Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 11:05 PM GMT

PDB ID	:	5DA8
Title	:	Crystal structure of chaperonin GroEL from
Authors	:	Chang, C.; Marshall, N.; Feldmann, B.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2015-08-19
Resolution	:	3.00 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

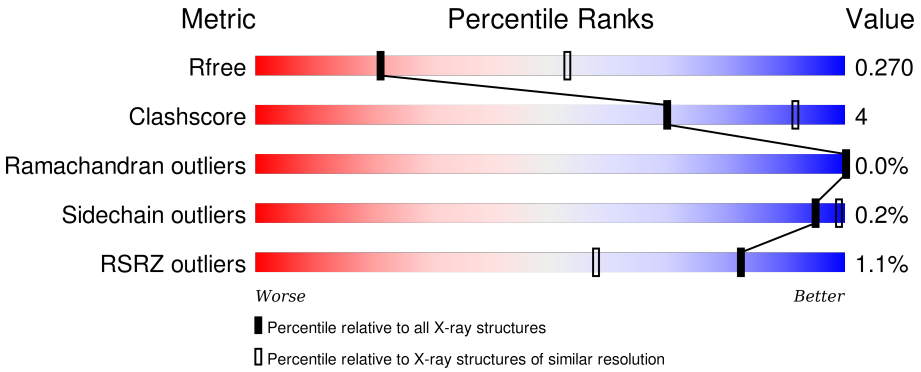
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	545	72% 19% 8%
1	B	545	81% 14% 5%
1	C	545	% 78% 9% 12%
1	D	545	% 83% 12% 5%
1	E	545	2% 83% 10% 7%

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Mol	Chain	Length	Quality of chain
1	F	545	80% 11% 9%
1	G	545	80% 12% 8%
1	H	545	82% 13% 6%
1	I	545	83% 11% 6%
1	J	545	82% 11% 7%
1	K	545	2% 71% 9% 21%
1	L	545	4% 79% 10% 11%
1	M	545	76% 9% 15%
1	N	545	82% 11% 6%
1	O	545	2% 81% 9% 10%
1	P	545	87% 9%
1	Q	545	78% 14% 8%
1	R	545	83% 9% 8%
1	S	545	83% 11% 6%
1	T	545	80% 11% 9%
1	U	545	83% 12% 5%
1	V	545	2% 77% 14% 8%
1	W	545	2% 84% 10% 5%
1	X	545	83% 10% 8%
1	Y	545	86% 8% 6%
1	Z	545	82% 13% 5%
1	a	545	2% 96%
1	b	545	77% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	601	-	-	-	X
2	SO4	B	601	-	-	-	X
2	SO4	D	601	-	-	-	X
2	SO4	F	601	-	-	-	X
2	SO4	G	601	-	-	-	X
2	SO4	J	601	-	-	-	X
2	SO4	K	601	-	-	-	X
2	SO4	N	601	-	-	-	X
2	SO4	P	601	-	-	-	X
2	SO4	R	602	-	-	-	X
2	SO4	T	602	-	-	-	X
2	SO4	V	602	-	-	-	X
2	SO4	Z	601	-	-	-	X
2	SO4	b	601	-	-	-	X
4	MG	M	601	-	-	-	X
4	MG	Q	601	-	-	-	X
4	MG	V	601	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 99552 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	499	Total	C	N	O	S	0	0	0
			3601	2242	631	720	8			
1	B	519	Total	C	N	O	S	0	0	0
			3706	2296	655	745	10			
1	C	478	Total	C	N	O	S	0	0	0
			3335	2066	591	670	8			
1	D	517	Total	C	N	O	S	0	0	0
			3721	2316	654	743	8			
1	E	509	Total	C	N	O	S	0	0	0
			3631	2254	641	727	9			
1	F	497	Total	C	N	O	S	0	0	0
			3560	2201	630	720	9			
1	G	499	Total	C	N	O	S	0	0	0
			3500	2168	621	703	8			
1	H	515	Total	C	N	O	S	0	0	0
			3766	2342	659	757	8			
1	I	512	Total	C	N	O	S	0	0	0
			3697	2298	646	745	8			
1	J	507	Total	C	N	O	S	0	0	0
			3525	2175	624	719	7			
1	K	433	Total	C	N	O	S	0	0	0
			2968	1831	536	597	4			
1	L	484	Total	C	N	O	S	0	0	0
			3309	2033	591	679	6			
1	M	463	Total	C	N	O	S	0	0	0
			3247	2012	577	651	7			
1	N	511	Total	C	N	O	S	0	0	0
			3603	2232	638	725	8			
1	O	492	Total	C	N	O	S	0	0	0
			3451	2131	609	704	7			
1	P	522	Total	C	N	O	S	0	0	0
			3780	2350	661	760	9			

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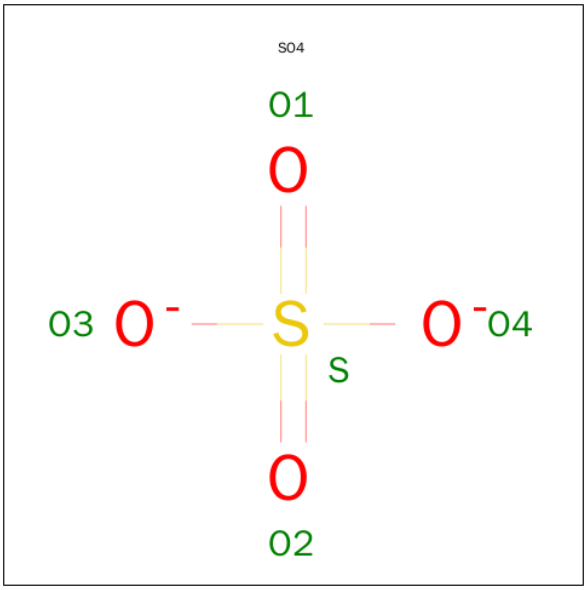
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	502	Total	C	N	O	S	0	0	0
			3585	2229	633	715	8			
1	R	502	Total	C	N	O	S	0	0	0
			3576	2218	628	722	8			
1	S	512	Total	C	N	O	S	0	0	0
			3677	2286	646	737	8			
1	T	497	Total	C	N	O	S	0	0	0
			3494	2163	617	707	7			
1	U	518	Total	C	N	O	S	0	0	0
			3718	2315	648	746	9			
1	V	500	Total	C	N	O	S	0	0	0
			3575	2215	626	725	9			
1	W	517	Total	C	N	O	S	0	0	0
			3661	2269	647	737	8			
1	X	504	Total	C	N	O	S	0	0	0
			3581	2218	637	721	5			
1	Y	512	Total	C	N	O	S	0	0	0
			3695	2298	647	741	9			
1	Z	518	Total	C	N	O	S	0	0	0
			3703	2294	654	746	9			
1	a	522	Total	C	N	O	S	0	0	0
			3743	2324	658	752	9			
1	b	423	Total	C	N	O	S	0	0	0
			2961	1831	525	598	7			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	N	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0
2	T	1	Total O S 5 4 1	0	0
2	U	1	Total O S 5 4 1	0	0
2	V	1	Total O S 5 4 1	0	0
2	Y	1	Total O S 5 4 1	0	0
2	Z	1	Total O S 5 4 1	0	0
2	a	1	Total O S 5 4 1	0	0
2	b	1	Total O S 5 4 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	J	1	Total Ca 1 1	0	0
3	Q	1	Total Ca 1 1	0	0
3	K	1	Total Ca 1 1	0	0
3	a	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	I	1	Total Ca 1 1	0	0
3	V	1	Total Ca 1 1	0	0
3	Z	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	T	1	Total Ca 1 1	0	0
3	U	1	Total Ca 1 1	0	0
3	O	1	Total Ca 1 1	0	0
3	R	1	Total Ca 1 1	0	0
3	Y	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	M	1	Total Ca 1 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	V	1	Total Mg 1 1	0	0
4	T	1	Total Mg 1 1	0	0
4	R	1	Total Mg 1 1	0	0
4	S	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	B	2	Total O 2 2	0	0
5	C	1	Total O 1 1	0	0
5	D	2	Total O 2 2	0	0
5	E	2	Total O 2 2	0	0
5	F	2	Total O 2 2	0	0
5	H	1	Total O 1 1	0	0
5	I	3	Total O 3 3	0	0
5	J	3	Total O 3 3	0	0
5	L	3	Total O 3 3	0	0
5	N	2	Total O 2 2	0	0
5	O	3	Total O 3 3	0	0
5	P	2	Total O 2 2	0	0
5	Q	3	Total O 3 3	0	0

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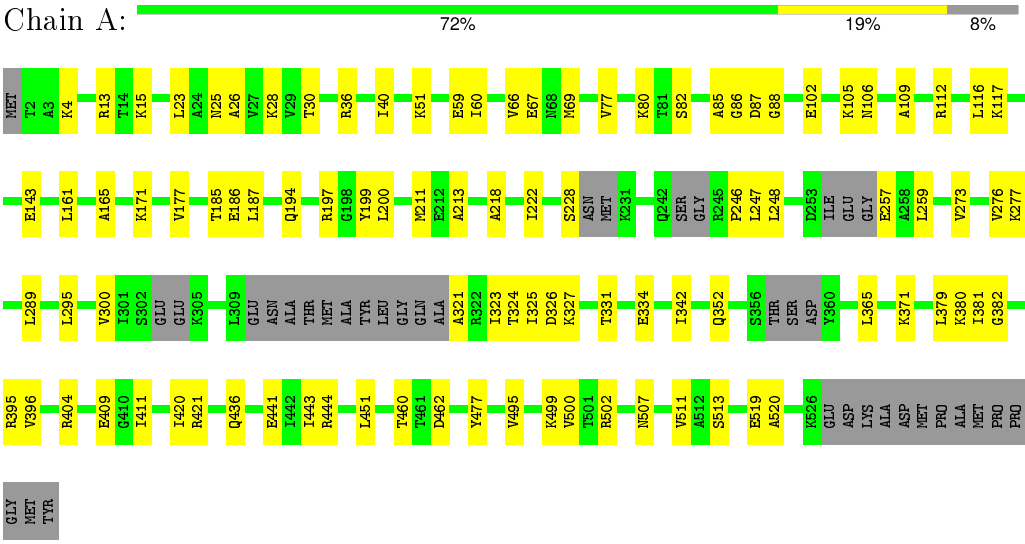
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	1	Total O 1 1	0	0
5	S	3	Total O 3 3	0	0
5	U	1	Total O 1 1	0	0
5	V	2	Total O 2 2	0	0
5	W	2	Total O 2 2	0	0
5	X	5	Total O 5 5	0	0
5	Y	3	Total O 3 3	0	0
5	Z	1	Total O 1 1	0	0
5	a	1	Total O 1 1	0	0
5	b	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

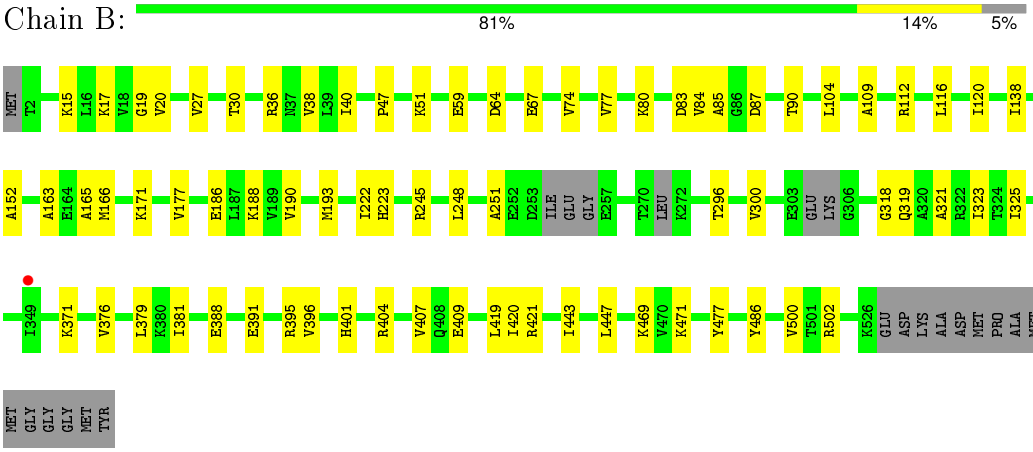
- Molecule 1: 60 kDa chaperonin

Chain A:



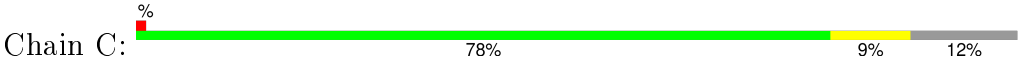
- Molecule 1: 60 kDa chaperonin

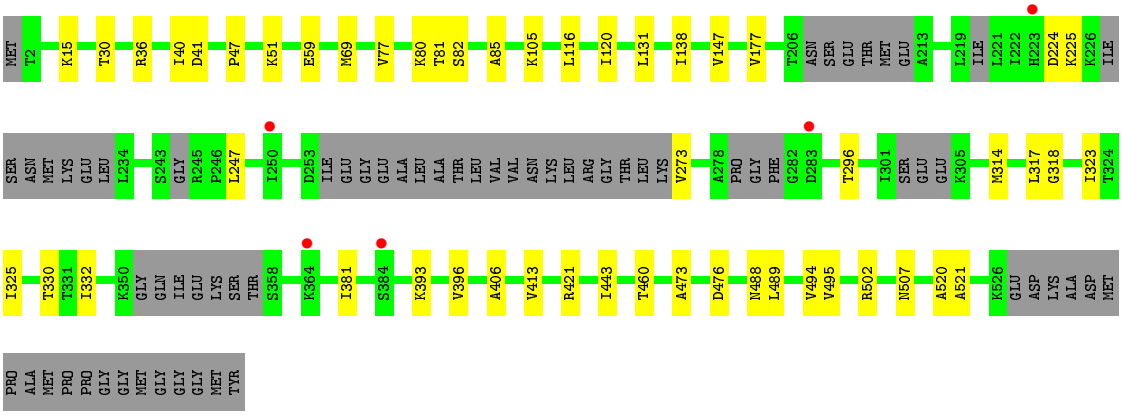
Chain B:



- Molecule 1: 60 kDa chaperonin

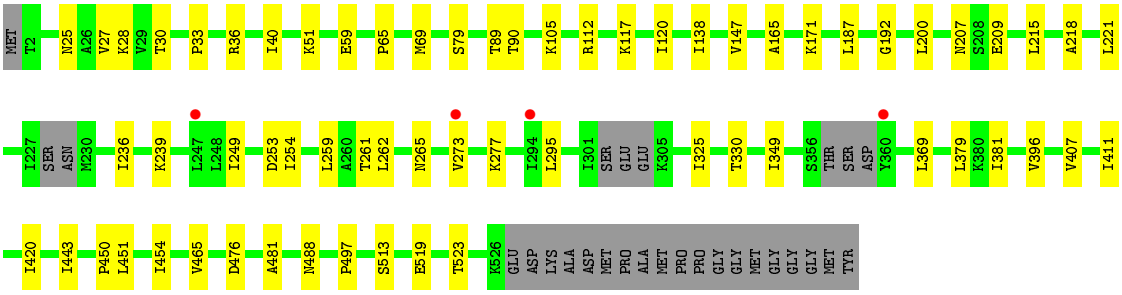
Chain C:





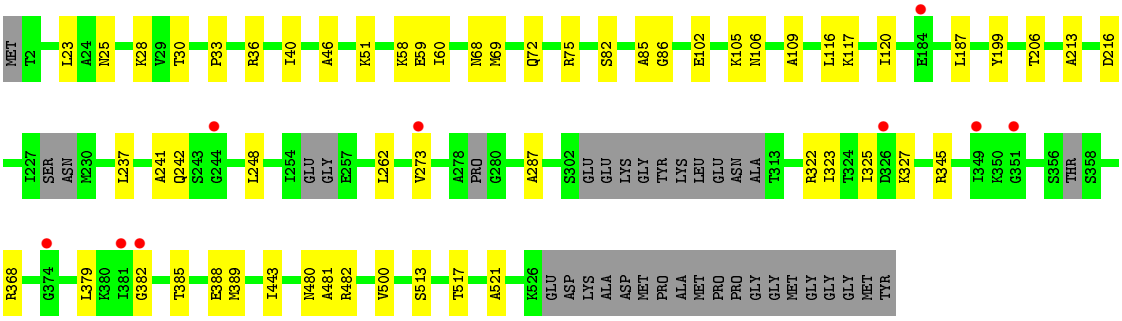
• Molecule 1: 60 kDa chaperonin

Chain D:



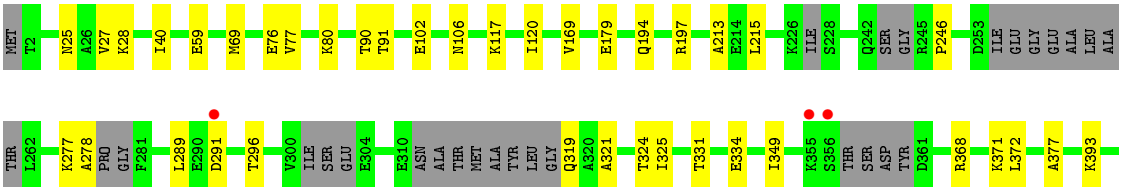
• Molecule 1: 60 kDa chaperonin

Chain E:



• Molecule 1: 60 kDa chaperonin

Chain F:

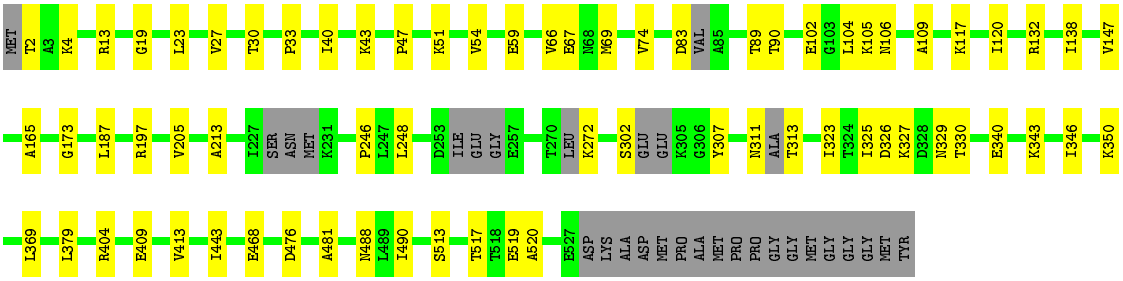


• Molecule 1: 60 kDa chaperonin

Chain G:

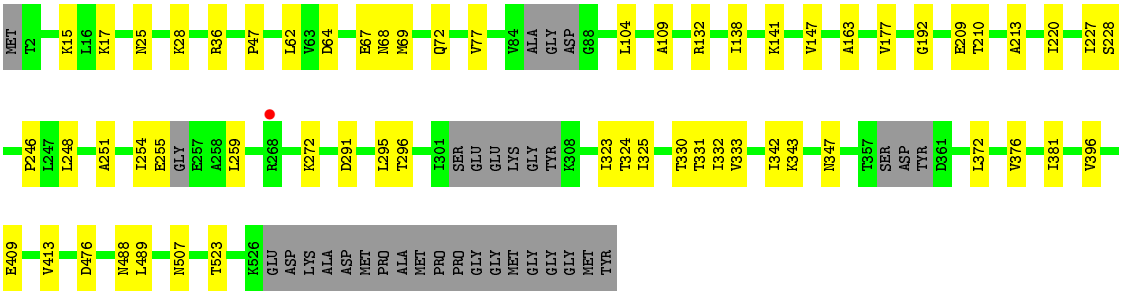
• Molecule 1: 60 kDa chaperonin

Chain H:



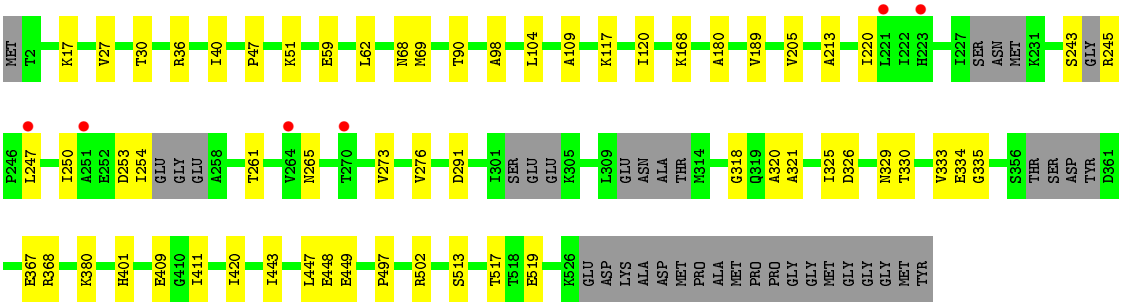
• Molecule 1: 60 kDa chaperonin

Chain I:



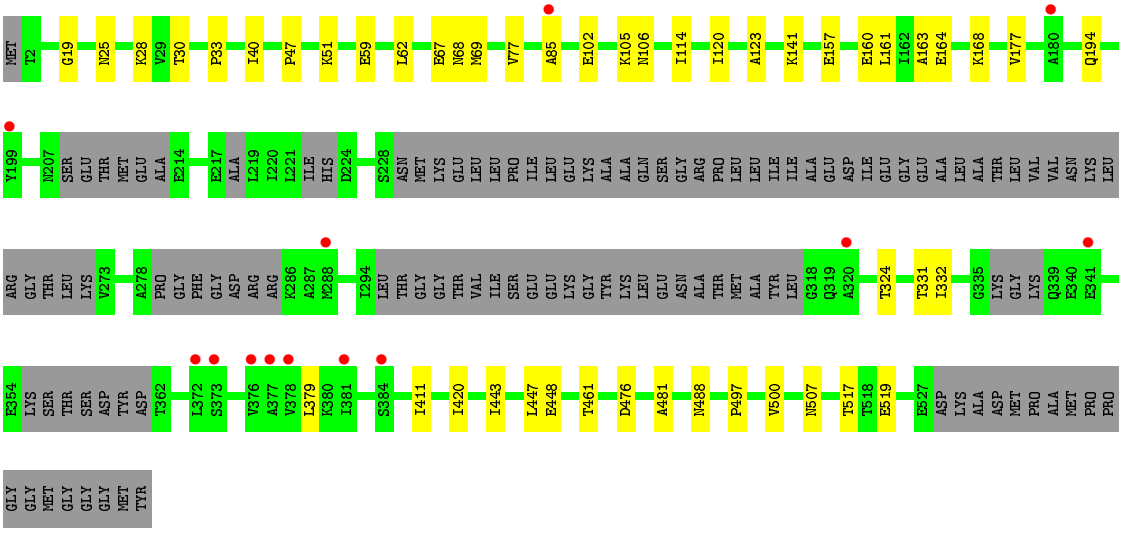
• Molecule 1: 60 kDa chaperonin

Chain J:



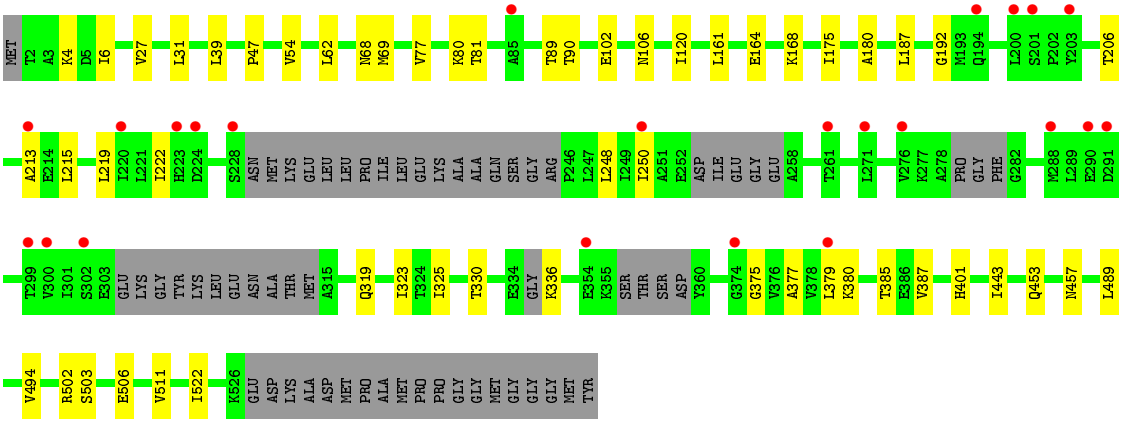
• Molecule 1: 60 kDa chaperonin

Chain K:



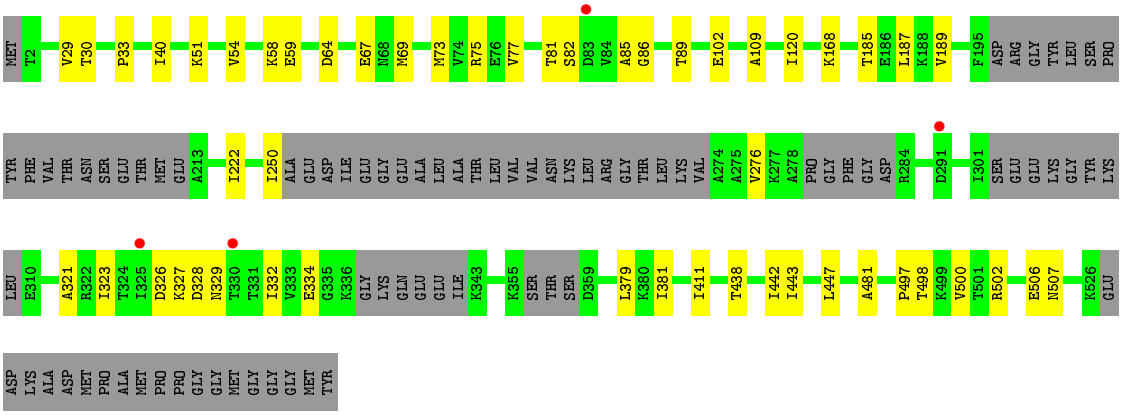
• Molecule 1: 60 kDa chaperonin

Chain L:



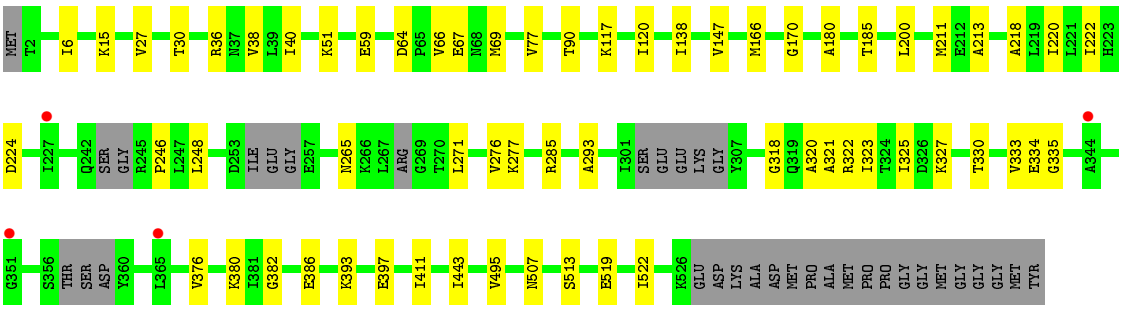
• Molecule 1: 60 kDa chaperonin

Chain M:



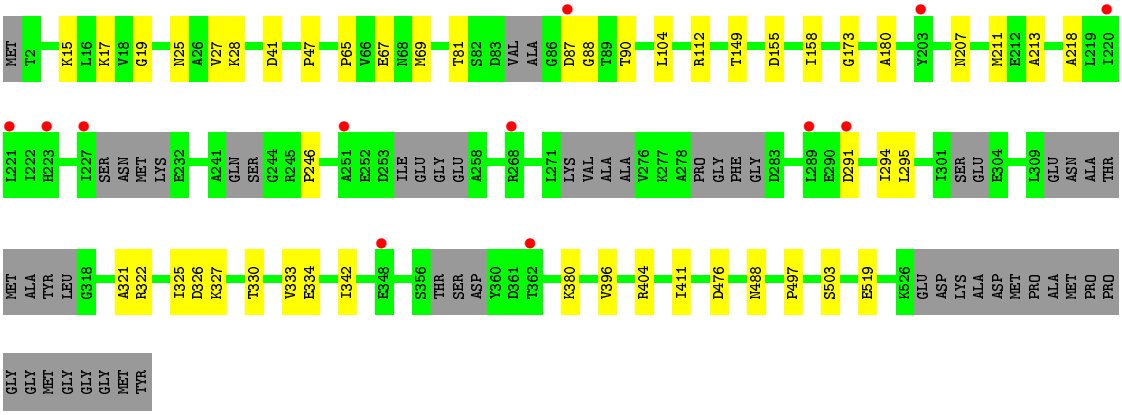
• Molecule 1: 60 kDa chaperonin

Chain N:



• Molecule 1: 60 kDa chaperonin

Chain O:

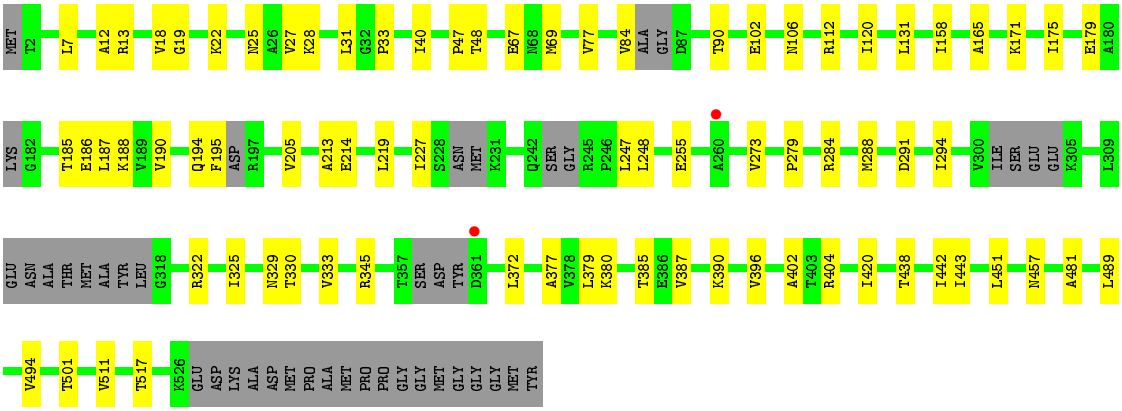


• Molecule 1: 60 kDa chaperonin

Chain P:

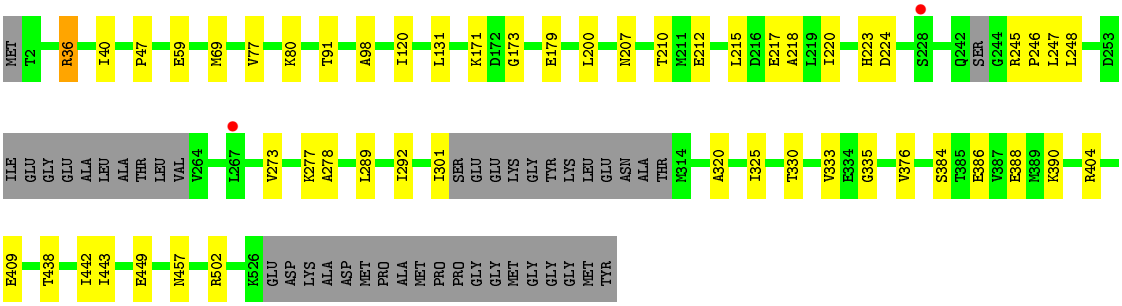
- Molecule 1: 60 kDa chaperonin

Chain Q:



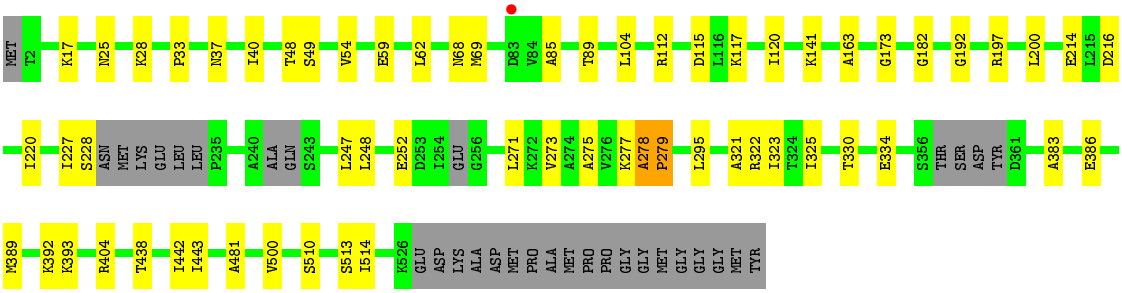
- Molecule 1: 60 kDa chaperonin

Chain R:



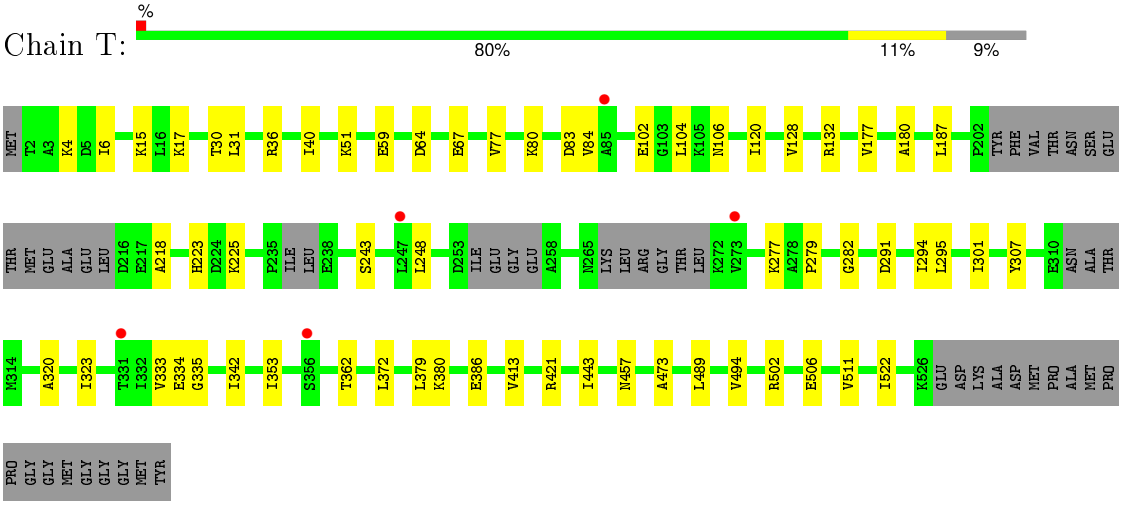
- Molecule 1: 60 kDa chaperonin

Chain S:



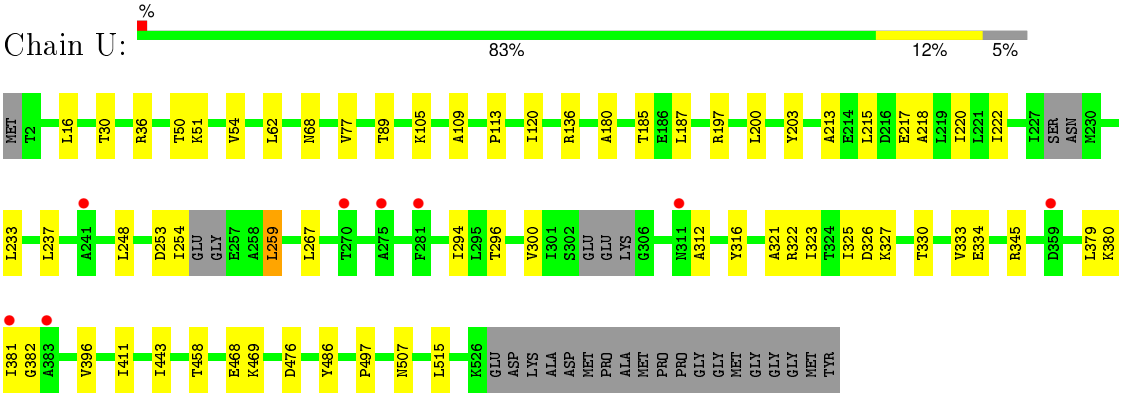
- Molecule 1: 60 kDa chaperonin

Chain T:



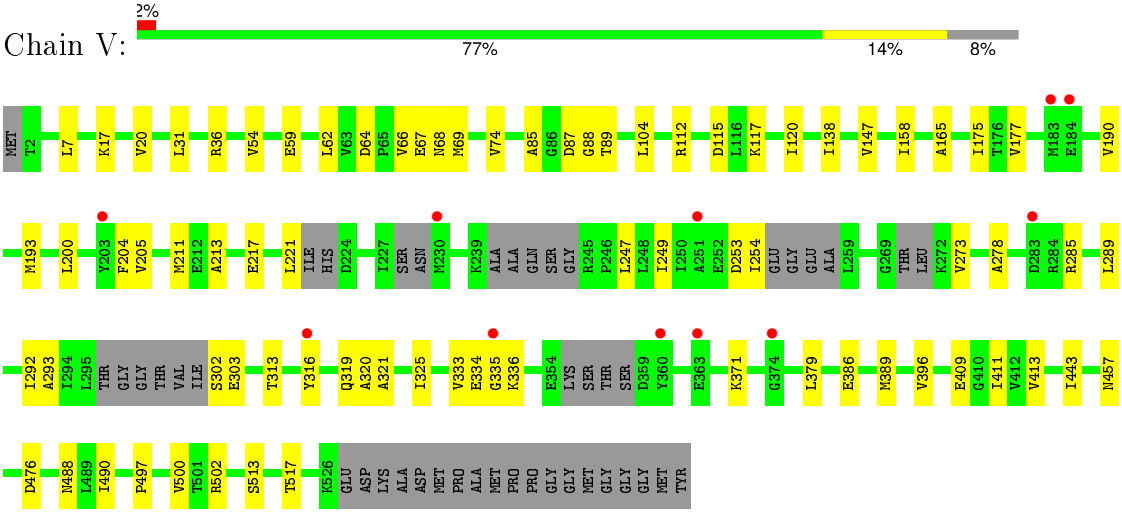
• Molecule 1: 60 kDa chaperonin

Chain U:



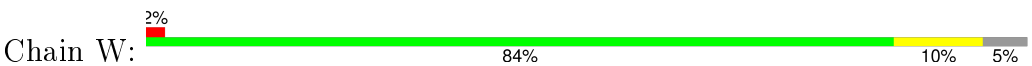
• Molecule 1: 60 kDa chaperonin

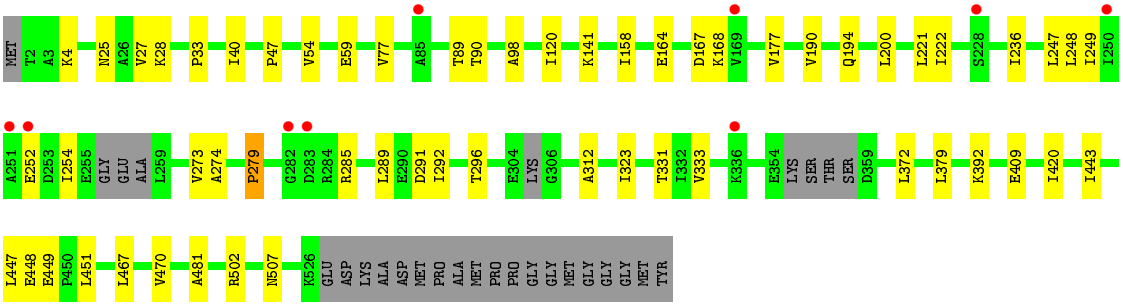
Chain V:



• Molecule 1: 60 kDa chaperonin

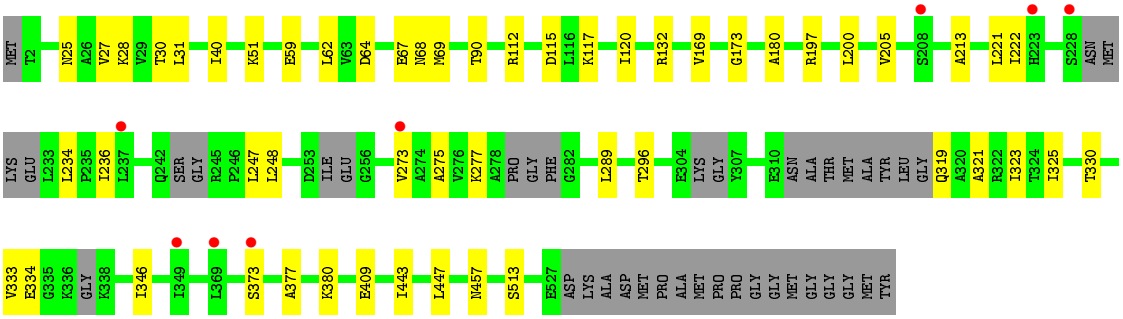
Chain W:





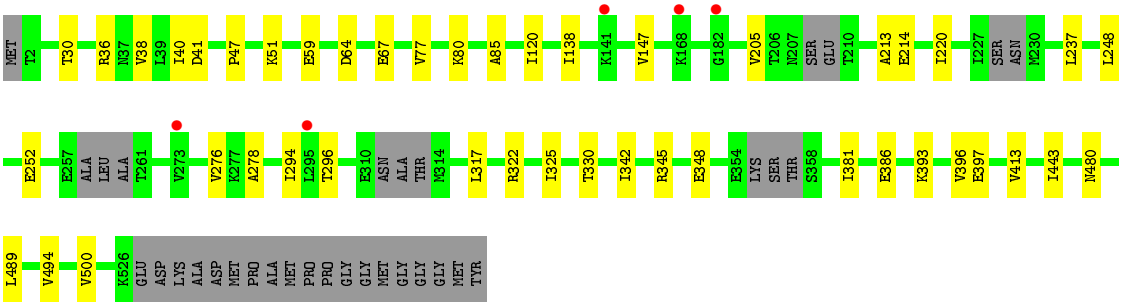
- Molecule 1: 60 kDa chaperonin

Chain X:



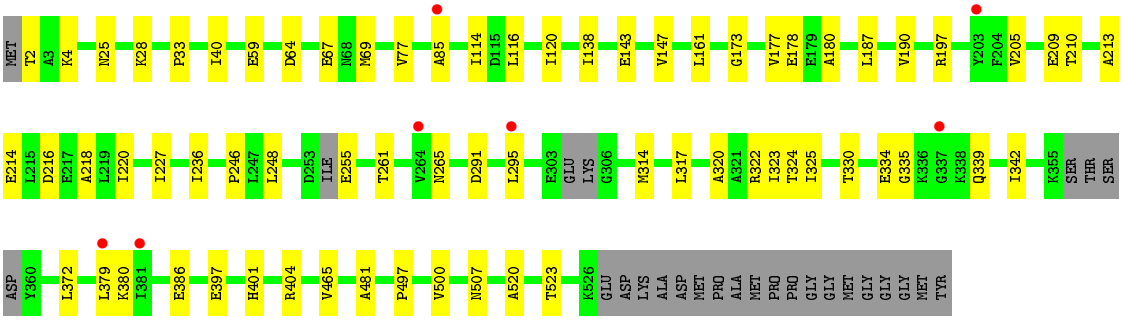
- Molecule 1: 60 kDa chaperonin

Chain Y:



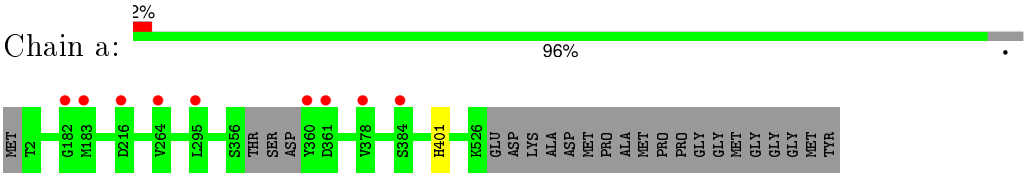
- Molecule 1: 60 kDa chaperonin

Chain Z:



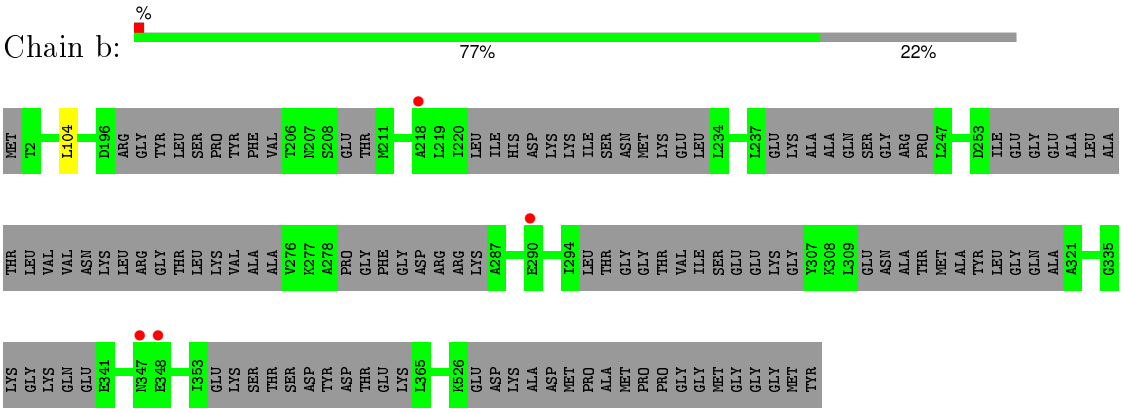
- Molecule 1: 60 kDa chaperonin

Chain a:



- Molecule 1: 60 kDa chaperonin

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	139.00Å 159.78Å 228.82Å 75.46° 90.51° 91.22°	Depositor
Resolution (Å)	48.60 – 3.00 49.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (48.60-3.00) 88.7 (49.65-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.230 , 0.263 0.239 , 0.270	Depositor DCC
R_{free} test set	18192 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.2	EDS
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 365169 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	99552	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CA, SO4

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	0.23	0/3615	0.40	0/4880
1	B	0.23	0/3727	0.41	0/5041
1	C	0.23	0/3344	0.40	0/4527
1	D	0.23	0/3742	0.41	0/5062
1	E	0.23	0/3647	0.41	0/4933
1	F	0.23	0/3574	0.41	0/4827
1	G	0.23	0/3514	0.42	0/4756
1	H	0.23	0/3785	0.40	0/5106
1	I	0.23	0/3715	0.41	0/5024
1	J	0.23	0/3541	0.41	0/4799
1	K	0.23	0/2974	0.41	0/4025
1	L	0.23	0/3319	0.40	0/4501
1	M	0.23	0/3257	0.40	0/4407
1	N	0.23	0/3620	0.41	0/4902
1	O	0.23	0/3462	0.41	0/4684
1	P	0.23	0/3803	0.41	0/5142
1	Q	0.23	0/3600	0.41	0/4862
1	R	0.23	0/3595	0.41	0/4867
1	S	0.23	0/3697	0.42	1/5001 (0.0%)
1	T	0.23	0/3508	0.43	1/4751 (0.0%)
1	U	0.23	0/3739	0.42	0/5062
1	V	0.23	0/3591	0.42	0/4854
1	W	0.23	0/3679	0.42	1/4981 (0.0%)
1	X	0.23	0/3597	0.40	0/4865
1	Y	0.23	0/3715	0.41	0/5017
1	Z	0.23	0/3723	0.42	0/5039
1	a	0.23	0/3766	0.42	0/5099
1	b	0.22	0/2965	0.40	0/4007
All	All	0.23	0/99814	0.41	3/135021 (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	J	0	1
1	T	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	279	PRO	N-CA-CB	6.36	110.93	103.30
1	W	279	PRO	N-CA-CB	6.24	110.78	103.30
1	T	279	PRO	N-CA-CB	6.05	110.56	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	367	GLU	Peptide
1	T	243	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3601	0	3651	64	0
1	B	3706	0	3668	49	0
1	C	3335	0	3252	32	0
1	D	3721	0	3751	38	0
1	E	3631	0	3624	35	0
1	F	3560	0	3514	33	0
1	G	3500	0	3438	37	0
1	H	3766	0	3823	40	0
1	I	3697	0	3728	37	0
1	J	3525	0	3391	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2968	0	2840	33	0
1	L	3309	0	3145	32	0
1	M	3247	0	3211	30	0
1	N	3603	0	3541	38	0
1	O	3451	0	3335	27	0
1	P	3780	0	3812	29	0
1	Q	3585	0	3577	43	0
1	R	3576	0	3541	31	0
1	S	3677	0	3683	34	0
1	T	3494	0	3435	35	0
1	U	3718	0	3723	37	0
1	V	3575	0	3506	44	0
1	W	3661	0	3601	32	0
1	X	3581	0	3504	30	0
1	Y	3695	0	3689	27	0
1	Z	3703	0	3669	43	0
1	a	3743	0	3741	0	0
1	b	2961	0	2899	0	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	G	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	P	5	0	0	0	0
2	R	5	0	0	1	0
2	T	5	0	0	0	0
2	U	5	0	0	0	0
2	V	5	0	0	0	0
2	Y	5	0	0	0	0
2	Z	5	0	0	0	0
2	a	5	0	0	0	0
2	b	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
3	a	1	0	0	0	0
4	H	1	0	0	0	0
4	M	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	V	1	0	0	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	H	1	0	0	0	0
5	I	3	0	0	0	0
5	J	3	0	0	0	0
5	L	3	0	0	0	0
5	N	2	0	0	0	0
5	O	3	0	0	0	0
5	P	2	0	0	0	0
5	Q	3	0	0	1	0
5	R	1	0	0	0	0
5	S	3	0	0	0	0
5	U	1	0	0	0	0
5	V	2	0	0	0	0
5	W	2	0	0	0	0
5	X	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	3	0	0	0	0
5	Z	1	0	0	0	0
5	a	1	0	0	0	0
5	b	2	0	0	0	0
All	All	99552	0	98292	878	0

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

All (878) 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:K:85:ALA:HB1	1:K:500:VAL:HG22	1.67	0.77
1:Y:252:GLU:HA	1:Y:278:ALA:HB2	1.68	0.75
1:X:333:VAL:HG12	1:X:334:GLU:HG3	1.69	0.74
1:Y:47:PRO:HG3	1:Z:69:MET:HG3	1.69	0.73
1:D:325:ILE:HG12	1:D:330:THR:HG23	1.71	0.72
1:U:200:LEU:HB3	1:U:259:LEU:HD11	1.73	0.71
1:O:207:ASN:HB3	1:O:211:MET:HA	1.73	0.70
1:W:200:LEU:HD11	1:W:254:ILE:HB	1.73	0.70
1:V:333:VAL:HG12	1:V:334:GLU:HG2	1.73	0.69
1:C:138:ILE:HD13	1:C:147:VAL:HG21	1.74	0.69
1:O:213:ALA:HB3	1:O:325:ILE:HB	1.75	0.68
1:F:169:VAL:HG21	1:F:377:ALA:HB2	1.75	0.68
1:Q:205:VAL:HA	1:Q:213:ALA:HB2	1.75	0.68
1:D:381:ILE:HG12	1:D:396:VAL:HG21	1.76	0.68
1:Z:339:GLN:HA	1:Z:342:ILE:HG12	1.76	0.68
1:S:173:GLY:O	1:S:404:ARG:NH1	2.26	0.68
1:K:120:ILE:HG23	1:K:443:ILE:HD11	1.76	0.67
1:M:85:ALA:HB1	1:M:500:VAL:HG22	1.76	0.67
1:J:321:ALA:HB3	1:J:334:GLU:HG3	1.76	0.67
1:A:460:THR:HG22	1:A:462:ASP:H	1.58	0.66
1:T:294:ILE:HG22	1:T:342:ILE:HG12	1.77	0.66
1:M:120:ILE:HG23	1:M:443:ILE:HD11	1.76	0.66
1:C:421:ARG:NH2	1:C:473:ALA:O	2.29	0.66
1:E:40:ILE:HD13	1:E:59:GLU:HG3	1.76	0.66
1:A:248:LEU:HD22	1:A:323:ILE:HG21	1.78	0.66
1:B:47:PRO:HG3	1:V:69:MET:HG3	177.43	0.65
1:M:40:ILE:HD13	1:M:59:GLU:HG3	1.78	0.65
1:V:190:VAL:HB	1:V:334:GLU:HB3	1.79	0.64
1:A:197:ARG:NH2	1:Z:386:GLU:OE1	57.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:HG12	1:B:330:THR:HG23	1.80	0.64
1:K:123:ALA:HB3	1:K:443:ILE:HD12	1.79	0.64
1:A:211:MET:HB3	1:A:327:LYS:HE2	1.77	0.64
1:Z:85:ALA:HB1	1:Z:500:VAL:HG22	1.79	0.64
1:O:180:ALA:HB2	1:O:380:LYS:HB3	1.79	0.64
1:C:120:ILE:HG23	1:C:443:ILE:HD11	1.80	0.63
1:Y:40:ILE:HD13	1:Y:59:GLU:HG3	1.79	0.63
1:Z:325:ILE:HG12	1:Z:330:THR:HG23	1.80	0.63
1:N:320:ALA:HA	1:N:335:GLY:HA2	1.80	0.63
1:A:186:GLU:HB2	1:A:380:LYS:HE2	2.71	0.63
1:N:320:ALA:HB3	1:N:323:ILE:HD11	1.80	0.63
1:Z:173:GLY:O	1:Z:404:ARG:NH2	2.32	0.63
1:R:120:ILE:HG23	1:R:443:ILE:HD11	1.81	0.63
1:M:185:THR:HG23	1:M:381:ILE:HA	1.80	0.63
1:A:185:THR:HG22	1:A:382:GLY:H	1.63	0.62
1:W:291:ASP:HB3	1:W:372:LEU:HD21	1.80	0.62
1:I:248:LEU:HD22	1:I:323:ILE:HG21	1.81	0.62
1:K:164:GLU:HB3	1:K:168:LYS:HE3	1.81	0.62
1:B:381:ILE:HG12	1:B:396:VAL:HG21	1.81	0.62
1:G:42:LYS:NZ	1:G:48:THR:OG1	2.31	0.62
1:X:40:ILE:HD13	1:X:59:GLU:HG3	1.82	0.61
1:J:326:ASP:HB2	1:J:329:ASN:HB2	1.81	0.61
1:X:112:ARG:NH1	1:X:115:ASP:OD2	2.33	0.61
1:N:185:THR:HG22	1:N:382:GLY:H	1.66	0.61
1:U:120:ILE:HG23	1:U:443:ILE:HD11	1.82	0.61
1:V:289:LEU:HD23	1:V:292:ILE:HD11	1.82	0.61
1:I:324:THR:HG1	1:I:331:THR:HG1	1.44	0.61
1:T:36:ARG:HH12	1:U:113:PRO:HG2	1.66	0.61
1:W:164:GLU:OE2	1:W:168:LYS:NZ	2.34	0.61
1:W:177:VAL:HG22	1:W:379:LEU:HD12	1.83	0.61
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.83	0.61
1:E:85:ALA:HB1	1:E:500:VAL:HG22	1.80	0.61
1:J:40:ILE:HD13	1:J:59:GLU:HG3	1.82	0.61
1:T:295:LEU:HD23	1:T:342:ILE:HD13	1.83	0.61
1:Z:320:ALA:HA	1:Z:335:GLY:HA2	1.83	0.61
1:T:40:ILE:HD13	1:T:59:GLU:HG3	1.83	0.61
1:N:325:ILE:HG12	1:N:330:THR:HG23	1.84	0.60
1:H:23:LEU:HD23	1:H:74:VAL:HG23	1.82	0.60
1:I:47:PRO:HG3	1:J:69:MET:HG3	1.81	0.60
1:Y:213:ALA:HB3	1:Y:325:ILE:HB	1.83	0.60
1:Z:227:ILE:O	1:Z:255:GLU:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:173:GLY:O	1:R:404:ARG:NH2	2.31	0.60
1:M:222:ILE:HG12	1:M:250:ILE:HD11	1.84	0.60
1:C:105:LYS:HG2	1:J:109:ALA:HA	1.82	0.60
1:H:248:LEU:HD22	1:H:323:ILE:HG21	1.84	0.60
1:A:120:ILE:HG23	1:A:443:ILE:HD11	1.93	0.60
1:S:247:LEU:HB3	1:S:273:VAL:HG12	1.82	0.60
1:F:291:ASP:HB3	1:F:372:LEU:HD11	1.84	0.60
1:R:223:HIS:HA	1:R:301:ILE:HG12	1.82	0.60
1:Y:248:LEU:HD11	1:Y:276:VAL:HG23	1.83	0.60
1:G:197:ARG:HE	1:G:279:PRO:HA	1.65	0.60
1:D:105:LYS:HG2	1:I:109:ALA:HA	1.84	0.60
1:O:322:ARG:HB3	1:O:333:VAL:HB	1.84	0.60
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.84	0.59
1:E:72:GLN:OE1	1:E:75:ARG:NH1	2.36	0.59
1:H:197:ARG:NH2	1:N:386:GLU:OE1	2.35	0.59
1:Q:284:ARG:O	1:Q:288:MET:N	2.36	0.59
1:A:40:ILE:HD13	1:A:59:GLU:HG3	2.02	0.59
1:G:120:ILE:HG23	1:G:443:ILE:HD11	1.82	0.59
1:Q:27:VAL:HG12	1:Q:90:THR:HG23	1.84	0.59
1:X:117:LYS:HG3	1:X:513:SER:HB3	1.84	0.59
1:Q:77:VAL:HG11	1:Q:511:VAL:HB	1.85	0.59
1:T:248:LEU:HD22	1:T:323:ILE:HG21	1.85	0.59
1:U:220:ILE:HD12	1:U:296:THR:HG21	1.84	0.59
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.85	0.59
1:A:194:GLN:O	1:A:371:LYS:NZ	2.34	0.59
1:L:206:THR:HB	1:L:213:ALA:HA	1.85	0.59
1:V:165:ALA:HB1	1:V:175:ILE:HD12	1.85	0.59
1:S:112:ARG:NH1	1:S:115:ASP:OD2	2.36	0.58
1:J:291:ASP:OD2	1:J:368:ARG:NH2	2.37	0.58
1:R:47:PRO:HG3	1:S:69:MET:HG3	1.85	0.58
1:B:296:THR:HG23	1:B:318:GLY:HA3	1.84	0.58
1:A:213:ALA:HB3	1:A:325:ILE:HB	1.85	0.58
1:X:248:LEU:HD22	1:X:323:ILE:HG21	1.86	0.58
1:I:36:ARG:HD3	1:J:519:GLU:HG3	1.85	0.58
1:J:180:ALA:HB2	1:J:380:LYS:HB3	1.84	0.58
1:Q:190:VAL:HG21	1:Q:333:VAL:HG13	1.84	0.58
1:H:138:ILE:HG12	1:H:147:VAL:HG21	1.84	0.58
1:K:40:ILE:HD13	1:K:59:GLU:HG3	1.86	0.58
1:N:120:ILE:HG23	1:N:443:ILE:HD11	1.85	0.58
1:G:40:ILE:HD13	1:G:59:GLU:HG3	1.85	0.58
1:B:120:ILE:HG23	1:B:443:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:325:ILE:HG12	1:S:330:THR:HG23	1.86	0.58
1:P:294:ILE:HD12	1:P:345:ARG:HD2	1.86	0.58
1:V:221:LEU:HD23	1:V:249:ILE:HG23	1.85	0.58
1:R:386:GLU:OE1	1:S:197:ARG:NH2	2.37	0.58
1:W:54:VAL:HG22	1:W:89:THR:HG21	1.86	0.57
1:V:59:GLU:HG3	1:W:4:LYS:HE2	1.85	0.57
1:A:138:ILE:HG23	1:A:143:GLU:HG3	1.86	0.57
1:G:248:LEU:HD22	1:G:323:ILE:HG21	1.85	0.57
1:L:187:LEU:HD13	1:L:379:LEU:HD23	1.84	0.57
1:G:262:LEU:HD22	1:G:273:VAL:HG11	1.86	0.57
1:Q:186:GLU:OE1	1:Q:188:LYS:NZ	2.37	0.57
1:Q:187:LEU:HD13	1:Q:379:LEU:HD23	1.86	0.57
1:T:77:VAL:HG21	1:T:511:VAL:HB	1.86	0.57
1:N:211:MET:O	1:N:327:LYS:NZ	2.38	0.57
1:F:40:ILE:HD13	1:F:59:GLU:HG3	1.87	0.57
1:Q:489:LEU:HB3	1:Q:494:VAL:HB	1.87	0.57
1:V:413:VAL:HG12	1:V:490:ILE:HG13	1.87	0.57
1:K:47:PRO:HG3	1:L:69:MET:HG3	1.87	0.57
1:Y:393:LYS:NZ	1:Y:397:GLU:OE2	2.38	0.57
1:O:325:ILE:HG12	1:O:330:THR:HG23	1.86	0.57
1:R:40:ILE:HD13	1:R:59:GLU:HG3	1.86	0.57
1:L:120:ILE:HG23	1:L:443:ILE:HD11	1.87	0.57
1:F:120:ILE:HG23	1:F:443:ILE:HD11	1.86	0.57
1:A:441:GLU:HG2	1:A:444:ARG:HH21	1.69	0.57
1:X:120:ILE:HG23	1:X:443:ILE:HD11	1.86	0.56
1:N:322:ARG:HB3	1:N:333:VAL:HB	1.87	0.56
1:E:248:LEU:HD22	1:E:323:ILE:HD13	1.87	0.56
1:V:247:LEU:HB3	1:V:273:VAL:HG12	1.87	0.56
1:O:27:VAL:HG12	1:O:90:THR:HG23	1.87	0.56
1:F:213:ALA:HB3	1:F:325:ILE:HB	1.87	0.56
1:I:138:ILE:HG12	1:I:147:VAL:HG21	1.87	0.56
1:M:82:SER:HA	1:M:86:GLY:HA2	1.86	0.56
1:W:47:PRO:HG3	1:X:69:MET:HG2	1.88	0.56
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.87	0.56
1:G:353:ILE:HG22	1:G:354:GLU:HG3	1.88	0.56
1:F:194:GLN:O	1:F:371:LYS:NZ	2.28	0.56
1:T:17:LYS:HD2	1:T:104:LEU:HD12	1.87	0.56
1:Z:214:GLU:HG2	1:Z:324:THR:HG22	1.86	0.56
1:S:214:GLU:OE1	1:S:322:ARG:NH2	2.39	0.56
1:V:17:LYS:HD2	1:V:104:LEU:HD12	1.87	0.56
1:A:105:LYS:HG2	1:U:109:ALA:HA	70.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:120:ILE:HG23	1:Q:443:ILE:HD11	1.87	0.56
1:N:218:ALA:HB2	1:N:246:PRO:HG2	1.88	0.56
1:B:248:LEU:HD22	1:B:323:ILE:HG21	1.88	0.56
1:B:17:LYS:HD2	1:B:104:LEU:HD12	1.88	0.56
1:Y:381:ILE:HG12	1:Y:396:VAL:HG21	1.87	0.56
1:U:180:ALA:HB2	1:U:380:LYS:HB3	1.87	0.56
1:A:82:SER:HA	1:A:86:GLY:H	1.70	0.56
1:P:120:ILE:HG23	1:P:443:ILE:HD11	1.88	0.56
1:Z:177:VAL:HG21	1:Z:397:GLU:HG2	1.88	0.56
1:P:47:PRO:HG3	1:Q:69:MET:HG2	1.86	0.55
1:H:302:SER:H	1:H:307:TYR:HB2	1.71	0.55
1:T:120:ILE:HG23	1:T:443:ILE:HD11	1.88	0.55
1:I:192:GLY:HA2	1:I:295:LEU:HD21	1.89	0.55
1:M:58:LYS:HA	1:M:75:ARG:HH21	1.71	0.55
1:F:450:PRO:O	1:F:454:ILE:HG12	2.05	0.55
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.89	0.55
1:O:173:GLY:O	1:O:404:ARG:NH2	2.39	0.55
1:H:47:PRO:HG3	1:I:69:MET:HG2	1.88	0.55
1:B:109:ALA:HA	1:K:105:LYS:HG2	1.87	0.55
1:S:182:GLY:HA2	1:T:282:GLY:HA2	1.89	0.55
1:N:213:ALA:HB3	1:N:325:ILE:HB	1.87	0.55
1:T:218:ALA:HB3	1:T:323:ILE:HD12	1.89	0.55
1:B:40:ILE:HD13	1:B:59:GLU:HG3	1.94	0.55
1:I:343:LYS:O	1:I:347:ASN:ND2	2.35	0.55
1:P:248:LEU:HD22	1:P:323:ILE:HG21	1.88	0.55
1:A:392:LYS:HG2	1:A:395:ARG:HH21	1.72	0.55
1:B:77:VAL:HA	1:B:80:LYS:HE2	1.87	0.55
1:V:213:ALA:HB3	1:V:325:ILE:HB	1.88	0.55
1:N:66:VAL:HA	1:N:69:MET:HE2	1.89	0.55
1:E:213:ALA:HB3	1:E:325:ILE:HB	1.88	0.55
1:V:87:ASP:OD1	1:V:88:GLY:N	2.39	0.55
1:T:386:GLU:OE1	1:U:197:ARG:NH2	2.32	0.55
1:E:120:ILE:HG23	1:E:443:ILE:HD11	1.88	0.55
1:S:200:LEU:HD12	1:S:275:ALA:HB1	1.87	0.55
1:C:247:LEU:O	1:C:273:VAL:N	2.40	0.55
1:F:215:LEU:HD23	1:F:246:PRO:HB2	1.87	0.55
1:P:255:GLU:HA	1:P:259:LEU:HB2	1.87	0.55
1:R:325:ILE:HG12	1:R:330:THR:HG23	1.88	0.55
1:V:319:GLN:O	1:V:336:LYS:N	2.27	0.55
1:H:173:GLY:O	1:H:404:ARG:NH2	2.39	0.54
1:A:324:THR:HG1	1:A:331:THR:HG1	5.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:120:ILE:HG23	1:Y:443:ILE:HD11	1.89	0.54
1:A:218:ALA:HB2	1:A:246:PRO:HG2	2.04	0.54
1:C:314:MET:HA	1:C:317:LEU:HD13	1.90	0.54
1:L:47:PRO:HG3	1:M:69:MET:HG3	1.89	0.54
1:Y:220:ILE:HD12	1:Y:296:THR:HG21	1.89	0.54
1:U:325:ILE:HG22	1:U:330:THR:HG23	1.90	0.54
1:T:333:VAL:HG12	1:T:334:GLU:HG2	1.90	0.54
1:U:322:ARG:HB3	1:U:333:VAL:HB	1.90	0.54
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.90	0.54
1:A:66:VAL:HA	1:A:69:MET:HE2	1.96	0.54
1:B:409:GLU:OE2	1:B:502:ARG:NH2	2.61	0.54
1:A:295:LEU:HD12	1:A:342:ILE:HD13	1.90	0.54
1:W:248:LEU:HD22	1:W:323:ILE:HG21	1.88	0.54
1:F:324:THR:OG1	1:F:331:THR:OG1	2.24	0.54
1:E:109:ALA:HA	1:H:105:LYS:HG2	1.90	0.54
1:J:120:ILE:HG23	1:J:443:ILE:HD11	1.89	0.54
1:V:292:ILE:HG13	1:V:293:ALA:H	1.73	0.54
1:Z:40:ILE:HD13	1:Z:59:GLU:HG3	1.89	0.54
1:T:102:GLU:O	1:T:106:ASN:ND2	2.41	0.54
1:B:177:VAL:HG22	1:B:379:LEU:HD12	2.48	0.53
1:I:246:PRO:HB3	1:I:272:LYS:HB3	1.90	0.53
1:L:164:GLU:OE2	1:L:168:LYS:NZ	2.36	0.53
1:Q:40:ILE:HB	1:Q:48:THR:HB	1.90	0.53
1:X:180:ALA:HB2	1:X:380:LYS:HB3	1.89	0.53
1:V:112:ARG:NH1	1:V:115:ASP:OD2	2.40	0.53
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.90	0.53
1:U:16:LEU:HD13	1:U:515:LEU:HD22	1.90	0.53
1:Y:294:ILE:HG22	1:Y:342:ILE:HD13	1.89	0.53
1:P:326:ASP:OD1	1:P:329:ASN:N	2.39	0.53
1:U:381:ILE:HG12	1:U:396:VAL:HG21	1.89	0.53
1:X:169:VAL:HG21	1:X:377:ALA:HB2	1.91	0.53
1:P:192:GLY:HA2	1:P:295:LEU:HD21	1.90	0.53
1:F:349:ILE:HD12	1:F:368:ARG:HH12	1.74	0.53
1:H:325:ILE:HG12	1:H:330:THR:HG23	1.89	0.53
1:Z:236:ILE:HD11	1:Z:317:LEU:HD11	1.90	0.53
1:A:77:VAL:HG12	1:A:507:ASN:HB3	1.90	0.53
1:B:333:VAL:HG22	1:B:376:VAL:HG11	1.91	0.53
1:T:413:VAL:HG23	1:T:489:LEU:HB2	1.91	0.53
1:H:413:VAL:HG22	1:H:490:ILE:HD11	1.90	0.53
1:E:345:ARG:HH21	1:E:368:ARG:HH22	1.56	0.53
1:V:278:ALA:HB3	1:V:285:ARG:HE	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:GLU:O	1:F:106:ASN:ND2	2.40	0.53
1:L:215:LEU:HB2	1:L:323:ILE:HG23	1.89	0.53
1:S:117:LYS:HG3	1:S:513:SER:HB3	1.91	0.53
1:N:40:ILE:HD13	1:N:59:GLU:HG3	1.89	0.53
1:U:333:VAL:HG12	1:U:334:GLU:HG3	1.90	0.53
1:H:33:PRO:HG2	1:H:481:ALA:HB3	1.91	0.53
1:H:246:PRO:HB3	1:H:272:LYS:HB3	1.90	0.53
1:B:186:GLU:OE1	1:B:188:LYS:NZ	2.36	0.53
1:N:218:ALA:HB3	1:N:323:ILE:HD13	1.91	0.53
1:M:81:THR:OG1	1:M:507:ASN:ND2	2.38	0.53
1:A:117:LYS:HG3	1:A:513:SER:HB3	2.18	0.53
1:B:419:LEU:HD22	1:B:447:LEU:HD22	2.33	0.52
1:G:381:ILE:HG12	1:G:396:VAL:HG21	1.91	0.52
1:A:247:LEU:HB3	1:A:273:VAL:HG12	1.91	0.52
1:Y:386:GLU:OE1	1:Z:197:ARG:NH2	2.40	0.52
1:Z:218:ALA:HB2	1:Z:246:PRO:HG2	1.91	0.52
1:C:77:VAL:HA	1:C:80:LYS:HE2	1.92	0.52
1:Q:84:VAL:HG22	1:Q:402:ALA:HA	1.90	0.52
1:D:40:ILE:HD13	1:D:59:GLU:HG3	1.91	0.52
1:Z:25:ASN:HA	1:Z:28:LYS:HE2	1.92	0.52
1:L:77:VAL:HG21	1:L:511:VAL:HB	1.91	0.52
1:W:120:ILE:HG23	1:W:443:ILE:HD11	1.91	0.52
1:L:180:ALA:HA	1:L:380:LYS:HE3	1.91	0.52
1:E:216:ASP:OD1	1:E:322:ARG:NH1	2.43	0.52
1:A:200:LEU:HD23	1:A:259:LEU:HD12	1.92	0.52
1:B:152:ALA:O	1:B:395:ARG:NH1	2.43	0.52
1:U:468:GLU:HG2	1:Z:465:VAL:HG11	1.91	0.52
1:T:421:ARG:NH1	1:T:473:ALA:O	2.43	0.52
1:X:197:ARG:HE	1:X:277:LYS:HB2	1.74	0.52
1:S:33:PRO:HG2	1:S:481:ALA:HB3	1.92	0.52
1:B:245:ARG:NH2	1:B:319:GLN:OE1	2.37	0.52
1:C:296:THR:HB	1:C:318:GLY:HA3	1.92	0.52
1:M:168:LYS:HG2	1:M:189:VAL:HG21	1.92	0.52
1:G:141:LYS:HD2	1:G:167:ASP:HB2	1.91	0.52
1:H:346:ILE:HG22	1:H:350:LYS:HE2	1.91	0.52
1:X:325:ILE:HG13	1:X:330:THR:HG23	1.93	0.52
1:A:85:ALA:HB1	1:A:500:VAL:HG22	1.91	0.52
1:B:138:ILE:HG12	1:B:147:VAL:HG21	1.92	0.51
1:B:15:LYS:NZ	1:B:67:GLU:OE2	3.08	0.51
1:M:502:ARG:NH1	1:M:506:GLU:OE1	2.43	0.51
1:I:381:ILE:HG12	1:I:396:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:138:ILE:HG13	1:Z:143:GLU:HB3	1.92	0.51
1:G:77:VAL:HA	1:G:80:LYS:HE2	1.91	0.51
1:M:250:ILE:HG22	1:M:276:VAL:HB	1.92	0.51
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.93	0.51
1:Q:33:PRO:HG2	1:Q:481:ALA:HB3	1.93	0.51
1:R:247:LEU:HB3	1:R:273:VAL:HG12	1.92	0.51
1:X:169:VAL:HG12	1:X:173:GLY:HA3	1.91	0.51
1:V:138:ILE:HG12	1:V:147:VAL:HG21	1.93	0.51
1:H:66:VAL:HA	1:H:69:MET:HE2	1.93	0.51
1:U:469:LYS:HD3	1:U:486:TYR:CZ	2.45	0.51
1:A:87:ASP:OD1	1:A:88:GLY:N	2.43	0.51
1:Q:385:THR:HG22	1:Q:387:VAL:H	1.75	0.51
1:W:27:VAL:HG12	1:W:90:THR:HG23	1.92	0.51
1:N:77:VAL:HG12	1:N:507:ASN:HB3	1.93	0.51
1:I:413:VAL:HG23	1:I:489:LEU:HB2	1.92	0.51
1:K:102:GLU:O	1:K:106:ASN:ND2	2.42	0.51
1:F:77:VAL:HA	1:F:80:LYS:HE2	1.93	0.51
1:Z:248:LEU:HD22	1:Z:323:ILE:HG21	1.92	0.51
1:P:382:GLY:O	1:P:392:LYS:NZ	2.40	0.51
1:A:381:ILE:HG12	1:A:396:VAL:HG21	1.93	0.51
1:N:321:ALA:HB3	1:N:334:GLU:HB3	1.93	0.50
1:A:109:ALA:HA	1:U:105:LYS:HG2	62.71	0.50
1:K:411:ILE:HD13	1:K:497:PRO:HA	1.92	0.50
1:O:81:THR:HG23	1:O:503:SER:HB2	1.92	0.50
1:B:36:ARG:HB3	1:V:517:THR:O	181.75	0.50
1:Q:171:LYS:O	1:Q:404:ARG:NH1	2.44	0.50
1:G:25:ASN:HA	1:G:28:LYS:HE2	1.94	0.50
1:I:255:GLU:HA	1:I:259:LEU:HB2	1.92	0.50
1:E:58:LYS:HA	1:E:75:ARG:HH21	1.77	0.50
1:V:386:GLU:HA	1:V:389:MET:HG2	1.93	0.50
1:Y:345:ARG:NH1	1:Y:348:GLU:OE1	2.43	0.50
1:M:29:VAL:HG11	1:N:519:GLU:HB2	1.93	0.50
1:K:33:PRO:HG2	1:K:481:ALA:HB3	1.92	0.50
1:U:203:TYR:HB3	1:U:267:LEU:HD21	1.94	0.50
1:C:41:ASP:HB2	1:D:523:THR:HG22	1.92	0.50
1:H:54:VAL:HG22	1:H:89:THR:HG21	1.93	0.50
1:D:120:ILE:HG23	1:D:443:ILE:HD11	1.92	0.50
1:U:185:THR:HG22	1:U:382:GLY:H	1.76	0.50
1:A:228:SER:HG	1:A:257:GLU:N	2.09	0.50
1:U:248:LEU:HD22	1:U:323:ILE:HG21	1.94	0.50
1:P:254:ILE:HD13	1:P:275:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HA	1:A:80:LYS:HE2	1.94	0.50
1:B:171:LYS:O	1:B:404:ARG:NH1	2.45	0.50
1:R:36:ARG:NH2	1:R:457:ASN:OD1	2.44	0.50
1:G:291:ASP:OD1	1:G:368:ARG:NH2	2.44	0.50
1:R:220:ILE:HG22	1:R:248:LEU:HB3	1.94	0.50
1:V:205:VAL:HA	1:V:213:ALA:HB2	1.94	0.50
1:S:85:ALA:HB1	1:S:500:VAL:HG22	1.94	0.50
1:H:120:ILE:HG23	1:H:443:ILE:HD11	1.94	0.50
1:B:85:ALA:HB1	1:B:500:VAL:HG22	2.05	0.50
1:U:411:ILE:HD13	1:U:497:PRO:HA	1.94	0.50
1:R:384:SER:OG	1:R:388:GLU:OE2	2.28	0.50
1:N:411:ILE:HD12	1:N:495:VAL:HG21	1.93	0.50
1:L:62:LEU:HB2	1:L:68:ASN:HB2	1.93	0.50
1:Z:295:LEU:HD11	1:Z:372:LEU:HG	1.93	0.50
1:M:54:VAL:HG22	1:M:89:THR:HG21	1.94	0.50
1:L:77:VAL:HA	1:L:80:LYS:HE2	1.93	0.49
1:S:17:LYS:HD2	1:S:104:LEU:HD12	1.94	0.49
1:O:149:THR:HG23	1:O:155:ASP:H	1.77	0.49
1:S:383:ALA:HB2	1:S:392:LYS:HD3	1.94	0.49
1:N:64:ASP:HB3	1:N:67:GLU:HB2	1.94	0.49
1:X:64:ASP:HB3	1:X:67:GLU:HB2	1.93	0.49
1:D:450:PRO:O	1:D:454:ILE:HG12	2.12	0.49
1:U:215:LEU:HB2	1:U:323:ILE:HB	1.93	0.49
1:D:33:PRO:HG2	1:D:481:ALA:HB3	1.95	0.49
1:V:411:ILE:HD13	1:V:497:PRO:HA	1.93	0.49
1:Z:190:VAL:HG21	1:Z:334:GLU:HB2	1.95	0.49
1:J:325:ILE:HG12	1:J:330:THR:HG23	1.94	0.49
1:J:243:SER:O	1:J:245:ARG:N	2.46	0.49
1:Y:237:LEU:HD11	1:Y:317:LEU:HD11	1.95	0.49
1:W:247:LEU:HB3	1:W:273:VAL:HG23	1.93	0.49
1:E:382:GLY:HA2	1:E:389:MET:HG2	1.93	0.49
1:J:333:VAL:HG12	1:J:334:GLU:HG2	1.94	0.49
1:J:47:PRO:HG3	1:K:69:MET:HG2	1.94	0.49
1:G:31:LEU:O	1:G:457:ASN:ND2	2.46	0.49
1:Z:2:THR:O	1:Z:4:LYS:NZ	2.44	0.49
1:N:265:ASN:O	1:N:271:LEU:N	2.46	0.49
1:L:502:ARG:NH1	1:L:506:GLU:OE1	2.46	0.49
1:H:102:GLU:O	1:H:106:ASN:ND2	2.43	0.49
1:W:33:PRO:HG2	1:W:481:ALA:HB3	1.95	0.49
1:G:165:ALA:HB2	1:G:379:LEU:HD21	1.95	0.49
1:X:221:LEU:HB2	1:X:247:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:TYR:OH	1:A:327:LYS:NZ	2.33	0.49
1:B:165:ALA:HB2	1:B:379:LEU:HD21	1.95	0.49
1:S:216:ASP:OD1	1:S:322:ARG:NH1	2.45	0.49
1:D:192:GLY:HA2	1:D:295:LEU:HD21	1.94	0.49
1:T:353:ILE:HG23	1:T:362:THR:HG23	1.95	0.49
1:H:2:THR:O	1:H:4:LYS:NZ	2.40	0.49
1:H:311:ASN:O	1:H:313:THR:N	2.46	0.49
1:W:236:ILE:HG21	1:W:312:ALA:HB3	1.94	0.49
1:M:326:ASP:OD1	1:M:327:LYS:N	2.39	0.49
1:G:16:LEU:HD13	1:G:515:LEU:HD22	1.95	0.49
1:R:179:GLU:OE1	1:R:390:LYS:NZ	2.44	0.49
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.94	0.49
1:X:27:VAL:HG12	1:X:90:THR:HG23	1.94	0.48
1:O:112:ARG:NH1	1:U:458:THR:O	2.44	0.48
1:D:165:ALA:HB2	1:D:379:LEU:HD21	1.95	0.48
1:Q:175:ILE:HG12	1:Q:377:ALA:HB3	1.95	0.48
1:W:289:LEU:HD23	1:W:292:ILE:HD12	1.95	0.48
1:R:289:LEU:HD23	1:R:292:ILE:HD12	1.94	0.48
1:J:36:ARG:HH12	1:K:114:ILE:HB	1.76	0.48
1:Q:25:ASN:HA	1:Q:28:LYS:HE2	1.95	0.48
1:S:25:ASN:HA	1:S:28:LYS:HE2	1.96	0.48
1:S:37:ASN:OD1	1:S:49:SER:OG	2.28	0.48
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.94	0.48
1:C:47:PRO:HG3	1:D:69:MET:HG2	1.94	0.48
1:R:200:LEU:HD21	1:R:277:LYS:HE3	1.95	0.48
1:T:301:ILE:HG23	1:T:307:TYR:HB3	1.96	0.48
1:V:62:LEU:HB2	1:V:68:ASN:HB2	1.95	0.48
1:V:200:LEU:HB2	1:V:204:PHE:HE2	1.77	0.48
1:P:411:ILE:HD13	1:P:497:PRO:HA	1.96	0.48
1:J:168:LYS:HG2	1:J:189:VAL:HG21	1.95	0.48
1:Z:314:MET:HG2	1:Z:317:LEU:HD12	1.96	0.48
1:P:458:THR:HB	1:Q:112:ARG:HH21	1.79	0.48
1:Y:64:ASP:HB3	1:Y:67:GLU:HB2	1.96	0.48
1:J:253:ASP:OD1	1:J:254:ILE:N	2.46	0.48
1:D:262:LEU:HD22	1:D:273:VAL:HG11	1.94	0.48
1:G:219:LEU:O	1:G:248:LEU:N	2.28	0.48
1:U:233:LEU:HD23	1:U:237:LEU:HB2	1.95	0.48
1:R:207:ASN:HB3	1:R:210:THR:HG22	1.95	0.48
1:U:213:ALA:HB3	1:U:325:ILE:HG12	1.94	0.48
1:J:62:LEU:HB2	1:J:68:ASN:HB2	1.96	0.48
1:Q:227:ILE:HB	1:Q:255:GLU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:187:LEU:HD13	1:T:379:LEU:HD23	1.94	0.48
1:J:17:LYS:HD2	1:J:104:LEU:HD12	1.96	0.48
1:D:253:ASP:OD1	1:D:254:ILE:N	2.47	0.48
1:N:276:VAL:HG22	1:N:277:LYS:H	1.79	0.48
1:A:85:ALA:HA	1:A:499:LYS:HE3	5.45	0.48
1:C:489:LEU:HB3	1:C:494:VAL:HB	1.94	0.48
1:E:25:ASN:HA	1:E:28:LYS:HE2	1.95	0.48
1:V:253:ASP:OD1	1:V:254:ILE:N	2.45	0.48
1:K:157:GLU:O	1:K:161:LEU:N	2.47	0.48
1:Z:220:ILE:HG22	1:Z:248:LEU:HB3	1.96	0.48
1:N:248:LEU:HD22	1:N:323:ILE:HG21	1.96	0.47
1:T:15:LYS:NZ	1:T:64:ASP:OD2	2.46	0.47
1:P:220:ILE:HD12	1:P:296:THR:HG21	1.95	0.47
1:I:141:LYS:HG3	1:I:163:ALA:HB1	1.96	0.47
1:C:40:ILE:HD13	1:C:59:GLU:HG3	1.95	0.47
1:U:187:LEU:HD13	1:U:379:LEU:HD23	1.96	0.47
1:D:117:LYS:HG3	1:D:513:SER:HB3	1.96	0.47
1:K:497:PRO:HB2	1:K:500:VAL:HG23	1.96	0.47
1:M:328:ASP:OD1	1:M:329:ASN:N	2.42	0.47
1:L:222:ILE:HG13	1:L:250:ILE:HD12	1.97	0.47
1:Q:294:ILE:HD12	1:Q:345:ARG:HH11	1.79	0.47
1:H:132:ARG:NH2	1:H:409:GLU:OE1	2.48	0.47
1:O:87:ASP:OD2	1:O:88:GLY:N	2.47	0.47
1:J:117:LYS:HG3	1:J:513:SER:HB3	1.96	0.47
1:W:252:GLU:HG3	1:W:285:ARG:HH11	1.80	0.47
1:S:386:GLU:OE2	1:T:277:LYS:NZ	2.43	0.47
1:H:117:LYS:HG3	1:H:513:SER:HB3	1.96	0.47
1:C:116:LEU:O	1:C:120:ILE:HG12	2.14	0.47
1:Q:420:ILE:HD12	1:Q:451:LEU:HD13	1.97	0.47
1:V:302:SER:OG	1:V:303:GLU:N	2.44	0.47
1:A:4:LYS:NZ	1:G:59:GLU:OE1	2.46	0.47
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.96	0.47
1:R:91:THR:N	2:R:602:SO4:O3	2.43	0.47
1:L:219:LEU:O	1:L:248:LEU:N	2.47	0.47
1:I:132:ARG:HH22	1:I:409:GLU:HB3	1.79	0.47
1:P:349:ILE:HG21	1:P:369:LEU:HB2	1.97	0.47
1:A:23:LEU:HD12	1:A:60:ILE:HD12	4.16	0.47
1:B:27:VAL:HG22	1:B:90:THR:HG23	4.19	0.47
1:C:69:MET:HE1	1:C:521:ALA:HB1	1.97	0.47
1:X:132:ARG:HH22	1:X:409:GLU:HB3	1.78	0.47
1:C:413:VAL:HG23	1:C:489:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:321:ALA:HB3	1:S:334:GLU:HB3	1.97	0.47
1:G:6:ILE:HG12	1:G:522:ILE:HG12	1.97	0.47
1:O:25:ASN:HA	1:O:28:LYS:HE2	1.97	0.47
1:A:187:LEU:HD13	1:A:379:LEU:HD23	1.96	0.47
1:Q:165:ALA:HB2	1:Q:379:LEU:HD21	1.97	0.46
1:I:295:LEU:HA	1:I:342:ILE:HD11	1.97	0.46
1:X:25:ASN:HA	1:X:28:LYS:HE2	1.97	0.46
1:J:220:ILE:O	1:J:318:GLY:N	2.47	0.46
1:X:205:VAL:HA	1:X:213:ALA:HB2	1.97	0.46
1:U:294:ILE:HD12	1:U:345:ARG:HD2	1.97	0.46
1:T:291:ASP:HB3	1:T:372:LEU:HD21	1.96	0.46
1:T:77:VAL:HA	1:T:80:LYS:HE2	1.96	0.46
1:E:105:LYS:HG2	1:H:109:ALA:HA	1.96	0.46
1:U:62:LEU:HB2	1:U:68:ASN:HB2	1.97	0.46
1:F:69:MET:HE1	1:F:521:ALA:HB1	1.97	0.46
1:F:296:THR:O	1:F:319:GLN:N	2.48	0.46
1:A:326:ASP:OD1	1:A:327:LYS:N	2.45	0.46
1:T:177:VAL:HG22	1:T:379:LEU:HD12	1.98	0.46
1:A:165:ALA:HB2	1:A:379:LEU:HD21	2.11	0.46
1:U:222:ILE:HG21	1:U:300:VAL:HG22	1.98	0.46
1:S:438:THR:O	1:S:442:ILE:HG12	2.16	0.46
1:Q:7:LEU:HD23	1:Q:12:ALA:HA	1.97	0.46
1:E:23:LEU:HD12	1:E:60:ILE:HD12	1.96	0.46
1:N:224:ASP:O	1:N:285:ARG:NH2	2.47	0.46
1:V:120:ILE:HG23	1:V:443:ILE:HD11	1.97	0.46
1:B:421:ARG:NH2	1:B:477:TYR:O	2.92	0.46
1:X:234:LEU:O	1:X:236:ILE:N	2.44	0.46
1:F:419:LEU:HD22	1:F:447:LEU:HD22	1.98	0.46
1:R:438:THR:O	1:R:442:ILE:HG12	2.16	0.46
1:Q:31:LEU:O	1:Q:457:ASN:ND2	2.44	0.46
1:N:117:LYS:HG3	1:N:513:SER:HB3	1.96	0.46
1:S:389:MET:HG2	1:S:393:LYS:HG3	1.96	0.46
1:Z:77:VAL:HG12	1:Z:507:ASN:HB3	1.97	0.46
1:F:117:LYS:HG3	1:F:513:SER:HB2	1.96	0.46
1:W:25:ASN:HA	1:W:28:LYS:HE2	1.97	0.46
1:Q:247:LEU:HB3	1:Q:273:VAL:HG12	1.97	0.46
1:B:222:ILE:HG21	1:B:300:VAL:HG22	1.98	0.46
1:A:25:ASN:HA	1:A:28:LYS:HE2	2.06	0.46
1:Y:77:VAL:HA	1:Y:80:LYS:HE2	1.98	0.46
1:F:480:ASN:HD22	1:F:494:VAL:HG21	1.81	0.46
1:A:388:GLU:O	1:A:392:LYS:N	3.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:THR:N	2:F:601:SO4:O3	2.46	0.46
1:W:40:ILE:HD13	1:W:59:GLU:HG3	1.98	0.46
1:S:227:ILE:HG23	1:S:228:SER:H	1.80	0.46
1:O:294:ILE:HG22	1:O:342:ILE:HD13	1.98	0.46
1:Z:116:LEU:O	1:Z:120:ILE:HG12	2.15	0.46
1:X:247:LEU:HB3	1:X:273:VAL:HG12	1.97	0.45
1:D:262:LEU:HD13	1:D:273:VAL:HG11	1.97	0.45
1:S:141:LYS:HG3	1:S:163:ALA:HB1	1.97	0.45
1:Y:36:ARG:HH12	1:Z:114:ILE:HB	1.80	0.45
1:L:175:ILE:HG12	1:L:377:ALA:HB3	1.97	0.45
1:Z:33:PRO:HG2	1:Z:481:ALA:HB3	1.97	0.45
1:V:193:MET:HB2	1:V:371:LYS:HB3	1.97	0.45
1:I:69:MET:HE1	1:I:523:THR:HB	1.99	0.45
1:E:206:THR:H	1:E:213:ALA:HA	1.82	0.45
1:M:77:VAL:HG12	1:M:507:ASN:HB3	1.98	0.45
1:Z:261:THR:O	1:Z:265:ASN:ND2	2.50	0.45
1:X:62:LEU:HB2	1:X:68:ASN:HB2	1.98	0.45
1:T:30:THR:HB	1:T:51:LYS:O	2.16	0.45
1:D:465:VAL:HG21	1:H:468:GLU:HG3	1.98	0.45
1:K:160:GLU:HA	1:K:163:ALA:HB2	1.97	0.45
1:D:261:THR:O	1:D:265:ASN:ND2	2.31	0.45
1:I:333:VAL:HG22	1:I:376:VAL:HG11	1.98	0.45
1:S:252:GLU:HA	1:S:278:ALA:HB2	1.99	0.45
1:V:85:ALA:HB1	1:V:500:VAL:HG22	1.99	0.45
1:R:77:VAL:HA	1:R:80:LYS:HE2	1.97	0.45
1:W:158:ILE:HD11	1:W:392:LYS:HE3	1.98	0.45
1:J:261:THR:O	1:J:265:ASN:ND2	2.49	0.45
1:Q:102:GLU:O	1:Q:106:ASN:ND2	2.45	0.45
1:B:223:HIS:O	1:B:251:ALA:HA	2.16	0.45
1:K:77:VAL:HG12	1:K:507:ASN:HB3	1.97	0.45
1:E:117:LYS:HG3	1:E:513:SER:HB3	1.99	0.45
1:N:393:LYS:NZ	1:N:397:GLU:OE2	2.45	0.45
1:I:15:LYS:HE3	1:I:67:GLU:HG3	1.98	0.45
1:G:205:VAL:HA	1:G:213:ALA:HB2	1.99	0.45
1:V:64:ASP:HB3	1:V:67:GLU:HB2	1.99	0.45
1:V:117:LYS:HG3	1:V:513:SER:HB3	1.99	0.45
1:V:313:THR:H	1:V:316:TYR:HD2	1.64	0.45
1:B:116:LEU:O	1:B:120:ILE:HG12	2.16	0.45
1:U:215:LEU:HB3	1:U:218:ALA:HB2	1.98	0.45
1:E:33:PRO:HG2	1:E:481:ALA:HB3	1.97	0.45
1:M:33:PRO:HG2	1:M:481:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:85:ALA:HB1	1:Y:500:VAL:HG22	1.99	0.45
1:N:333:VAL:HG22	1:N:376:VAL:HG11	1.98	0.45
1:J:443:ILE:O	1:J:447:LEU:HG	2.16	0.45
1:B:64:ASP:HB3	1:B:67:GLU:HB2	2.23	0.45
1:G:222:ILE:HG21	1:G:300:VAL:HG12	1.99	0.45
1:S:248:LEU:HD22	1:S:323:ILE:HG21	1.98	0.45
1:T:502:ARG:NH1	1:T:506:GLU:OE1	2.42	0.45
1:F:25:ASN:HA	1:F:28:LYS:HE2	1.97	0.45
1:T:180:ALA:HB2	1:T:380:LYS:HB3	1.99	0.45
1:M:64:ASP:HB3	1:M:67:GLU:HB2	1.98	0.45
1:L:161:LEU:HD11	1:L:187:LEU:HB2	1.98	0.45
1:Q:438:THR:O	1:Q:442:ILE:HG12	2.17	0.45
1:J:205:VAL:HA	1:J:213:ALA:HB2	1.98	0.45
1:U:136:ARG:NH2	1:U:476:ASP:OD2	2.48	0.45
1:Q:214:GLU:OE1	1:Q:322:ARG:NH1	2.50	0.45
1:X:321:ALA:HB3	1:X:334:GLU:HB2	1.99	0.45
1:Z:291:ASP:HB3	1:Z:372:LEU:HD11	1.98	0.45
1:O:158:ILE:HG23	1:O:396:VAL:HG22	1.98	0.45
1:N:222:ILE:HD12	1:N:293:ALA:HB2	1.98	0.45
1:D:200:LEU:HD11	1:D:277:LYS:HG3	1.99	0.45
1:I:77:VAL:HG12	1:I:507:ASN:HB3	1.99	0.45
1:T:31:LEU:O	1:T:457:ASN:ND2	2.45	0.45
1:S:120:ILE:HG23	1:S:443:ILE:HD11	1.97	0.45
1:P:116:LEU:O	1:P:120:ILE:HG12	2.17	0.45
1:B:321:ALA:HB3	1:B:334:GLU:HB3	1.99	0.45
1:M:438:THR:O	1:M:442:ILE:HG12	2.17	0.45
1:N:15:LYS:NZ	1:N:67:GLU:OE2	2.50	0.44
1:E:187:LEU:HD13	1:E:379:LEU:HD23	1.99	0.44
1:V:20:VAL:HG13	1:V:74:VAL:HG21	1.99	0.44
1:X:346:ILE:HD13	1:X:373:SER:HB2	1.98	0.44
1:V:292:ILE:HG13	1:V:293:ALA:N	2.32	0.44
1:U:321:ALA:HB3	1:U:334:GLU:HB2	1.98	0.44
1:P:64:ASP:HB3	1:P:67:GLU:HB2	1.99	0.44
1:P:476:ASP:HB2	1:P:488:ASN:ND2	2.32	0.44
1:Y:413:VAL:HG23	1:Y:489:LEU:HB2	1.98	0.44
1:L:81:THR:HG23	1:L:503:SER:HB2	1.98	0.44
1:D:420:ILE:HD12	1:D:451:LEU:HD13	1.98	0.44
1:Q:291:ASP:HB3	1:Q:372:LEU:HD11	2.00	0.44
1:H:326:ASP:OD1	1:H:329:ASN:N	2.41	0.44
1:P:490:ILE:HD13	1:P:495:VAL:HG12	1.99	0.44
1:A:15:LYS:HE3	1:A:67:GLU:HG3	3.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:ALA:O	1:E:368:ARG:NH2	2.51	0.44
1:F:278:ALA:HB1	1:F:289:LEU:HD11	1.99	0.44
1:O:321:ALA:HB3	1:O:334:GLU:HB3	2.00	0.44
1:G:187:LEU:HD13	1:G:379:LEU:HD23	1.99	0.44
1:G:210:THR:HG23	1:G:212:GLU:HG2	1.99	0.44
1:Q:47:PRO:HB3	1:R:69:MET:HG2	2.00	0.44
1:Y:38:VAL:HG22	1:Z:520:ALA:HB3	1.98	0.44
1:W:77:VAL:HG12	1:W:507:ASN:HB3	1.99	0.44
1:Q:194:GLN:HE21	1:Q:329:ASN:HB3	1.83	0.44
1:I:25:ASN:HA	1:I:28:LYS:HE2	2.00	0.44
1:M:411:ILE:HD13	1:M:497:PRO:HA	2.00	0.44
1:A:411:ILE:HD12	1:A:495:VAL:HG21	5.00	0.44
1:V:31:LEU:O	1:V:457:ASN:ND2	2.43	0.44
1:W:141:LYS:HD2	1:W:167:ASP:HB2	1.99	0.44
1:Z:216:ASP:OD1	1:Z:322:ARG:NE	2.50	0.44
1:L:161:LEU:HG	1:L:379:LEU:HD22	1.99	0.44
1:C:381:ILE:HG12	1:C:396:VAL:HG21	1.99	0.44
1:H:517:THR:O	1:N:36:ARG:HB3	2.18	0.44
1:H:340:GLU:HA	1:H:343:LYS:HE2	1.99	0.44
1:W:221:LEU:HD23	1:W:249:ILE:HG12	2.00	0.44
1:H:205:VAL:HA	1:H:213:ALA:HB2	2.00	0.44
1:V:7:LEU:HD12	1:V:66:VAL:HG21	2.00	0.44
1:R:333:VAL:HG22	1:R:376:VAL:HG11	1.99	0.44
1:G:105:LYS:HG2	1:M:109:ALA:HA	2.00	0.44
1:B:193:MET:HB2	1:B:371:LYS:HB3	1.99	0.44
1:K:59:GLU:OE1	1:L:4:LYS:NZ	2.50	0.44
1:U:77:VAL:HG12	1:U:507:ASN:HB3	1.98	0.44
1:O:218:ALA:HB2	1:O:246:PRO:HG2	2.00	0.44
1:N:30:THR:HB	1:N:51:LYS:O	2.18	0.44
1:D:349:ILE:HG22	1:D:369:LEU:HD12	1.99	0.44
1:Y:138:ILE:HG12	1:Y:147:VAL:HG21	2.00	0.43
1:Q:195:PHE:CD1	1:Q:279:PRO:HG3	2.53	0.43
1:I:227:ILE:HG23	1:I:228:SER:H	1.83	0.43
1:O:411:ILE:HD13	1:O:497:PRO:HA	2.00	0.43
1:B:166:MET:HE1	1:B:407:VAL:HG11	3.06	0.43
1:A:420:ILE:HD12	1:A:451:LEU:HD13	2.05	0.43
1:S:192:GLY:HA2	1:S:295:LEU:HD21	1.98	0.43
1:G:488:ASN:HB3	1:G:491:GLU:HG2	2.00	0.43
1:Z:138:ILE:HG12	1:Z:147:VAL:HG21	2.00	0.43
1:D:25:ASN:HA	1:D:28:LYS:HE2	2.00	0.43
1:P:222:ILE:HG21	1:P:300:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ILE:HG12	1:D:147:VAL:HG21	2.00	0.43
1:G:66:VAL:HA	1:G:69:MET:HE2	2.00	0.43
1:S:200:LEU:HD21	1:S:277:LYS:HG2	2.01	0.43
1:B:190:VAL:HG21	1:B:333:VAL:HG13	2.64	0.43
1:I:64:ASP:HB3	1:I:67:GLU:HB2	1.99	0.43
1:B:83:ASP:OD1	1:B:84:VAL:N	3.90	0.43
1:O:47:PRO:HG3	1:P:69:MET:HG3	2.01	0.43
1:G:469:LYS:HD2	1:G:486:TYR:CZ	2.53	0.43
1:Z:180:ALA:HA	1:Z:380:LYS:HE2	2.00	0.43
1:Z:205:VAL:HA	1:Z:213:ALA:HB2	1.99	0.43
1:B:321:ALA:N	1:B:334:GLU:O	2.79	0.43
1:Y:214:GLU:OE1	1:Y:322:ARG:NH2	2.50	0.43
1:K:62:LEU:HB2	1:K:68:ASN:HB2	2.01	0.43
1:D:79:SER:HA	1:D:89:THR:HG22	2.00	0.43
1:H:165:ALA:HB2	1:H:379:LEU:HD21	2.01	0.43
1:A:421:ARG:NH2	1:A:477:TYR:O	2.68	0.43
1:B:177:VAL:HG13	1:B:381:ILE:HD13	2.01	0.43
1:P:102:GLU:O	1:P:106:ASN:ND2	2.50	0.43
1:A:13:ARG:NH2	1:A:519:GLU:OE2	3.90	0.43
1:Q:219:LEU:O	1:Q:248:LEU:N	2.34	0.43
1:R:171:LYS:O	1:R:404:ARG:NH1	2.52	0.43
1:D:187:LEU:HD13	1:D:379:LEU:HD23	1.99	0.43
1:C:476:ASP:HB2	1:C:488:ASN:ND2	2.33	0.43
1:X:222:ILE:HG23	1:X:289:LEU:HD22	2.01	0.43
1:G:123:ALA:HB2	1:G:440:ILE:HD13	2.01	0.43
1:Y:30:THR:HB	1:Y:51:LYS:O	2.18	0.43
1:P:438:THR:O	1:P:442:ILE:HG12	2.19	0.43
1:W:194:GLN:NE2	1:W:331:THR:OG1	2.50	0.43
1:J:420:ILE:HD11	1:J:448:GLU:HA	2.00	0.43
1:B:321:ALA:N	1:B:333:VAL:O	3.33	0.43
1:M:102:GLU:HB2	1:M:442:ILE:HG23	2.00	0.43
1:P:469:LYS:HD3	1:P:486:TYR:CZ	2.54	0.43
1:E:262:LEU:HD22	1:E:273:VAL:HG11	1.99	0.43
1:B:87:ASP:HB3	2:B:601:SO4:O1	6.20	0.43
1:H:13:ARG:HB3	1:H:104:LEU:HD21	2.00	0.43
1:R:98:ALA:HB2	1:R:449:GLU:HG2	2.01	0.43
1:Y:205:VAL:HA	1:Y:213:ALA:HB2	2.01	0.43
1:C:77:VAL:HG12	1:C:507:ASN:HB3	2.01	0.43
1:R:278:ALA:HB1	1:R:289:LEU:HD21	2.00	0.43
1:D:254:ILE:HG22	1:D:259:LEU:HB2	1.99	0.43
1:O:295:LEU:HA	1:O:342:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:519:GLU:HG3	1:N:36:ARG:CZ	2.48	0.43
1:A:222:ILE:HG21	1:A:300:VAL:HG12	2.00	0.43
1:Z:161:LEU:HD11	1:Z:187:LEU:HB2	2.00	0.43
1:Q:19:GLY:HA3	1:Q:67:GLU:O	2.19	0.43
1:B:141:LYS:HG3	1:B:163:ALA:HB1	2.72	0.43
1:D:221:LEU:HD23	1:D:249:ILE:HG12	2.00	0.43
1:N:6:ILE:HD12	1:N:522:ILE:HG12	2.01	0.43
1:B:420:ILE:HG21	1:B:471:LYS:HG2	2.01	0.43
1:T:489:LEU:HB3	1:T:494:VAL:HB	2.01	0.43
1:Y:36:ARG:HH22	1:Z:114:ILE:HB	1.84	0.43
1:A:122:ARG:NH1	1:A:436:GLN:OE1	2.52	0.43
1:F:469:LYS:HD2	1:F:486:TYR:CZ	2.54	0.43
1:W:409:GLU:OE2	1:W:502:ARG:NH2	2.51	0.43
1:K:324:THR:O	1:K:331:THR:N	2.51	0.43
1:V:177:VAL:HG22	1:V:379:LEU:HD12	2.01	0.43
1:W:222:ILE:HG23	1:W:289:LEU:HD22	2.01	0.43
1:E:36:ARG:CZ	1:F:519:GLU:HG3	2.48	0.43
1:K:420:ILE:HD11	1:K:448:GLU:HA	2.00	0.43
1:I:68:ASN:O	1:I:72:GLN:HG2	2.19	0.43
1:F:476:ASP:HB2	1:F:488:ASN:ND2	2.34	0.43
1:I:251:ALA:HB3	1:I:254:ILE:HG12	1.99	0.43
1:E:82:SER:HA	1:E:86:GLY:H	1.84	0.43
1:J:250:ILE:HG12	1:J:276:VAL:HB	2.01	0.43
1:C:30:THR:HB	1:C:51:LYS:O	2.19	0.43
1:R:320:ALA:HA	1:R:335:GLY:HA2	2.00	0.43
1:W:448:GLU:HB3	1:W:467:LEU:HD21	2.01	0.43
1:I:291:ASP:HB3	1:I:372:LEU:HD11	2.01	0.43
1:H:187:LEU:HD13	1:H:379:LEU:HD23	2.01	0.42
1:H:83:ASP:OD2	1:H:327:LYS:NZ	2.34	0.42
1:T:320:ALA:HA	1:T:335:GLY:HA2	2.00	0.42
1:L:54:VAL:HG22	1:L:89:THR:HG21	2.00	0.42
1:A:352:GLN:HB2	1:A:365:LEU:HD21	2.01	0.42
1:G:206:THR:HB	1:G:214:GLU:H	1.84	0.42
1:P:443:ILE:O	1:P:447:LEU:HG	2.19	0.42
1:G:33:PRO:HG2	1:G:481:ALA:HB3	2.02	0.42
1:R:409:GLU:OE2	1:R:502:ARG:NH2	2.49	0.42
1:I:177:VAL:HG13	1:I:381:ILE:HD13	2.00	0.42
1:J:36:ARG:HD2	1:K:519:GLU:HG2	2.02	0.42
1:A:222:ILE:HG21	1:A:300:VAL:HG22	5.51	0.42
1:I:62:LEU:HB2	1:I:68:ASN:HB2	2.01	0.42
1:D:215:LEU:HB3	1:D:218:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:30:THR:HB	1:M:51:LYS:O	2.18	0.42
1:A:102:GLU:O	1:A:106:ASN:ND2	2.48	0.42
1:Q:179:GLU:OE2	1:Q:390:LYS:NZ	2.41	0.42
1:L:385:THR:HG22	1:L:387:VAL:H	1.84	0.42
1:O:19:GLY:HA3	1:O:67:GLU:O	2.20	0.42
1:H:19:GLY:HA3	1:H:67:GLU:O	2.19	0.42
1:O:41:ASP:HB3	1:P:523:THR:HA	2.00	0.42
1:G:158:ILE:HG23	1:G:396:VAL:HG22	2.01	0.42
1:J:36:ARG:HB3	1:K:517:THR:O	2.20	0.42
1:G:476:ASP:HB2	1:G:488:ASN:ND2	2.34	0.42
1:W:420:ILE:HD11	1:W:448:GLU:HA	2.00	0.42
1:N:220:ILE:N	1:N:318:GLY:O	2.42	0.42
1:I:213:ALA:HB3	1:I:325:ILE:HB	2.00	0.42
1:D:171:LYS:HE3	1:D:407:VAL:HG12	2.02	0.42
1:X:200:LEU:HB2	1:X:275:ALA:HB3	2.00	0.42
1:P:30:THR:HB	1:P:51:LYS:O	2.20	0.42
1:H:43:LYS:HB2	1:H:43:LYS:HE2	1.90	0.42
1:M:443:ILE:O	1:M:447:LEU:HG	2.20	0.42
1:H:346:ILE:HG23	1:H:369:LEU:HD11	2.01	0.42
1:Z:178:GLU:HG3	1:Z:322:ARG:CZ	2.49	0.42
1:O:17:LYS:HD2	1:O:104:LEU:HD12	2.01	0.42
1:O:476:ASP:HB2	1:O:488:ASN:ND2	2.34	0.42
1:K:476:ASP:HB2	1:K:488:ASN:ND2	2.35	0.42
1:V:217:GLU:N	1:V:321:ALA:O	2.41	0.42
1:B:469:LYS:HD2	1:B:486:TYR:CZ	2.54	0.42
1:B:20:VAL:HG13	1:B:74:VAL:HG21	2.01	0.42
1:L:489:LEU:HB3	1:L:494:VAL:HB	2.01	0.42
1:R:218:ALA:HB2	1:R:246:PRO:HG2	2.00	0.42
1:T:6:ILE:HG12	1:T:522:ILE:HG12	2.01	0.42
1:F:443:ILE:O	1:F:447:LEU:HG	2.20	0.42
1:M:187:LEU:HD13	1:M:379:LEU:HD23	2.02	0.42
1:E:237:LEU:O	1:E:241:ALA:N	2.53	0.42
1:G:443:ILE:O	1:G:447:LEU:HG	2.20	0.42
1:A:77:VAL:HG21	1:A:511:VAL:HB	2.01	0.42
1:A:161:LEU:HG	1:A:379:LEU:HD22	2.01	0.42
1:P:196:ASP:OD1	1:P:197:ARG:NH1	2.53	0.42
1:W:190:VAL:HG21	1:W:333:VAL:HG13	2.02	0.42
1:B:30:THR:HB	1:B:51:LYS:O	2.22	0.42
1:Z:64:ASP:HB3	1:Z:67:GLU:HB2	2.02	0.42
1:C:138:ILE:HD12	1:C:406:ALA:HB1	2.02	0.42
1:P:136:ARG:NH2	1:P:476:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:131:LEU:HD23	1:R:502:ARG:HB3	2.02	0.42
1:O:15:LYS:NZ	1:O:67:GLU:OE2	2.53	0.42
1:C:82:SER:HA	1:C:85:ALA:HB3	2.01	0.42
1:Y:41:ASP:HB2	1:Z:523:THR:HG22	2.01	0.42
1:Q:158:ILE:HG23	1:Q:396:VAL:HG22	2.01	0.42
1:V:54:VAL:HG22	1:V:89:THR:HG21	2.00	0.42
1:A:520:ALA:HB3	1:G:38:VAL:HG22	2.02	0.42
1:U:54:VAL:HG22	1:U:89:THR:HG21	2.02	0.42
1:L:319:GLN:O	1:L:336:LYS:N	2.52	0.42
1:A:460:THR:HG22	1:B:112:ARG:HD2	5.79	0.42
1:E:116:LEU:O	1:E:120:ILE:HG12	2.20	0.42
1:M:498:THR:O	1:M:502:ARG:HG2	2.20	0.42
1:W:273:VAL:HG22	1:W:274:ALA:H	1.85	0.42
1:O:65:PRO:O	1:O:69:MET:HG3	2.20	0.42
1:U:312:ALA:HB1	1:U:316:TYR:HD2	1.84	0.42
1:E:102:GLU:O	1:E:106:ASN:ND2	2.49	0.42
1:L:6:ILE:HG12	1:L:522:ILE:HG12	2.01	0.42
1:J:320:ALA:HA	1:J:335:GLY:HA2	2.01	0.42
1:F:179:GLU:HG2	1:F:393:LYS:HD2	2.01	0.42
1:A:222:ILE:HG23	1:A:289:LEU:HD22	2.07	0.41
1:R:215:LEU:HB3	1:R:218:ALA:HB2	2.02	0.41
1:C:460:THR:HG22	1:D:112:ARG:HD2	2.02	0.41
1:E:30:THR:HB	1:E:51:LYS:O	2.20	0.41
1:V:476:ASP:HB2	1:V:488:ASN:ND2	2.34	0.41
1:Q:18:VAL:HG12	1:Q:22:LYS:HE2	2.01	0.41
1:A:112:ARG:HH22	1:G:484:GLU:CD	2.23	0.41
1:C:81:THR:O	1:C:85:ALA:HB2	2.20	0.41
1:M:323:ILE:HD12	1:M:332:ILE:HG12	2.02	0.41
1:A:409:GLU:OE2	1:A:502:ARG:NH2	2.54	0.41
1:F:439:GLY:HA2	1:F:442:ILE:HD12	2.01	0.41
1:X:296:THR:O	1:X:319:GLN:N	2.52	0.41
1:A:382:GLY:HA2	1:A:389:MET:HG2	2.02	0.41
1:E:68:ASN:O	1:E:72:GLN:HG2	2.19	0.41
1:R:210:THR:HG23	1:R:212:GLU:H	1.85	0.41
1:A:171:LYS:O	1:A:404:ARG:NH1	2.53	0.41
1:Y:480:ASN:HD22	1:Y:494:VAL:HG21	1.85	0.41
1:H:40:ILE:HD13	1:H:59:GLU:HG3	2.02	0.41
1:D:65:PRO:O	1:D:69:MET:HB2	2.21	0.41
1:E:385:THR:HG23	1:E:388:GLU:H	1.85	0.41
1:Q:131:LEU:HD21	1:Q:501:THR:HG22	2.02	0.41
1:S:62:LEU:HB2	1:S:68:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:180:ALA:HB2	1:N:380:LYS:HB3	2.02	0.41
1:Z:497:PRO:HB2	1:Z:500:VAL:HG23	2.02	0.41
1:G:141:LYS:HA	1:G:141:LYS:HD3	1.88	0.41
1:V:36:ARG:NH2	1:V:457:ASN:OD1	2.53	0.41
1:T:128:VAL:O	1:T:132:ARG:HG2	2.21	0.41
1:C:177:VAL:HG12	1:C:393:LYS:HE2	2.02	0.41
1:E:199:TYR:CE2	1:E:327:LYS:HA	2.56	0.41
1:H:520:ALA:HB3	1:N:38:VAL:HG22	2.01	0.41
1:P:36:ARG:HB3	1:Q:517:THR:O	2.20	0.41
1:W:443:ILE:O	1:W:447:LEU:HG	2.20	0.41
1:W:292:ILE:O	1:W:296:THR:OG1	2.30	0.41
1:K:177:VAL:HG22	1:K:379:LEU:HD12	2.01	0.41
1:I:209:GLU:HG2	1:I:210:THR:HG23	2.03	0.41
1:L:102:GLU:O	1:L:106:ASN:ND2	2.48	0.41
1:V:320:ALA:HA	1:V:335:GLY:HA2	2.02	0.41
1:R:217:GLU:O	1:R:245:ARG:NH1	2.53	0.41
1:Y:325:ILE:HG12	1:Y:330:THR:HG23	2.02	0.41
1:A:177:VAL:HG13	1:A:381:ILE:HD13	2.02	0.41
1:A:26:ALA:HB3	1:A:60:ILE:HD11	2.85	0.41
1:S:220:ILE:HD11	1:S:323:ILE:HD11	2.03	0.41
1:K:25:ASN:HA	1:K:28:LYS:HE2	2.03	0.41
1:Q:185:THR:HG23	1:Q:380:LYS:O	2.21	0.41
1:N:138:ILE:HG12	1:N:147:VAL:HG21	2.03	0.41
1:J:30:THR:HB	1:J:51:LYS:O	2.21	0.41
1:X:31:LEU:O	1:X:457:ASN:ND2	2.53	0.41
1:C:131:LEU:HD23	1:C:502:ARG:HB3	2.03	0.41
1:P:25:ASN:HA	1:P:28:LYS:HE2	2.03	0.41
1:B:443:ILE:O	1:B:447:LEU:HG	2.26	0.41
1:X:443:ILE:O	1:X:447:LEU:HG	2.21	0.41
1:K:141:LYS:HE3	1:K:163:ALA:HB1	2.01	0.41
1:F:321:ALA:HB3	1:F:334:GLU:HB3	2.02	0.41
1:I:17:LYS:HD2	1:I:104:LEU:HD12	2.02	0.41
1:T:223:HIS:NE2	1:T:225:LYS:HB2	2.36	0.41
1:L:31:LEU:O	1:L:457:ASN:ND2	2.52	0.41
1:C:224:ASP:OD1	1:C:225:LYS:N	2.54	0.41
1:U:326:ASP:OD1	1:U:327:LYS:N	2.47	0.41
1:O:326:ASP:OD1	1:O:327:LYS:N	2.46	0.41
1:O:519:GLU:HG3	1:U:36:ARG:HD2	2.02	0.41
1:S:40:ILE:HB	1:S:48:THR:HB	2.03	0.41
1:B:38:VAL:HG13	1:C:520:ALA:HB3	2.03	0.41
1:W:98:ALA:HB2	1:W:449:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:323:ILE:HD12	1:I:332:ILE:HG12	2.02	0.41
1:K:164:GLU:O	1:K:168:LYS:HG2	2.21	0.41
1:R:224:ASP:H	1:R:301:ILE:HD11	1.84	0.41
1:V:205:VAL:HG11	1:V:211:MET:HA	2.02	0.41
1:B:19:GLY:HA3	1:B:67:GLU:O	2.25	0.41
1:B:222:ILE:HG22	1:B:300:VAL:HG13	2.03	0.41
1:C:476:ASP:HB2	1:C:488:ASN:HD21	1.85	0.41
1:I:325:ILE:HG13	1:I:330:THR:HG23	2.02	0.41
1:Q:158:ILE:HD12	1:Q:396:VAL:HG22	2.03	0.41
1:A:321:ALA:HB3	1:A:334:GLU:HB3	2.07	0.41
1:Q:13:ARG:NH1	5:Q:701:HOH:O	2.53	0.41
1:A:30:THR:HB	1:A:51:LYS:O	2.20	0.41
1:C:323:ILE:HD12	1:C:332:ILE:HG12	2.02	0.41
1:H:30:THR:HB	1:H:51:LYS:O	2.19	0.41
1:Q:325:ILE:HG22	1:Q:330:THR:HG23	2.02	0.41
1:D:36:ARG:HB3	1:E:517:THR:O	2.21	0.41
1:I:476:ASP:HB2	1:I:488:ASN:ND2	2.36	0.41
1:C:15:LYS:HB3	1:C:15:LYS:HE3	1.94	0.41
1:E:242:GLN:H	1:E:242:GLN:HG2	1.68	0.41
1:K:59:GLU:O	1:L:4:LYS:HG3	2.21	0.41
1:F:455:VAL:O	1:F:458:THR:OG1	2.29	0.41
1:A:277:LYS:HG2	1:A:278:ALA:H	1.85	0.41
1:J:411:ILE:HD13	1:J:497:PRO:HA	2.03	0.41
1:D:236:ILE:HA	1:D:239:LYS:HZ2	1.86	0.41
1:S:54:VAL:HG22	1:S:89:THR:HG21	2.03	0.41
1:Z:209:GLU:HG3	1:Z:210:THR:HG23	2.03	0.41
1:D:30:THR:HB	1:D:51:LYS:O	2.21	0.41
1:K:164:GLU:O	1:K:168:LYS:N	2.53	0.40
1:Z:187:LEU:HD13	1:Z:379:LEU:HD23	2.02	0.40
1:S:510:SER:O	1:S:514:ILE:HG12	2.20	0.40
1:H:476:ASP:HB2	1:H:488:ASN:ND2	2.36	0.40
1:X:197:ARG:HD2	1:X:197:ARG:HA	1.92	0.40
1:I:227:ILE:HG23	1:I:228:SER:N	2.35	0.40
1:L:453:GLN:NE2	1:L:457:ASN:OD1	2.54	0.40
1:X:30:THR:HB	1:X:51:LYS:O	2.20	0.40
1:W:451:LEU:HD11	1:W:470:VAL:HG11	2.03	0.40
1:D:476:ASP:HB2	1:D:488:ASN:ND2	2.36	0.40
1:N:166:MET:O	1:N:170:GLY:N	2.54	0.40
1:E:69:MET:HE1	1:E:521:ALA:HB1	2.03	0.40
1:J:409:GLU:OE2	1:J:502:ARG:NH2	2.48	0.40
1:U:253:ASP:OD1	1:U:254:ILE:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:HG21	1:A:325:ILE:HD12	2.03	0.40
1:T:15:LYS:NZ	1:T:67:GLU:OE2	2.54	0.40
1:K:30:THR:HB	1:K:51:LYS:O	2.22	0.40
1:E:46:ALA:HB2	1:F:76:GLU:HG3	2.02	0.40
1:D:207:ASN:HB2	1:D:209:GLU:OE1	2.22	0.40
1:E:480:ASN:OD1	1:E:482:ARG:HG2	2.21	0.40
1:V:409:GLU:OE2	1:V:502:ARG:NH2	2.52	0.40
1:D:411:ILE:HD13	1:D:497:PRO:HA	2.03	0.40
1:C:36:ARG:HD3	1:D:519:GLU:HB2	2.03	0.40
1:B:388:GLU:HA	1:B:391:GLU:HG2	4.26	0.40
1:I:220:ILE:HG13	1:I:296:THR:HG21	2.03	0.40
1:K:443:ILE:O	1:K:447:LEU:HG	2.21	0.40
1:A:116:LEU:O	1:A:120:ILE:HG12	3.99	0.40
1:E:36:ARG:HB3	1:F:517:THR:O	2.20	0.40
1:T:83:ASP:OD1	1:T:84:VAL:N	2.49	0.40
1:V:158:ILE:HD12	1:V:396:VAL:HG22	2.03	0.40
1:L:192:GLY:H	1:L:375:GLY:HA2	1.86	0.40
1:S:59:GLU:O	1:T:4:LYS:HG3	2.20	0.40
1:U:30:THR:HB	1:U:51:LYS:O	2.21	0.40
1:K:19:GLY:HA3	1:K:67:GLU:O	2.22	0.40
1:K:194:GLN:HA	1:K:332:ILE:O	2.21	0.40
1:J:98:ALA:HB2	1:J:449:GLU:HG3	2.03	0.40
1:I:36:ARG:HB3	1:J:517:THR:O	2.22	0.40
1:F:77:VAL:HG12	1:F:507:ASN:HB3	2.04	0.40
1:Z:161:LEU:HG	1:Z:379:LEU:HD22	2.04	0.40
1:M:321:ALA:HB3	1:M:334:GLU:HB2	2.04	0.40
1:F:197:ARG:HB3	1:F:277:LYS:HB2	2.03	0.40
1:J:247:LEU:HB3	1:J:273:VAL:HG12	2.02	0.40
1:L:39:LEU:HD13	1:M:73:MET:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	483/545 (89%)	472 (98%)	11 (2%)	0	100	100
1	B	511/545 (94%)	496 (97%)	15 (3%)	0	100	100
1	C	460/545 (84%)	448 (97%)	12 (3%)	0	100	100
1	D	509/545 (93%)	497 (98%)	12 (2%)	0	100	100
1	E	497/545 (91%)	479 (96%)	18 (4%)	0	100	100
1	F	481/545 (88%)	468 (97%)	13 (3%)	0	100	100
1	G	485/545 (89%)	467 (96%)	18 (4%)	0	100	100
1	H	501/545 (92%)	489 (98%)	12 (2%)	0	100	100
1	I	502/545 (92%)	490 (98%)	12 (2%)	0	100	100
1	J	493/545 (90%)	477 (97%)	16 (3%)	0	100	100
1	K	415/545 (76%)	399 (96%)	16 (4%)	0	100	100
1	L	470/545 (86%)	456 (97%)	14 (3%)	0	100	100
1	M	449/545 (82%)	434 (97%)	15 (3%)	0	100	100
1	N	499/545 (92%)	480 (96%)	19 (4%)	0	100	100
1	O	472/545 (87%)	449 (95%)	23 (5%)	0	100	100
1	P	516/545 (95%)	497 (96%)	19 (4%)	0	100	100
1	Q	484/545 (89%)	469 (97%)	15 (3%)	0	100	100
1	R	494/545 (91%)	475 (96%)	19 (4%)	0	100	100
1	S	502/545 (92%)	485 (97%)	15 (3%)	2 (0%)	39	80
1	T	485/545 (89%)	466 (96%)	19 (4%)	0	100	100
1	U	510/545 (94%)	498 (98%)	12 (2%)	0	100	100
1	V	484/545 (89%)	465 (96%)	19 (4%)	0	100	100
1	W	509/545 (93%)	476 (94%)	32 (6%)	1 (0%)	52	88
1	X	488/545 (90%)	469 (96%)	19 (4%)	0	100	100
1	Y	500/545 (92%)	486 (97%)	14 (3%)	0	100	100
1	Z	510/545 (94%)	487 (96%)	23 (4%)	0	100	100
1	a	518/545 (95%)	497 (96%)	21 (4%)	0	100	100
1	b	401/545 (74%)	386 (96%)	15 (4%)	0	100	100
All	All	13628/15260 (89%)	13157 (96%)	468 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	279	PRO
1	W	279	PRO
1	S	278	ALA

5.3.2 Protein sidechains (i)

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	360/427 (84%)	359 (100%)	1 (0%)	94 98
1	B	358/427 (84%)	357 (100%)	1 (0%)	94 98
1	C	310/427 (73%)	309 (100%)	1 (0%)	94 98
1	D	367/427 (86%)	367 (100%)	0	100 100
1	E	353/427 (83%)	353 (100%)	0	100 100
1	F	347/427 (81%)	347 (100%)	0	100 100
1	G	331/427 (78%)	330 (100%)	1 (0%)	94 98
1	H	381/427 (89%)	381 (100%)	0	100 100
1	I	369/427 (86%)	369 (100%)	0	100 100
1	J	328/427 (77%)	327 (100%)	1 (0%)	94 98
1	K	266/427 (62%)	265 (100%)	1 (0%)	93 98
1	L	299/427 (70%)	298 (100%)	1 (0%)	94 98
1	M	307/427 (72%)	307 (100%)	0	100 100
1	N	343/427 (80%)	343 (100%)	0	100 100
1	O	324/427 (76%)	323 (100%)	1 (0%)	94 98
1	P	378/427 (88%)	378 (100%)	0	100 100
1	Q	349/427 (82%)	349 (100%)	0	100 100
1	R	347/427 (81%)	346 (100%)	1 (0%)	94 98
1	S	362/427 (85%)	361 (100%)	1 (0%)	94 98
1	T	332/427 (78%)	332 (100%)	0	100 100
1	U	366/427 (86%)	363 (99%)	3 (1%)	86 96
1	V	345/427 (81%)	345 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	W	348/427 (82%)	348 (100%)	0	100 100
1	X	340/427 (80%)	340 (100%)	0	100 100
1	Y	362/427 (85%)	362 (100%)	0	100 100
1	Z	359/427 (84%)	358 (100%)	1 (0%)	94 98
1	a	368/427 (86%)	367 (100%)	1 (0%)	94 98
1	b	279/427 (65%)	278 (100%)	1 (0%)	93 98
All	All	9578/11956 (80%)	9562 (100%)	16 (0%)	95 99

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	B	401	HIS
1	C	495	VAL
1	G	401	HIS
1	J	401	HIS
1	K	461	THR
1	L	401	HIS
1	O	291	ASP
1	R	36	ARG
1	S	271	LEU
1	U	50	THR
1	U	217	GLU
1	U	259	LEU
1	Z	401	HIS
1	a	401	HIS
1	b	104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	507	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 25 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	C	601	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	D	601	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	E	601	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	F	601	-	4,4,4	0.25	0	6,6,6	0.05	0
2	SO4	G	601	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	J	601	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	K	601	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	L	601	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	M	602	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	N	601	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	P	601	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	R	602	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	T	602	-	4,4,4	0.25	0	6,6,6	0.06	0
2	SO4	U	601	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	V	602	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	Y	601	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	Z	601	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	a	601	-	4,4,4	0.25	0	6,6,6	0.07	0
2	SO4	b	601	-	4,4,4	0.25	0	6,6,6	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	601	-	-	0/0/0/0	0/0/0/0
2	SO4	B	601	-	-	0/0/0/0	0/0/0/0
2	SO4	C	601	-	-	0/0/0/0	0/0/0/0
2	SO4	D	601	-	-	0/0/0/0	0/0/0/0
2	SO4	E	601	-	-	0/0/0/0	0/0/0/0
2	SO4	F	601	-	-	0/0/0/0	0/0/0/0
2	SO4	G	601	-	-	0/0/0/0	0/0/0/0
2	SO4	J	601	-	-	0/0/0/0	0/0/0/0
2	SO4	K	601	-	-	0/0/0/0	0/0/0/0
2	SO4	L	601	-	-	0/0/0/0	0/0/0/0
2	SO4	M	602	-	-	0/0/0/0	0/0/0/0
2	SO4	N	601	-	-	0/0/0/0	0/0/0/0
2	SO4	P	601	-	-	0/0/0/0	0/0/0/0
2	SO4	R	602	-	-	0/0/0/0	0/0/0/0
2	SO4	T	602	-	-	0/0/0/0	0/0/0/0
2	SO4	U	601	-	-	0/0/0/0	0/0/0/0
2	SO4	V	602	-	-	0/0/0/0	0/0/0/0
2	SO4	Y	601	-	-	0/0/0/0	0/0/0/0
2	SO4	Z	601	-	-	0/0/0/0	0/0/0/0
2	SO4	a	601	-	-	0/0/0/0	0/0/0/0
2	SO4	b	601	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	SO4	1	0
2	F	601	SO4	1	0
2	R	602	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	499/545 (91%)	-0.19	0 100 100	18, 51, 104, 115	0
1	B	519/545 (95%)	-0.24	1 (0%) 95 87	14, 44, 104, 121	0
1	C	478/545 (87%)	-0.12	5 (1%) 84 60	18, 52, 103, 127	0
1	D	517/545 (94%)	-0.10	4 (0%) 87 67	18, 58, 110, 129	0
1	E	509/545 (93%)	-0.10	9 (1%) 71 43	20, 66, 110, 123	0
1	F	497/545 (91%)	-0.19	3 (0%) 90 73	16, 46, 102, 122	0
1	G	499/545 (91%)	-0.15	3 (0%) 90 73	19, 59, 113, 125	0
1	H	515/545 (94%)	-0.19	0 100 100	18, 60, 102, 111	0
1	I	512/545 (93%)	-0.27	1 (0%) 95 87	17, 52, 97, 116	0
1	J	507/545 (93%)	-0.11	6 (1%) 81 55	18, 63, 116, 133	0
1	K	433/545 (79%)	-0.02	13 (3%) 54 25	20, 54, 121, 138	0
1	L	484/545 (88%)	-0.02	23 (4%) 34 14	21, 53, 125, 136	0
1	M	463/545 (84%)	-0.14	4 (0%) 85 64	24, 55, 108, 129	0
1	N	511/545 (93%)	-0.08	4 (0%) 87 67	21, 65, 112, 129	0
1	O	492/545 (90%)	-0.06	12 (2%) 62 32	20, 50, 122, 132	0
1	P	522/545 (95%)	-0.28	1 (0%) 95 87	15, 49, 92, 116	0
1	Q	502/545 (92%)	-0.22	2 (0%) 93 80	11, 44, 110, 134	0
1	R	502/545 (92%)	-0.24	2 (0%) 93 80	11, 37, 106, 125	0
1	S	512/545 (93%)	-0.20	1 (0%) 95 87	15, 61, 100, 118	0
1	T	497/545 (91%)	-0.14	5 (1%) 84 60	23, 62, 98, 111	0
1	U	518/545 (95%)	-0.10	8 (1%) 76 49	24, 74, 106, 124	0
1	V	500/545 (91%)	-0.06	11 (2%) 65 35	15, 49, 119, 139	0
1	W	517/545 (94%)	-0.08	9 (1%) 73 45	14, 55, 119, 127	0
1	X	504/545 (92%)	-0.07	8 (1%) 74 47	15, 61, 125, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	512/545 (93%)	-0.11	5 (0%) 84 60	21, 58, 110, 139	0
1	Z	518/545 (95%)	-0.05	7 (1%) 78 51	25, 75, 113, 124	0
1	a	522/545 (95%)	-0.01	9 (1%) 73 45	27, 74, 111, 126	0
1	b	423/545 (77%)	-0.08	4 (0%) 85 64	19, 49, 119, 136	0
All	All	13984/15260 (91%)	-0.13	160 (1%) 82 58	11, 56, 113, 144	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	282	GLY	4.8
1	S	83	ASP	4.5
1	V	335	GLY	4.1
1	K	180	ALA	4.1
1	L	201	SER	4.0
1	X	373	SER	4.0
1	a	384	SER	4.0
1	K	320	ALA	3.9
1	T	85	ALA	3.8
1	X	208	SER	3.8
1	E	374	GLY	3.6
1	U	359	ASP	3.6
1	X	237	LEU	3.5
1	K	199	TYR	3.4
1	L	220	ILE	3.4
1	C	223	HIS	3.4
1	E	381	ILE	3.4
1	L	290	GLU	3.3
1	L	250	ILE	3.3
1	N	365	LEU	3.1
1	U	281	PHE	3.1
1	W	283	ASP	3.1
1	V	374	GLY	3.1
1	G	376	VAL	3.1
1	L	194	GLN	3.1
1	a	183	MET	3.1
1	Q	260	ALA	3.1
1	T	247	LEU	3.0
1	L	213	ALA	3.0
1	V	251	ALA	3.0
1	a	361	ASP	3.0
1	J	264	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	U	383	ALA	2.9
1	L	85	ALA	2.9
1	Y	295	LEU	2.8
1	b	218	ALA	2.8
1	W	252	GLU	2.8
1	X	273	VAL	2.8
1	K	381	ILE	2.8
1	X	228	SER	2.8
1	a	216	ASP	2.8
1	U	275	ALA	2.8
1	L	374	GLY	2.7
1	E	273	VAL	2.7
1	V	184	GLU	2.7
1	J	221	LEU	2.7
1	V	363	GLU	2.7
1	G	251	ALA	2.7
1	O	203	TYR	2.7
1	O	251	ALA	2.7
1	V	203	TYR	2.7
1	Z	264	VAL	2.7
1	W	251	ALA	2.7
1	L	354	GLU	2.6
1	O	227	ILE	2.6
1	C	283	ASP	2.6
1	N	351	GLY	2.6
1	L	261	THR	2.6
1	L	271	LEU	2.5
1	J	251	ALA	2.5
1	O	289	LEU	2.5
1	U	270	THR	2.5
1	V	360	TYR	2.5
1	W	336	LYS	2.5
1	a	182	GLY	2.5
1	E	349	ILE	2.5
1	K	377	ALA	2.5
1	L	223	HIS	2.5
1	K	384	SER	2.5
1	L	200	LEU	2.4
1	a	295	LEU	2.4
1	Z	85	ALA	2.4
1	E	184	GLU	2.4
1	M	83	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	O	220	ILE	2.4
1	O	221	LEU	2.4
1	W	228	SER	2.4
1	I	268	ARG	2.4
1	O	362	THR	2.4
1	P	381	ILE	2.4
1	V	183	MET	2.4
1	F	356	SER	2.4
1	K	288	MET	2.4
1	M	291	ASP	2.4
1	O	291	ASP	2.4
1	Y	141	LYS	2.4
1	U	311	ASN	2.4
1	K	373	SER	2.4
1	L	302	SER	2.3
1	T	356	SER	2.3
1	O	223	HIS	2.3
1	L	291	ASP	2.3
1	D	247	LEU	2.3
1	D	294	ILE	2.3
1	W	85	ALA	2.3
1	Z	381	ILE	2.3
1	J	223	HIS	2.3
1	X	223	HIS	2.3
1	D	360	TYR	2.3
1	K	372	LEU	2.3
1	X	349	ILE	2.3
1	N	344	ALA	2.3
1	Z	203	TYR	2.3
1	K	378	VAL	2.3
1	b	290	GLU	2.3
1	F	291	ASP	2.3
1	J	247	LEU	2.3
1	L	224	ASP	2.3
1	a	264	VAL	2.3
1	L	288	MET	2.3
1	L	203	TYR	2.3
1	L	300	VAL	2.3
1	L	276	VAL	2.3
1	T	331	THR	2.3
1	N	227	ILE	2.3
1	K	341	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	230	MET	2.2
1	C	250	ILE	2.2
1	T	273	VAL	2.2
1	U	381	ILE	2.2
1	O	268	ARG	2.2
1	B	349	ILE	2.2
1	b	347	ASN	2.2
1	C	384	SER	2.2
1	E	382	GLY	2.2
1	L	379	LEU	2.2
1	D	273	VAL	2.2
1	E	326	ASP	2.2
1	V	283	ASP	2.2
1	K	376	VAL	2.2
1	L	299	THR	2.2
1	Y	273	VAL	2.2
1	Z	337	GLY	2.2
1	L	228	SER	2.2
1	G	261	THR	2.2
1	R	267	LEU	2.1
1	R	228	SER	2.1
1	C	364	LYS	2.1
1	W	169	VAL	2.1
1	K	85	ALA	2.1
1	Y	168	LYS	2.1
1	b	348	GLU	2.1
1	V	316	TYR	2.1
1	a	378	VAL	2.1
1	F	355	LYS	2.1
1	Z	295	LEU	2.1
1	U	241	ALA	2.1
1	Q	361	ASP	2.1
1	M	330	THR	2.1
1	E	351	GLY	2.1
1	O	87	ASP	2.1
1	M	325	ILE	2.0
1	Y	182	GLY	2.0
1	Z	379	LEU	2.0
1	a	360	TYR	2.0
1	J	270	THR	2.0
1	O	348	GLU	2.0
1	E	244	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	W	250	ILE	2.0
1	X	369	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	Q	601	1/1	0.30	0.50	8.71	67,67,67,67	0
4	MG	V	601	1/1	0.82	0.38	8.64	61,61,61,61	0
2	SO4	K	601	5/5	0.63	0.42	6.64	42,55,61,61	5
2	SO4	B	601	5/5	0.81	0.32	5.92	24,30,35,36	5
2	SO4	G	601	5/5	0.82	0.28	4.32	36,48,56,57	5
2	SO4	N	601	5/5	0.86	0.29	4.23	41,47,51,54	5
2	SO4	D	601	5/5	0.82	0.33	3.68	33,44,50,50	5
2	SO4	F	601	5/5	0.86	0.26	3.57	25,34,38,38	5
2	SO4	A	601	5/5	0.68	0.36	3.37	37,61,63,70	5
2	SO4	V	602	5/5	0.79	0.33	3.36	34,35,45,48	5
2	SO4	Z	601	5/5	0.79	0.37	3.00	49,51,72,74	5
2	SO4	P	601	5/5	0.72	0.35	2.96	29,35,57,64	5
2	SO4	b	601	5/5	0.83	0.40	2.71	62,84,95,96	0
2	SO4	T	602	5/5	0.77	0.31	2.47	37,47,50,59	5
2	SO4	R	602	5/5	0.88	0.29	2.41	23,33,34,34	5
2	SO4	J	601	5/5	0.84	0.28	2.20	33,42,51,52	5
4	MG	M	601	1/1	0.56	0.26	2.03	53,53,53,53	0
2	SO4	E	601	5/5	0.80	0.27	1.52	43,47,62,63	5
2	SO4	Y	601	5/5	0.82	0.26	1.15	34,41,58,58	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	L	601	5/5	0.76	0.29	1.09	38,55,60,64	5
2	SO4	M	602	5/5	0.80	0.28	0.97	54,55,71,77	5
2	SO4	U	601	5/5	0.74	0.26	0.90	55,62,75,80	5
2	SO4	C	601	5/5	0.80	0.26	0.86	41,46,67,74	5
3	CA	M	603	1/1	0.91	0.19	-0.34	78,78,78,78	0
2	SO4	a	601	5/5	0.89	0.20	-0.59	50,53,63,69	5
4	MG	H	601	1/1	0.85	0.16	-0.64	51,51,51,51	0
3	CA	R	603	1/1	0.97	0.06	-2.71	64,64,64,64	0
4	MG	T	601	1/1	0.84	0.15	-	58,58,58,58	0
3	CA	I	601	1/1	0.93	0.09	-	79,79,79,79	0
3	CA	A	602	1/1	0.92	0.07	-	72,72,72,72	0
3	CA	a	602	1/1	0.90	0.08	-	78,78,78,78	0
4	MG	R	601	1/1	0.76	0.24	-	34,34,34,34	0
3	CA	J	602	1/1	0.82	0.12	-	72,72,72,72	0
3	CA	Y	602	1/1	0.80	0.10	-	72,72,72,72	0
3	CA	Q	602	1/1	0.79	0.08	-	78,78,78,78	0
3	CA	Z	602	1/1	0.81	0.10	-	92,92,92,92	0
4	MG	S	601	1/1	0.40	0.31	-	54,54,54,54	0
3	CA	V	603	1/1	0.95	0.13	-	70,70,70,70	0
3	CA	B	602	1/1	0.71	0.12	-	77,77,77,77	0
3	CA	P	602	1/1	0.75	0.14	-	71,71,71,71	0
3	CA	F	602	1/1	0.84	0.09	-	77,77,77,77	0
3	CA	G	602	1/1	0.89	0.15	-	76,76,76,76	0
3	CA	K	602	1/1	0.85	0.08	-	82,82,82,82	0
3	CA	U	602	1/1	0.97	0.11	-	62,62,62,62	0
3	CA	T	603	1/1	0.95	0.19	-	69,69,69,69	0
3	CA	O	601	1/1	0.78	0.09	-	73,73,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.