



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 AM GMT

PDB ID : 2NWC
Title : A 3.02 angstrom crystal structure of wild-type apo GroEL in a monoclinic space group
Authors : Kiser, P.D.; Lodowski, D.T.; Palczewski, K.
Deposited on : 2006-11-14
Resolution : 3.02 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

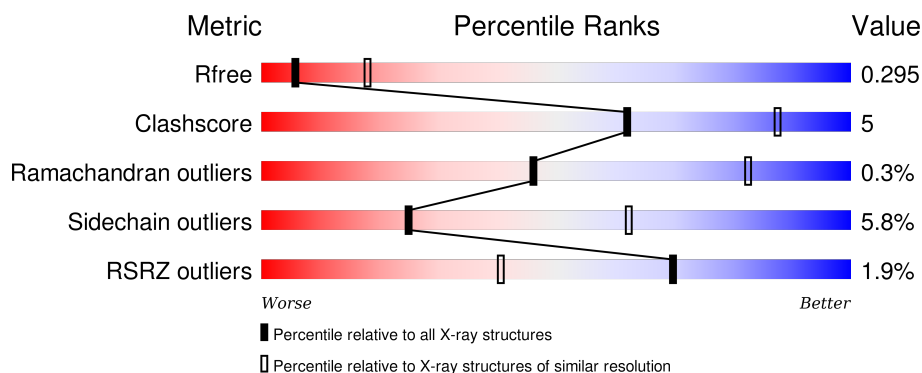
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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.



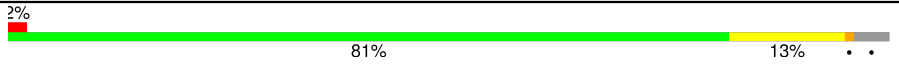

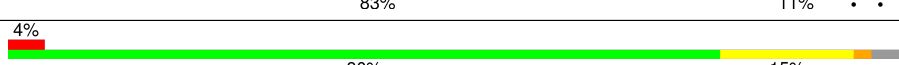


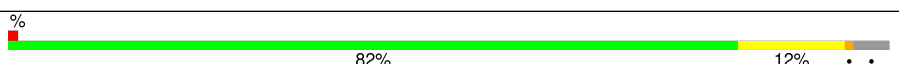



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	547	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 15% ... </div> </div>
1	B	547	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 2% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 82% 13% ... </div> </div>
1	C	547	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 14% ... </div> </div>
1	D	547	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 79% 14% ... </div> </div>
1	E	547	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> 3% </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 14% ... </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53970 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.

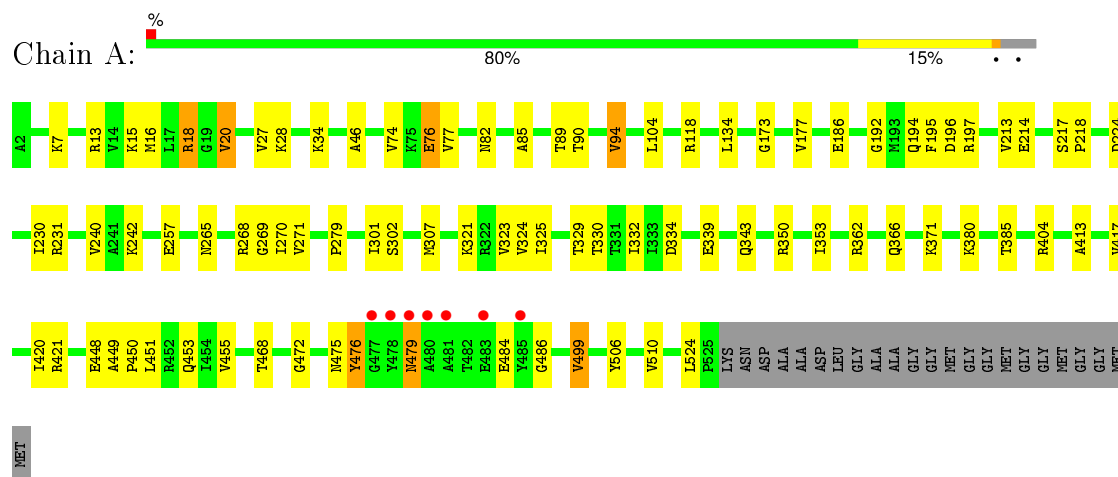
- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

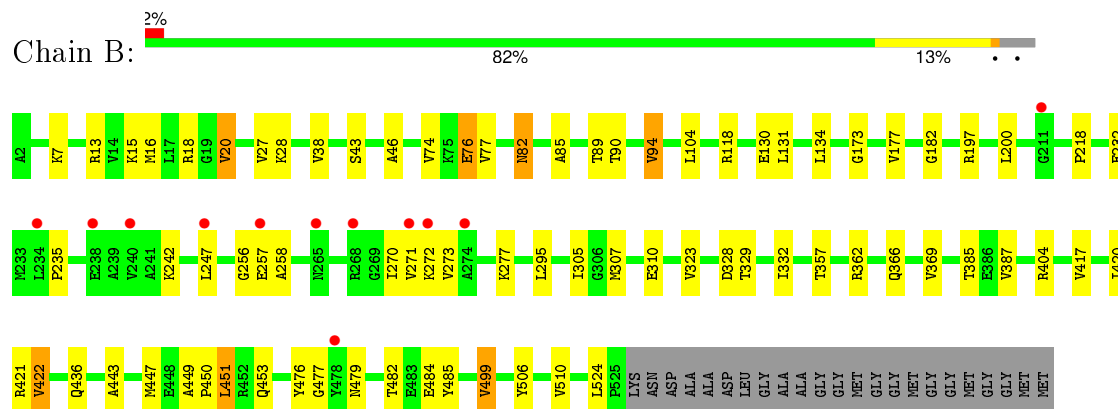
3 Residue-property plots

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

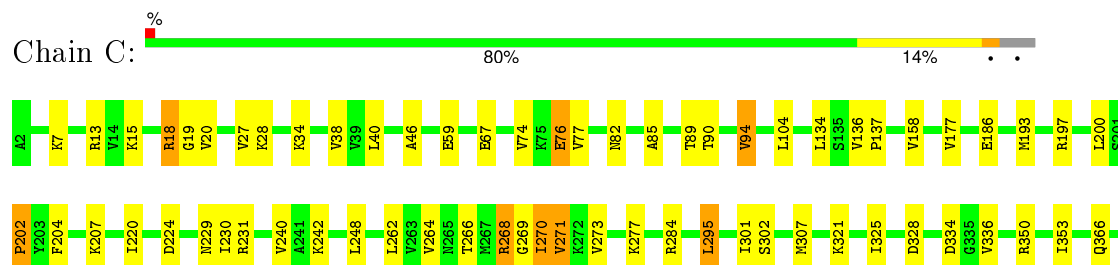
- Molecule 1: 60 kDa chaperonin

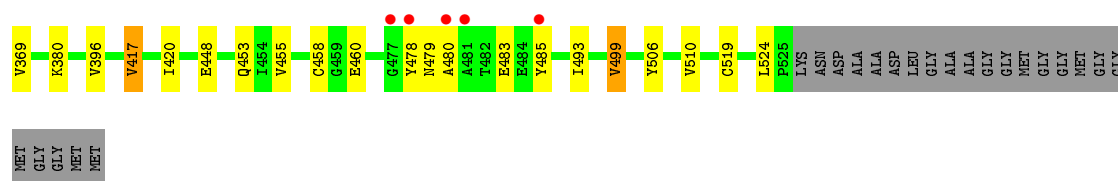


- Molecule 1: 60 kDa chaperonin



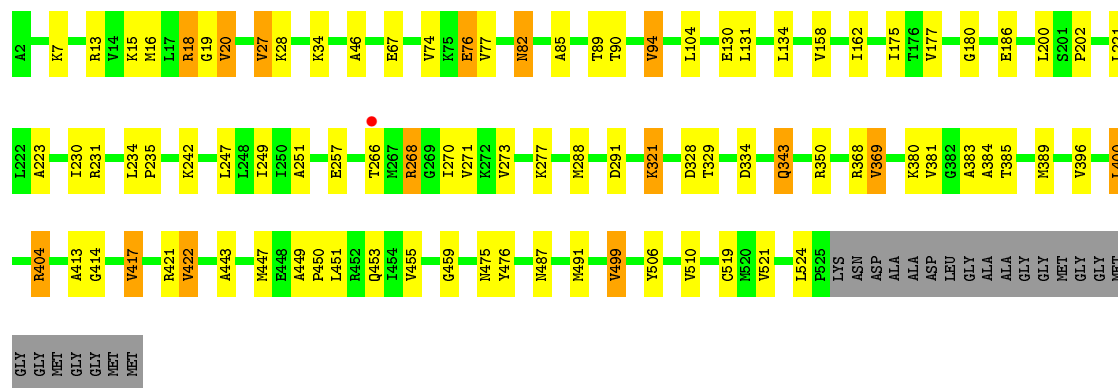
- Molecule 1: 60 kDa chaperonin





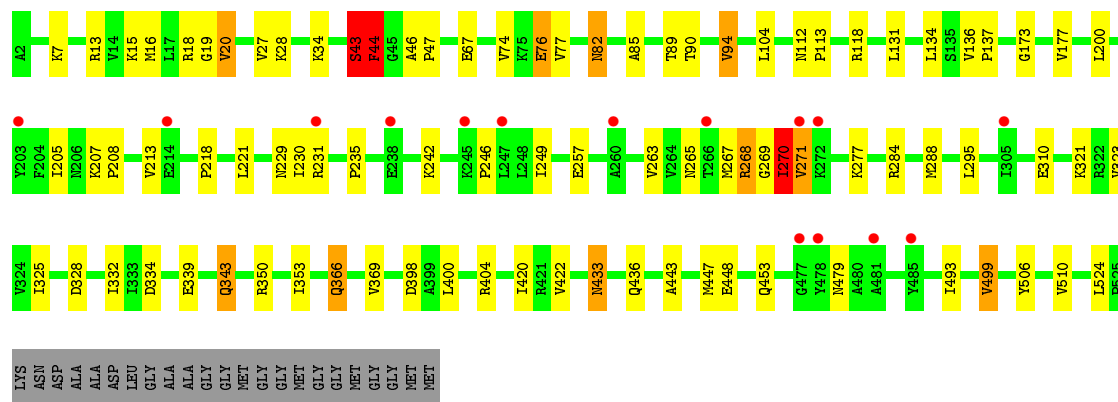
• Molecule 1: 60 kDa chaperonin

Chain D: 79% 14%



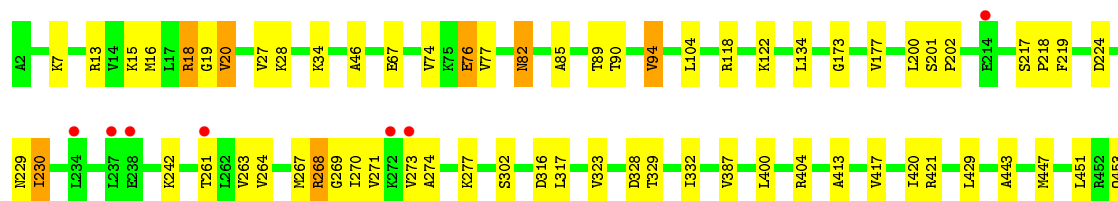
• Molecule 1: 60 kDa chaperonin

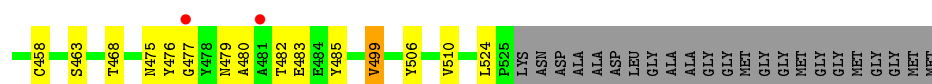
Chain E: 3% 80% 14%



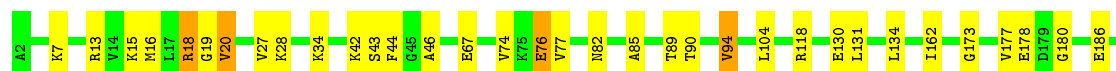
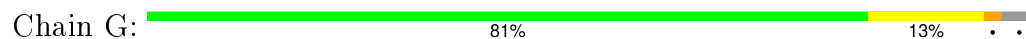
• Molecule 1: 60 kDa chaperonin

Chain F: 2% 81% 13%

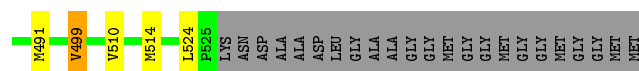
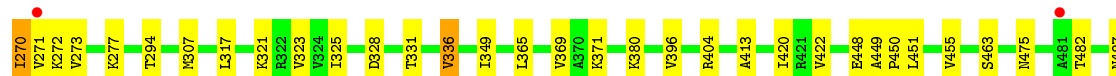
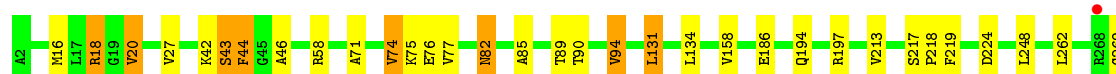
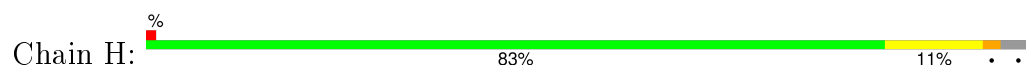




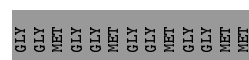
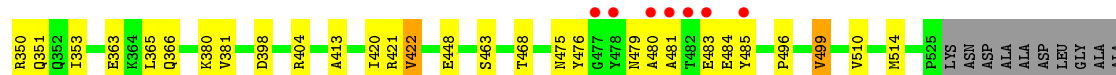
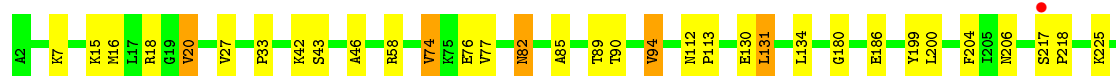
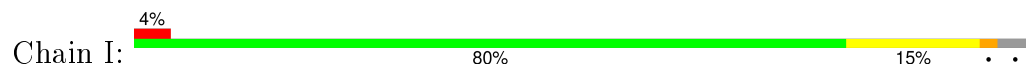
- Molecule 1: 60 kDa chaperonin



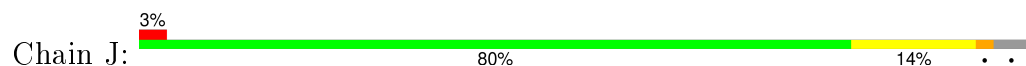
- Molecule 1: 60 kDa chaperonin

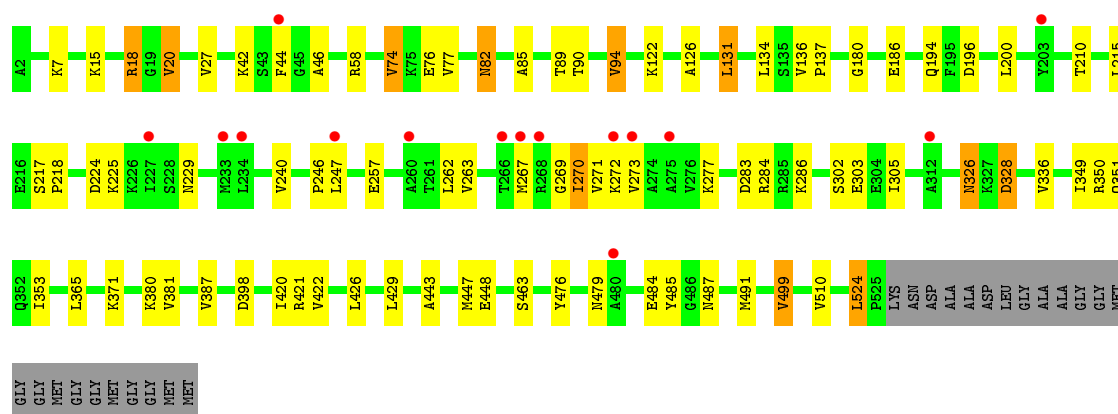


- Molecule 1: 60 kDa chaperonin

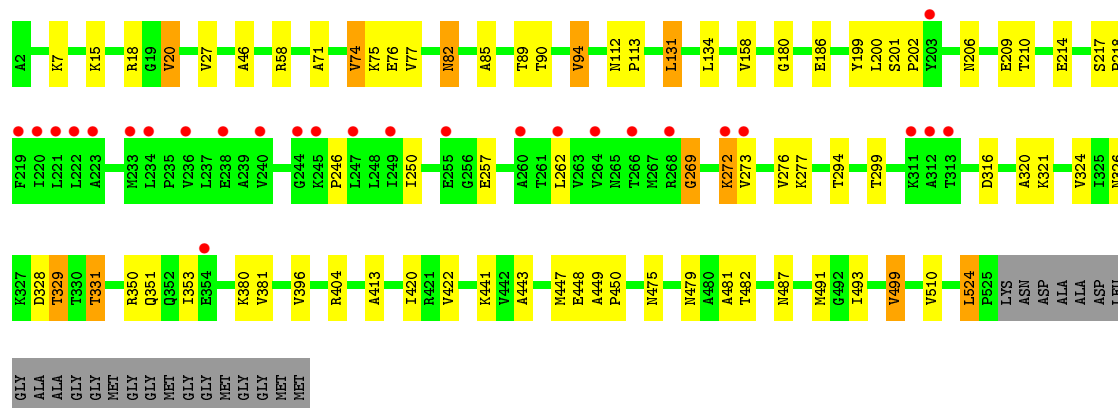
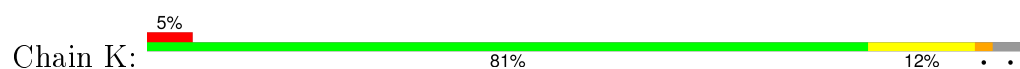


- Molecule 1: 60 kDa chaperonin

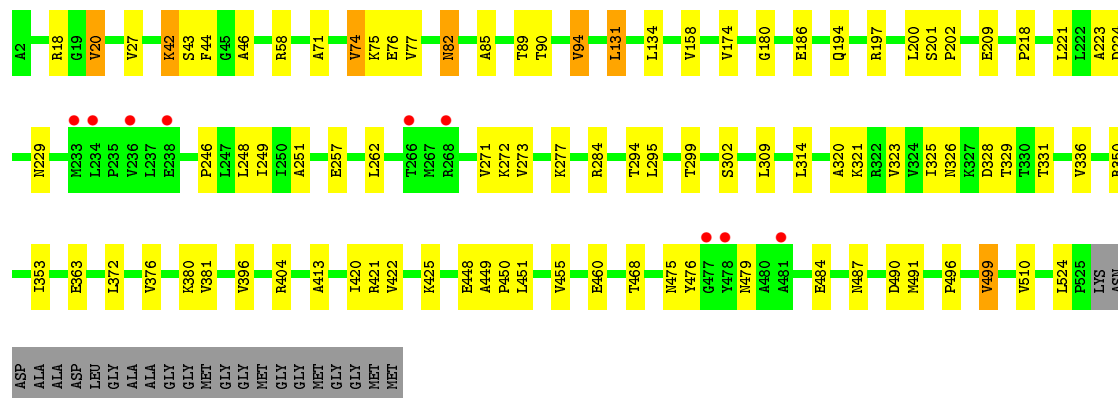
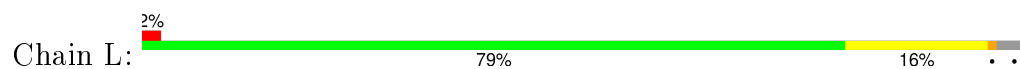




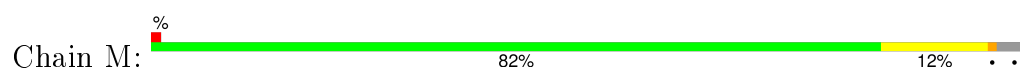
- Molecule 1: 60 kDa chaperonin

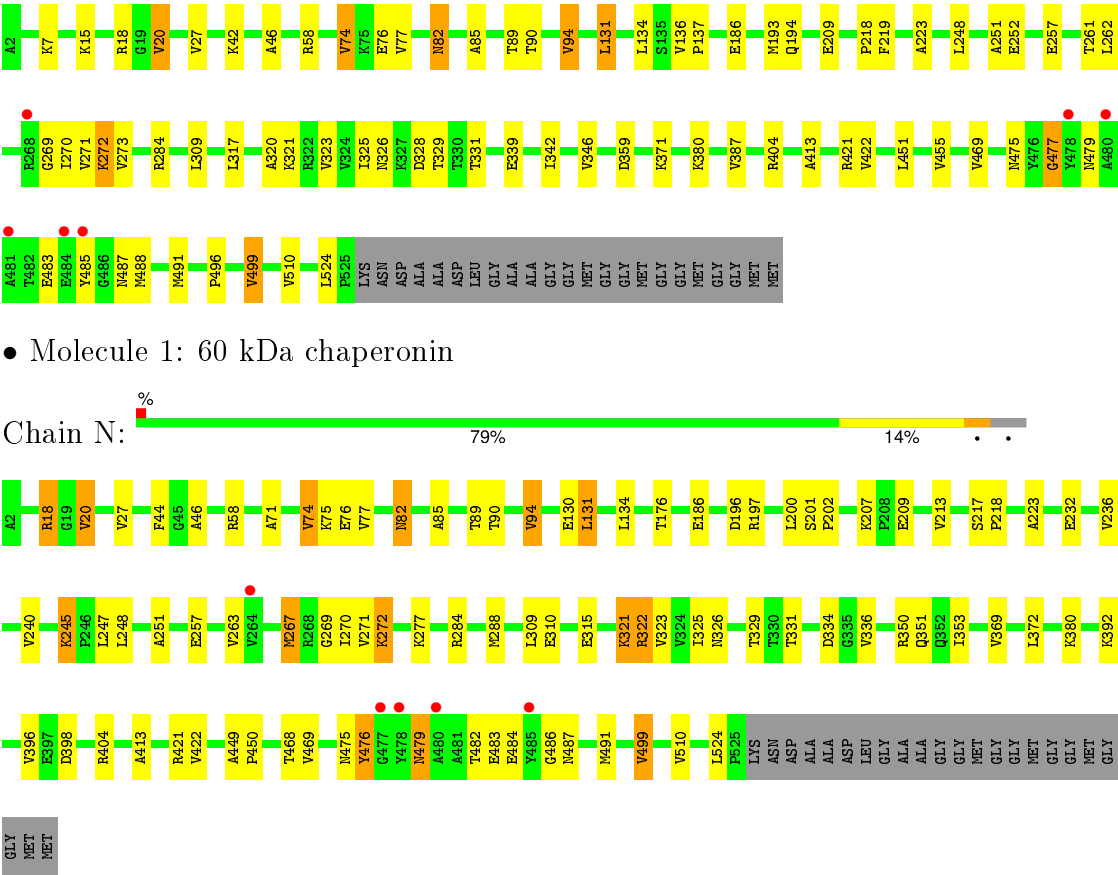


- Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin





• Molecule 1: 60 kDa chaperonin

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.42Å 262.25Å 147.07Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	30.00 – 3.02 49.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.02) 99.0 (49.32-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.227 , 0.263 0.268 , 0.295	Depositor DCC
R_{free} test set	10045 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 12.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 201615 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	53970	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.32	0/3883	0.50	0/5243
1	B	0.45	2/3883 (0.1%)	0.49	1/5243 (0.0%)
1	C	0.33	0/3883	0.49	0/5243
1	D	0.34	0/3883	0.50	0/5243
1	E	0.34	0/3883	0.55	2/5243 (0.0%)
1	F	0.32	0/3883	0.50	0/5243
1	G	0.33	0/3883	0.62	3/5243 (0.1%)
1	H	0.32	0/3883	0.49	0/5243
1	I	0.36	1/3883 (0.0%)	0.50	0/5243
1	J	0.32	0/3883	0.49	0/5243
1	K	0.32	0/3883	0.48	0/5243
1	L	0.33	0/3883	0.50	0/5243
1	M	0.33	0/3883	0.49	0/5243
1	N	0.34	0/3883	0.49	0/5243
All	All	0.34	3/54362 (0.0%)	0.51	6/73402 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	I	0	1
1	K	0	1
1	M	0	2
1	N	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	GLU	CD-OE2	16.33	1.43	1.25
1	B	232	GLU	CD-OE1	9.88	1.36	1.25
1	I	327	LYS	CE-NZ	8.56	1.70	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	18	ARG	NE-CZ-NH1	-18.59	111.01	120.30
1	G	18	ARG	NE-CZ-NH2	17.59	129.09	120.30
1	E	43	SER	N-CA-CB	-13.09	90.87	110.50
1	E	43	SER	N-CA-C	8.90	135.04	111.00
1	G	18	ARG	CD-NE-CZ	7.90	134.66	123.60
1	B	232	GLU	OE1-CD-OE2	5.51	129.91	123.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLY	Peptide
1	C	269	GLY	Peptide
1	D	268	ARG	Peptide
1	E	43	SER	Peptide
1	F	269	GLY	Peptide
1	I	269	GLY	Peptide
1	K	269	GLY	Peptide
1	M	269	GLY	Peptide
1	M	270	ILE	Peptide
1	N	269	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3976	48	0
1	B	3855	0	3976	43	0
1	C	3855	0	3976	52	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3855	0	3976	58	0
1	E	3855	0	3976	56	0
1	F	3855	0	3976	42	0
1	G	3855	0	3976	40	0
1	H	3855	0	3976	34	0
1	I	3855	0	3976	44	0
1	J	3855	0	3976	43	0
1	K	3855	0	3976	43	0
1	L	3855	0	3976	47	0
1	M	3855	0	3976	35	0
1	N	3855	0	3976	46	0
All	All	53970	0	55664	587	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 5.

All (587) 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:I:327:LYS:CE	1:I:327:LYS:NZ	1.70	1.49
1:E:46:ALA:HB2	1:F:76:GLU:HG3	1.24	1.09
1:A:46:ALA:HB2	1:B:76:GLU:HG3	1.35	1.07
1:F:46:ALA:HB2	1:G:76:GLU:HG3	1.41	0.99
1:A:76:GLU:HG3	1:G:46:ALA:HB2	1.50	0.93
1:D:46:ALA:HB2	1:E:76:GLU:HG3	1.53	0.89
1:D:46:ALA:CB	1:E:76:GLU:HG3	2.01	0.89
1:I:479:ASN:HB3	1:I:484:GLU:H	1.35	0.89
1:D:384:ALA:C	1:D:385:THR:CG2	2.41	0.88
1:M:477:GLY:O	1:M:485:TYR:HA	1.73	0.88
1:H:76:GLU:HG3	1:N:46:ALA:HB2	1.56	0.87
1:K:326:ASN:HB2	1:K:329:THR:HG22	1.55	0.86
1:L:46:ALA:HB2	1:M:76:GLU:HG3	1.58	0.86
1:E:44:PHE:O	1:E:44:PHE:CD1	2.30	0.84
1:K:46:ALA:HB2	1:L:76:GLU:HG3	1.58	0.83
1:E:44:PHE:O	1:E:44:PHE:CG	2.33	0.82
1:E:46:ALA:CB	1:F:76:GLU:HG3	2.10	0.81
1:I:46:ALA:HB2	1:J:76:GLU:HG3	1.63	0.81
1:F:46:ALA:CB	1:G:76:GLU:HG3	2.11	0.80
1:J:46:ALA:HB2	1:K:76:GLU:HG3	1.61	0.80
1:A:76:GLU:HG3	1:G:46:ALA:CB	2.13	0.78
1:M:413:ALA:HB1	1:M:488:MET:HG2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ALA:C	1:D:385:THR:HG23	2.06	0.76
1:D:384:ALA:O	1:D:385:THR:HG22	1.86	0.75
1:H:46:ALA:HB2	1:I:76:GLU:HG3	1.67	0.75
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.69	0.74
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.70	0.74
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.70	0.73
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.70	0.73
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.70	0.73
1:C:270:ILE:HG22	1:C:271:VAL:HG22	1.71	0.73
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.71	0.72
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.72	0.71
1:N:479:ASN:HB3	1:N:484:GLU:H	1.54	0.71
1:J:420:ILE:HG13	1:J:448:GLU:HG2	1.73	0.71
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.73	0.70
1:B:46:ALA:CB	1:C:76:GLU:HG3	2.21	0.70
1:D:384:ALA:HB3	1:D:385:THR:HG23	1.74	0.70
1:A:339:GLU:O	1:A:343:GLN:HG2	1.92	0.70
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.73	0.70
1:N:270:ILE:HG22	1:N:271:VAL:HG23	1.75	0.69
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.75	0.69
1:H:270:ILE:HG22	1:H:271:VAL:HG23	1.73	0.69
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.75	0.69
1:J:479:ASN:HB3	1:J:484:GLU:H	1.58	0.69
1:C:13:ARG:HD3	1:C:104:LEU:HD22	1.75	0.69
1:I:327:LYS:CD	1:I:327:LYS:NZ	2.55	0.68
1:B:118:ARG:HB3	1:B:436:GLN:HE21	1.58	0.68
1:E:13:ARG:HD3	1:E:104:LEU:HD22	1.75	0.68
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.76	0.68
1:K:487:ASN:O	1:K:491:MET:HG2	1.93	0.68
1:B:13:ARG:HD3	1:B:104:LEU:HD22	1.76	0.68
1:F:270:ILE:O	1:G:229:ASN:ND2	2.24	0.68
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.76	0.68
1:G:13:ARG:HD3	1:G:104:LEU:HD22	1.74	0.68
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.76	0.68
1:D:384:ALA:C	1:D:385:THR:HG22	2.15	0.68
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.75	0.68
1:C:46:ALA:CB	1:D:76:GLU:HG3	2.24	0.67
1:D:13:ARG:HD3	1:D:104:LEU:HD22	1.76	0.67
1:M:326:ASN:HD22	1:M:329:THR:HB	1.59	0.67
1:A:13:ARG:HD3	1:A:104:LEU:HD22	1.75	0.67
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:262:LEU:HD22	1:K:273:VAL:HG11	1.77	0.67
1:F:13:ARG:HD3	1:F:104:LEU:HD22	1.76	0.67
1:N:218:PRO:HG3	1:N:323:VAL:HG12	1.77	0.66
1:J:270:ILE:HG22	1:J:271:VAL:HG23	1.77	0.66
1:E:265:ASN:O	1:E:270:ILE:HG13	1.96	0.66
1:E:44:PHE:C	1:E:44:PHE:CD1	2.68	0.66
1:E:269:GLY:O	1:E:270:ILE:C	2.34	0.66
1:K:180:GLY:HA3	1:K:381:VAL:O	1.97	0.65
1:A:420:ILE:HG12	1:A:448:GLU:HG2	1.79	0.65
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.79	0.65
1:E:479:ASN:HD22	1:E:493:ILE:HD11	1.62	0.65
1:D:27:VAL:HG13	1:D:90:THR:HG23	1.79	0.65
1:N:176:THR:CG2	1:N:322:ARG:HH12	2.10	0.64
1:I:326:ASN:HB2	1:I:329:THR:HB	1.80	0.64
1:C:46:ALA:HB2	1:D:76:GLU:HG3	1.78	0.63
1:L:479:ASN:HB3	1:L:484:GLU:H	1.62	0.63
1:K:218:PRO:HD2	1:K:320:ALA:O	1.98	0.63
1:E:27:VAL:HG13	1:E:90:THR:HG23	1.80	0.63
1:E:28:LYS:HE2	1:E:453:GLN:OE1	1.98	0.63
1:D:288:MET:HG2	1:D:368:ARG:HD3	1.81	0.63
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.81	0.62
1:M:248:LEU:HD22	1:M:323:VAL:HG11	1.82	0.62
1:C:27:VAL:HG13	1:C:90:THR:HG23	1.81	0.62
1:K:46:ALA:HB2	1:L:76:GLU:CG	2.29	0.61
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.82	0.61
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.82	0.61
1:C:321:LYS:HB2	1:C:334:ASP:HB3	1.83	0.61
1:D:384:ALA:CB	1:D:385:THR:HG23	2.31	0.61
1:G:130:GLU:HB3	1:G:422:VAL:HG22	1.83	0.61
1:F:28:LYS:HE2	1:F:453:GLN:OE1	2.01	0.60
1:G:27:VAL:HG13	1:G:90:THR:HG23	1.82	0.60
1:F:27:VAL:HG13	1:F:90:THR:HG23	1.82	0.60
1:B:27:VAL:HG13	1:B:90:THR:HG23	1.81	0.60
1:M:262:LEU:HD22	1:M:273:VAL:HG11	1.81	0.60
1:L:248:LEU:HD22	1:L:323:VAL:HG21	1.84	0.60
1:C:193:MET:HB2	1:C:295:LEU:HD13	1.82	0.60
1:A:27:VAL:HG13	1:A:90:THR:HG23	1.82	0.60
1:C:479:ASN:HB3	1:C:493:ILE:CD1	2.32	0.60
1:H:269:GLY:HA3	1:I:257:GLU:HB2	1.84	0.60
1:D:28:LYS:HE2	1:D:453:GLN:OE1	2.01	0.59
1:B:28:LYS:HE2	1:B:453:GLN:OE1	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ASP:OD2	1:D:368:ARG:HD2	2.03	0.59
1:I:130:GLU:HB3	1:I:422:VAL:HG22	1.85	0.58
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.85	0.58
1:A:34:LYS:HE3	1:B:118:ARG:HH22	1.68	0.58
1:M:194:GLN:HG3	1:M:331:THR:HB	1.86	0.58
1:D:186:GLU:HB2	1:D:380:LYS:HB2	1.85	0.58
1:A:421:ARG:NH2	1:A:476:TYR:O	2.36	0.58
1:D:34:LYS:HE3	1:E:118:ARG:HH22	1.67	0.58
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.85	0.58
1:H:194:GLN:O	1:H:371:LYS:HE3	2.04	0.58
1:L:131:LEU:HD13	1:L:422:VAL:HG21	1.86	0.58
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.86	0.57
1:D:221:LEU:HD23	1:D:249:ILE:HG23	1.85	0.57
1:D:130:GLU:HB3	1:D:422:VAL:HG22	1.86	0.57
1:I:204:PHE:HD1	1:I:266:THR:HG21	1.68	0.57
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.86	0.57
1:J:262:LEU:HD22	1:J:273:VAL:HG11	1.86	0.57
1:D:175:ILE:H	1:D:404:ARG:HH22	1.53	0.57
1:F:230:ILE:HG13	1:F:261:THR:HG21	1.86	0.57
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.86	0.57
1:H:131:LEU:HD13	1:H:422:VAL:HG21	1.87	0.57
1:I:186:GLU:HB2	1:I:380:LYS:HB2	1.87	0.56
1:J:131:LEU:HD13	1:J:422:VAL:HG21	1.85	0.56
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.35	0.56
1:A:28:LYS:HE2	1:A:453:GLN:OE1	2.05	0.56
1:D:268:ARG:HG3	1:D:270:ILE:CD1	2.35	0.56
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.36	0.56
1:E:321:LYS:HB3	1:E:334:ASP:HB3	1.86	0.56
1:D:343:GLN:HE21	1:D:343:GLN:HA	1.70	0.56
1:E:350:ARG:HA	1:E:353:ILE:HD12	1.87	0.56
1:K:46:ALA:CB	1:L:76:GLU:HG3	2.33	0.56
1:M:131:LEU:HD13	1:M:422:VAL:HG21	1.88	0.56
1:I:479:ASN:CB	1:I:484:GLU:H	2.15	0.56
1:D:421:ARG:NH2	1:D:476:TYR:O	2.39	0.56
1:A:194:GLN:HG3	1:A:329:THR:HG23	1.88	0.55
1:G:180:GLY:HA3	1:G:381:VAL:O	2.06	0.55
1:D:268:ARG:HG3	1:D:270:ILE:HD12	1.87	0.55
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.36	0.55
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.36	0.55
1:J:269:GLY:HA3	1:K:257:GLU:HB2	1.89	0.55
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HD22	1:C:59:GLU:HG3	1.87	0.55
1:E:366:GLN:HA	1:E:369:VAL:HG22	1.88	0.55
1:G:413:ALA:HB2	1:G:475:ASN:HD22	1.72	0.55
1:L:218:PRO:HG3	1:L:323:VAL:HG12	1.90	0.54
1:H:18:ARG:HH11	1:H:18:ARG:HB3	1.73	0.54
1:N:131:LEU:HD13	1:N:422:VAL:HG21	1.90	0.54
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.37	0.54
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.37	0.54
1:D:180:GLY:HA3	1:D:381:VAL:O	2.07	0.54
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.89	0.54
1:I:131:LEU:HD13	1:I:422:VAL:HG21	1.90	0.54
1:B:182:GLY:HA2	1:C:284:ARG:HH21	1.73	0.54
1:I:217:SER:N	1:I:218:PRO:HD3	2.23	0.53
1:I:204:PHE:CD1	1:I:266:THR:HG21	2.43	0.53
1:J:476:TYR:OH	1:J:485:TYR:HB3	2.09	0.53
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.90	0.53
1:D:270:ILE:O	1:E:229:ASN:ND2	2.42	0.53
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.91	0.53
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.90	0.53
1:E:34:LYS:HE3	1:F:118:ARG:HH22	1.74	0.53
1:D:131:LEU:HD13	1:D:422:VAL:HG21	1.91	0.53
1:A:77:VAL:HG21	1:A:510:VAL:HB	1.90	0.53
1:N:240:VAL:HG11	1:N:247:LEU:HB2	1.90	0.53
1:K:479:ASN:HD21	1:K:481:ALA:HB3	1.74	0.53
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.91	0.53
1:J:18:ARG:HH11	1:J:18:ARG:HB3	1.74	0.53
1:J:283:ASP:HA	1:J:286:LYS:HE2	1.90	0.53
1:K:350:ARG:HA	1:K:353:ILE:HD12	1.92	0.52
1:E:263:VAL:O	1:E:267:MET:HB2	2.08	0.52
1:L:18:ARG:HH11	1:L:18:ARG:HB3	1.74	0.52
1:K:413:ALA:HB2	1:K:475:ASN:HD22	1.75	0.52
1:L:224:ASP:CB	1:L:302:SER:HA	2.40	0.52
1:C:458:CYS:SG	1:C:480:ALA:HB1	2.50	0.52
1:K:131:LEU:HD13	1:K:422:VAL:HG21	1.91	0.52
1:N:18:ARG:HH11	1:N:18:ARG:HB3	1.75	0.52
1:E:221:LEU:HD23	1:E:249:ILE:HG23	1.92	0.52
1:F:77:VAL:HG21	1:F:510:VAL:HB	1.91	0.52
1:J:350:ARG:HA	1:J:353:ILE:HD12	1.91	0.52
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.92	0.52
1:M:223:ALA:O	1:M:251:ALA:HA	2.10	0.52
1:I:413:ALA:HB2	1:I:475:ASN:HD22	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:197:ARG:HD2	1:L:277:LYS:HB2	1.91	0.52
1:N:248:LEU:HD22	1:N:323:VAL:HG21	1.92	0.52
1:M:46:ALA:HB2	1:N:76:GLU:HG3	1.92	0.52
1:M:487:ASN:O	1:M:491:MET:HG2	2.10	0.52
1:I:18:ARG:HB3	1:I:18:ARG:HH11	1.75	0.52
1:D:82:ASN:HB2	1:D:89:THR:OG1	2.10	0.51
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.10	0.51
1:I:90:THR:O	1:I:94:VAL:HG13	2.10	0.51
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.92	0.51
1:B:417:VAL:HG12	1:B:451:LEU:CD1	2.40	0.51
1:M:18:ARG:HH11	1:M:18:ARG:HB3	1.75	0.51
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.92	0.51
1:J:487:ASN:O	1:J:491:MET:HG2	2.10	0.51
1:D:77:VAL:HG21	1:D:510:VAL:HB	1.92	0.51
1:D:443:ALA:O	1:D:447:MET:HG3	2.10	0.51
1:A:224:ASP:HB3	1:A:302:SER:HA	1.91	0.51
1:H:76:GLU:CG	1:N:46:ALA:HB2	2.36	0.51
1:B:77:VAL:HG21	1:B:510:VAL:HB	1.91	0.51
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.93	0.51
1:N:413:ALA:HB2	1:N:475:ASN:HD22	1.76	0.51
1:L:223:ALA:HB3	1:L:251:ALA:HB2	1.92	0.51
1:B:197:ARG:HD2	1:B:277:LYS:HB2	1.92	0.51
1:N:321:LYS:HB2	1:N:334:ASP:HB3	1.93	0.51
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.11	0.51
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.93	0.51
1:F:173:GLY:O	1:F:404:ARG:NH2	2.44	0.51
1:K:18:ARG:HB3	1:K:18:ARG:HH11	1.76	0.51
1:B:46:ALA:HB2	1:C:76:GLU:HG3	1.91	0.51
1:B:82:ASN:HB2	1:B:89:THR:OG1	2.11	0.51
1:G:77:VAL:HG21	1:G:510:VAL:HB	1.92	0.51
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.93	0.51
1:B:270:ILE:O	1:C:229:ASN:ND2	2.37	0.51
1:F:218:PRO:HG3	1:F:323:VAL:HG22	1.93	0.50
1:G:463:SER:O	1:G:467:ASN:HB2	2.11	0.50
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.92	0.50
1:H:43:SER:O	1:H:44:PHE:HB3	2.11	0.50
1:C:366:GLN:HA	1:C:369:VAL:HG22	1.92	0.50
1:L:421:ARG:NH2	1:L:476:TYR:O	2.42	0.50
1:L:420:ILE:HG12	1:L:448:GLU:HG2	1.93	0.50
1:D:223:ALA:O	1:D:251:ALA:HA	2.12	0.50
1:B:131:LEU:HD13	1:B:422:VAL:HG21	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LYS:HE3	1:B:15:LYS:HE3	1.93	0.50
1:B:479:ASN:HB3	1:B:484:GLU:H	1.76	0.50
1:L:158:VAL:HG13	1:L:396:VAL:HG22	1.94	0.50
1:K:217:SER:N	1:K:218:PRO:HD3	2.26	0.50
1:E:343:GLN:HE21	1:E:343:GLN:HA	1.76	0.50
1:K:218:PRO:HB3	1:K:246:PRO:HB2	1.93	0.50
1:F:7:LYS:HE3	1:F:15:LYS:HE3	1.94	0.50
1:M:271:VAL:HG12	1:M:272:LYS:N	2.27	0.50
1:B:366:GLN:HA	1:B:369:VAL:HG22	1.93	0.50
1:C:40:LEU:HD23	1:D:521:VAL:HB	1.94	0.50
1:N:326:ASN:HD22	1:N:329:THR:HB	1.76	0.50
1:B:479:ASN:CG	1:B:482:THR:HG22	2.30	0.50
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.94	0.50
1:K:479:ASN:ND2	1:K:493:ILE:HD11	2.26	0.50
1:I:270:ILE:O	1:J:229:ASN:ND2	2.45	0.50
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.93	0.50
1:E:265:ASN:O	1:E:270:ILE:CG1	2.60	0.49
1:J:421:ARG:NH2	1:J:476:TYR:O	2.45	0.49
1:B:130:GLU:HB3	1:B:422:VAL:HG22	1.94	0.49
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.94	0.49
1:A:192:GLY:HA2	1:A:332:ILE:O	2.12	0.49
1:C:82:ASN:HB2	1:C:89:THR:OG1	2.12	0.49
1:L:42:LYS:HG3	1:L:44:PHE:CZ	2.47	0.49
1:A:362:ARG:HG2	1:A:366:GLN:HE21	1.77	0.49
1:J:218:PRO:HB3	1:J:246:PRO:HB2	1.94	0.49
1:A:213:VAL:HB	1:A:325:ILE:HB	1.94	0.49
1:G:7:LYS:HE3	1:G:15:LYS:HE3	1.95	0.49
1:N:284:ARG:O	1:N:288:MET:HG3	2.12	0.49
1:C:455:VAL:CG1	1:C:460:GLU:HB2	2.43	0.49
1:L:90:THR:O	1:L:94:VAL:HG13	2.13	0.49
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.95	0.49
1:E:7:LYS:HE3	1:E:15:LYS:HE3	1.95	0.49
1:N:90:THR:O	1:N:94:VAL:HG13	2.12	0.49
1:E:82:ASN:HB2	1:E:89:THR:OG1	2.12	0.49
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.94	0.49
1:B:305:ILE:HD12	1:B:307:MET:HE2	1.95	0.49
1:L:224:ASP:HB3	1:L:302:SER:HA	1.94	0.49
1:D:247:LEU:O	1:D:273:VAL:HG13	2.13	0.49
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.95	0.48
1:C:28:LYS:HE2	1:C:453:GLN:OE1	2.13	0.48
1:E:479:ASN:HD22	1:E:493:ILE:CD1	2.26	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:262:LEU:HD22	1:L:273:VAL:HG11	1.96	0.48
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.94	0.48
1:K:90:THR:O	1:K:94:VAL:HG13	2.13	0.48
1:N:223:ALA:O	1:N:251:ALA:HA	2.13	0.48
1:B:477:GLY:O	1:B:485:TYR:HA	2.14	0.48
1:A:82:ASN:HB2	1:A:89:THR:OG1	2.12	0.48
1:I:476:TYR:CE2	1:I:485:TYR:HB3	2.48	0.48
1:A:7:LYS:HE3	1:A:15:LYS:HE3	1.95	0.48
1:K:404:ARG:HH11	1:K:404:ARG:HA	1.78	0.48
1:J:90:THR:O	1:J:94:VAL:HG13	2.13	0.48
1:C:455:VAL:HG13	1:C:460:GLU:HB2	1.95	0.48
1:N:232:GLU:HA	1:N:310:GLU:HG3	1.95	0.48
1:M:46:ALA:HB2	1:N:76:GLU:CG	2.44	0.48
1:F:264:VAL:O	1:F:268:ARG:HG3	2.14	0.48
1:B:421:ARG:NH2	1:B:476:TYR:O	2.41	0.48
1:K:420:ILE:HG13	1:K:448:GLU:HG2	1.95	0.48
1:E:77:VAL:HG12	1:E:506:TYR:HB3	1.96	0.48
1:L:413:ALA:HB2	1:L:475:ASN:HD22	1.78	0.48
1:L:326:ASN:HB2	1:L:329:THR:HB	1.96	0.48
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.96	0.47
1:I:420:ILE:HG12	1:I:448:GLU:HG2	1.95	0.47
1:G:173:GLY:O	1:G:404:ARG:NH2	2.47	0.47
1:H:90:THR:O	1:H:94:VAL:HG13	2.14	0.47
1:F:122:LYS:HE2	1:F:429:LEU:HD11	1.95	0.47
1:J:270:ILE:HG22	1:J:271:VAL:N	2.30	0.47
1:D:7:LYS:HE3	1:D:15:LYS:HE3	1.95	0.47
1:E:43:SER:HB2	1:E:44:PHE:HB3	1.96	0.47
1:A:323:VAL:HG12	1:A:332:ILE:HA	1.97	0.47
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.95	0.47
1:B:357:THR:HA	1:B:362:ARG:HH22	1.78	0.47
1:L:174:VAL:HB	1:L:376:VAL:HG22	1.95	0.47
1:J:225:LYS:HE2	1:J:303:GLU:HB3	1.95	0.47
1:D:459:GLY:HA3	1:E:112:ASN:HD22	1.80	0.47
1:I:218:PRO:HB3	1:I:246:PRO:HB2	1.95	0.47
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.96	0.47
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.96	0.47
1:A:479:ASN:HB3	1:A:484:GLU:H	1.80	0.47
1:I:180:GLY:HA3	1:I:381:VAL:O	2.13	0.47
1:F:323:VAL:HG12	1:F:332:ILE:HA	1.97	0.47
1:F:477:GLY:O	1:F:485:TYR:HA	2.15	0.47
1:G:202:PRO:O	1:G:203:TYR:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.97	0.47
1:C:350:ARG:HA	1:C:353:ILE:HD12	1.96	0.47
1:M:90:THR:O	1:M:94:VAL:HG13	2.14	0.47
1:F:217:SER:N	1:F:218:PRO:HD3	2.30	0.47
1:A:321:LYS:HB2	1:A:334:ASP:HB3	1.96	0.47
1:J:326:ASN:HD22	1:J:328:ASP:H	1.63	0.47
1:M:248:LEU:HD13	1:M:325:ILE:HD11	1.97	0.47
1:C:34:LYS:HD2	1:C:458:CYS:HA	1.96	0.47
1:L:271:VAL:O	1:L:273:VAL:HG23	2.15	0.47
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.95	0.47
1:F:413:ALA:HB2	1:F:475:ASN:HD22	1.79	0.47
1:C:7:LYS:HE3	1:C:15:LYS:HE3	1.96	0.47
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.98	0.46
1:E:269:GLY:C	1:F:229:ASN:HD21	2.18	0.46
1:D:321:LYS:HB3	1:D:334:ASP:HB3	1.97	0.46
1:I:33:PRO:HG3	1:I:480:ALA:HB1	1.98	0.46
1:L:194:GLN:HG3	1:L:331:THR:HB	1.96	0.46
1:M:421:ARG:NH1	1:M:469:VAL:O	2.45	0.46
1:I:350:ARG:HA	1:I:353:ILE:HD12	1.96	0.46
1:C:197:ARG:HD2	1:C:277:LYS:HB2	1.98	0.46
1:L:487:ASN:O	1:L:491:MET:HG2	2.16	0.46
1:F:224:ASP:HB3	1:F:302:SER:HA	1.97	0.46
1:M:20:VAL:HB	1:M:74:VAL:HG11	1.97	0.46
1:C:479:ASN:HB3	1:C:493:ILE:HD13	1.97	0.46
1:K:200:LEU:HG	1:K:276:VAL:HA	1.97	0.46
1:M:272:LYS:N	1:M:272:LYS:HD3	2.31	0.46
1:G:28:LYS:HE2	1:G:453:GLN:OE1	2.16	0.46
1:F:34:LYS:HE3	1:G:118:ARG:HH22	1.81	0.46
1:D:34:LYS:HE3	1:E:118:ARG:NH2	2.31	0.46
1:A:194:GLN:O	1:A:371:LYS:HE3	2.16	0.46
1:N:350:ARG:HA	1:N:353:ILE:HD12	1.97	0.46
1:D:414:GLY:O	1:D:417:VAL:HG13	2.15	0.46
1:F:458:CYS:SG	1:F:480:ALA:HB1	2.55	0.46
1:H:270:ILE:HG22	1:H:271:VAL:N	2.30	0.46
1:G:42:LYS:O	1:G:44:PHE:N	2.49	0.46
1:H:213:VAL:HB	1:H:325:ILE:HB	1.96	0.46
1:J:443:ALA:O	1:J:447:MET:HG3	2.16	0.46
1:E:90:THR:O	1:E:94:VAL:HG13	2.17	0.45
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.98	0.45
1:E:284:ARG:O	1:E:288:MET:HG3	2.15	0.45
1:N:236:VAL:O	1:N:240:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:VAL:HB	1:L:74:VAL:HG11	1.97	0.45
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.98	0.45
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.98	0.45
1:K:272:LYS:HB2	1:K:272:LYS:HE3	1.62	0.45
1:A:34:LYS:HE3	1:B:118:ARG:NH2	2.32	0.45
1:M:326:ASN:HB2	1:M:329:THR:HB	1.98	0.45
1:C:193:MET:HB2	1:C:295:LEU:CD1	2.44	0.45
1:I:20:VAL:HB	1:I:74:VAL:HG11	1.98	0.45
1:B:218:PRO:HG3	1:B:323:VAL:HG22	1.98	0.45
1:H:349:ILE:HG23	1:H:365:LEU:HD22	1.98	0.45
1:E:218:PRO:HB3	1:E:246:PRO:HB2	1.98	0.45
1:J:194:GLN:O	1:J:371:LYS:HE3	2.17	0.45
1:D:90:THR:O	1:D:94:VAL:HG13	2.17	0.45
1:J:20:VAL:HB	1:J:74:VAL:HG11	1.98	0.45
1:E:173:GLY:O	1:E:404:ARG:NH2	2.49	0.45
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.98	0.45
1:B:479:ASN:HB2	1:B:484:GLU:O	2.16	0.45
1:J:215:LEU:HD22	1:J:246:PRO:HB3	1.98	0.45
1:K:20:VAL:HB	1:K:74:VAL:HG11	1.97	0.45
1:H:218:PRO:HG3	1:H:323:VAL:HG12	1.99	0.45
1:H:248:LEU:HD22	1:H:323:VAL:HG21	1.99	0.45
1:J:180:GLY:HA3	1:J:381:VAL:O	2.16	0.45
1:F:421:ARG:NH2	1:F:476:TYR:O	2.50	0.45
1:N:20:VAL:HB	1:N:74:VAL:HG11	1.97	0.45
1:H:20:VAL:HB	1:H:74:VAL:HG11	1.98	0.45
1:A:194:GLN:HG3	1:A:329:THR:CG2	2.46	0.45
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.47	0.45
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.99	0.45
1:E:213:VAL:HB	1:E:325:ILE:HB	1.97	0.45
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.99	0.45
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.47	0.45
1:A:350:ARG:HA	1:A:353:ILE:HD12	1.98	0.45
1:F:90:THR:O	1:F:94:VAL:HG13	2.17	0.45
1:A:218:PRO:HG3	1:A:323:VAL:HG22	1.99	0.45
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.47	0.45
1:C:224:ASP:HB2	1:C:302:SER:HA	1.99	0.45
1:E:323:VAL:HG12	1:E:332:ILE:HA	1.99	0.45
1:E:443:ALA:O	1:E:447:MET:HG3	2.17	0.45
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.99	0.44
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.47	0.44
1:G:178:GLU:HA	1:G:393:LYS:HE3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:VAL:HG13	1:D:396:VAL:HG22	1.99	0.44
1:B:323:VAL:HG12	1:B:332:ILE:HA	1.99	0.44
1:L:180:GLY:HA3	1:L:381:VAL:O	2.17	0.44
1:A:46:ALA:HB2	1:B:76:GLU:CG	2.26	0.44
1:E:268:ARG:HD2	1:E:270:ILE:HD11	1.99	0.44
1:G:77:VAL:HG12	1:G:506:TYR:HB3	1.98	0.44
1:D:487:ASN:O	1:D:491:MET:HG3	2.17	0.44
1:A:214:GLU:HG3	1:A:324:VAL:HG22	1.99	0.44
1:C:336:VAL:O	1:C:336:VAL:HG12	2.17	0.44
1:G:131:LEU:HD13	1:G:422:VAL:HG21	1.98	0.44
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.98	0.44
1:C:186:GLU:HB2	1:C:380:LYS:HB2	2.00	0.44
1:N:479:ASN:ND2	1:N:482:THR:OG1	2.51	0.44
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.98	0.44
1:E:270:ILE:HG12	1:E:270:ILE:H	1.66	0.44
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.99	0.44
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.99	0.44
1:C:248:LEU:HD13	1:C:325:ILE:HD11	2.00	0.44
1:I:232:GLU:HB3	1:I:309:LEU:HB2	2.00	0.44
1:J:224:ASP:HB3	1:J:302:SER:HB3	2.00	0.44
1:G:193:MET:HB2	1:G:295:LEU:CD1	2.48	0.44
1:H:451:LEU:O	1:H:455:VAL:HG23	2.16	0.44
1:M:218:PRO:HD2	1:M:320:ALA:O	2.17	0.44
1:F:479:ASN:ND2	1:F:482:THR:OG1	2.51	0.43
1:H:262:LEU:HD22	1:H:273:VAL:HG11	2.00	0.43
1:C:38:VAL:HG22	1:D:519:CYS:HB3	2.00	0.43
1:N:248:LEU:HD13	1:N:325:ILE:HD11	1.99	0.43
1:C:220:ILE:HG12	1:C:248:LEU:HB3	2.01	0.43
1:G:16:MET:O	1:G:20:VAL:HG13	2.18	0.43
1:L:295:LEU:HD23	1:L:372:LEU:HD12	2.00	0.43
1:N:82:ASN:HB2	1:N:89:THR:OG1	2.18	0.43
1:C:479:ASN:CB	1:C:493:ILE:CD1	2.97	0.43
1:H:82:ASN:HB2	1:H:89:THR:OG1	2.18	0.43
1:J:349:ILE:HG23	1:J:365:LEU:HD22	2.00	0.43
1:I:272:LYS:HA	1:I:272:LYS:HD3	1.83	0.43
1:N:217:SER:HB3	1:N:245:LYS:HD3	1.99	0.43
1:N:263:VAL:O	1:N:267:MET:HB2	2.17	0.43
1:B:38:VAL:HG22	1:C:519:CYS:HB3	2.00	0.43
1:H:197:ARG:HD2	1:H:277:LYS:HB2	2.00	0.43
1:F:77:VAL:HG12	1:F:506:TYR:HB3	2.00	0.43
1:C:417:VAL:HA	1:C:420:ILE:HG22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:206:ASN:HD21	1:K:214:GLU:H	1.66	0.43
1:I:349:ILE:HG23	1:I:365:LEU:HD22	2.01	0.43
1:N:336:VAL:HG12	1:N:336:VAL:O	2.19	0.43
1:B:90:THR:O	1:B:94:VAL:HG13	2.19	0.43
1:A:90:THR:O	1:A:94:VAL:HG13	2.18	0.43
1:C:202:PRO:C	1:C:204:PHE:H	2.22	0.43
1:J:240:VAL:HG21	1:J:247:LEU:HD22	1.99	0.43
1:D:16:MET:O	1:D:20:VAL:HG13	2.19	0.43
1:L:350:ARG:HA	1:L:353:ILE:HD12	2.00	0.43
1:G:215:LEU:HB2	1:G:323:VAL:HG22	1.99	0.43
1:C:90:THR:O	1:C:94:VAL:HG13	2.19	0.43
1:F:201:SER:HA	1:F:202:PRO:HD3	1.89	0.43
1:N:176:THR:HG21	1:N:322:ARG:HH12	1.81	0.43
1:F:273:VAL:HG12	1:F:274:ALA:N	2.34	0.43
1:F:417:VAL:HA	1:F:420:ILE:HG22	2.00	0.43
1:J:326:ASN:ND2	1:J:328:ASP:H	2.17	0.42
1:I:301:ILE:HG23	1:I:307:MET:HB2	2.01	0.42
1:H:158:VAL:HG13	1:H:396:VAL:HG22	2.00	0.42
1:B:16:MET:O	1:B:20:VAL:HG13	2.19	0.42
1:K:82:ASN:HB2	1:K:89:THR:OG1	2.19	0.42
1:M:479:ASN:HB3	1:M:483:GLU:N	2.34	0.42
1:C:18:ARG:HE	1:C:18:ARG:HB2	1.62	0.42
1:A:472:GLY:HA3	1:A:476:TYR:CD2	2.54	0.42
1:N:130:GLU:HB3	1:N:422:VAL:HG13	2.01	0.42
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.49	0.42
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.49	0.42
1:B:173:GLY:O	1:B:404:ARG:NH2	2.52	0.42
1:C:264:VAL:O	1:C:268:ARG:HG3	2.20	0.42
1:K:324:VAL:HB	1:K:331:THR:HG23	2.01	0.42
1:G:487:ASN:O	1:G:491:MET:HG3	2.19	0.42
1:L:82:ASN:HB2	1:L:89:THR:OG1	2.19	0.42
1:A:118:ARG:HH22	1:G:34:LYS:HE3	1.84	0.42
1:E:270:ILE:HB	1:E:271:VAL:H	1.50	0.42
1:L:218:PRO:HD2	1:L:320:ALA:O	2.19	0.42
1:D:383:ALA:HB3	1:D:389:MET:HB2	2.01	0.42
1:H:270:ILE:CG2	1:H:271:VAL:HG23	2.45	0.42
1:N:197:ARG:HD2	1:N:277:LYS:HB2	2.01	0.42
1:D:413:ALA:HB2	1:D:475:ASN:HD22	1.83	0.42
1:A:451:LEU:O	1:A:455:VAL:HG23	2.19	0.42
1:D:350:ARG:HG3	1:D:369:VAL:HG11	2.01	0.42
1:N:71:ALA:O	1:N:75:LYS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:ASN:HA	1:E:113:PRO:HD3	1.95	0.42
1:G:42:LYS:C	1:G:44:PHE:H	2.23	0.42
1:M:342:ILE:O	1:M:346:VAL:HG23	2.19	0.42
1:I:82:ASN:HB2	1:I:89:THR:OG1	2.19	0.42
1:H:16:MET:HB3	1:H:514:MET:HE3	2.02	0.42
1:M:451:LEU:O	1:M:455:VAL:HG23	2.19	0.42
1:A:192:GLY:CA	1:A:332:ILE:O	2.68	0.42
1:H:217:SER:N	1:H:218:PRO:HD3	2.35	0.42
1:N:421:ARG:NH1	1:N:469:VAL:O	2.52	0.42
1:A:195:PHE:HB2	1:A:279:PRO:HB3	2.01	0.42
1:E:420:ILE:HG13	1:E:448:GLU:HG2	2.02	0.42
1:C:271:VAL:O	1:C:273:VAL:HG23	2.20	0.42
1:K:158:VAL:HG13	1:K:396:VAL:HG22	2.02	0.42
1:E:207:LYS:HA	1:E:208:PRO:HD3	1.92	0.42
1:M:413:ALA:HB2	1:M:475:ASN:HD22	1.84	0.42
1:M:496:PRO:HB2	1:M:499:VAL:HG13	2.02	0.42
1:I:421:ARG:NH2	1:I:476:TYR:O	2.51	0.42
1:F:479:ASN:O	1:F:483:GLU:HA	2.20	0.42
1:F:263:VAL:O	1:F:267:MET:HB2	2.19	0.42
1:H:413:ALA:HB2	1:H:475:ASN:HD22	1.84	0.42
1:J:82:ASN:HB2	1:J:89:THR:OG1	2.20	0.42
1:I:16:MET:HB3	1:I:514:MET:HE3	2.02	0.42
1:N:487:ASN:O	1:N:491:MET:HG2	2.19	0.42
1:K:443:ALA:O	1:K:447:MET:HG3	2.19	0.42
1:H:71:ALA:O	1:H:75:LYS:HB2	2.20	0.42
1:E:46:ALA:HA	1:E:47:PRO:HD3	1.95	0.42
1:H:420:ILE:HG13	1:H:448:GLU:HG2	2.01	0.42
1:D:451:LEU:O	1:D:455:VAL:HG23	2.20	0.42
1:I:363:GLU:HA	1:I:366:GLN:HB2	2.02	0.42
1:F:18:ARG:HE	1:F:18:ARG:HB2	1.61	0.42
1:N:213:VAL:HB	1:N:325:ILE:HB	2.02	0.41
1:M:82:ASN:HB2	1:M:89:THR:OG1	2.20	0.41
1:I:199:TYR:OH	1:I:327:LYS:HG2	2.20	0.41
1:A:476:TYR:C	1:A:476:TYR:CD2	2.93	0.41
1:L:487:ASN:HB3	1:L:490:ASP:HB2	2.03	0.41
1:D:266:THR:HA	1:D:271:VAL:O	2.20	0.41
1:C:136:VAL:HA	1:C:137:PRO:HD3	1.90	0.41
1:I:342:ILE:O	1:I:346:VAL:HG23	2.21	0.41
1:K:524:LEU:HA	1:K:524:LEU:HD12	1.98	0.41
1:H:487:ASN:O	1:H:491:MET:HG2	2.21	0.41
1:J:42:LYS:C	1:J:44:PHE:H	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:LEU:N	1:G:235:PRO:HD2	2.35	0.41
1:G:288:MET:HG2	1:G:368:ARG:HD3	2.01	0.41
1:D:234:LEU:N	1:D:235:PRO:HD2	2.36	0.41
1:K:441:LYS:HA	1:K:441:LYS:HD3	1.87	0.41
1:N:476:TYR:C	1:N:476:TYR:CD2	2.93	0.41
1:I:496:PRO:HB2	1:I:499:VAL:HG13	2.01	0.41
1:N:217:SER:N	1:N:218:PRO:CD	2.83	0.41
1:G:90:THR:O	1:G:94:VAL:HG13	2.19	0.41
1:M:7:LYS:HE2	1:M:15:LYS:HE3	2.02	0.41
1:C:262:LEU:O	1:C:266:THR:HG22	2.20	0.41
1:D:162:ILE:HG12	1:D:400:LEU:HD23	2.02	0.41
1:F:16:MET:O	1:F:20:VAL:HG13	2.21	0.41
1:K:201:SER:HA	1:K:202:PRO:HD3	1.92	0.41
1:J:263:VAL:O	1:J:267:MET:HB2	2.20	0.41
1:A:18:ARG:HE	1:A:18:ARG:HB2	1.61	0.41
1:H:219:PHE:HB3	1:H:317:LEU:HD23	2.02	0.41
1:C:200:LEU:HD21	1:C:277:LYS:HG3	2.02	0.41
1:A:195:PHE:CE2	1:A:197:ARG:HB2	2.55	0.41
1:D:19:GLY:HA3	1:D:67:GLU:O	2.20	0.41
1:J:524:LEU:HD12	1:J:524:LEU:HA	1.98	0.41
1:L:229:ASN:N	1:L:229:ASN:HD22	2.18	0.41
1:N:392:LYS:O	1:N:396:VAL:HG23	2.20	0.41
1:L:218:PRO:HB3	1:L:246:PRO:HB2	2.03	0.41
1:I:112:ASN:HA	1:I:113:PRO:HD3	1.94	0.41
1:A:16:MET:O	1:A:20:VAL:HG13	2.21	0.41
1:B:256:GLY:C	1:B:258:ALA:H	2.24	0.41
1:I:7:LYS:HE2	1:I:15:LYS:HE3	2.03	0.41
1:L:496:PRO:HB2	1:L:499:VAL:HG13	2.03	0.41
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.50	0.41
1:J:7:LYS:HE2	1:J:15:LYS:HE3	2.02	0.41
1:J:122:LYS:HG2	1:J:429:LEU:HD21	2.02	0.41
1:E:433:ASN:ND2	1:E:436:GLN:HG3	2.35	0.41
1:G:19:GLY:HA3	1:G:67:GLU:O	2.20	0.41
1:E:19:GLY:HA3	1:E:67:GLU:O	2.21	0.41
1:K:71:ALA:O	1:K:75:LYS:HB2	2.21	0.41
1:J:126:ALA:HB1	1:J:426:LEU:HD22	2.02	0.41
1:I:284:ARG:O	1:I:288:MET:HG3	2.21	0.41
1:L:420:ILE:HD12	1:L:451:LEU:HD13	2.03	0.41
1:A:301:ILE:HG23	1:A:307:MET:HB3	2.03	0.41
1:E:136:VAL:HA	1:E:137:PRO:HD3	1.91	0.41
1:D:18:ARG:HB2	1:D:18:ARG:HE	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:199:TYR:HA	1:K:276:VAL:HG12	2.03	0.40
1:G:162:ILE:HG12	1:G:400:LEU:HD23	2.04	0.40
1:J:136:VAL:HA	1:J:137:PRO:HD3	1.89	0.40
1:B:443:ALA:O	1:B:447:MET:HG3	2.21	0.40
1:K:7:LYS:HE2	1:K:15:LYS:HE3	2.02	0.40
1:F:19:GLY:HA3	1:F:67:GLU:O	2.21	0.40
1:L:71:ALA:O	1:L:75:LYS:HB2	2.21	0.40
1:M:136:VAL:HA	1:M:137:PRO:HD3	1.88	0.40
1:G:301:ILE:HG23	1:G:307:MET:HB3	2.03	0.40
1:L:248:LEU:HD13	1:L:325:ILE:HD11	2.03	0.40
1:C:19:GLY:HA3	1:C:67:GLU:O	2.21	0.40
1:L:221:LEU:HD23	1:L:249:ILE:HG23	2.03	0.40
1:A:194:GLN:HA	1:A:330:THR:O	2.21	0.40
1:K:479:ASN:HD22	1:K:493:ILE:HD11	1.85	0.40
1:J:217:SER:N	1:J:218:PRO:HD3	2.36	0.40
1:G:358:SER:HB3	1:G:361:ASP:HB2	2.02	0.40
1:L:201:SER:HA	1:L:202:PRO:HD3	1.97	0.40
1:D:449:ALA:HB3	1:D:450:PRO:HD3	2.03	0.40
1:A:173:GLY:O	1:A:404:ARG:NH2	2.54	0.40
1:E:16:MET:O	1:E:20:VAL:HG13	2.22	0.40
1:D:384:ALA:CA	1:D:385:THR:HG23	2.52	0.40
1:F:443:ALA:O	1:F:447:MET:HG3	2.21	0.40
1:L:455:VAL:HG13	1:L:460:GLU:HB2	2.04	0.40
1:I:248:LEU:HD22	1:I:323:VAL:HG21	2.04	0.40
1:K:112:ASN:HA	1:K:113:PRO:HD3	1.96	0.40
1:N:272:LYS:HB2	1:N:272:LYS:HE3	1.74	0.40
1:C:478:TYR:HB2	1:C:485:TYR:CE2	2.56	0.40
1:A:476:TYR:HA	1:A:486:GLY:O	2.21	0.40
1:C:301:ILE:HG23	1:C:307:MET:HB3	2.02	0.40
1:N:201:SER:HA	1:N:202:PRO:HD3	1.98	0.40
1:A:413:ALA:HB2	1:A:475:ASN:HD22	1.87	0.40
1:E:235:PRO:HG3	1:E:310:GLU:HG3	2.03	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	522/547 (95%)	505 (97%)	15 (3%)	2 (0%)	39	79
1	B	522/547 (95%)	507 (97%)	13 (2%)	2 (0%)	39	79
1	C	522/547 (95%)	507 (97%)	13 (2%)	2 (0%)	39	79
1	D	522/547 (95%)	512 (98%)	9 (2%)	1 (0%)	52	87
1	E	522/547 (95%)	501 (96%)	19 (4%)	2 (0%)	39	79
1	F	522/547 (95%)	507 (97%)	15 (3%)	0	100	100
1	G	522/547 (95%)	509 (98%)	11 (2%)	2 (0%)	39	79
1	H	522/547 (95%)	508 (97%)	11 (2%)	3 (1%)	30	71
1	I	522/547 (95%)	496 (95%)	22 (4%)	4 (1%)	24	65
1	J	522/547 (95%)	505 (97%)	16 (3%)	1 (0%)	52	87
1	K	522/547 (95%)	507 (97%)	14 (3%)	1 (0%)	52	87
1	L	522/547 (95%)	504 (97%)	17 (3%)	1 (0%)	52	87
1	M	522/547 (95%)	505 (97%)	16 (3%)	1 (0%)	52	87
1	N	522/547 (95%)	508 (97%)	12 (2%)	2 (0%)	39	79
All	All	7308/7658 (95%)	7081 (97%)	203 (3%)	24 (0%)	46	82

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	44	PHE
1	E	270	ILE
1	H	44	PHE
1	I	483	GLU
1	G	43	SER
1	G	256	GLY
1	H	43	SER
1	I	43	SER
1	B	257	GLU
1	I	481	ALA
1	K	269	GLY
1	N	479	ASN
1	H	336	VAL
1	L	43	SER
1	N	486	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	479	ASN
1	C	202	PRO
1	C	483	GLU
1	M	477	GLY
1	B	43	SER
1	D	202	PRO
1	A	270	ILE
1	J	336	VAL
1	I	256	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/414 (98%)	381 (94%)	23 (6%)	25	63
1	B	404/414 (98%)	384 (95%)	20 (5%)	30	69
1	C	404/414 (98%)	384 (95%)	20 (5%)	30	69
1	D	404/414 (98%)	380 (94%)	24 (6%)	24	61
1	E	404/414 (98%)	378 (94%)	26 (6%)	22	58
1	F	404/414 (98%)	382 (95%)	22 (5%)	27	65
1	G	404/414 (98%)	381 (94%)	23 (6%)	25	63
1	H	404/414 (98%)	380 (94%)	24 (6%)	24	61
1	I	404/414 (98%)	381 (94%)	23 (6%)	25	63
1	J	404/414 (98%)	381 (94%)	23 (6%)	25	63
1	K	404/414 (98%)	382 (95%)	22 (5%)	27	65
1	L	404/414 (98%)	379 (94%)	25 (6%)	23	59
1	M	404/414 (98%)	381 (94%)	23 (6%)	25	63
1	N	404/414 (98%)	373 (92%)	31 (8%)	16	48
All	All	5656/5796 (98%)	5327 (94%)	329 (6%)	25	62

All (329) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	20	VAL
1	A	74	VAL
1	A	76	GLU
1	A	94	VAL
1	A	134	LEU
1	A	177	VAL
1	A	196	ASP
1	A	217	SER
1	A	230	ILE
1	A	231	ARG
1	A	240	VAL
1	A	242	LYS
1	A	257	GLU
1	A	265	ASN
1	A	268	ARG
1	A	271	VAL
1	A	385	THR
1	A	417	VAL
1	A	468	THR
1	A	476	TYR
1	A	499	VAL
1	A	524	LEU
1	B	18	ARG
1	B	20	VAL
1	B	74	VAL
1	B	76	GLU
1	B	82	ASN
1	B	94	VAL
1	B	134	LEU
1	B	177	VAL
1	B	242	LYS
1	B	271	VAL
1	B	272	LYS
1	B	295	LEU
1	B	328	ASP
1	B	329	THR
1	B	385	THR
1	B	387	VAL
1	B	422	VAL
1	B	451	LEU
1	B	499	VAL
1	B	524	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	18	ARG
1	C	20	VAL
1	C	74	VAL
1	C	76	GLU
1	C	94	VAL
1	C	134	LEU
1	C	177	VAL
1	C	207	LYS
1	C	230	ILE
1	C	231	ARG
1	C	240	VAL
1	C	242	LYS
1	C	268	ARG
1	C	270	ILE
1	C	271	VAL
1	C	295	LEU
1	C	328	ASP
1	C	417	VAL
1	C	499	VAL
1	C	524	LEU
1	D	18	ARG
1	D	20	VAL
1	D	27	VAL
1	D	74	VAL
1	D	76	GLU
1	D	82	ASN
1	D	94	VAL
1	D	134	LEU
1	D	177	VAL
1	D	230	ILE
1	D	231	ARG
1	D	242	LYS
1	D	257	GLU
1	D	321	LYS
1	D	328	ASP
1	D	329	THR
1	D	343	GLN
1	D	369	VAL
1	D	400	LEU
1	D	404	ARG
1	D	417	VAL
1	D	422	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	499	VAL
1	D	524	LEU
1	E	18	ARG
1	E	20	VAL
1	E	44	PHE
1	E	74	VAL
1	E	76	GLU
1	E	82	ASN
1	E	94	VAL
1	E	134	LEU
1	E	177	VAL
1	E	230	ILE
1	E	231	ARG
1	E	242	LYS
1	E	257	GLU
1	E	268	ARG
1	E	270	ILE
1	E	271	VAL
1	E	295	LEU
1	E	328	ASP
1	E	339	GLU
1	E	343	GLN
1	E	366	GLN
1	E	398	ASP
1	E	400	LEU
1	E	433	ASN
1	E	499	VAL
1	E	524	LEU
1	F	18	ARG
1	F	20	VAL
1	F	74	VAL
1	F	76	GLU
1	F	82	ASN
1	F	94	VAL
1	F	134	LEU
1	F	177	VAL
1	F	230	ILE
1	F	242	LYS
1	F	268	ARG
1	F	271	VAL
1	F	316	ASP
1	F	328	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	329	THR
1	F	387	VAL
1	F	400	LEU
1	F	451	LEU
1	F	463	SER
1	F	468	THR
1	F	499	VAL
1	F	524	LEU
1	G	18	ARG
1	G	20	VAL
1	G	74	VAL
1	G	76	GLU
1	G	94	VAL
1	G	134	LEU
1	G	177	VAL
1	G	230	ILE
1	G	231	ARG
1	G	257	GLU
1	G	271	VAL
1	G	295	LEU
1	G	321	LYS
1	G	328	ASP
1	G	336	VAL
1	G	369	VAL
1	G	398	ASP
1	G	400	LEU
1	G	417	VAL
1	G	420	ILE
1	G	422	VAL
1	G	499	VAL
1	G	524	LEU
1	H	18	ARG
1	H	20	VAL
1	H	42	LYS
1	H	58	ARG
1	H	74	VAL
1	H	82	ASN
1	H	94	VAL
1	H	131	LEU
1	H	134	LEU
1	H	224	ASP
1	H	270	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	272	LYS
1	H	294	THR
1	H	307	MET
1	H	321	LYS
1	H	328	ASP
1	H	331	THR
1	H	336	VAL
1	H	369	VAL
1	H	404	ARG
1	H	463	SER
1	H	482	THR
1	H	499	VAL
1	H	524	LEU
1	I	20	VAL
1	I	42	LYS
1	I	58	ARG
1	I	74	VAL
1	I	82	ASN
1	I	94	VAL
1	I	131	LEU
1	I	134	LEU
1	I	206	ASN
1	I	225	LYS
1	I	231	ARG
1	I	272	LYS
1	I	294	THR
1	I	321	LYS
1	I	328	ASP
1	I	331	THR
1	I	351	GLN
1	I	398	ASP
1	I	404	ARG
1	I	422	VAL
1	I	463	SER
1	I	468	THR
1	I	499	VAL
1	J	18	ARG
1	J	20	VAL
1	J	58	ARG
1	J	74	VAL
1	J	82	ASN
1	J	94	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	131	LEU
1	J	134	LEU
1	J	196	ASP
1	J	210	THR
1	J	257	GLU
1	J	270	ILE
1	J	272	LYS
1	J	284	ARG
1	J	305	ILE
1	J	326	ASN
1	J	328	ASP
1	J	351	GLN
1	J	387	VAL
1	J	398	ASP
1	J	463	SER
1	J	499	VAL
1	J	524	LEU
1	K	20	VAL
1	K	58	ARG
1	K	74	VAL
1	K	82	ASN
1	K	94	VAL
1	K	131	LEU
1	K	134	LEU
1	K	209	GLU
1	K	210	THR
1	K	250	ILE
1	K	272	LYS
1	K	294	THR
1	K	299	THR
1	K	316	ASP
1	K	321	LYS
1	K	328	ASP
1	K	329	THR
1	K	331	THR
1	K	351	GLN
1	K	482	THR
1	K	499	VAL
1	K	524	LEU
1	L	20	VAL
1	L	42	LYS
1	L	58	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	74	VAL
1	L	82	ASN
1	L	94	VAL
1	L	131	LEU
1	L	134	LEU
1	L	209	GLU
1	L	257	GLU
1	L	272	LYS
1	L	284	ARG
1	L	294	THR
1	L	299	THR
1	L	309	LEU
1	L	314	LEU
1	L	321	LYS
1	L	328	ASP
1	L	336	VAL
1	L	363	GLU
1	L	404	ARG
1	L	425	LYS
1	L	468	THR
1	L	499	VAL
1	L	524	LEU
1	M	20	VAL
1	M	42	LYS
1	M	58	ARG
1	M	74	VAL
1	M	82	ASN
1	M	94	VAL
1	M	131	LEU
1	M	134	LEU
1	M	209	GLU
1	M	252	GLU
1	M	257	GLU
1	M	261	THR
1	M	272	LYS
1	M	284	ARG
1	M	309	LEU
1	M	321	LYS
1	M	328	ASP
1	M	339	GLU
1	M	359	ASP
1	M	387	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	404	ARG
1	M	499	VAL
1	M	524	LEU
1	N	18	ARG
1	N	20	VAL
1	N	44	PHE
1	N	58	ARG
1	N	74	VAL
1	N	82	ASN
1	N	94	VAL
1	N	131	LEU
1	N	134	LEU
1	N	196	ASP
1	N	207	LYS
1	N	209	GLU
1	N	245	LYS
1	N	257	GLU
1	N	267	MET
1	N	272	LYS
1	N	309	LEU
1	N	315	GLU
1	N	321	LYS
1	N	322	ARG
1	N	331	THR
1	N	351	GLN
1	N	369	VAL
1	N	372	LEU
1	N	398	ASP
1	N	404	ARG
1	N	468	THR
1	N	476	TYR
1	N	483	GLU
1	N	499	VAL
1	N	524	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	343	GLN
1	A	366	GLN
1	A	475	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	GLN
1	B	343	GLN
1	B	401	HIS
1	B	475	ASN
1	C	146	GLN
1	C	265	ASN
1	C	343	GLN
1	C	401	HIS
1	C	475	ASN
1	D	146	GLN
1	D	194	GLN
1	D	265	ASN
1	D	343	GLN
1	D	475	ASN
1	E	146	GLN
1	E	343	GLN
1	E	433	ASN
1	E	475	ASN
1	F	146	GLN
1	F	194	GLN
1	F	229	ASN
1	F	343	GLN
1	F	432	GLN
1	F	475	ASN
1	F	479	ASN
1	G	146	GLN
1	G	265	ASN
1	G	475	ASN
1	H	146	GLN
1	H	351	GLN
1	H	475	ASN
1	I	146	GLN
1	I	265	ASN
1	I	475	ASN
1	J	146	GLN
1	J	326	ASN
1	J	475	ASN
1	K	146	GLN
1	K	229	ASN
1	K	475	ASN
1	K	479	ASN
1	L	146	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	229	ASN
1	L	265	ASN
1	L	475	ASN
1	M	146	GLN
1	M	326	ASN
1	M	351	GLN
1	M	401	HIS
1	M	475	ASN
1	N	146	GLN
1	N	265	ASN
1	N	290	GLN
1	N	326	ASN
1	N	475	ASN
1	N	479	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](#)

There are no ligands in this entry.

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	524/547 (95%)	-0.09	7 (1%) 79 52	64, 70, 74, 93	0
1	B	524/547 (95%)	0.10	12 (2%) 64 33	63, 70, 74, 89	0
1	C	524/547 (95%)	-0.03	5 (0%) 84 60	64, 70, 74, 91	0
1	D	524/547 (95%)	-0.01	1 (0%) 95 87	60, 70, 74, 84	0
1	E	524/547 (95%)	0.13	15 (2%) 55 25	62, 70, 74, 90	0
1	F	524/547 (95%)	0.10	9 (1%) 73 44	62, 70, 74, 91	0
1	G	524/547 (95%)	-0.07	1 (0%) 95 87	61, 70, 74, 85	0
1	H	524/547 (95%)	-0.04	3 (0%) 90 73	62, 71, 73, 90	0
1	I	524/547 (95%)	0.15	23 (4%) 38 15	62, 71, 73, 96	0
1	J	524/547 (95%)	0.08	15 (2%) 55 25	62, 71, 73, 90	0
1	K	524/547 (95%)	0.20	27 (5%) 31 12	61, 70, 73, 87	0
1	L	524/547 (95%)	0.06	9 (1%) 73 44	61, 71, 73, 92	0
1	M	524/547 (95%)	-0.02	6 (1%) 82 57	61, 70, 73, 96	0
1	N	524/547 (95%)	-0.07	5 (0%) 84 60	62, 71, 74, 93	0
All	All	7336/7658 (95%)	0.04	138 (1%) 70 40	60, 70, 74, 96	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	481	ALA	5.9
1	K	266	THR	5.5
1	M	481	ALA	5.1
1	A	481	ALA	4.9
1	A	480	ALA	4.7
1	I	480	ALA	4.7
1	E	478	TYR	4.5
1	K	233	MET	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	483	GLU	4.2
1	J	44	PHE	4.2
1	F	477	GLY	4.2
1	C	478	TYR	3.9
1	K	223	ALA	3.9
1	K	312	ALA	3.9
1	I	477	GLY	3.8
1	E	272	LYS	3.8
1	L	266	THR	3.8
1	K	273	VAL	3.7
1	M	480	ALA	3.5
1	A	478	TYR	3.5
1	I	266	THR	3.5
1	K	264	VAL	3.5
1	K	234	LEU	3.5
1	D	266	THR	3.2
1	F	234	LEU	3.2
1	J	480	ALA	3.1
1	J	234	LEU	3.1
1	J	233	MET	3.1
1	K	245	LYS	3.0
1	K	203	TYR	3.0
1	K	313	THR	3.0
1	A	479	ASN	2.9
1	E	245	LYS	2.9
1	I	270	ILE	2.9
1	E	481	ALA	2.9
1	L	233	MET	2.9
1	M	485	TYR	2.8
1	L	481	ALA	2.8
1	L	268	ARG	2.8
1	B	240	VAL	2.8
1	N	477	GLY	2.8
1	E	271	VAL	2.8
1	J	260	ALA	2.8
1	J	227	ILE	2.7
1	C	485	TYR	2.7
1	J	266	THR	2.7
1	E	238	GLU	2.7
1	J	203	TYR	2.7
1	A	477	GLY	2.6
1	C	480	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	478	TYR	2.6
1	I	246	PRO	2.6
1	B	268	ARG	2.6
1	B	257	GLU	2.6
1	E	485	TYR	2.6
1	B	211	GLY	2.6
1	I	217	SER	2.6
1	I	268	ARG	2.5
1	K	272	LYS	2.5
1	M	478	TYR	2.5
1	B	272	LYS	2.5
1	H	481	ALA	2.5
1	K	268	ARG	2.5
1	M	268	ARG	2.5
1	K	354	GLU	2.5
1	F	481	ALA	2.5
1	L	236	VAL	2.5
1	F	272	LYS	2.5
1	E	214	GLU	2.5
1	K	238	GLU	2.5
1	N	480	ALA	2.5
1	E	203	TYR	2.5
1	K	255	GLU	2.5
1	K	219	PHE	2.5
1	K	311	LYS	2.5
1	F	261	THR	2.4
1	I	482	THR	2.4
1	I	264	VAL	2.4
1	L	478	TYR	2.4
1	B	271	VAL	2.4
1	K	220	ILE	2.4
1	J	273	VAL	2.4
1	E	247	LEU	2.4
1	L	238	GLU	2.4
1	J	272	LYS	2.4
1	K	236	VAL	2.4
1	K	262	LEU	2.4
1	L	234	LEU	2.4
1	C	477	GLY	2.4
1	E	305	ILE	2.4
1	I	233	MET	2.3
1	A	483	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	247	LEU	2.3
1	H	268	ARG	2.3
1	K	244	GLY	2.3
1	B	265	ASN	2.3
1	C	481	ALA	2.3
1	E	477	GLY	2.3
1	I	271	VAL	2.3
1	J	247	LEU	2.3
1	K	222	LEU	2.3
1	E	231	ARG	2.3
1	I	485	TYR	2.3
1	J	268	ARG	2.3
1	B	238	GLU	2.3
1	F	238	GLU	2.3
1	B	247	LEU	2.3
1	I	236	VAL	2.3
1	I	247	LEU	2.2
1	F	273	VAL	2.2
1	L	477	GLY	2.2
1	I	478	TYR	2.2
1	I	272	LYS	2.2
1	I	319	GLN	2.2
1	F	237	LEU	2.2
1	J	267	MET	2.2
1	J	312	ALA	2.2
1	A	485	TYR	2.1
1	B	274	ALA	2.1
1	F	214	GLU	2.1
1	I	262	LEU	2.1
1	E	260	ALA	2.1
1	K	240	VAL	2.1
1	E	266	THR	2.1
1	G	203	TYR	2.1
1	N	485	TYR	2.1
1	N	478	TYR	2.1
1	K	260	ALA	2.1
1	K	249	ILE	2.1
1	I	267	MET	2.1
1	K	221	LEU	2.0
1	I	255	GLU	2.0
1	I	313	THR	2.0
1	M	484	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	275	ALA	2.0
1	B	234	LEU	2.0
1	H	271	VAL	2.0
1	N	264	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.