3	-3.85	103.05	109.98
2	K	501	1AZ	C1-C2-C3	-3.82	117.93	120.46
2	F	501	1AZ	C10-C9-N3	-3.81	103.12	109.98
2	B	501	1AZ	C10-C9-N3	-3.79	103.16	109.98
2	I	501	1AZ	C1-C2-C3	-3.69	118.01	120.46
2	I	501	1AZ	C10-C9-N3	-3.67	103.38	109.98
2	G	501	1AZ	C1-C2-C3	-3.61	118.06	120.46
2	C	501	1AZ	C1-C2-C3	-3.52	118.12	120.46
2	K	501	1AZ	C10-C9-N3	-3.51	103.66	109.98
2	F	501	1AZ	C1-C2-C3	-3.50	118.14	120.46
2	E	501	1AZ	C10-C9-N3	-3.40	103.86	109.98
2	J	501	1AZ	C1-C2-C3	-3.35	118.24	120.46
2	H	501	1AZ	C1-C2-C3	-3.29	118.28	120.46
2	D	501	1AZ	C1-C2-C3	-3.22	118.33	120.46
2	H	501	1AZ	C11-C12-N3	-3.13	104.35	109.98
2	L	501	1AZ	C6-C5-N1	-3.02	118.43	120.52
2	L	501	1AZ	C11-C12-N3	-2.86	104.84	109.98
2	A	501	1AZ	C1-C2-C3	-2.84	118.58	120.46
2	K	501	1AZ	C11-C12-N3	-2.83	104.89	109.98
2	J	501	1AZ	C11-C12-N3	-2.82	104.90	109.98
2	I	501	1AZ	C11-C12-N3	-2.78	104.97	109.98
2	F	501	1AZ	C11-C12-N3	-2.68	105.16	109.98
2	B	501	1AZ	C11-C12-N3	-2.50	105.48	109.98
2	J	501	1AZ	C6-C5-N1	-2.44	118.82	120.52
2	C	501	1AZ	C6-C5-N1	-2.40	118.85	120.52
2	D	501	1AZ	C6-C5-N1	-2.32	118.91	120.52
2	D	501	1AZ	C6-C13-N4	-2.32	106.11	110.68
2	A	501	1AZ	C6-C13-N4	-2.23	106.27	110.68
2	G	501	1AZ	C11-C12-N3	-2.23	105.97	109.98
2	E	501	1AZ	C6-C13-N4	-2.16	106.41	110.68
2	A	501	1AZ	C6-C5-N1	-2.12	119.05	120.52
2	C	501	1AZ	C11-C12-N3	-2.11	106.18	109.98
2	H	501	1AZ	C5-C6-C13	-2.10	118.48	119.92
2	D	501	1AZ	C11-C12-N3	-2.08	106.23	109.98
2	J	501	1AZ	C6-C13-N4	-2.08	106.58	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	1AZ	C6-C13-N4	-2.05	106.64	110.68
2	E	501	1AZ	C11-C12-N3	-2.04	106.30	109.98
2	B	501	1AZ	C6-C13-N4	-2.02	106.70	110.68
2	K	501	1AZ	C6-C13-N4	-2.02	106.70	110.68
2	C	501	1AZ	C6-C13-N4	-2.00	106.73	110.68
2	E	501	1AZ	C4-N1-C5	2.00	120.21	117.79
2	K	501	1AZ	C16-C3-C2	2.01	121.40	118.53
2	F	501	1AZ	C4-N1-C5	2.04	120.26	117.79
2	B	501	1AZ	C16-C3-C2	2.05	121.45	118.53
2	J	501	1AZ	C14-N5-C13	2.06	121.25	118.31
2	D	501	1AZ	C14-N5-C13	2.06	121.25	118.31
2	H	501	1AZ	C14-N5-C13	2.10	121.31	118.31
2	D	501	1AZ	C4-N1-C5	2.11	120.34	117.79
2	C	501	1AZ	C16-C3-C2	2.16	121.62	118.53
2	C	501	1AZ	C14-N5-C13	2.23	121.49	118.31
2	A	501	1AZ	C4-N1-C5	2.28	120.54	117.79
2	K	501	1AZ	C4-N1-C5	2.33	120.61	117.79
2	A	501	1AZ	C14-N5-C13	2.36	121.67	118.31
2	H	501	1AZ	C4-N1-C5	3.06	121.48	117.79

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	463/486 (95%)	0.60	46 (9%) 8 8	22, 38, 70, 99	0
1	B	463/486 (95%)	0.59	50 (10%) 6 6	22, 39, 70, 99	0
1	C	463/486 (95%)	0.69	66 (14%) 3 3	22, 39, 70, 99	0
1	D	463/486 (95%)	0.61	44 (9%) 9 9	22, 39, 70, 99	0
1	E	463/486 (95%)	0.63	41 (8%) 10 11	22, 38, 70, 99	0
1	F	463/486 (95%)	0.73	44 (9%) 9 9	22, 38, 70, 99	0
1	G	463/486 (95%)	0.62	49 (10%) 7 7	22, 38, 70, 99	0
1	H	463/486 (95%)	0.69	48 (10%) 7 7	22, 38, 70, 99	0
1	I	463/486 (95%)	0.65	57 (12%) 5 4	22, 39, 70, 99	0
1	J	463/486 (95%)	1.05	82 (17%) 2 1	22, 39, 70, 99	0
1	K	463/486 (95%)	0.64	53 (11%) 6 5	22, 39, 70, 99	0
1	L	463/486 (95%)	0.71	49 (10%) 7 7	22, 38, 70, 99	0
All	All	5556/5832 (95%)	0.68	629 (11%) 6 5	22, 39, 71, 99	0

All (629) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	333	GLY	12.7
1	I	334	TYR	11.1
1	L	61	PHE	9.7
1	J	296	ALA	9.5
1	C	414	ALA	9.2
1	I	61	PHE	9.1
1	J	347	ARG	9.1
1	J	334	TYR	9.0
1	L	413	ALA	8.9
1	H	58	ILE	8.8
1	G	414	ALA	8.7

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Mol	Chain	Res	Type	RSRZ
1	J	414	ALA	8.6
1	H	59	ARG	8.6
1	H	413	ALA	8.4
1	I	333	GLY	8.4
1	L	99	PHE	8.4
1	A	58	ILE	8.3
1	J	403	LYS	8.2
1	J	60	GLY	8.0
1	J	59	ARG	8.0
1	A	413	ALA	8.0
1	J	413	ALA	8.0
1	I	414	ALA	7.8
1	L	334	TYR	7.7
1	L	60	GLY	7.7
1	H	56	SER	7.7
1	F	99	PHE	7.7
1	E	414	ALA	7.6
1	A	414	ALA	7.6
1	H	57	SER	7.4
1	K	414	ALA	7.4
1	J	57	SER	7.4
1	C	99	PHE	7.3
1	H	61	PHE	7.3
1	K	332	PRO	7.3
1	A	404	ASP	7.2
1	J	401	VAL	7.1
1	F	404	ASP	7.1
1	J	61	PHE	7.1
1	K	333	GLY	7.1
1	B	58	ILE	7.1
1	G	99	PHE	7.0
1	B	413	ALA	6.9
1	E	415	SER	6.8
1	D	334	TYR	6.8
1	G	67	SER	6.8
1	A	403	LYS	6.8
1	A	334	TYR	6.7
1	E	334	TYR	6.7
1	F	413	ALA	6.6
1	J	58	ILE	6.6
1	F	61	PHE	6.6
1	L	58	ILE	6.6

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Mol	Chain	Res	Type	RSRZ
1	D	413	ALA	6.6
1	B	56	SER	6.5
1	L	403	LYS	6.5
1	D	333	GLY	6.5
1	C	347	ARG	6.4
1	D	99	PHE	6.4
1	J	402	ASP	6.3
1	C	332	PRO	6.3
1	H	347	ARG	6.3
1	B	414	ALA	6.2
1	B	61	PHE	6.2
1	H	67	SER	6.2
1	D	403	LYS	6.2
1	J	404	ASP	6.1
1	A	61	PHE	6.1
1	C	355	ILE	6.1
1	A	347	ARG	6.0
1	F	56	SER	6.0
1	G	61	PHE	5.9
1	C	403	LYS	5.9
1	H	404	ASP	5.9
1	F	334	TYR	5.9
1	F	335	GLU	5.8
1	F	58	ILE	5.8
1	F	403	LYS	5.8
1	J	415	SER	5.8
1	E	67	SER	5.8
1	C	357	GLY	5.7
1	B	404	ASP	5.7
1	C	334	TYR	5.7
1	F	414	ALA	5.7
1	I	413	ALA	5.7
1	J	56	SER	5.7
1	H	332	PRO	5.7
1	G	413	ALA	5.6
1	B	59	ARG	5.6
1	I	67	SER	5.6
1	H	55	GLY	5.6
1	B	347	ARG	5.5
1	H	333	GLY	5.5
1	H	334	TYR	5.5
1	A	99	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	L	56	SER	5.5
1	D	347	ARG	5.5
1	I	355	ILE	5.5
1	J	292	GLU	5.4
1	K	62	GLN	5.4
1	F	62	GLN	5.4
1	H	403	LYS	5.4
1	J	184	GLY	5.4
1	E	333	GLY	5.4
1	C	413	ALA	5.4
1	H	414	ALA	5.4
1	D	58	ILE	5.4
1	J	293	THR	5.4
1	I	56	SER	5.3
1	H	335	GLU	5.3
1	F	401	VAL	5.3
1	D	404	ASP	5.3
1	B	99	PHE	5.3
1	J	416	ILE	5.3
1	J	356	THR	5.3
1	E	403	LYS	5.3
1	C	404	ASP	5.3
1	C	358	SER	5.3
1	D	60	GLY	5.2
1	D	415	SER	5.2
1	B	62	GLN	5.2
1	F	333	GLY	5.2
1	J	358	SER	5.2
1	D	61	PHE	5.2
1	L	404	ASP	5.2
1	L	57	SER	5.2
1	H	184	GLY	5.2
1	D	332	PRO	5.2
1	J	346	ASN	5.2
1	L	45	SER	5.1
1	L	59	ARG	5.1
1	B	336	ALA	5.1
1	C	335	GLU	5.1
1	J	295	TYR	5.1
1	B	335	GLU	5.1
1	G	347	ARG	5.1
1	J	355	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	403	LYS	5.0
1	K	334	TYR	5.0
1	F	68	ASP	5.0
1	L	335	GLU	5.0
1	J	332	PRO	4.9
1	G	334	TYR	4.9
1	C	333	GLY	4.9
1	J	357	GLY	4.9
1	D	335	GLU	4.9
1	K	58	ILE	4.9
1	K	293	THR	4.9
1	D	414	ALA	4.9
1	A	335	GLU	4.9
1	L	414	ALA	4.9
1	I	403	LYS	4.8
1	K	345	ARG	4.8
1	B	334	TYR	4.8
1	L	68	ASP	4.8
1	H	62	GLN	4.8
1	J	122	THR	4.8
1	J	345	ARG	4.7
1	A	333	GLY	4.7
1	I	99	PHE	4.7
1	G	335	GLU	4.6
1	B	332	PRO	4.6
1	G	403	LYS	4.6
1	D	345	ARG	4.6
1	A	67	SER	4.6
1	D	55	GLY	4.6
1	I	332	PRO	4.6
1	H	99	PHE	4.6
1	G	293	THR	4.5
1	I	402	ASP	4.5
1	G	404	ASP	4.5
1	C	331	VAL	4.5
1	J	398	GLN	4.5
1	F	57	SER	4.5
1	G	415	SER	4.5
1	H	415	SER	4.5
1	I	358	SER	4.5
1	B	333	GLY	4.5
1	D	416	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	67	SER	4.4
1	C	401	VAL	4.4
1	C	61	PHE	4.4
1	K	347	ARG	4.4
1	K	358	SER	4.4
1	E	58	ILE	4.4
1	E	332	PRO	4.4
1	J	341	VAL	4.4
1	B	57	SER	4.4
1	F	415	SER	4.4
1	H	60	GLY	4.3
1	L	358	SER	4.3
1	E	5	THR	4.3
1	K	335	GLU	4.3
1	D	59	ARG	4.3
1	J	399	ALA	4.3
1	K	415	SER	4.3
1	A	345	ARG	4.3
1	A	57	SER	4.2
1	C	62	GLN	4.2
1	A	401	VAL	4.2
1	C	415	SER	4.2
1	D	170	ALA	4.2
1	A	62	GLN	4.2
1	C	45	SER	4.2
1	J	335	GLU	4.2
1	L	62	GLN	4.1
1	D	62	GLN	4.1
1	I	62	GLN	4.1
1	E	345	ARG	4.1
1	J	99	PHE	4.1
1	H	401	VAL	4.1
1	J	362	ALA	4.1
1	I	335	GLU	4.1
1	H	345	ARG	4.1
1	I	184	GLY	4.1
1	E	335	GLU	4.1
1	B	5	THR	4.1
1	E	336	ALA	4.0
1	J	45	SER	4.0
1	J	120	ILE	4.0
1	D	57	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	62	GLN	4.0
1	C	67	SER	3.9
1	B	101	LEU	3.9
1	E	309	LEU	3.9
1	J	62	GLN	3.9
1	A	336	ALA	3.9
1	I	69	MET	3.9
1	B	55	GLY	3.9
1	B	415	SER	3.9
1	G	56	SER	3.9
1	J	449	GLU	3.9
1	E	404	ASP	3.8
1	B	293	THR	3.8
1	K	57	SER	3.8
1	I	404	ASP	3.8
1	B	68	ASP	3.8
1	A	358	SER	3.8
1	F	59	ARG	3.8
1	J	342	TYR	3.8
1	C	346	ASN	3.8
1	C	56	SER	3.8
1	K	300	ASP	3.7
1	K	362	ALA	3.7
1	E	61	PHE	3.7
1	I	59	ARG	3.7
1	I	170	ALA	3.7
1	A	402	ASP	3.7
1	J	55	GLY	3.7
1	K	67	SER	3.6
1	C	183	LYS	3.6
1	G	449	GLU	3.6
1	C	360	PRO	3.6
1	E	413	ALA	3.6
1	J	284	ASP	3.6
1	D	56	SER	3.5
1	J	291	ASP	3.5
1	K	403	LYS	3.5
1	K	404	ASP	3.5
1	C	293	THR	3.5
1	C	336	ALA	3.5
1	J	348	SER	3.5
1	J	344	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	293	THR	3.5
1	A	415	SER	3.5
1	D	100	THR	3.5
1	G	100	THR	3.5
1	I	415	SER	3.5
1	E	347	ARG	3.5
1	C	416	ILE	3.5
1	C	59	ARG	3.5
1	E	45	SER	3.4
1	L	415	SER	3.4
1	B	346	ASN	3.4
1	F	347	ARG	3.4
1	C	402	ASP	3.4
1	F	60	GLY	3.4
1	B	345	ARG	3.4
1	K	367	PHE	3.4
1	I	293	THR	3.4
1	I	347	ARG	3.4
1	D	402	ASP	3.4
1	H	358	SER	3.4
1	F	332	PRO	3.4
1	C	285	GLY	3.4
1	K	59	ARG	3.4
1	K	336	ALA	3.4
1	A	101	LEU	3.3
1	L	100	THR	3.3
1	L	55	GLY	3.3
1	G	355	ILE	3.3
1	F	346	ASN	3.3
1	K	184	GLY	3.3
1	E	351	VAL	3.3
1	J	67	SER	3.3
1	H	100	THR	3.3
1	L	54	ASP	3.3
1	I	5	THR	3.3
1	F	277	CYS	3.3
1	G	285	GLY	3.2
1	I	58	ILE	3.2
1	A	56	SER	3.2
1	F	101	LEU	3.2
1	G	333	GLY	3.2
1	J	418	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	360	PRO	3.2
1	C	48	ASP	3.2
1	J	118	TYR	3.2
1	A	416	ILE	3.2
1	L	332	PRO	3.2
1	I	292	GLU	3.2
1	D	401	VAL	3.2
1	G	416	ILE	3.1
1	J	400	PRO	3.1
1	G	59	ARG	3.1
1	H	416	ILE	3.1
1	F	402	ASP	3.1
1	H	5	THR	3.1
1	K	61	PHE	3.1
1	I	55	GLY	3.1
1	I	435	GLU	3.1
1	C	345	ARG	3.1
1	A	170	ALA	3.1
1	J	450	THR	3.1
1	J	417	PRO	3.0
1	L	454	PHE	3.0
1	D	186	TYR	3.0
1	B	183	LYS	3.0
1	E	383	MET	3.0
1	A	295	TYR	3.0
1	C	286	ALA	3.0
1	F	45	SER	3.0
1	B	54	ASP	3.0
1	C	291	ASP	3.0
1	K	99	PHE	3.0
1	H	170	ALA	3.0
1	L	101	LEU	3.0
1	A	59	ARG	3.0
1	H	101	LEU	3.0
1	E	99	PHE	3.0
1	L	416	ILE	3.0
1	C	290	TYR	3.0
1	D	45	SER	3.0
1	B	67	SER	3.0
1	C	6	PRO	3.0
1	I	97	ASP	2.9
1	J	283	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	449	GLU	2.9
1	C	7	ASP	2.9
1	B	17	LYS	2.9
1	G	101	LEU	2.9
1	J	102	GLU	2.9
1	E	449	GLU	2.9
1	I	284	ASP	2.9
1	K	445	ASN	2.9
1	J	44	LYS	2.9
1	F	454	PHE	2.9
1	L	347	ARG	2.9
1	B	450	THR	2.9
1	C	5	THR	2.9
1	B	60	GLY	2.8
1	C	338	ILE	2.8
1	K	416	ILE	2.8
1	F	67	SER	2.8
1	J	290	TYR	2.8
1	F	358	SER	2.8
1	H	69	MET	2.8
1	K	444	THR	2.8
1	K	291	ASP	2.8
1	J	304	HIS	2.8
1	K	304	HIS	2.8
1	J	42	PHE	2.8
1	G	300	ASP	2.8
1	B	357	GLY	2.8
1	L	333	GLY	2.8
1	K	350	CYS	2.8
1	F	54	ASP	2.8
1	K	5	THR	2.8
1	L	67	SER	2.8
1	J	183	LYS	2.8
1	B	100	THR	2.8
1	C	170	ALA	2.8
1	I	100	THR	2.8
1	I	101	LEU	2.8
1	E	352	ARG	2.8
1	A	332	PRO	2.8
1	C	98	PRO	2.8
1	J	11	LYS	2.7
1	G	358	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	30	GLY	2.7
1	A	293	THR	2.7
1	K	101	LEU	2.7
1	L	365	LEU	2.7
1	H	48	ASP	2.7
1	B	98	PRO	2.7
1	E	7	ASP	2.7
1	J	300	ASP	2.7
1	G	332	PRO	2.7
1	L	170	ALA	2.7
1	B	338	ILE	2.7
1	B	290	TYR	2.7
1	I	44	LYS	2.7
1	A	186	TYR	2.7
1	A	285	GLY	2.7
1	C	294	GLY	2.7
1	B	291	ASP	2.7
1	L	351	VAL	2.7
1	E	358	SER	2.7
1	F	351	VAL	2.6
1	C	356	THR	2.6
1	C	450	THR	2.6
1	G	170	ALA	2.6
1	J	121	SER	2.6
1	G	55	GLY	2.6
1	J	297	GLY	2.6
1	C	49	ASP	2.6
1	G	345	ARG	2.6
1	J	351	VAL	2.6
1	F	100	THR	2.6
1	L	346	ASN	2.6
1	G	58	ILE	2.6
1	H	68	ASP	2.6
1	A	450	THR	2.6
1	D	336	ALA	2.6
1	G	184	GLY	2.6
1	J	441	GLY	2.6
1	C	97	ASP	2.6
1	I	8	ASP	2.6
1	L	277	CYS	2.6
1	K	413	ALA	2.6
1	G	284	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	15	ASP	2.6
1	C	392	LYS	2.6
1	G	5	THR	2.6
1	H	351	VAL	2.6
1	H	8	ASP	2.6
1	F	336	ALA	2.6
1	A	98	PRO	2.6
1	D	309	LEU	2.6
1	E	380	PHE	2.6
1	L	285	GLY	2.6
1	C	435	GLU	2.6
1	J	435	GLU	2.6
1	F	367	PHE	2.5
1	C	184	GLY	2.5
1	K	126	ASP	2.5
1	I	416	ILE	2.5
1	A	360	PRO	2.5
1	C	300	ASP	2.5
1	G	183	LYS	2.5
1	L	350	CYS	2.5
1	L	345	ARG	2.5
1	C	126	ASP	2.5
1	C	282	TRP	2.5
1	G	402	ASP	2.5
1	K	100	THR	2.5
1	J	46	VAL	2.5
1	J	294	GLY	2.5
1	C	292	GLU	2.5
1	I	173	SER	2.5
1	F	399	ALA	2.5
1	G	286	ALA	2.5
1	J	285	GLY	2.5
1	E	62	GLN	2.5
1	A	355	ILE	2.5
1	C	58	ILE	2.5
1	A	100	THR	2.5
1	F	55	GLY	2.5
1	B	126	ASP	2.4
1	G	97	ASP	2.4
1	D	360	PRO	2.4
1	J	445	ASN	2.4
1	K	357	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	4	LYS	2.4
1	I	309	LEU	2.4
1	B	184	GLY	2.4
1	D	346	ASN	2.4
1	F	376	PRO	2.4
1	H	183	LYS	2.4
1	K	6	PRO	2.4
1	C	101	LEU	2.4
1	A	40	SER	2.4
1	B	102	GLU	2.4
1	D	284	ASP	2.4
1	H	367	PHE	2.4
1	C	295	TYR	2.4
1	H	449	GLU	2.4
1	I	432	ALA	2.4
1	B	4	LYS	2.4
1	J	298	LEU	2.4
1	I	345	ARG	2.4
1	A	284	ASP	2.4
1	H	292	GLU	2.4
1	I	16	GLU	2.4
1	H	11	LYS	2.4
1	K	402	ASP	2.4
1	F	170	ALA	2.4
1	C	57	SER	2.4
1	F	309	LEU	2.4
1	I	294	GLY	2.3
1	I	360	PRO	2.3
1	J	303	ARG	2.3
1	K	69	MET	2.3
1	K	295	TYR	2.3
1	A	453	SER	2.3
1	J	361	LYS	2.3
1	D	49	ASP	2.3
1	J	54	ASP	2.3
1	J	126	ASP	2.3
1	I	57	SER	2.3
1	K	45	SER	2.3
1	H	54	ASP	2.3
1	B	360	PRO	2.3
1	L	376	PRO	2.3
1	A	132	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	170	ALA	2.3
1	E	379	ALA	2.3
1	I	357	GLY	2.3
1	G	282	TRP	2.3
1	J	69	MET	2.3
1	F	26	CYS	2.3
1	A	55	GLY	2.3
1	D	17	LYS	2.3
1	G	398	GLN	2.3
1	E	376	PRO	2.3
1	A	338	ILE	2.3
1	G	294	GLY	2.3
1	H	402	ASP	2.3
1	K	122	THR	2.3
1	E	417	PRO	2.3
1	F	24	ARG	2.3
1	D	31	ILE	2.3
1	E	284	ASP	2.3
1	E	367	PHE	2.3
1	G	7	ASP	2.3
1	I	49	ASP	2.3
1	D	331	VAL	2.2
1	H	7	ASP	2.2
1	E	170	ALA	2.2
1	J	338	ILE	2.2
1	K	292	GLU	2.2
1	E	360	PRO	2.2
1	D	398	GLN	2.2
1	J	390	GLY	2.2
1	G	351	VAL	2.2
1	I	7	ASP	2.2
1	A	449	GLU	2.2
1	C	215	LYS	2.2
1	I	286	ALA	2.2
1	I	356	THR	2.2
1	G	71	LEU	2.2
1	H	186	TYR	2.2
1	C	171	ASP	2.2
1	I	449	GLU	2.2
1	C	100	THR	2.2
1	K	282	TRP	2.2
1	K	346	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	44	LYS	2.2
1	G	372	SER	2.2
1	J	453	SER	2.2
1	B	7	ASP	2.2
1	K	186	TYR	2.2
1	K	290	TYR	2.2
1	K	348	SER	2.2
1	C	351	VAL	2.2
1	G	275	MET	2.2
1	L	8	ASP	2.2
1	L	25	PHE	2.2
1	L	183	LYS	2.2
1	G	277	CYS	2.2
1	G	360	PRO	2.2
1	L	309	LEU	2.2
1	F	242	MET	2.2
1	A	4	LYS	2.2
1	H	286	ALA	2.2
1	K	284	ASP	2.2
1	C	400	PRO	2.2
1	E	59	ARG	2.2
1	H	350	CYS	2.2
1	B	358	SER	2.2
1	B	453	SER	2.2
1	K	56	SER	2.2
1	G	186	TYR	2.1
1	B	294	GLY	2.1
1	F	374	GLY	2.1
1	F	416	ILE	2.1
1	L	184	GLY	2.1
1	B	53	PHE	2.1
1	I	367	PHE	2.1
1	D	340	LEU	2.1
1	C	284	ASP	2.1
1	I	54	ASP	2.1
1	J	359	ASN	2.1
1	E	184	GLY	2.1
1	A	376	PRO	2.1
1	K	215	LYS	2.1
1	D	358	SER	2.1
1	D	351	VAL	2.1
1	I	401	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	287	PRO	2.1
1	L	49	ASP	2.1
1	L	51	LEU	2.1
1	C	432	ALA	2.1
1	D	399	ALA	2.1
1	C	376	PRO	2.1
1	A	97	ASP	2.1
1	B	11	LYS	2.1
1	E	416	ILE	2.1
1	L	71	LEU	2.1
1	G	435	GLU	2.1
1	L	69	MET	2.1
1	E	306	ILE	2.1
1	I	285	GLY	2.1
1	E	331	VAL	2.0
1	K	320	THR	2.0
1	B	45	SER	2.0
1	I	446	ASP	2.0
1	G	461	GLU	2.0
1	I	186	TYR	2.0
1	L	370	PRO	2.0
1	I	11	LYS	2.0
1	L	336	ALA	2.0
1	H	46	VAL	2.0
1	I	123	GLY	2.0
1	F	353	ILE	2.0
1	A	290	TYR	2.0
1	E	443	PHE	2.0
1	C	431	GLU	2.0
1	E	8	ASP	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	1AZ	C	501	28/28	0.88	0.25	1.96	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	-0.08	46,47,48,50	0
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 [i](#)

There are no such residues in this entry.