



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:54 AM UTC

PDB ID : 2NWC / pdb_00002nwc
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

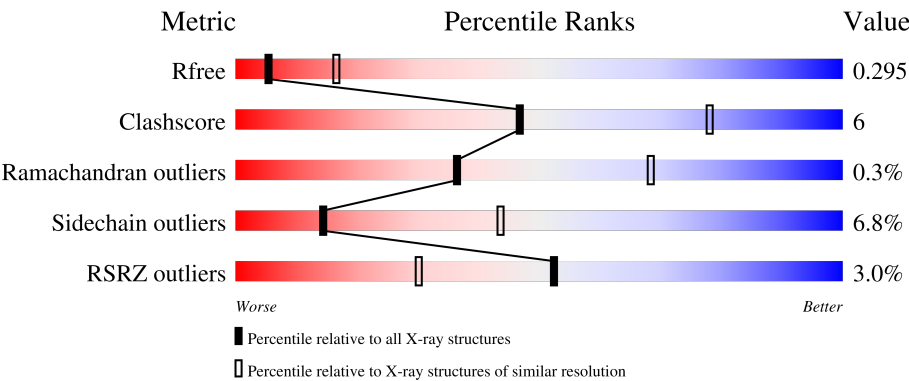
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 80% 15% ...
1	B	547	3% 80% 14% ...
1	C	547	% 79% 14% ...
1	D	547	% 78% 15% ...
1	E	547	5% 79% 14% ...

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Mol	Chain	Length	Quality of chain
1	F	547	4% 80% 14% . .
1	G	547	% 81% 13% . .
1	H	547	% 82% 11% . .
1	I	547	4% 78% 16% . .
1	J	547	5% 79% 14% . .
1	K	547	7% 80% 12% . .
1	L	547	5% 78% 16% . .
1	M	547	% 81% 12% . .
1	N	547	% 78% 15% . .

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.

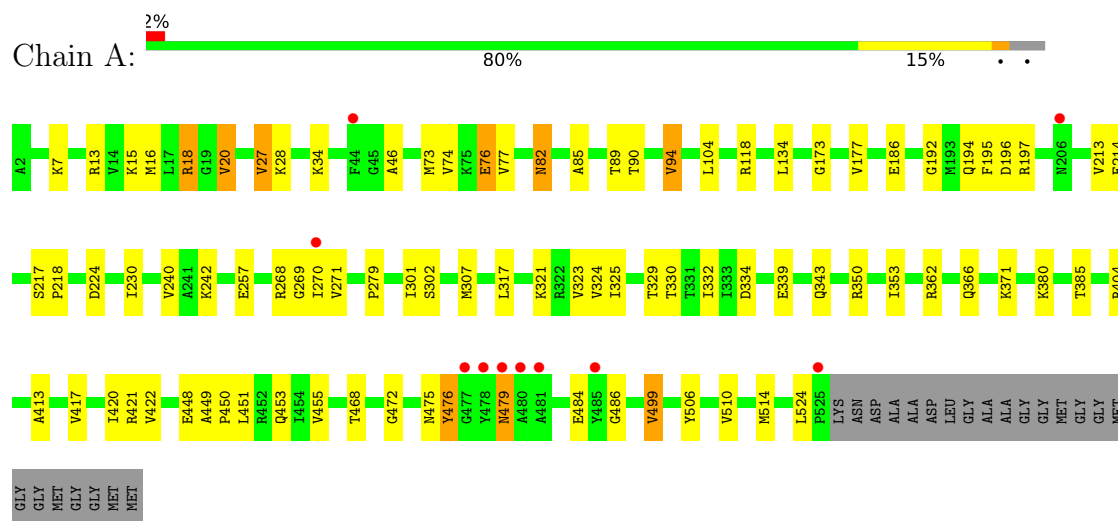
- Molecule 1 is a protein called 60 kDa chaperonin.

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			

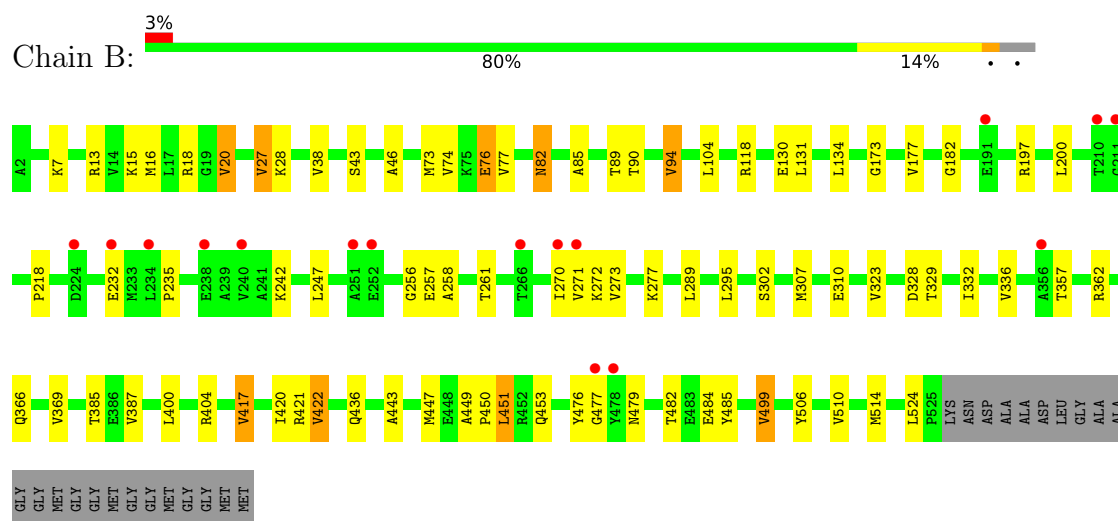
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

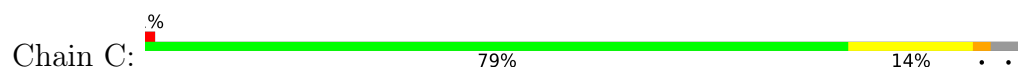
- Molecule 1: 60 kDa chaperonin

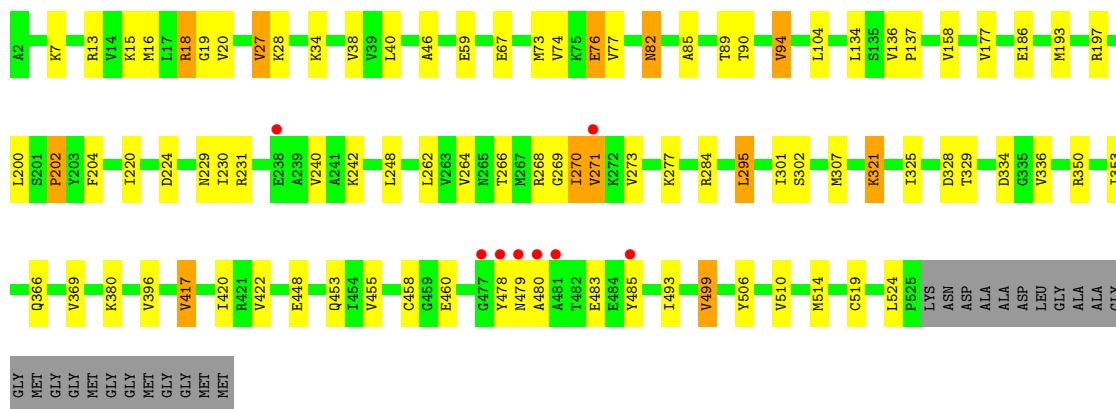


- Molecule 1: 60 kDa chaperonin

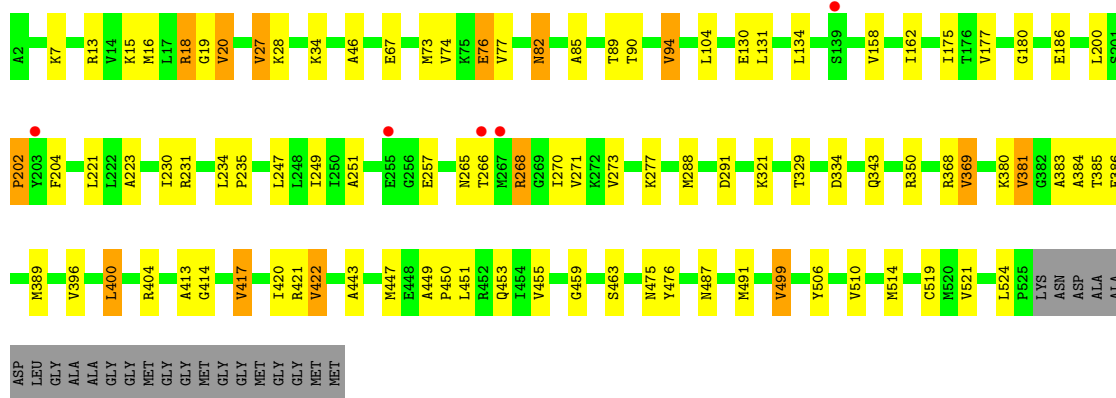
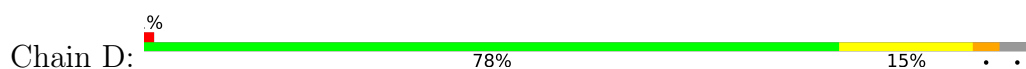


- Molecule 1: 60 kDa chaperonin

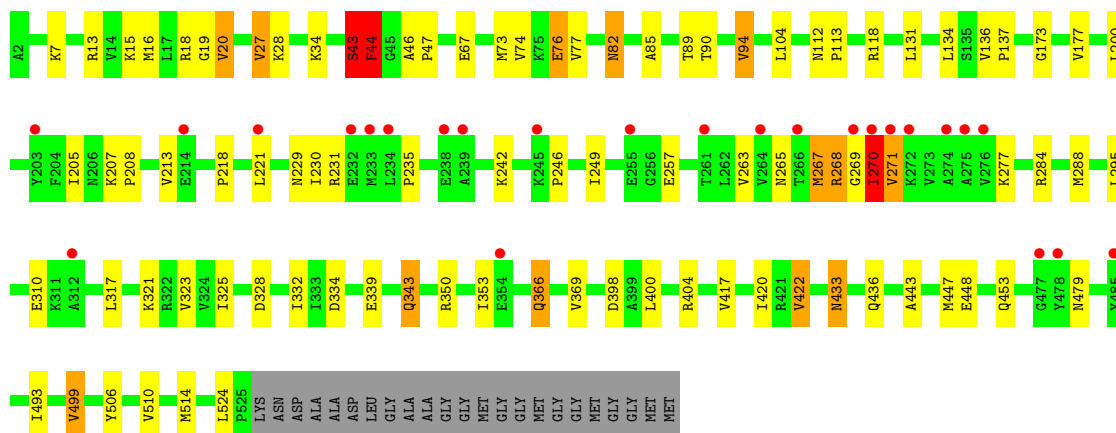
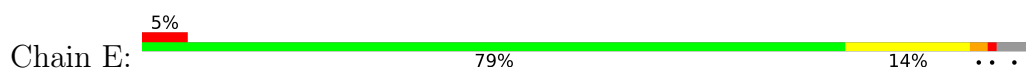




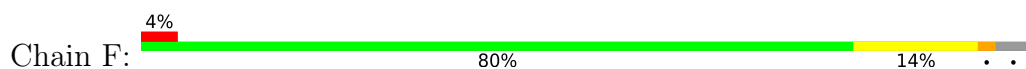
• Molecule 1: 60 kDa chaperonin

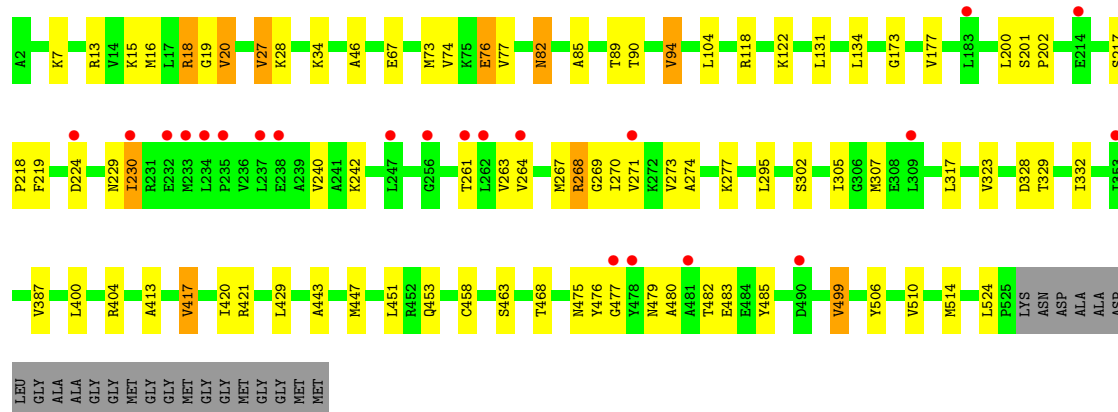


• Molecule 1: 60 kDa chaperonin

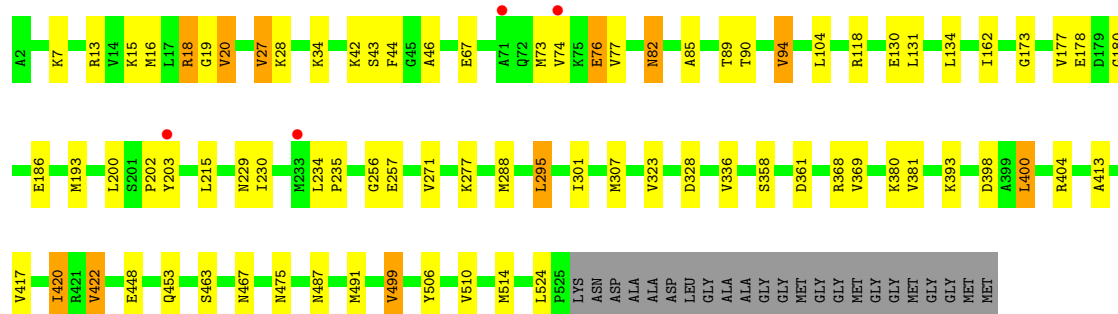
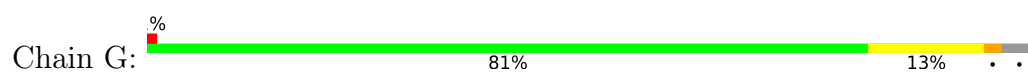


• Molecule 1: 60 kDa chaperonin

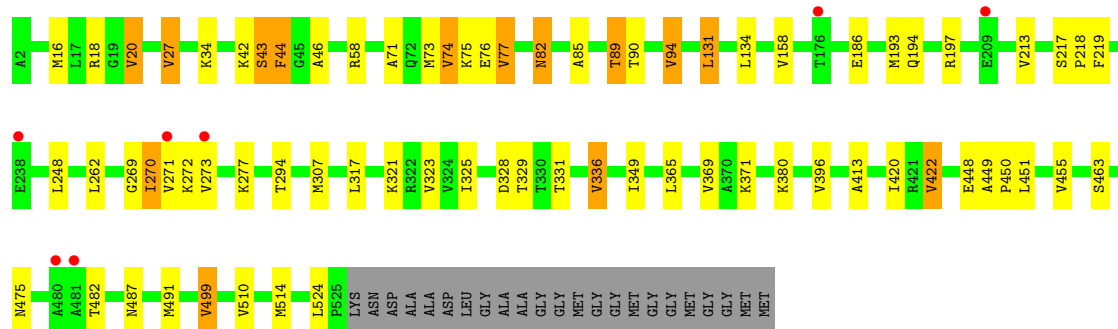
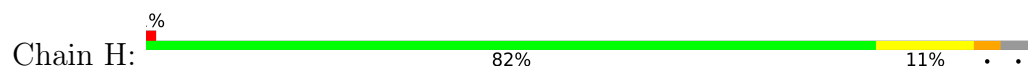




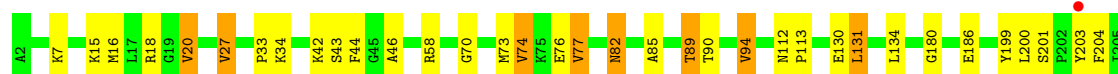
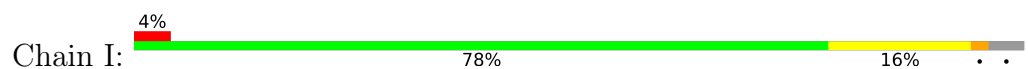
• Molecule 1: 60 kDa chaperonin

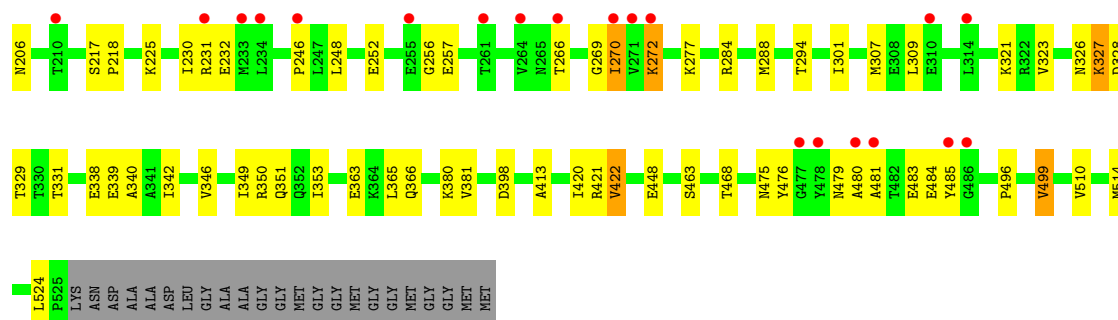


• Molecule 1: 60 kDa chaperonin

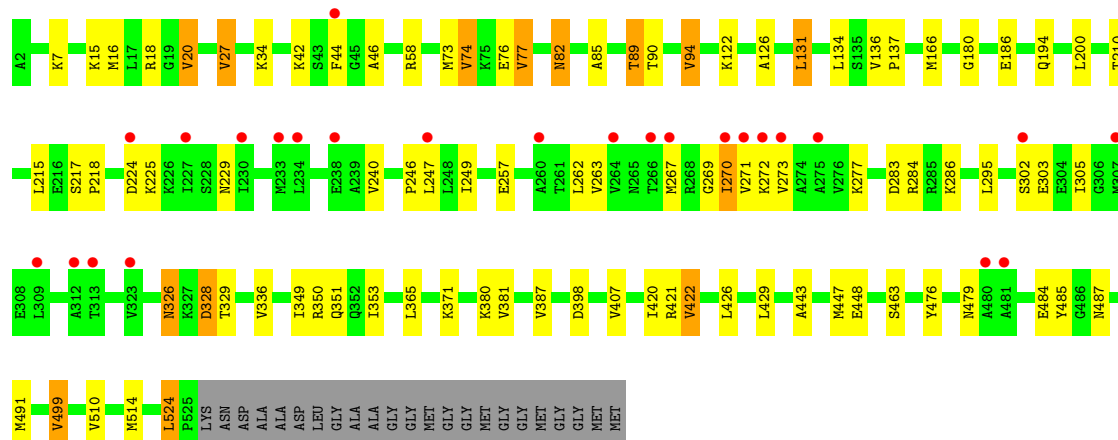
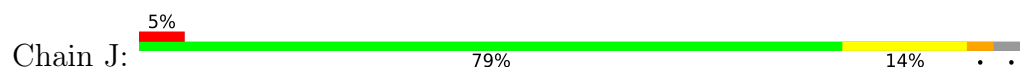


• Molecule 1: 60 kDa chaperonin

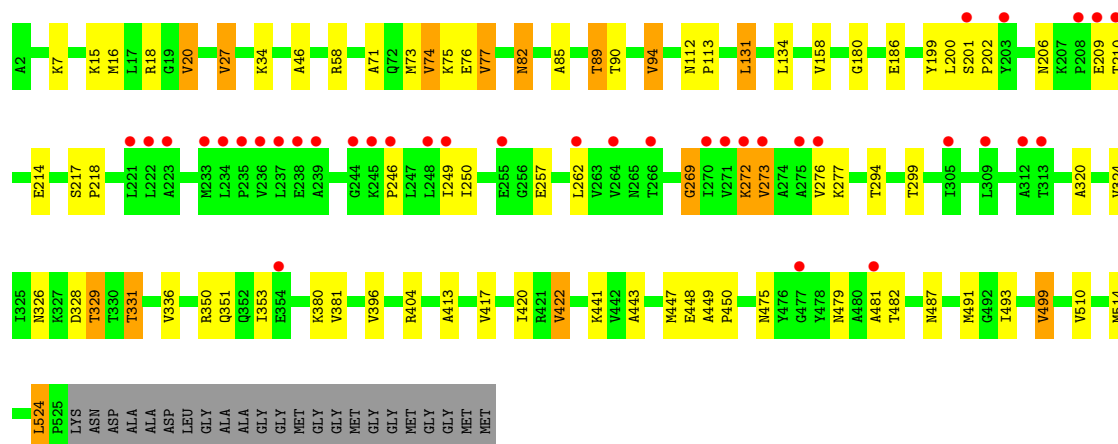
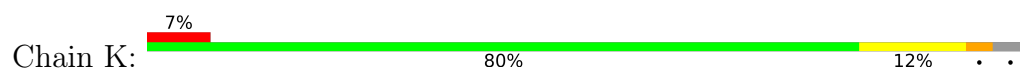




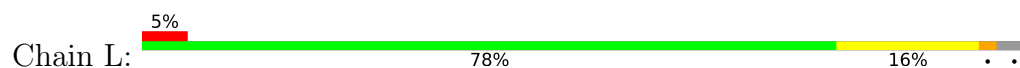
- Molecule 1: 60 kDa chaperonin



- 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 30.00 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-3.02) 99.6 (30.00-3.02)	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 0.270 , 0.295	Depositor DCC
R_{free} test set	10227 reflections (3.49%)	wwPDB-VP
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 , 8.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.46	0/3883	0.84	0/5243
1	B	0.49	2/3883 (0.1%)	0.82	0/5243
1	C	0.46	0/3883	0.84	0/5243
1	D	0.48	0/3883	0.85	0/5243
1	E	0.48	1/3883 (0.0%)	0.90	2/5243 (0.0%)
1	F	0.46	0/3883	0.84	0/5243
1	G	0.45	0/3883	0.87	3/5243 (0.1%)
1	H	0.45	0/3883	0.83	0/5243
1	I	0.47	1/3883 (0.0%)	0.84	0/5243
1	J	0.45	0/3883	0.83	0/5243
1	K	0.46	0/3883	0.83	0/5243
1	L	0.45	0/3883	0.85	1/5243 (0.0%)
1	M	0.47	0/3883	0.85	3/5243 (0.1%)
1	N	0.46	0/3883	0.84	0/5243
All	All	0.46	4/54362 (0.0%)	0.85	9/73402 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	232	GLU	CD-OE2	9.61	1.43	1.25
1	E	267	MET	SD-CE	7.53	1.98	1.79
1	I	327	LYS	CE-NZ	7.03	1.70	1.49
1	B	232	GLU	CD-OE1	5.88	1.36	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	43	SER	N-CA-C	18.05	135.04	113.20
1	E	43	SER	N-CA-CB	-12.07	90.87	110.42
1	G	18	ARG	NE-CZ-NH2	10.99	129.09	119.20
1	G	18	ARG	NE-CZ-NH1	-10.49	111.01	121.50
1	G	18	ARG	CD-NE-CZ	7.33	134.66	124.40
1	M	485	TYR	N-CA-C	6.21	118.53	108.34
1	L	484	GLU	N-CA-C	5.85	116.00	108.34
1	M	207	LYS	CA-C-N	5.67	125.13	119.24
1	M	207	LYS	C-N-CA	5.67	125.13	119.24

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	50	0
1	B	3855	0	3976	45	0
1	C	3855	0	3976	54	0
1	D	3855	0	3976	61	0
1	E	3855	0	3976	58	0
1	F	3855	0	3976	46	0
1	G	3855	0	3976	42	0
1	H	3855	0	3976	36	0
1	I	3855	0	3976	50	0
1	J	3855	0	3976	46	0
1	K	3855	0	3976	45	0
1	L	3855	0	3976	50	0
1	M	3855	0	3976	38	0
1	N	3855	0	3976	51	0
All	All	53970	0	55664	628	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 6.

All (628) 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:NZ	1:I:327:LYS:CE	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:D:384:ALA:C	1:D:385:THR:CG2	2.41	0.93
1:A:76:GLU:HG3	1:G:46:ALA:HB2	1.50	0.93
1:D:46:ALA:CB	1:E:76:GLU:HG3	2.01	0.89
1:D:46:ALA:HB2	1:E:76:GLU:HG3	1.53	0.89
1:I:479:ASN:HB3	1:I:484:GLU:H	1.35	0.89
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:D:384:ALA:C	1:D:385:THR:HG23	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:384:ALA:C	1:D:385:THR:HG22	2.15	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:E:44:PHE:CD1	1:E:44:PHE:C	2.68	0.71
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.73	0.70
1:E:269:GLY:O	1:E:270:ILE:C	2.34	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:NZ	1:I:327:LYS:CD	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:B:13:ARG:HD3	1:B:104:LEU:HD22	1.76	0.68
1:K:487:ASN:O	1:K:491:MET:HG2	1.93	0.68
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.76	0.68
1:F:270:ILE:O	1:G:229:ASN:ND2	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:13:ARG:HD3	1:F:104:LEU:HD22	1.76	0.67
1:K:262:LEU:HD22	1:K:273:VAL:HG11	1.77	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:A:420:ILE:HG12	1:A:448:GLU:HG2	1.79	0.65
1:K:180:GLY:HA3	1:K:381:VAL:O	1.97	0.65
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.79	0.65
1:K:16:MET:HB3	1:K:514:MET:HE3	1.78	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:J:16:MET:HB3	1:J:514:MET:HE3	1.79	0.64
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:I:16:MET:HB3	1:I:514:MET:HE3	1.81	0.63
1:D:288:MET:HG2	1:D:368:ARG:HD3	1.81	0.63
1:E:28:LYS:HE2	1:E:453:GLN:OE1	1.98	0.63
1:N:16:MET:HB3	1:N:514:MET:HE3	1.81	0.62
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:H:449:ALA:HB3	1:H:450:PRO:HD3	1.82	0.61
1:K:46:ALA:HB2	1:L:76:GLU:CG	2.29	0.61
1:L:16:MET:HB3	1:L:514:MET:HE3	1.83	0.61
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.82	0.61
1:H:16:MET:HB3	1:H:514:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:262:LEU:HD22	1:M:273:VAL:HG11	1.81	0.60
1:A:27:VAL:HG13	1:A:90:THR:HG23	1.82	0.60
1:C:193:MET:HB2	1:C:295:LEU:HD13	1.82	0.60
1:L:248:LEU:HD22	1:L:323:VAL:HG21	1.84	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
1:D:291:ASP:OD2	1:D:368:ARG:HD2	2.03	0.59
1:M:16:MET:HB3	1:M:514:MET:HE3	1.85	0.58
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:D:186:GLU:HB2	1:D:380:LYS:HB2	1.85	0.58
1:M:194:GLN:HG3	1:M:331:THR:HB	1.86	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: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:N:186:GLU:HB2	1:N:380:LYS:HB2	1.85	0.58
1:D:130:GLU:HB3	1:D:422:VAL:HG22	1.86	0.57
1:D:221:LEU:HD23	1:D:249:ILE:HG23	1.85	0.57
1:K:200:LEU:HD21	1:K:277:LYS:HG3	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: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:E:27:VAL:CG1	1:E:90:THR:HG23	2.35	0.56
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.36	0.56
1:D:343:GLN:HA	1:D:343:GLN:HE21	1.70	0.56
1:E:321:LYS:HB3	1:E:334:ASP:HB3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:166:MET:HE1	1:N:407:VAL:HG21	1.88	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:L:16:MET:SD	1:L:73:MET:HE1	2.47	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:B:16:MET:SD	1:B:73:MET:HE1	2.46	0.55
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.37	0.55
1:C:40:LEU:HD22	1:C:59:GLU:HG3	1.87	0.55
1:B:479:ASN:CG	1:B:482:THR:HG22	2.30	0.55
1:E:16:MET:SD	1:E:73:MET:HE1	2.47	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:G:16:MET:SD	1:G:73:MET:HE1	2.46	0.54
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.37	0.54
1:C:27:VAL:CG1	1:C: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:B:182:GLY:HA2	1:C:284:ARG:HH21	1.73	0.54
1:I:131:LEU:HD13	1:I:422:VAL:HG21	1.90	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:M:16:MET:SD	1:M:73:MET:HE1	2.49	0.53
1:D:270:ILE:O	1:E:229:ASN:ND2	2.42	0.53
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.90	0.53
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.91	0.53
1:E:34:LYS:HE3	1:F:118:ARG:HH22	1.74	0.53
1:A:77:VAL:HG21	1:A:510:VAL:HB	1.90	0.53
1:D:131:LEU:HD13	1:D:422:VAL:HG21	1.91	0.53
1:I:16:MET:SD	1:I:73:MET:HE1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:283:ASP:HA	1:J:286:LYS:HE2	1.90	0.53
1:K:479:ASN:HD21	1:K:481:ALA:HB3	1.74	0.53
1:N:240:VAL:HG11	1:N:247:LEU:HB2	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:HB3	1:L:18:ARG:HH11	1.74	0.52
1:K:413:ALA:HB2	1:K:475:ASN:HD22	1.75	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:L:224:ASP:CB	1:L:302:SER:HA	2.40	0.52
1:N:18:ARG:HB3	1:N:18:ARG:HH11	1.75	0.52
1:E:221:LEU:HD23	1:E:249:ILE:HG23	1.92	0.52
1:E:269:GLY:C	1:F:229:ASN:HD21	2.18	0.52
1:F:16:MET:SD	1:F:73:MET:HE1	2.49	0.52
1:C:16:MET:SD	1:C:73:MET:HE1	2.49	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:N:16:MET:SD	1:N:73:MET:HE1	2.50	0.52
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.92	0.52
1:I:413:ALA:HB2	1:I:475:ASN:HD22	1.74	0.52
1:M:223:ALA:O	1:M:251:ALA:HA	2.10	0.52
1:L:197:ARG:HD2	1:L:277:LYS:HB2	1.91	0.52
1:I:18:ARG:HH11	1:I:18:ARG:HB3	1.75	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:N:248:LEU:HD22	1:N:323:VAL:HG21	1.92	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:F:16:MET:HG2	1:F:514:MET:HE3	1.92	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:A:16:MET:SD	1:A:73:MET:HE1	2.50	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:A:224:ASP:HB3	1:A:302:SER:HA	1.91	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:J:487:ASN:O	1:J:491:MET:HG2	2.10	0.51
1:K:16:MET:SD	1:K:73:MET:HE1	2.49	0.51
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.92	0.51
1:B:77:VAL:HG21	1:B:510:VAL:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:GLU:CG	1:N:46:ALA:HB2	2.36	0.51
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.93	0.51
1:J:166:MET:HE1	1:J:407:VAL:HG21	1.91	0.51
1:L:223:ALA:HB3	1:L:251:ALA:HB2	1.92	0.51
1:N:413:ALA:HB2	1:N:475:ASN:HD22	1.76	0.51
1:B:197:ARG:HD2	1:B:277:LYS:HB2	1.92	0.51
1:F:173:GLY:O	1:F:404:ARG:NH2	2.44	0.51
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.11	0.51
1:K:18:ARG:HH11	1:K:18:ARG:HB3	1.76	0.51
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.93	0.51
1:N:321:LYS:HB2	1:N:334:ASP:HB3	1.93	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:16:MET:SD	1:J:73:MET:HE1	2.51	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:C:366:GLN:HA	1:C:369:VAL:HG22	1.92	0.50
1:D:16:MET:SD	1:D:73:MET:HE1	2.51	0.50
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:H:43:SER:O	1:H:44:PHE:HB3	2.11	0.50
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.92	0.50
1:L:420:ILE:HG12	1:L:448:GLU:HG2	1.93	0.50
1:L:421:ARG:NH2	1:L:476:TYR:O	2.42	0.50
1:D:223:ALA:O	1:D:251:ALA:HA	2.12	0.50
1:B:7:LYS:HE3	1:B:15:LYS:HE3	1.93	0.50
1:B:131:LEU:HD13	1:B:422:VAL:HG21	1.92	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:E:343:GLN:HE21	1:E:343:GLN:HA	1.76	0.50
1:K:217:SER:N	1:K:218:PRO:HD3	2.26	0.50
1:B:366:GLN:HA	1:B:369:VAL:HG22	1.93	0.50
1:F:7:LYS:HE3	1:F:15:LYS:HE3	1.94	0.50
1:K:218:PRO:HB3	1:K:246:PRO:HB2	1.93	0.50
1:M:271:VAL:HG12	1:M:272:LYS:N	2.27	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:N:77:VAL:HG21	1:N:510:VAL:HB	1.94	0.50
1:I:270:ILE:O	1:J:229:ASN:ND2	2.45	0.50
1:K:479:ASN:ND2	1:K:493:ILE:HD11	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.93	0.50
1:B:130:GLU:HB3	1:B:422:VAL:HG22	1.94	0.49
1:E:265:ASN:O	1:E:270:ILE:CG1	2.60	0.49
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.94	0.49
1:J:421:ARG:NH2	1:J:476:TYR:O	2.45	0.49
1:A:192:GLY:HA2	1:A:332:ILE:O	2.12	0.49
1:A:362:ARG:HG2	1:A:366:GLN:HE21	1.77	0.49
1:C:82:ASN:HB2	1:C:89:THR:OG1	2.12	0.49
1:J:218:PRO:HB3	1:J:246:PRO:HB2	1.94	0.49
1:L:42:LYS:HG3	1:L:44:PHE:CZ	2.47	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:E:7:LYS:HE3	1:E:15:LYS:HE3	1.95	0.49
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.95	0.49
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.94	0.49
1:E:82:ASN:HB2	1:E:89:THR:OG1	2.12	0.49
1:H:16:MET:SD	1:H:73:MET:HE1	2.53	0.49
1:N:90:THR:O	1:N:94:VAL:HG13	2.12	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:28:LYS:HE2	1:C:453:GLN:OE1	2.13	0.48
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.95	0.48
1:C:16:MET:HG2	1:C:514:MET:HE3	1.95	0.48
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.94	0.48
1:E:479:ASN:HD22	1:E:493:ILE:CD1	2.26	0.48
1:K:90:THR:O	1:K:94:VAL:HG13	2.13	0.48
1:L:262:LEU:HD22	1:L:273:VAL:HG11	1.96	0.48
1:A:82:ASN:HB2	1:A:89:THR:OG1	2.12	0.48
1:B:477:GLY:O	1:B:485:TYR:HA	2.14	0.48
1:I:476:TYR:CE2	1:I:485:TYR:HB3	2.48	0.48
1:N:223:ALA:O	1:N:251:ALA:HA	2.13	0.48
1:A:7:LYS:HE3	1:A:15:LYS:HE3	1.95	0.48
1:F:302:SER:H	1:F:307:MET:HE3	1.77	0.48
1:K:404:ARG:HA	1:K:404:ARG:HH11	1.78	0.48
1:A:16:MET:HG2	1:A:514:MET:HE3	1.96	0.48
1:E:16:MET:HG2	1:E:514:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:421:ARG:NH2	1:B:476:TYR:O	2.41	0.48
1:F:264:VAL:O	1:F:268:ARG:HG3	2.14	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:I:420:ILE:HG12	1:I:448:GLU:HG2	1.95	0.47
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.96	0.47
1:F:122:LYS:HE2	1:F:429:LEU:HD11	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:D:7:LYS:HE3	1:D:15:LYS:HE3	1.95	0.47
1:J:270:ILE:HG22	1:J:271:VAL:N	2.30	0.47
1:A:323:VAL:HG12	1:A:332:ILE:HA	1.97	0.47
1:B:357:THR:HA	1:B:362:ARG:HH22	1.78	0.47
1:E:43:SER:HB2	1:E:44:PHE:HB3	1.96	0.47
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.95	0.47
1:D:459:GLY:HA3	1:E:112:ASN:HD22	1.80	0.47
1:J:225:LYS:HE2	1:J:303:GLU:HB3	1.95	0.47
1:L:174:VAL:HB	1:L:376:VAL:HG22	1.95	0.47
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.96	0.47
1:A:479:ASN:HB3	1:A:484:GLU:H	1.80	0.47
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.96	0.47
1:I:180:GLY:HA3	1:I:381:VAL:O	2.13	0.47
1:I:218:PRO:HB3	1:I:246:PRO:HB2	1.95	0.47
1:C:350:ARG:HA	1:C:353:ILE:HD12	1.96	0.47
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.97	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
1:M:90:THR:O	1:M:94:VAL:HG13	2.14	0.47
1:N:193:MET:HE3	1:N:371:LYS:HD3	1.96	0.47
1:A:321:LYS:HB2	1:A:334:ASP:HB3	1.96	0.47
1:C:202:PRO:C	1:C:204:PHE:H	2.22	0.47
1:F:217:SER:N	1:F:218:PRO:HD3	2.30	0.47
1:G:42:LYS:C	1:G:44:PHE:H	2.23	0.47
1:J:326:ASN:HD22	1:J:328:ASP:H	1.63	0.47
1:C:7:LYS:HE3	1:C:15:LYS:HE3	1.96	0.47
1:C:34:LYS:HD2	1:C:458:CYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:271:VAL:O	1:L:273:VAL:HG23	2.15	0.47
1:M:248:LEU:HD13	1:M:325:ILE:HD11	1.97	0.47
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.98	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:A:476:TYR:C	1:A:476:TYR:CD2	2.93	0.46
1:I:350:ARG:HA	1:I:353:ILE:HD12	1.96	0.46
1:M:421:ARG:NH1	1:M:469:VAL:O	2.45	0.46
1:C:197:ARG:HD2	1:C:277:LYS:HB2	1.98	0.46
1:F:224:ASP:HB3	1:F:302:SER:HA	1.97	0.46
1:L:487:ASN:O	1:L:491:MET:HG2	2.16	0.46
1:M:20:VAL:HB	1:M:74:VAL:HG11	1.97	0.46
1:J:42:LYS:C	1:J:44:PHE:H	2.24	0.46
1:C:479:ASN:HB3	1:C:493:ILE:HD13	1.97	0.46
1:F:34:LYS:HE3	1:G:118:ARG:HH22	1.81	0.46
1:G:28:LYS:HE2	1:G:453:GLN:OE1	2.16	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:N:476:TYR:CD2	1:N:476:TYR:C	2.93	0.46
1:A:194:GLN:O	1:A:371:LYS:HE3	2.16	0.46
1:D:34:LYS:HE3	1:E:118:ARG:NH2	2.31	0.46
1:D:414:GLY:O	1:D:417:VAL:HG13	2.15	0.46
1:G:16:MET:HG2	1:G:514:MET:HE3	1.98	0.46
1:N:350:ARG:HA	1:N:353:ILE:HD12	1.97	0.46
1:F:458:CYS:SG	1:F:480:ALA:HB1	2.55	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:H:270:ILE:HG22	1:H:271:VAL:N	2.30	0.46
1:B:256:GLY:C	1:B:258:ALA:H	2.24	0.46
1:J:443:ALA:O	1:J:447:MET:HG3	2.16	0.46
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.98	0.45
1:E:90:THR:O	1:E:94:VAL:HG13	2.17	0.45
1:E:284:ARG:O	1:E:288:MET:HG3	2.15	0.45
1:F:305:ILE:HB	1:F:307:MET:HE2	1.98	0.45
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.98	0.45
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.98	0.45
1:K:272:LYS:HE3	1:K:272:LYS:HB2	1.62	0.45
1:L:20:VAL:HB	1:L:74:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:236:VAL:O	1:N:240:VAL:HG23	2.16	0.45
1:A:34:LYS:HE3	1:B:118:ARG:NH2	2.32	0.45
1:B:218:PRO:HG3	1:B:323:VAL:HG22	1.98	0.45
1:C:193:MET:HB2	1:C:295:LEU:CD1	2.44	0.45
1:E:218:PRO:HB3	1:E:246:PRO:HB2	1.98	0.45
1:H:349:ILE:HG23	1:H:365:LEU:HD22	1.98	0.45
1:I:20:VAL:HB	1:I:74:VAL:HG11	1.98	0.45
1:J:194:GLN:O	1:J:371:LYS:HE3	2.17	0.45
1:M:326:ASN:HB2	1:M:329:THR:HB	1.98	0.45
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.98	0.45
1:D:90:THR:O	1:D:94:VAL:HG13	2.17	0.45
1:E:173:GLY:O	1:E:404:ARG:NH2	2.49	0.45
1:J:20:VAL:HB	1:J:74:VAL:HG11	1.98	0.45
1:B:479:ASN:HB2	1:B:484:GLU:O	2.16	0.45
1:H:218:PRO:HG3	1:H:323:VAL:HG12	1.99	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: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:H:20:VAL:HB	1:H:74:VAL:HG11	1.98	0.45
1:N:20:VAL:HB	1:N:74:VAL:HG11	1.97	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:A:350:ARG:HA	1:A:353:ILE:HD12	1.98	0.45
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.99	0.45
1:E:213:VAL:HB	1:E:325:ILE:HB	1.97	0.45
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.47	0.45
1:A:218:PRO:HG3	1:A:323:VAL:HG22	1.99	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:F:90:THR:O	1:F:94:VAL:HG13	2.17	0.45
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.47	0.45
1:B:16:MET:HG2	1:B:514:MET:HE3	1.99	0.44
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.99	0.44
1:D:158:VAL:HG13	1:D:396:VAL:HG22	1.99	0.44
1:D:385:THR:O	1:D:386:GLU:C	2.60	0.44
1:G:178:GLU:HA	1:G:393:LYS:HE3	1.98	0.44
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:193:MET:HE3	1:H:371:LYS:HD3	1.99	0.44
1:A:214:GLU:HG3	1:A:324:VAL:HG22	1.99	0.44
1:C:336:VAL:HG12	1:C:336:VAL:O	2.17	0.44
1:D:487:ASN:O	1:D:491:MET:HG3	2.17	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:G:131:LEU:HD13	1:G:422:VAL:HG21	1.98	0.44
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.98	0.44
1:I:42:LYS:C	1:I:44:PHE:H	2.26	0.44
1:N:479:ASN:ND2	1:N:482:THR:OG1	2.51	0.44
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.99	0.44
1:E:270:ILE:H	1:E:270:ILE:HG12	1.66	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:D:16:MET:HG2	1:D:514:MET:HE3	1.98	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: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:M:218:PRO:HD2	1:M:320:ALA:O	2.17	0.44
1:C:38:VAL:HG22	1:D:519:CYS:HB3	2.00	0.43
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: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:N:248:LEU:HD13	1:N:325:ILE:HD11	1.99	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:I:201:SER:C	1:I:203:TYR:H	2.25	0.43
1:I:272:LYS:HA	1:I:272:LYS:HD3	1.83	0.43
1:J:349:ILE:HG23	1:J:365:LEU:HD22	2.00	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:N:217:SER:HB3	1:N:245:LYS:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:263:VAL:O	1:N:267:MET:HB2	2.17	0.43
1:C:417:VAL:HA	1:C:420:ILE:HG22	2.01	0.43
1:F:77:VAL:HG12	1:F:506:TYR:HB3	2.00	0.43
1:I:349:ILE:HG23	1:I:365:LEU:HD22	2.01	0.43
1:K:206:ASN:HD21	1:K:214:GLU:H	1.66	0.43
1:M:166:MET:HE1	1:M:407:VAL:HG21	2.00	0.43
1:N:336:VAL:HG12	1:N:336:VAL:O	2.19	0.43
1:A:90:THR:O	1:A:94:VAL:HG13	2.18	0.43
1:B:90:THR:O	1:B:94:VAL:HG13	2.19	0.43
1:D:16:MET:O	1:D:20:VAL:HG13	2.19	0.43
1:J:240:VAL:HG21	1:J:247:LEU:HD22	1.99	0.43
1:G:215:LEU:HB2	1:G:323:VAL:HG22	1.99	0.43
1:I:70:GLY:HA2	1:I:73:MET:HE3	2.01	0.43
1:L:350:ARG:HA	1:L:353:ILE:HD12	2.00	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: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:N:176:THR:HG21	1:N:322:ARG:HH12	1.81	0.43
1:B:16:MET:O	1:B:20:VAL:HG13	2.19	0.42
1:C:18:ARG:HE	1:C:18:ARG:HB2	1.62	0.42
1:H:158:VAL:HG13	1:H:396:VAL:HG22	2.00	0.42
1:I:301:ILE:HG23	1:I:307:MET:HB2	2.01	0.42
1:J:326:ASN:ND2	1:J:328:ASP:H	2.17	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:A:472:GLY:HA3	1:A:476:TYR:CD2	2.54	0.42
1:N:27:VAL:CG1	1:N:90:THR:HG23	2.49	0.42
1:N:130:GLU:HB3	1:N:422:VAL:HG13	2.01	0.42
1:A:118:ARG:HH22	1:G:34:LYS:HE3	1.84	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:G:487:ASN:O	1:G:491:MET:HG3	2.19	0.42
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.49	0.42
1:K:324:VAL:HB	1:K:331:THR:HG23	2.01	0.42
1:L:82:ASN:HB2	1:L:89:THR:OG1	2.19	0.42
1:B:302:SER:H	1:B:307:MET:HE3	1.85	0.42
1:D:383:ALA:HB3	1:D:389:MET:HB2	2.01	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:A:451:LEU:O	1:A:455:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:ARG:HG3	1:D:369:VAL:HG11	2.01	0.42
1:D:413:ALA:HB2	1:D:475:ASN:HD22	1.83	0.42
1:H:270:ILE:CG2	1:H:271:VAL:HG23	2.45	0.42
1:N:71:ALA:O	1:N:75:LYS:HB2	2.19	0.42
1:N:197:ARG:HD2	1:N:277:LYS:HB2	2.01	0.42
1:E:112:ASN:HA	1:E:113:PRO:HD3	1.95	0.42
1:I:82:ASN:HB2	1:I:89:THR:OG1	2.19	0.42
1:M:342:ILE:O	1:M:346:VAL:HG23	2.19	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: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: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:C:271:VAL:O	1:C:273:VAL:HG23	2.20	0.42
1:E:207:LYS:HA	1:E:208:PRO:HD3	1.92	0.42
1:K:158:VAL:HG13	1:K:396:VAL:HG22	2.02	0.42
1:F:263:VAL:O	1:F:267:MET:HB2	2.19	0.42
1:F:479:ASN:O	1:F:483:GLU:HA	2.20	0.42
1:H:71:ALA:O	1:H:75:LYS:HB2	2.20	0.42
1:H:413:ALA:HB2	1:H:475:ASN:HD22	1.84	0.42
1:I:421:ARG:NH2	1:I:476:TYR:O	2.51	0.42
1:J:82:ASN:HB2	1:J:89:THR:OG1	2.20	0.42
1:K:443:ALA:O	1:K:447:MET:HG3	2.19	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:N:487:ASN:O	1:N:491:MET:HG2	2.19	0.42
1:D:202:PRO:C	1:D:204:PHE:H	2.28	0.42
1:D:451:LEU:O	1:D:455:VAL:HG23	2.20	0.42
1:E:46:ALA:HA	1:E:47:PRO:HD3	1.95	0.42
1:F:18:ARG:HE	1:F:18:ARG:HB2	1.61	0.42
1:H:420:ILE:HG13	1:H:448:GLU:HG2	2.01	0.42
1:I:338:GLU:C	1:I:340:ALA:H	2.28	0.42
1:I:363:GLU:HA	1:I:366:GLN:HB2	2.02	0.42
1:M:82:ASN:HB2	1:M:89:THR:OG1	2.20	0.41
1:N:213:VAL:HB	1:N:325:ILE:HB	2.02	0.41
1:D:266:THR:HA	1:D:271:VAL:O	2.20	0.41
1:I:199:TYR:OH	1:I:327:LYS:HG2	2.20	0.41
1:L:487:ASN:HB3	1:L:490:ASP:HB2	2.03	0.41
1:C:136:VAL:HA	1:C:137:PRO:HD3	1.90	0.41
1:G:234:LEU:N	1:G:235:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:487:ASN:O	1:H:491:MET:HG2	2.21	0.41
1:I:342:ILE:O	1:I:346:VAL:HG23	2.21	0.41
1:K:524:LEU:HD12	1:K:524:LEU:HA	1.98	0.41
1:D:234:LEU:N	1:D:235:PRO:HD2	2.36	0.41
1:G:288:MET:HG2	1:G:368:ARG:HD3	2.01	0.41
1:K:441:LYS:HA	1:K:441:LYS:HD3	1.87	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:G:90:THR:O	1:G:94:VAL:HG13	2.19	0.41
1:I:496:PRO:HB2	1:I:499:VAL:HG13	2.01	0.41
1:M:7:LYS:HE2	1:M:15:LYS:HE3	2.02	0.41
1:N:217:SER:N	1:N:218:PRO:CD	2.83	0.41
1:A:18:ARG:HE	1:A:18:ARG:HB2	1.61	0.41
1:F:16:MET:O	1:F:20:VAL:HG13	2.21	0.41
1:H:219:PHE:HB3	1:H:317:LEU:HD23	2.02	0.41
1:J:263:VAL:O	1:J:267:MET:HB2	2.20	0.41
1:K:201:SER:HA	1:K:202:PRO:HD3	1.92	0.41
1:A:195:PHE:CE2	1:A:197:ARG:HB2	2.55	0.41
1:C:200:LEU:HD21	1:C:277:LYS:HG3	2.02	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:A:16:MET:O	1:A:20:VAL:HG13	2.21	0.41
1:I:7:LYS:HE2	1:I:15:LYS:HE3	2.03	0.41
1:I:112:ASN:HA	1:I:113:PRO:HD3	1.94	0.41
1:L:218:PRO:HB3	1:L:246:PRO:HB2	2.03	0.41
1:E:19:GLY:HA3	1:E:67:GLU:O	2.21	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:H:27:VAL:CG1	1:H:90:THR:HG23	2.50	0.41
1:I:230:ILE:C	1:I:232:GLU:H	2.29	0.41
1:I:284:ARG:O	1:I:288:MET:HG3	2.21	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:J:126:ALA:HB1	1:J:426:LEU:HD22	2.02	0.41
1:K:71:ALA:O	1:K:75:LYS:HB2	2.21	0.41
1:L:496:PRO:HB2	1:L:499:VAL:HG13	2.03	0.41
1:A:301:ILE:HG23	1:A:307:MET:HB3	2.03	0.41
1:D:18:ARG:HE	1:D:18:ARG:HB2	1.62	0.41
1:E:136:VAL:HA	1:E:137:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:420:ILE:HD12	1:L:451:LEU:HD13	2.03	0.41
1:B:443:ALA:O	1:B:447:MET:HG3	2.21	0.40
1:F:19:GLY:HA3	1:F:67:GLU:O	2.21	0.40
1:G:162:ILE:HG12	1:G:400:LEU:HD23	2.04	0.40
1:G:301:ILE:HG23	1:G:307:MET:HB3	2.03	0.40
1:J:136:VAL:HA	1:J:137:PRO:HD3	1.89	0.40
1:K:7:LYS:HE2	1:K:15:LYS:HE3	2.02	0.40
1:K:199:TYR:HA	1:K:276:VAL:HG12	2.03	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: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:L:248:LEU:HD13	1:L:325:ILE:HD11	2.03	0.40
1:L:476:TYR:CD2	1:L:476:TYR:C	3.00	0.40
1:A:173:GLY:O	1:A:404:ARG:NH2	2.54	0.40
1:A:194:GLN:HA	1:A:330:THR:O	2.21	0.40
1:D:449:ALA:HB3	1:D:450:PRO:HD3	2.03	0.40
1:E:16:MET:O	1:E:20:VAL:HG13	2.22	0.40
1:G:358:SER:HB3	1:G:361:ASP:HB2	2.02	0.40
1:J:217:SER:N	1:J:218:PRO:HD3	2.36	0.40
1:K:479:ASN:HD22	1:K:493:ILE:HD11	1.85	0.40
1:L:201:SER:HA	1:L:202:PRO:HD3	1.97	0.40
1:C:478:TYR:HB2	1:C:485:TYR:CE2	2.56	0.40
1:F:443:ALA:O	1:F:447:MET:HG3	2.21	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:L:455:VAL:HG13	1:L:460:GLU:HB2	2.04	0.40
1:N:209:GLU:CD	1:N:209:GLU:H	2.29	0.40
1:N:272:LYS:HB2	1:N:272:LYS:HE3	1.74	0.40
1:A:413:ALA:HB2	1:A:475:ASN:HD22	1.87	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:E:235:PRO:HG3	1:E:310:GLU:HG3	2.03	0.40
1:N:201:SER:HA	1:N:202:PRO:HD3	1.98	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%)	30	63
1	B	522/547 (95%)	507 (97%)	13 (2%)	2 (0%)	30	63
1	C	522/547 (95%)	507 (97%)	13 (2%)	2 (0%)	30	63
1	D	522/547 (95%)	512 (98%)	9 (2%)	1 (0%)	43	75
1	E	522/547 (95%)	501 (96%)	19 (4%)	2 (0%)	30	63
1	F	522/547 (95%)	507 (97%)	15 (3%)	0	100	100
1	G	522/547 (95%)	509 (98%)	11 (2%)	2 (0%)	30	63
1	H	522/547 (95%)	508 (97%)	11 (2%)	3 (1%)	21	54
1	I	522/547 (95%)	496 (95%)	22 (4%)	4 (1%)	16	48
1	J	522/547 (95%)	505 (97%)	16 (3%)	1 (0%)	43	75
1	K	522/547 (95%)	507 (97%)	14 (3%)	1 (0%)	43	75
1	L	522/547 (95%)	504 (97%)	17 (3%)	1 (0%)	43	75
1	M	522/547 (95%)	505 (97%)	16 (3%)	1 (0%)	43	75
1	N	522/547 (95%)	508 (97%)	12 (2%)	2 (0%)	30	63
All	All	7308/7658 (95%)	7081 (97%)	203 (3%)	24 (0%)	36	68

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

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Mol	Chain	Res	Type
1	I	481	ALA
1	K	269	GLY
1	N	479	ASN
1	H	336	VAL
1	L	43	SER
1	N	486	GLY
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%)	379 (94%)	25 (6%)	16	47
1	B	404/414 (98%)	378 (94%)	26 (6%)	16	46
1	C	404/414 (98%)	381 (94%)	23 (6%)	18	50
1	D	404/414 (98%)	381 (94%)	23 (6%)	18	50
1	E	404/414 (98%)	374 (93%)	30 (7%)	13	40
1	F	404/414 (98%)	378 (94%)	26 (6%)	16	46
1	G	404/414 (98%)	381 (94%)	23 (6%)	18	50
1	H	404/414 (98%)	377 (93%)	27 (7%)	15	44
1	I	404/414 (98%)	375 (93%)	29 (7%)	13	41
1	J	404/414 (98%)	375 (93%)	29 (7%)	13	41
1	K	404/414 (98%)	375 (93%)	29 (7%)	13	41
1	L	404/414 (98%)	372 (92%)	32 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	404/414 (98%)	378 (94%)	26 (6%)	16	46
1	N	404/414 (98%)	367 (91%)	37 (9%)	8	31
All	All	5656/5796 (98%)	5271 (93%)	385 (7%)	14	43

All (385) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	20	VAL
1	A	27	VAL
1	A	74	VAL
1	A	76	GLU
1	A	82	ASN
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	240	VAL
1	A	242	LYS
1	A	257	GLU
1	A	268	ARG
1	A	271	VAL
1	A	317	LEU
1	A	385	THR
1	A	417	VAL
1	A	422	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	27	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

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Mol	Chain	Res	Type
1	B	242	LYS
1	B	261	THR
1	B	271	VAL
1	B	272	LYS
1	B	289	LEU
1	B	295	LEU
1	B	328	ASP
1	B	329	THR
1	B	336	VAL
1	B	385	THR
1	B	387	VAL
1	B	400	LEU
1	B	417	VAL
1	B	422	VAL
1	B	451	LEU
1	B	499	VAL
1	B	524	LEU
1	C	18	ARG
1	C	20	VAL
1	C	27	VAL
1	C	74	VAL
1	C	76	GLU
1	C	82	ASN
1	C	94	VAL
1	C	134	LEU
1	C	177	VAL
1	C	230	ILE
1	C	231	ARG
1	C	240	VAL
1	C	242	LYS
1	C	270	ILE
1	C	271	VAL
1	C	295	LEU
1	C	321	LYS
1	C	328	ASP
1	C	329	THR
1	C	417	VAL
1	C	422	VAL
1	C	499	VAL
1	C	524	LEU
1	D	18	ARG
1	D	20	VAL

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Mol	Chain	Res	Type
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	257	GLU
1	D	265	ASN
1	D	329	THR
1	D	369	VAL
1	D	381	VAL
1	D	400	LEU
1	D	417	VAL
1	D	420	ILE
1	D	422	VAL
1	D	463	SER
1	D	499	VAL
1	D	524	LEU
1	E	18	ARG
1	E	20	VAL
1	E	27	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	317	LEU
1	E	328	ASP
1	E	339	GLU

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Mol	Chain	Res	Type
1	E	343	GLN
1	E	366	GLN
1	E	398	ASP
1	E	400	LEU
1	E	417	VAL
1	E	422	VAL
1	E	433	ASN
1	E	499	VAL
1	E	524	LEU
1	F	18	ARG
1	F	20	VAL
1	F	27	VAL
1	F	74	VAL
1	F	76	GLU
1	F	82	ASN
1	F	94	VAL
1	F	131	LEU
1	F	134	LEU
1	F	177	VAL
1	F	230	ILE
1	F	240	VAL
1	F	242	LYS
1	F	268	ARG
1	F	271	VAL
1	F	295	LEU
1	F	328	ASP
1	F	329	THR
1	F	387	VAL
1	F	400	LEU
1	F	417	VAL
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	27	VAL
1	G	74	VAL
1	G	76	GLU
1	G	82	ASN
1	G	94	VAL

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Mol	Chain	Res	Type
1	G	134	LEU
1	G	177	VAL
1	G	230	ILE
1	G	257	GLU
1	G	271	VAL
1	G	295	LEU
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	20	VAL
1	H	27	VAL
1	H	34	LYS
1	H	42	LYS
1	H	58	ARG
1	H	74	VAL
1	H	77	VAL
1	H	82	ASN
1	H	89	THR
1	H	94	VAL
1	H	131	LEU
1	H	134	LEU
1	H	270	ILE
1	H	272	LYS
1	H	294	THR
1	H	307	MET
1	H	321	LYS
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	336	VAL
1	H	369	VAL
1	H	422	VAL
1	H	463	SER
1	H	482	THR
1	H	499	VAL

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Mol	Chain	Res	Type
1	H	524	LEU
1	I	20	VAL
1	I	27	VAL
1	I	34	LYS
1	I	58	ARG
1	I	74	VAL
1	I	77	VAL
1	I	82	ASN
1	I	89	THR
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	252	GLU
1	I	270	ILE
1	I	272	LYS
1	I	294	THR
1	I	321	LYS
1	I	328	ASP
1	I	331	THR
1	I	339	GLU
1	I	351	GLN
1	I	398	ASP
1	I	422	VAL
1	I	463	SER
1	I	468	THR
1	I	499	VAL
1	I	524	LEU
1	J	20	VAL
1	J	27	VAL
1	J	34	LYS
1	J	58	ARG
1	J	74	VAL
1	J	77	VAL
1	J	82	ASN
1	J	89	THR
1	J	94	VAL
1	J	131	LEU
1	J	134	LEU
1	J	210	THR

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Mol	Chain	Res	Type
1	J	249	ILE
1	J	257	GLU
1	J	270	ILE
1	J	272	LYS
1	J	284	ARG
1	J	295	LEU
1	J	305	ILE
1	J	326	ASN
1	J	328	ASP
1	J	329	THR
1	J	351	GLN
1	J	387	VAL
1	J	398	ASP
1	J	422	VAL
1	J	463	SER
1	J	499	VAL
1	J	524	LEU
1	K	20	VAL
1	K	27	VAL
1	K	34	LYS
1	K	58	ARG
1	K	74	VAL
1	K	77	VAL
1	K	82	ASN
1	K	89	THR
1	K	94	VAL
1	K	131	LEU
1	K	134	LEU
1	K	209	GLU
1	K	210	THR
1	K	249	ILE
1	K	250	ILE
1	K	272	LYS
1	K	273	VAL
1	K	294	THR
1	K	299	THR
1	K	328	ASP
1	K	329	THR
1	K	331	THR
1	K	336	VAL
1	K	351	GLN
1	K	417	VAL

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Mol	Chain	Res	Type
1	K	422	VAL
1	K	482	THR
1	K	499	VAL
1	K	524	LEU
1	L	20	VAL
1	L	27	VAL
1	L	34	LYS
1	L	58	ARG
1	L	74	VAL
1	L	77	VAL
1	L	82	ASN
1	L	89	THR
1	L	94	VAL
1	L	131	LEU
1	L	134	LEU
1	L	207	LYS
1	L	209	GLU
1	L	229	ASN
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	317	LEU
1	L	328	ASP
1	L	329	THR
1	L	336	VAL
1	L	363	GLU
1	L	417	VAL
1	L	422	VAL
1	L	425	LYS
1	L	468	THR
1	L	499	VAL
1	L	524	LEU
1	M	20	VAL
1	M	27	VAL
1	M	34	LYS
1	M	42	LYS
1	M	58	ARG
1	M	74	VAL

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Mol	Chain	Res	Type
1	M	77	VAL
1	M	82	ASN
1	M	89	THR
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	309	LEU
1	M	328	ASP
1	M	339	GLU
1	M	343	GLN
1	M	387	VAL
1	M	417	VAL
1	M	422	VAL
1	M	499	VAL
1	M	524	LEU
1	N	20	VAL
1	N	27	VAL
1	N	34	LYS
1	N	43	SER
1	N	58	ARG
1	N	74	VAL
1	N	77	VAL
1	N	82	ASN
1	N	89	THR
1	N	94	VAL
1	N	131	LEU
1	N	134	LEU
1	N	209	GLU
1	N	210	THR
1	N	245	LYS
1	N	257	GLU
1	N	267	MET
1	N	270	ILE
1	N	272	LYS
1	N	294	THR
1	N	309	LEU
1	N	315	GLU

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Mol	Chain	Res	Type
1	N	317	LEU
1	N	321	LYS
1	N	329	THR
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	417	VAL
1	N	468	THR
1	N	476	TYR
1	N	483	GLU
1	N	499	VAL
1	N	524	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	82	ASN
1	A	146	GLN
1	A	343	GLN
1	A	366	GLN
1	A	475	ASN
1	B	82	ASN
1	B	146	GLN
1	B	153	ASN
1	B	343	GLN
1	B	348	GLN
1	B	475	ASN
1	C	82	ASN
1	C	146	GLN
1	C	153	ASN
1	C	265	ASN
1	C	343	GLN
1	C	401	HIS
1	C	453	GLN
1	D	37	ASN
1	D	82	ASN
1	D	146	GLN
1	D	265	ASN

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Mol	Chain	Res	Type
1	D	290	GLN
1	D	343	GLN
1	D	475	ASN
1	E	37	ASN
1	E	82	ASN
1	E	146	GLN
1	E	343	GLN
1	E	351	GLN
1	E	433	ASN
1	E	475	ASN
1	E	479	ASN
1	F	82	ASN
1	F	146	GLN
1	F	229	ASN
1	F	319	GLN
1	F	343	GLN
1	F	348	GLN
1	F	432	GLN
1	F	475	ASN
1	F	479	ASN
1	G	82	ASN
1	G	146	GLN
1	G	265	ASN
1	G	453	GLN
1	G	475	ASN
1	H	82	ASN
1	H	97	GLN
1	H	146	GLN
1	H	351	GLN
1	H	453	GLN
1	H	475	ASN
1	I	82	ASN
1	I	146	GLN
1	I	265	ASN
1	I	453	GLN
1	I	475	ASN
1	J	82	ASN
1	J	146	GLN
1	J	194	GLN
1	J	326	ASN
1	J	348	GLN
1	J	453	GLN

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Mol	Chain	Res	Type
1	J	475	ASN
1	K	82	ASN
1	K	453	GLN
1	K	475	ASN
1	K	479	ASN
1	L	82	ASN
1	L	146	GLN
1	L	229	ASN
1	L	265	ASN
1	L	290	GLN
1	L	343	GLN
1	L	352	GLN
1	L	475	ASN
1	M	82	ASN
1	M	146	GLN
1	M	194	GLN
1	M	326	ASN
1	M	351	GLN
1	M	475	ASN
1	N	82	ASN
1	N	229	ASN
1	N	265	ASN
1	N	290	GLN
1	N	326	ASN
1	N	352	GLN
1	N	475	ASN
1	N	479	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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%)	0.34	10 (1%) 66 43	64, 70, 74, 93	0
1	B	524/547 (95%)	0.48	16 (3%) 51 30	63, 70, 74, 89	0
1	C	524/547 (95%)	0.38	8 (1%) 72 49	64, 70, 74, 91	0
1	D	524/547 (95%)	0.44	5 (0%) 79 59	60, 70, 74, 84	0
1	E	524/547 (95%)	0.59	25 (4%) 35 18	62, 70, 74, 90	0
1	F	524/547 (95%)	0.55	22 (4%) 40 22	62, 70, 74, 91	0
1	G	524/547 (95%)	0.43	4 (0%) 82 64	61, 70, 74, 85	0
1	H	524/547 (95%)	0.32	7 (1%) 75 53	62, 71, 73, 90	0
1	I	524/547 (95%)	0.52	21 (4%) 42 23	62, 71, 73, 96	0
1	J	524/547 (95%)	0.55	25 (4%) 35 18	62, 71, 73, 90	0
1	K	524/547 (95%)	0.61	37 (7%) 22 11	61, 70, 73, 87	0
1	L	524/547 (95%)	0.51	27 (5%) 33 16	61, 70, 73, 92	0
1	M	524/547 (95%)	0.38	6 (1%) 78 57	61, 70, 73, 96	0
1	N	524/547 (95%)	0.39	7 (1%) 75 53	62, 71, 74, 93	0
All	All	7336/7658 (95%)	0.46	220 (2%) 52 30	60, 70, 74, 96	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	480	ALA	5.5
1	A	480	ALA	5.5
1	K	266	THR	5.4
1	N	480	ALA	4.7
1	I	477	GLY	4.7
1	E	271	VAL	4.6
1	J	480	ALA	4.6
1	M	480	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	271	VAL	4.3
1	I	481	ALA	4.3
1	K	233	MET	4.2
1	L	266	THR	4.1
1	M	478	TYR	4.0
1	C	478	TYR	4.0
1	K	234	LEU	4.0
1	H	480	ALA	3.9
1	E	478	TYR	3.8
1	J	233	MET	3.8
1	N	477	GLY	3.8
1	F	234	LEU	3.8
1	K	236	VAL	3.7
1	D	266	THR	3.7
1	K	223	ALA	3.6
1	H	481	ALA	3.6
1	E	272	LYS	3.5
1	F	214	GLU	3.4
1	K	275	ALA	3.4
1	K	264	VAL	3.4
1	A	479	ASN	3.3
1	K	271	VAL	3.3
1	A	481	ALA	3.3
1	K	312	ALA	3.3
1	A	478	TYR	3.3
1	E	270	ILE	3.3
1	B	478	TYR	3.2
1	N	478	TYR	3.2
1	K	273	VAL	3.2
1	L	270	ILE	3.2
1	K	238	GLU	3.2
1	E	203	TYR	3.2
1	M	481	ALA	3.2
1	F	477	GLY	3.2
1	L	477	GLY	3.1
1	F	309	LEU	3.1
1	J	44	PHE	3.1
1	K	208	PRO	3.1
1	L	271	VAL	3.1
1	F	261	THR	3.1
1	I	266	THR	3.1
1	L	234	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	477	GLY	3.0
1	K	244	GLY	3.0
1	B	271	VAL	3.0
1	C	479	ASN	3.0
1	G	203	TYR	3.0
1	D	255	GLU	2.9
1	H	238	GLU	2.9
1	J	481	ALA	2.9
1	L	236	VAL	2.9
1	B	224	ASP	2.9
1	D	203	TYR	2.9
1	E	269	GLY	2.9
1	L	309	LEU	2.9
1	E	245	LYS	2.9
1	L	203	TYR	2.9
1	I	270	ILE	2.9
1	E	477	GLY	2.9
1	L	233	MET	2.9
1	B	210	THR	2.8
1	L	238	GLU	2.8
1	J	273	VAL	2.8
1	E	312	ALA	2.8
1	E	264	VAL	2.8
1	A	477	GLY	2.8
1	B	270	ILE	2.8
1	L	485	TYR	2.8
1	L	481	ALA	2.8
1	K	222	LEU	2.8
1	E	233	MET	2.8
1	E	238	GLU	2.8
1	K	203	TYR	2.7
1	H	271	VAL	2.7
1	J	271	VAL	2.7
1	E	234	LEU	2.7
1	E	214	GLU	2.7
1	K	235	PRO	2.7
1	J	312	ALA	2.7
1	L	480	ALA	2.7
1	E	276	VAL	2.7
1	I	234	LEU	2.7
1	E	266	THR	2.7
1	B	240	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	221	LEU	2.7
1	I	478	TYR	2.7
1	K	270	ILE	2.6
1	L	301	ILE	2.6
1	I	233	MET	2.6
1	C	481	ALA	2.6
1	E	239	ALA	2.6
1	C	480	ALA	2.6
1	J	247	LEU	2.6
1	J	302	SER	2.6
1	K	245	LYS	2.6
1	K	255	GLU	2.6
1	J	313	THR	2.6
1	K	262	LEU	2.6
1	L	275	ALA	2.6
1	K	309	LEU	2.5
1	B	252	GLU	2.5
1	C	238	GLU	2.5
1	K	239	ALA	2.5
1	K	249	ILE	2.5
1	K	246	PRO	2.5
1	J	238	GLU	2.5
1	K	481	ALA	2.5
1	I	261	THR	2.5
1	L	210	THR	2.5
1	J	224	ASP	2.5
1	B	211	GLY	2.5
1	L	228	SER	2.5
1	I	210	THR	2.5
1	B	234	LEU	2.5
1	K	237	LEU	2.5
1	J	260	ALA	2.4
1	I	310	GLU	2.4
1	N	434	GLU	2.4
1	I	246	PRO	2.4
1	E	485	TYR	2.4
1	L	486	GLY	2.4
1	N	485	TYR	2.4
1	A	206	ASN	2.4
1	L	299	THR	2.4
1	L	264	VAL	2.4
1	A	270	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	275	ALA	2.4
1	B	238	GLU	2.4
1	B	477	GLY	2.4
1	F	271	VAL	2.4
1	I	264	VAL	2.4
1	B	356	ALA	2.3
1	K	272	LYS	2.3
1	C	485	TYR	2.3
1	M	485	TYR	2.3
1	N	490	ASP	2.3
1	J	234	LEU	2.3
1	M	304	GLU	2.3
1	F	264	VAL	2.3
1	J	309	LEU	2.3
1	K	221	LEU	2.3
1	F	233	MET	2.3
1	F	262	LEU	2.3
1	K	276	VAL	2.3
1	A	525	PRO	2.3
1	J	227	ILE	2.3
1	J	270	ILE	2.3
1	J	267	MET	2.3
1	I	485	TYR	2.3
1	D	267	MET	2.2
1	J	307	MET	2.2
1	K	248	LEU	2.2
1	F	232	GLU	2.2
1	F	230	ILE	2.2
1	E	275	ALA	2.2
1	L	307	MET	2.2
1	F	478	TYR	2.2
1	I	231	ARG	2.2
1	G	74	VAL	2.2
1	H	209	GLU	2.2
1	K	209	GLU	2.2
1	L	274	ALA	2.2
1	K	201	SER	2.2
1	I	314	LEU	2.2
1	K	354	GLU	2.2
1	F	256	GLY	2.2
1	K	477	GLY	2.2
1	K	210	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	191	GLU	2.2
1	J	272	LYS	2.2
1	C	271	VAL	2.1
1	K	313	THR	2.1
1	E	354	GLU	2.1
1	F	481	ALA	2.1
1	F	235	PRO	2.1
1	F	490	ASP	2.1
1	J	230	ILE	2.1
1	B	251	ALA	2.1
1	N	486	GLY	2.1
1	H	273	VAL	2.1
1	L	222	LEU	2.1
1	F	238	GLU	2.1
1	M	484	GLU	2.1
1	A	485	TYR	2.1
1	H	176	THR	2.1
1	J	266	THR	2.1
1	A	44	PHE	2.1
1	I	255	GLU	2.1
1	L	201	SER	2.1
1	K	305	ILE	2.1
1	B	266	THR	2.1
1	G	233	MET	2.1
1	L	478	TYR	2.1
1	G	71	ALA	2.1
1	J	323	VAL	2.0
1	F	183	LEU	2.0
1	F	247	LEU	2.0
1	F	353	ILE	2.0
1	L	229	ASN	2.0
1	I	486	GLY	2.0
1	E	232	GLU	2.0
1	E	255	GLU	2.0
1	I	272	LYS	2.0
1	J	264	VAL	2.0
1	F	237	LEU	2.0
1	D	139	SER	2.0
1	E	261	THR	2.0
1	E	274	ALA	2.0
1	L	241	ALA	2.0
1	I	203	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	224	ASP	2.0
1	B	232	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.