



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:11 AM UTC

PDB ID : 5DA8 / pdb_00005da8
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

<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
Mogul : 2022.3.0, CSD as543be (2022)
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

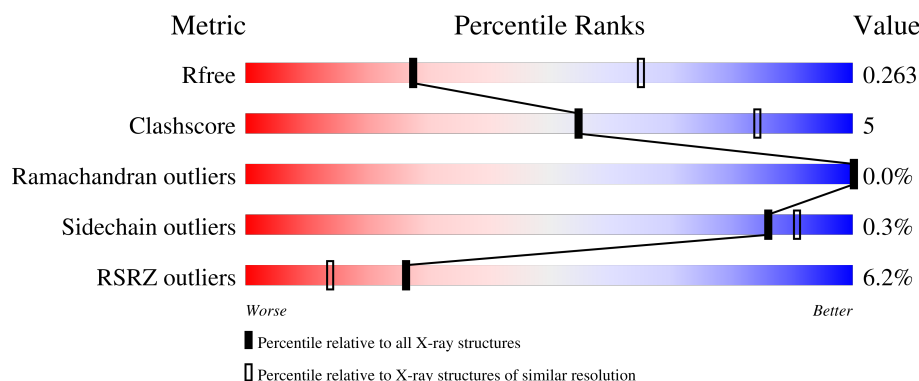
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	545	4% 78% 14% 8%
1	B	545	6% 86% 10% 5%
1	C	545	7% 78% 10% 12%
1	D	545	5% 83% 12% 5%
1	E	545	6% 82% 12% 7%

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Mol	Chain	Length	Quality of chain
1	F	545	
1	G	545	
1	H	545	
1	I	545	
1	J	545	
1	K	545	
1	L	545	
1	M	545	
1	N	545	
1	O	545	
1	P	545	
1	Q	545	
1	R	545	
1	S	545	
1	T	545	
1	U	545	
1	V	545	
1	W	545	
1	X	545	
1	Y	545	
1	Z	545	
1	a	545	
1	b	545	

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.

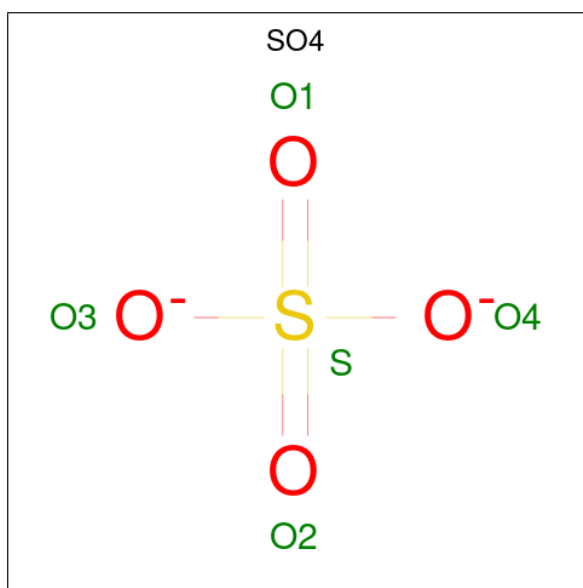
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3601	2242	631	720	8			
1	B	519	Total	C	N	O	S	0	0	0
			3706	2296	655	745	10			
1	C	478	Total	C	N	O	S	0	0	0
			3335	2066	591	670	8			
1	D	517	Total	C	N	O	S	0	0	0
			3721	2316	654	743	8			
1	E	509	Total	C	N	O	S	0	0	0
			3631	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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

- Molecule 5 is water.

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

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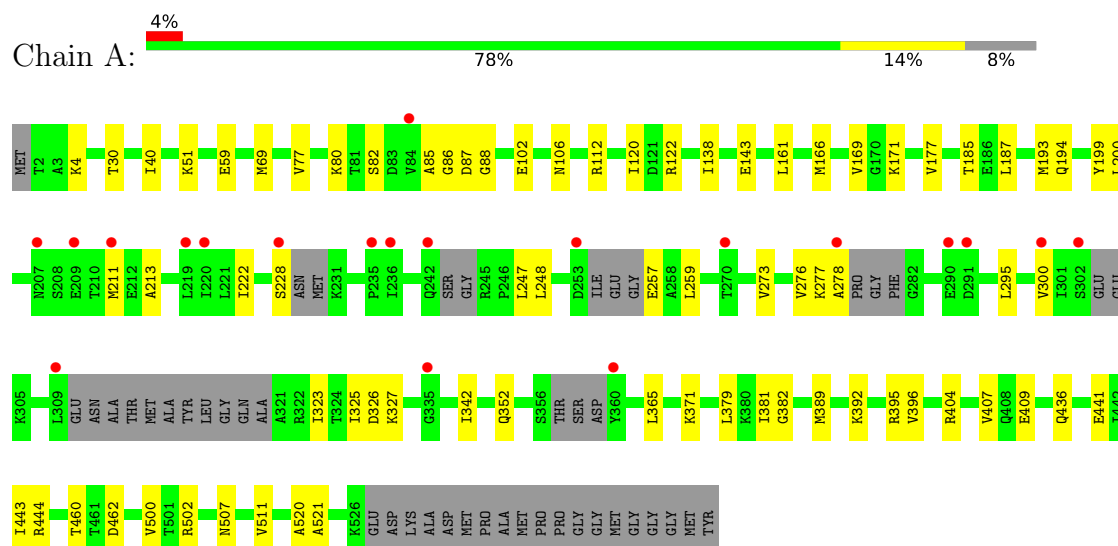
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	1	Total 1	O 1	0	0
5	S	3	Total 3	O 3	0	0
5	U	1	Total 1	O 1	0	0
5	V	2	Total 2	O 2	0	0
5	W	2	Total 2	O 2	0	0
5	X	5	Total 5	O 5	0	0
5	Y	3	Total 3	O 3	0	0
5	Z	1	Total 1	O 1	0	0
5	a	1	Total 1	O 1	0	0
5	b	2	Total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

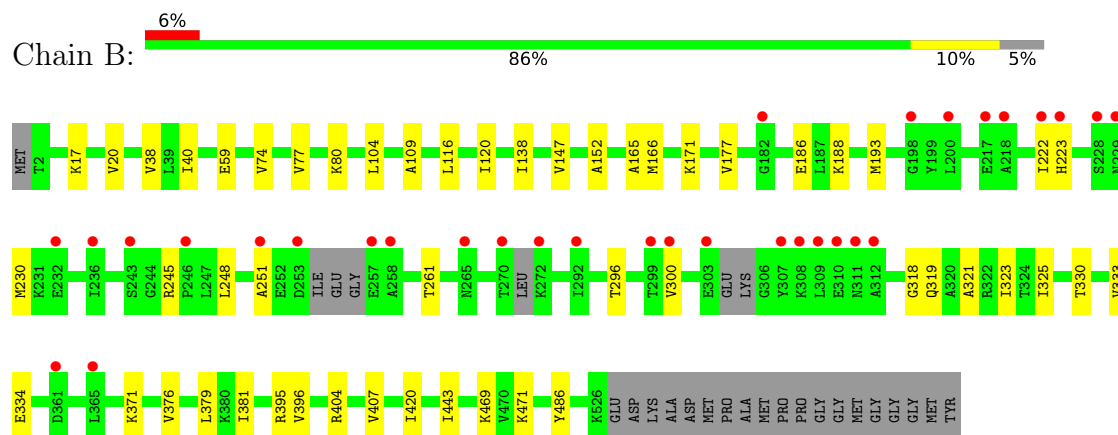
3 Residue-property plots [i](#)

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.

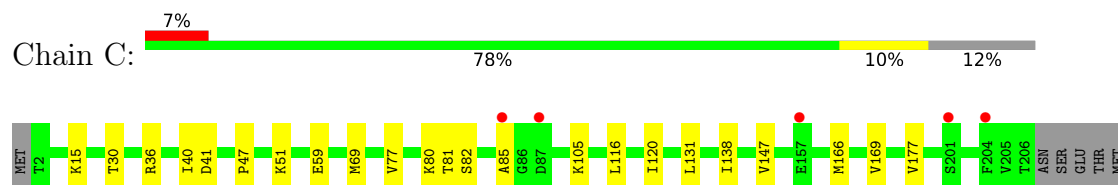
• Molecule 1: 60 kDa chaperonin

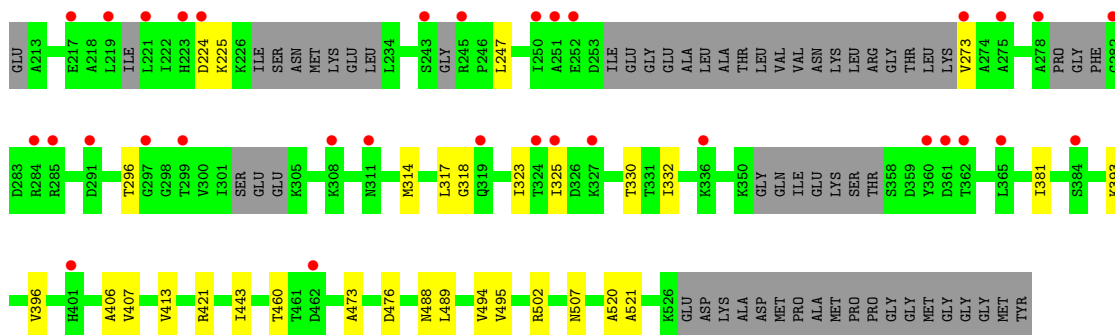


• Molecule 1: 60 kDa chaperonin

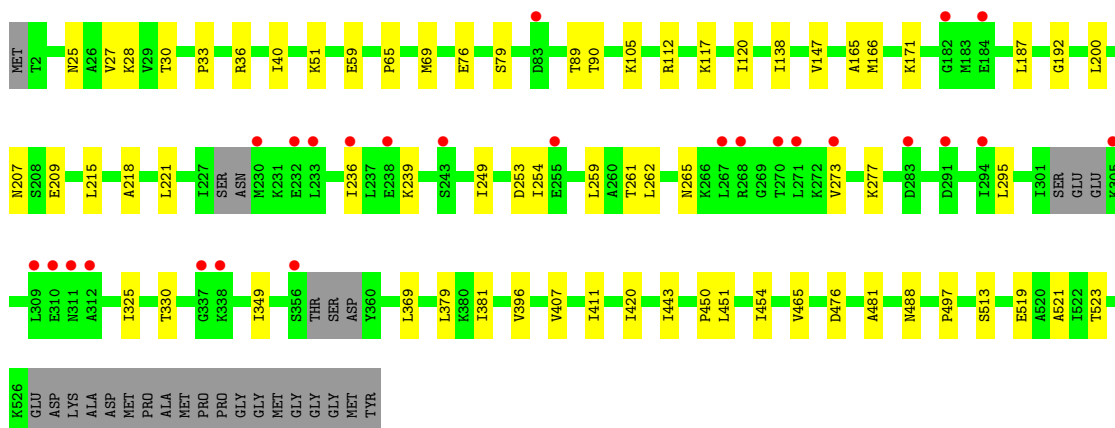
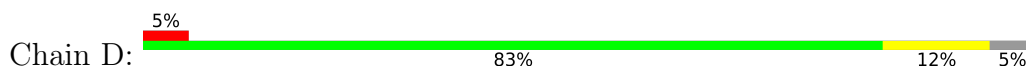


• Molecule 1: 60 kDa chaperonin

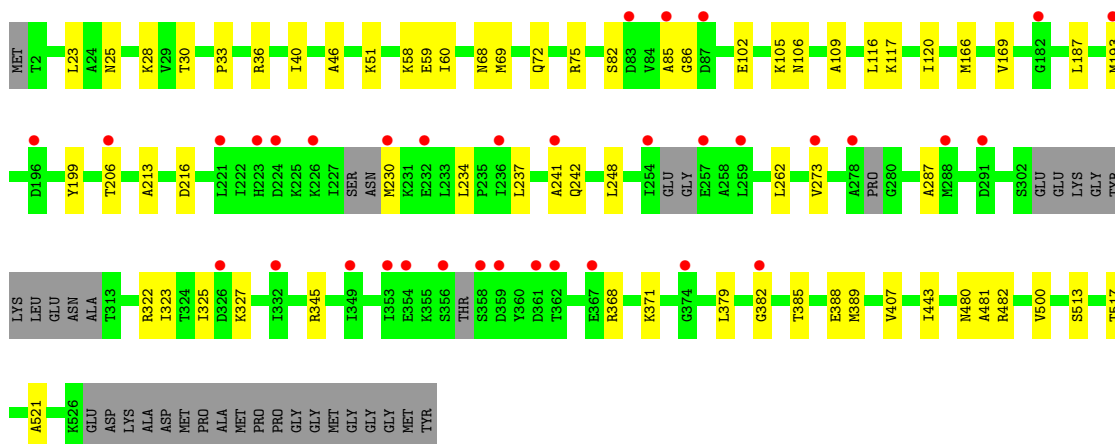
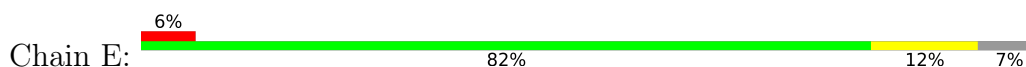




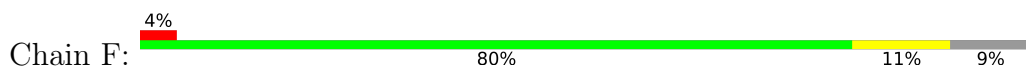
• Molecule 1: 60 kDa chaperonin

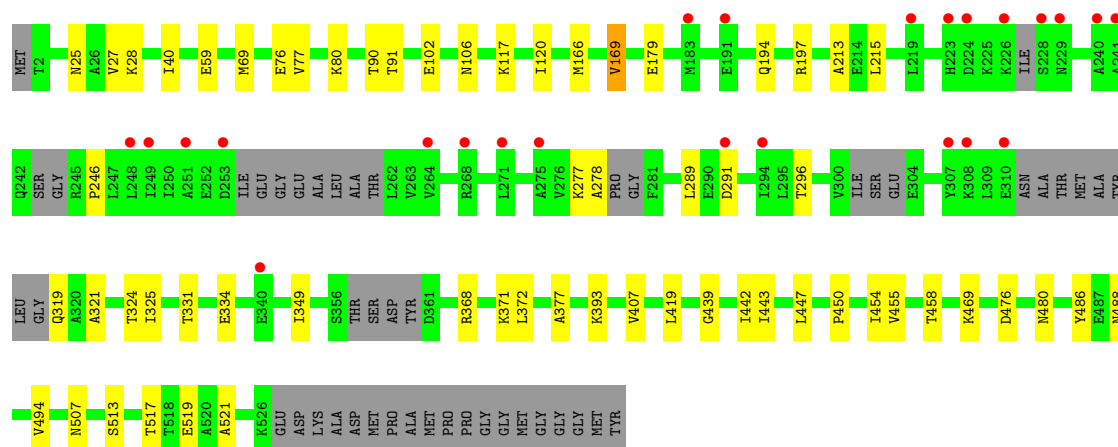


• Molecule 1: 60 kDa chaperonin

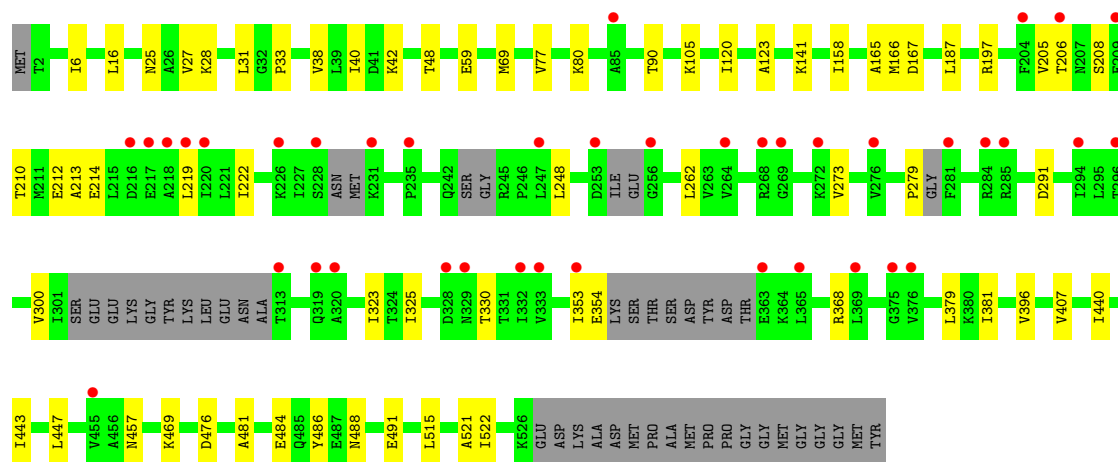
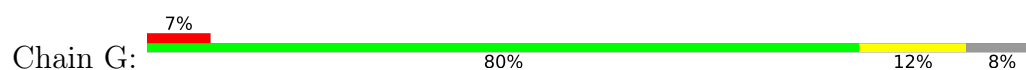


• Molecule 1: 60 kDa chaperonin

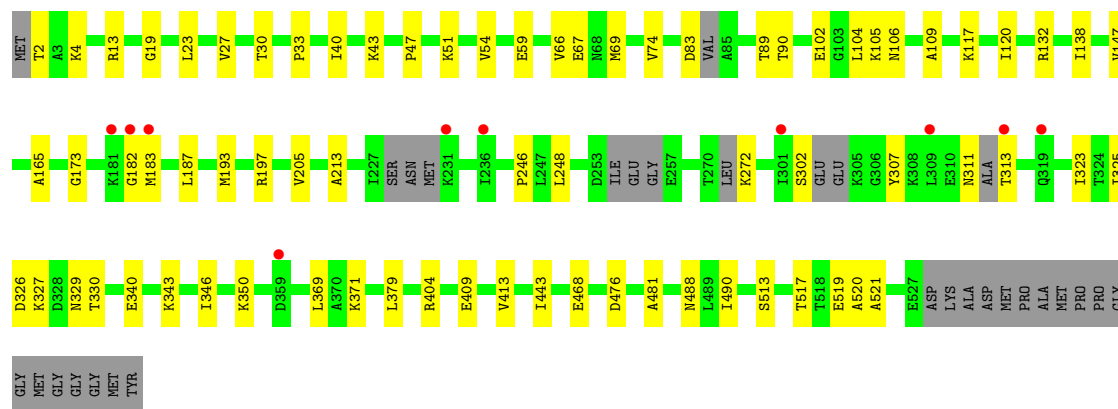
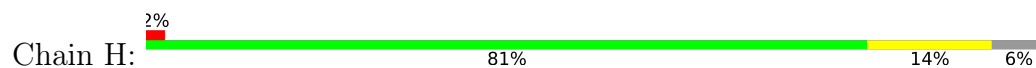




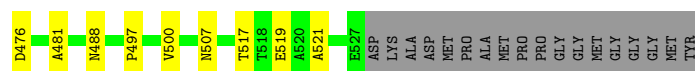
• Molecule 1: 60 kDa chaperonin



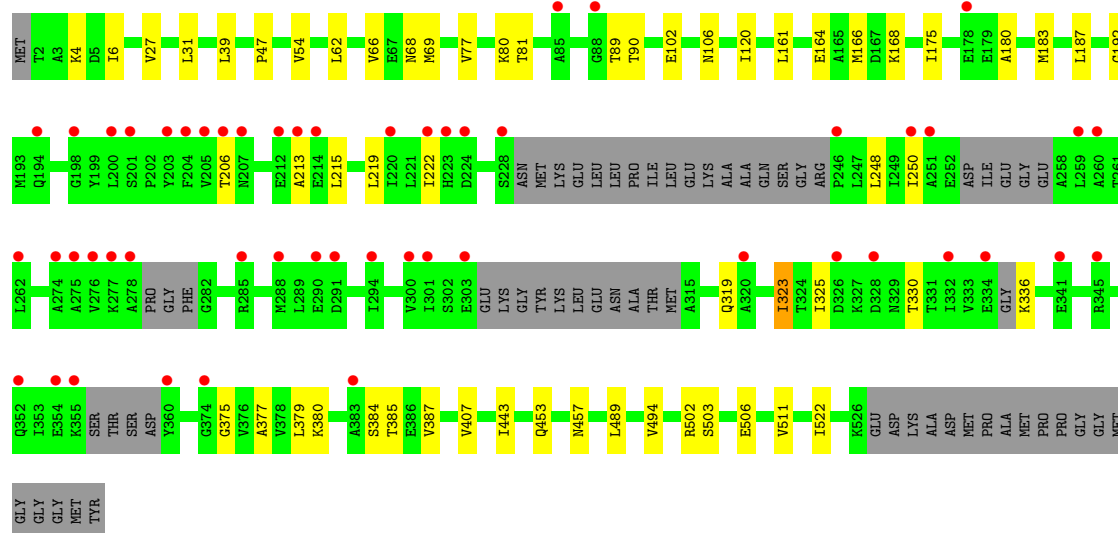
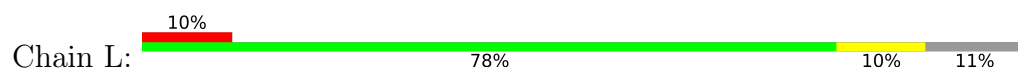
• Molecule 1: 60 kDa chaperonin



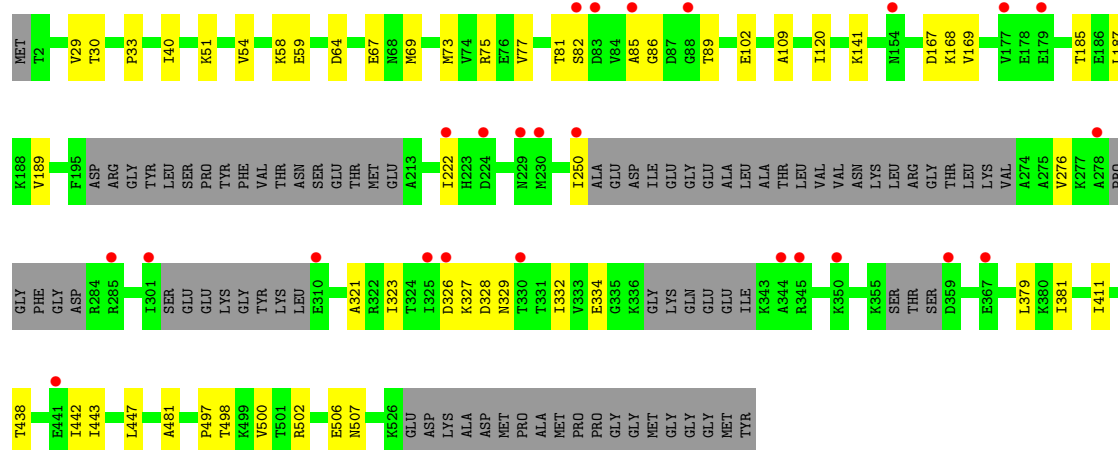
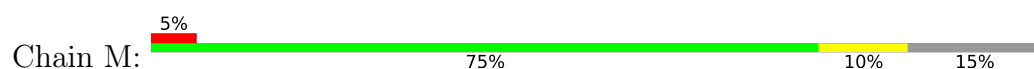
• Molecule 1: 60 kDa chaperonin



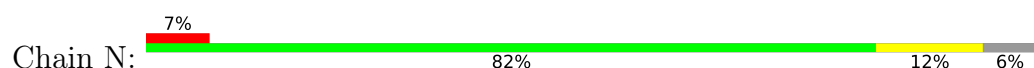
• Molecule 1: 60 kDa chaperonin

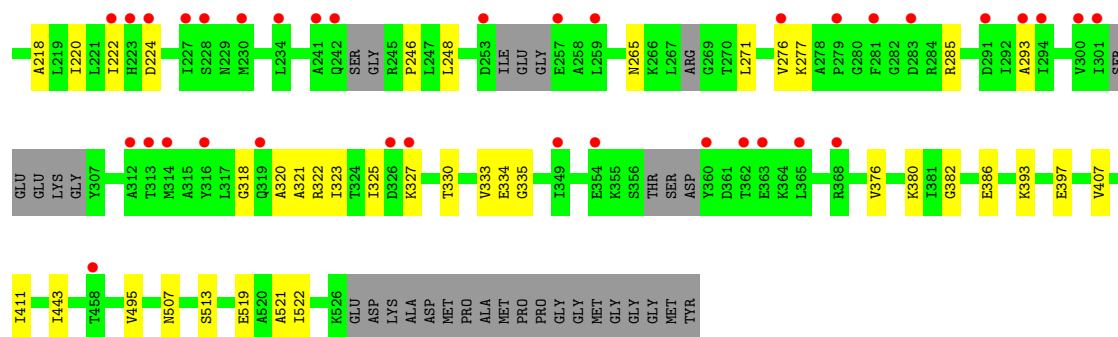


• Molecule 1: 60 kDa chaperonin

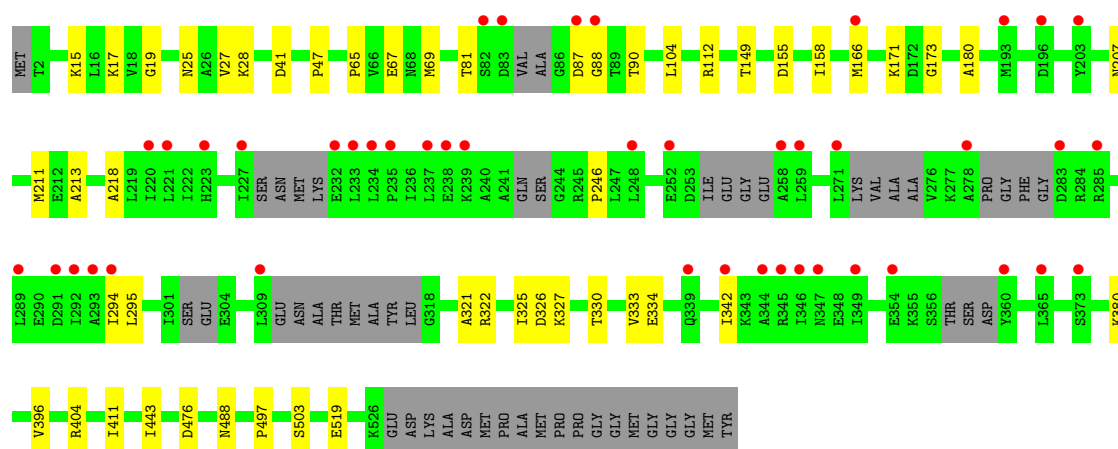
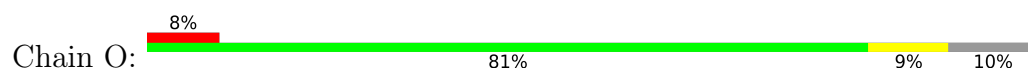


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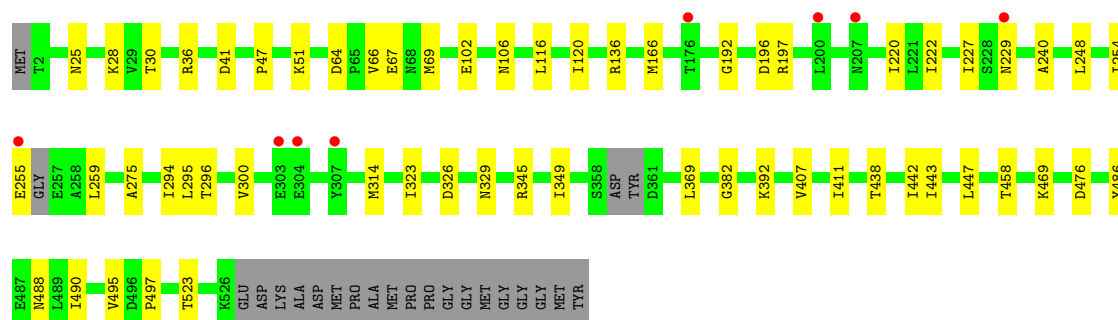
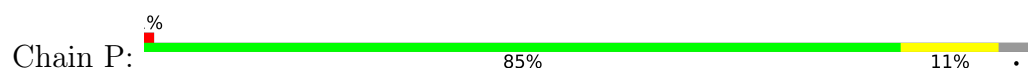




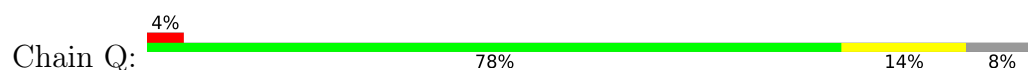
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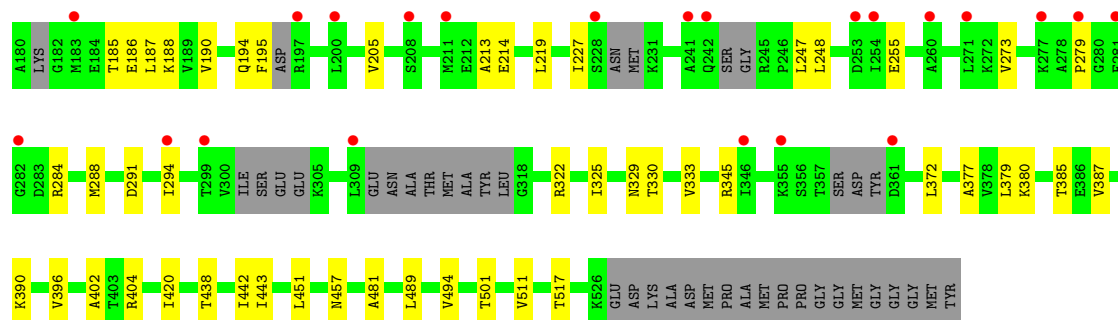


• Molecule 1: 60 kDa chaperonin

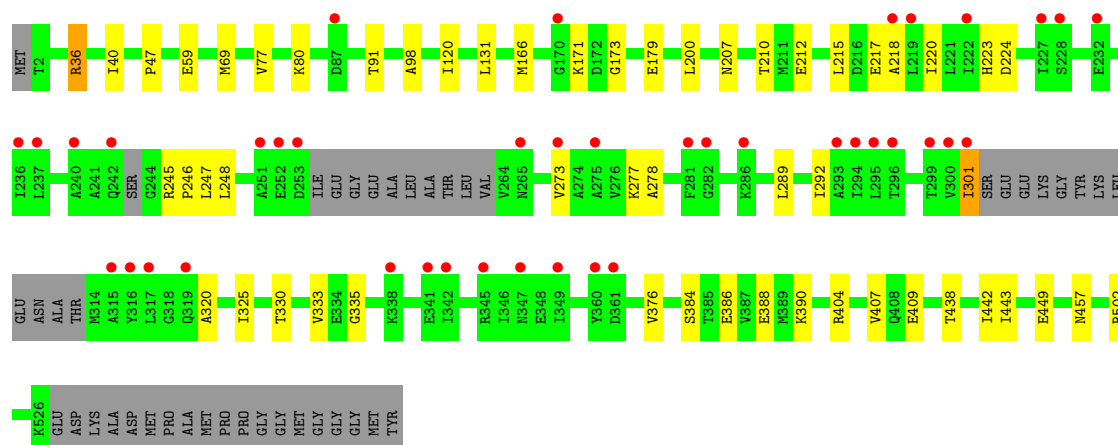
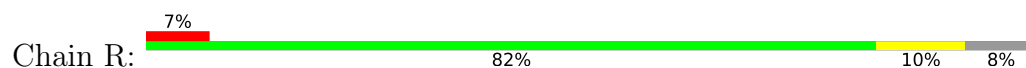


• Molecule 1: 60 kDa chaperonin

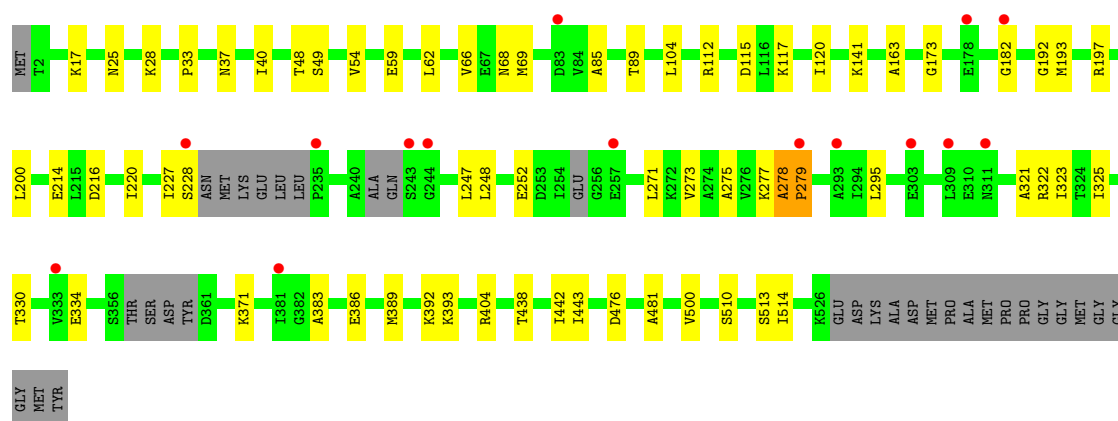
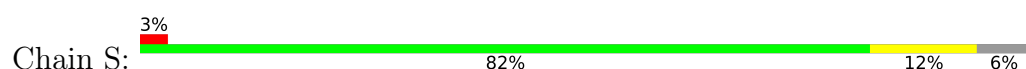




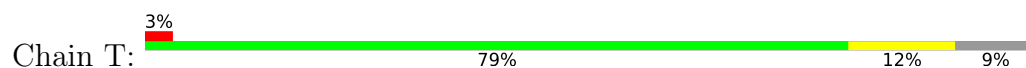
● Molecule 1: 60 kDa chaperonin

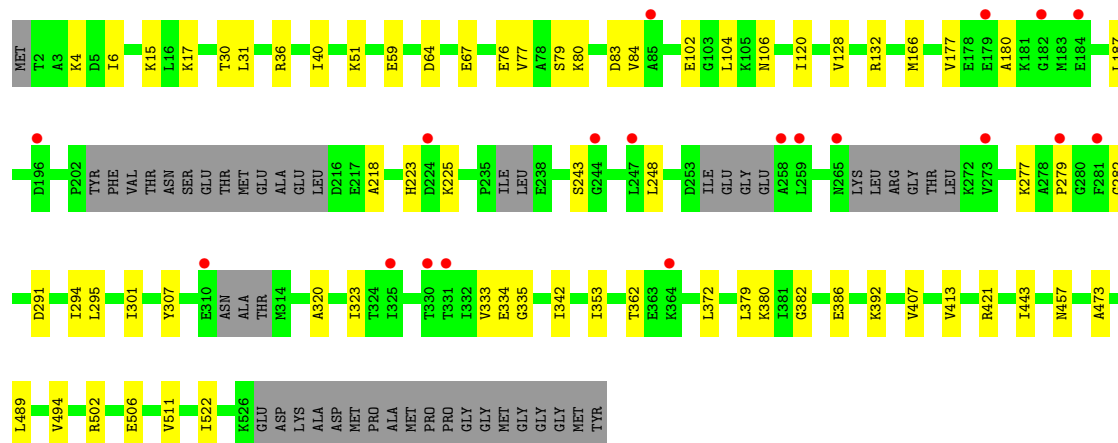


● Molecule 1: 60 kDa chaperonin

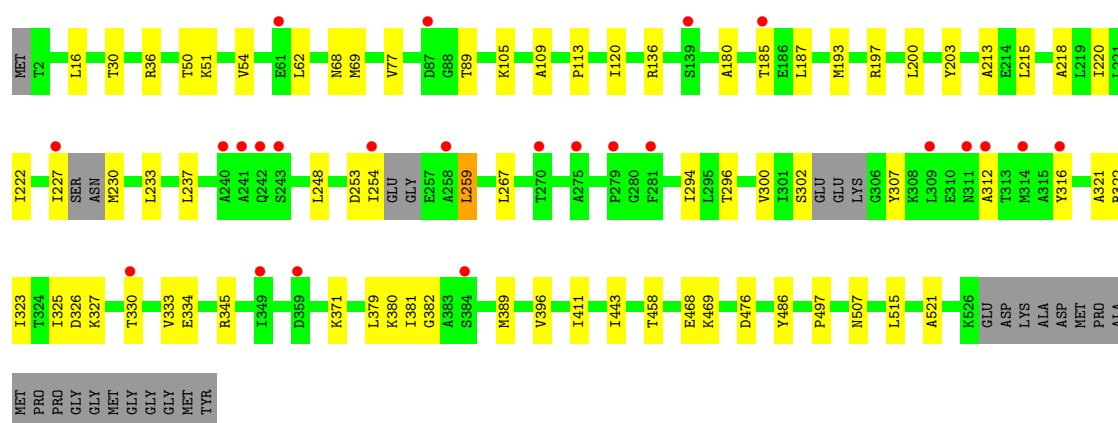
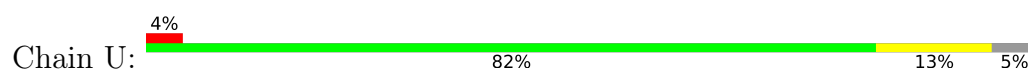


● Molecule 1: 60 kDa chaperonin

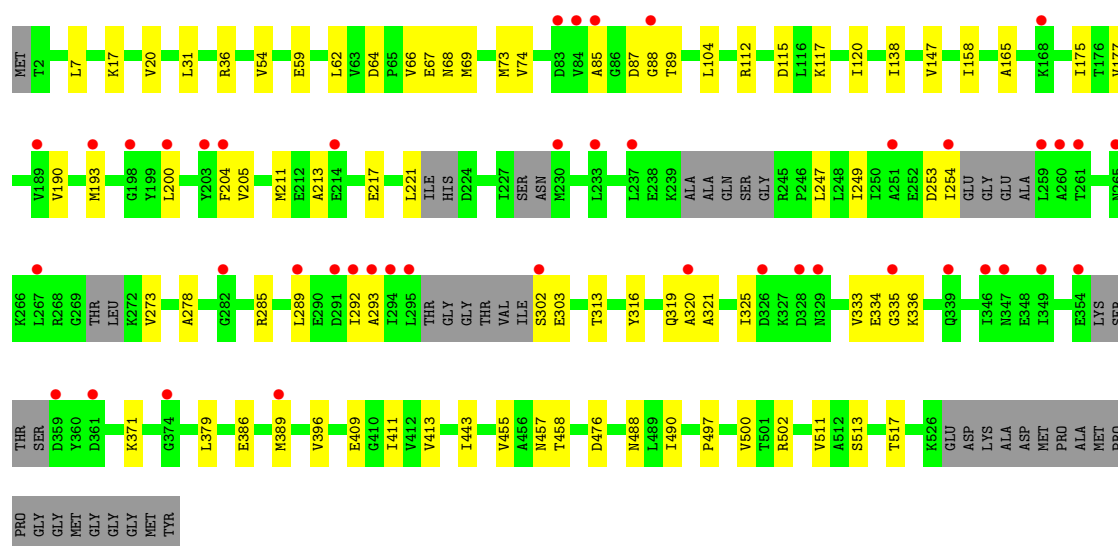
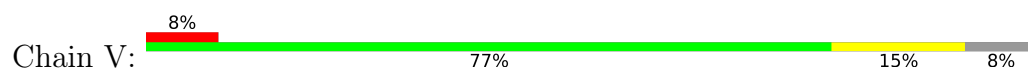




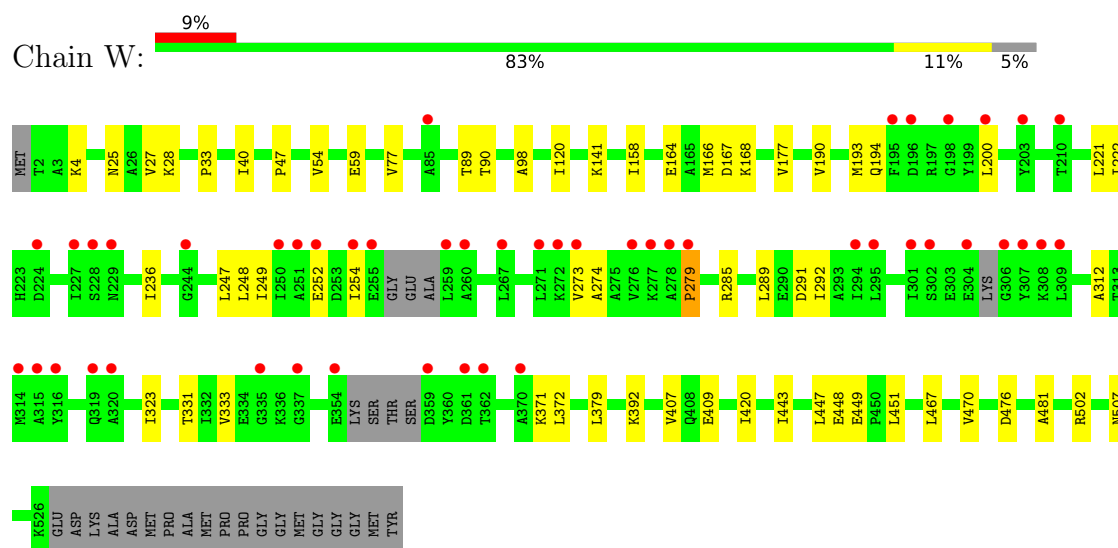
• Molecule 1: 60 kDa chaperonin



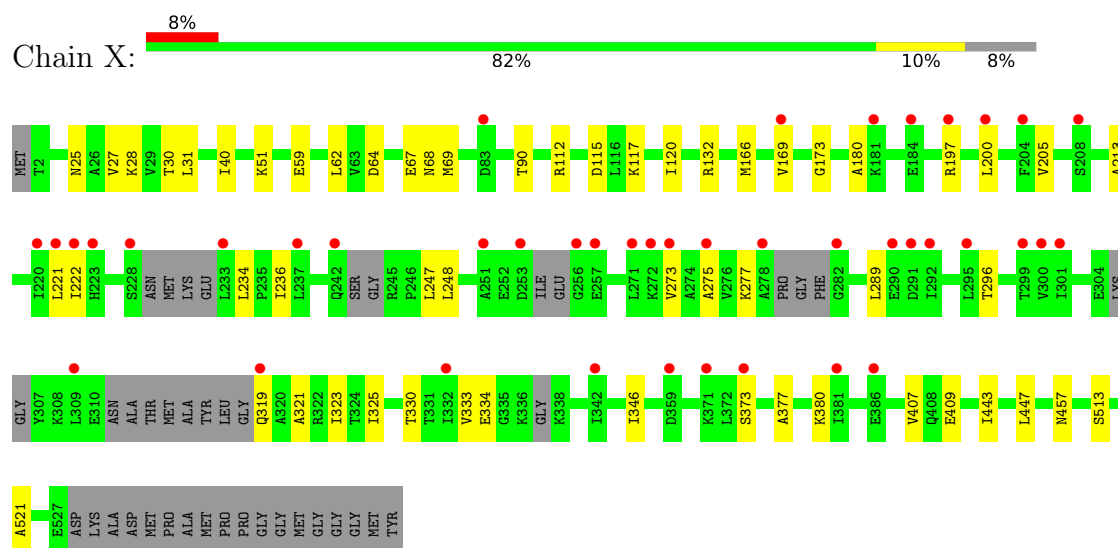
• Molecule 1: 60 kDa chaperonin



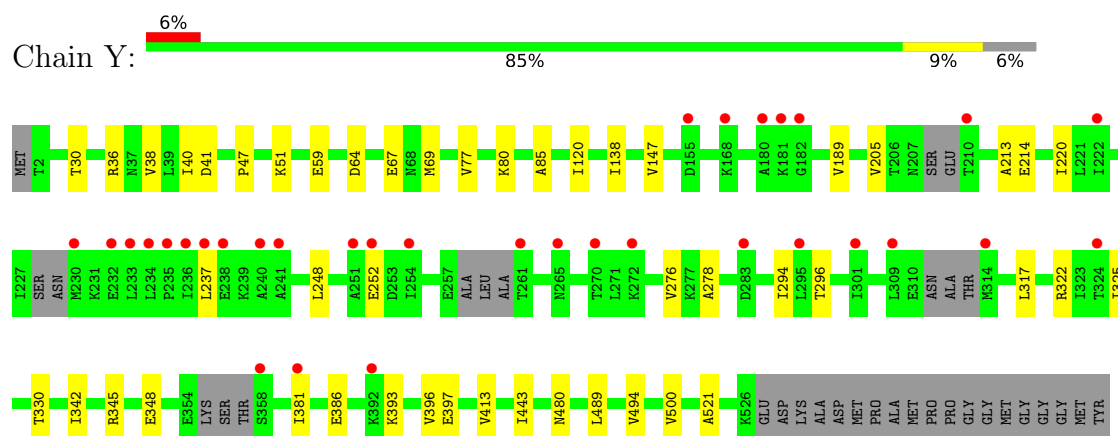
- Molecule 1: 60 kDa chaperonin



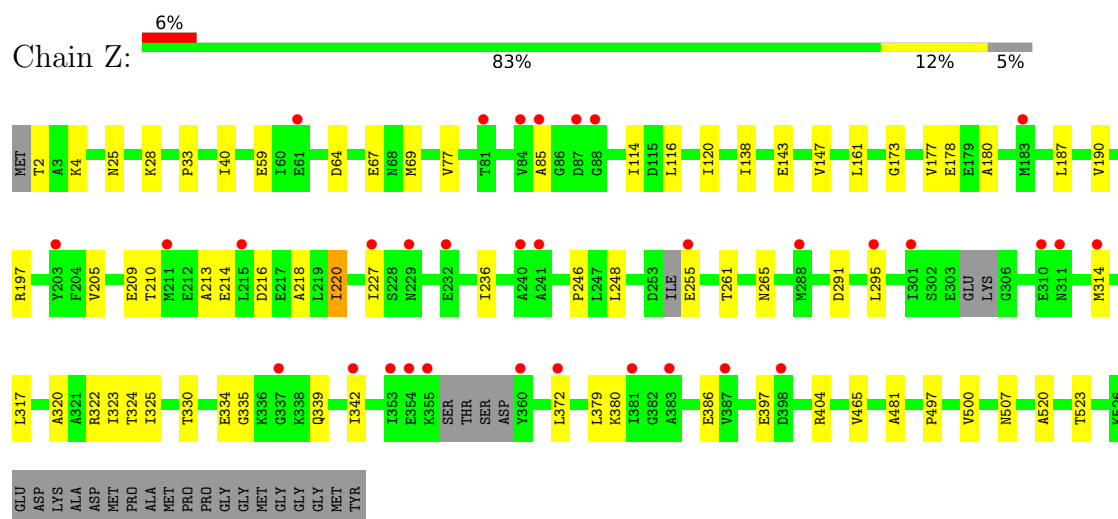
- Molecule 1: 60 kDa chaperonin



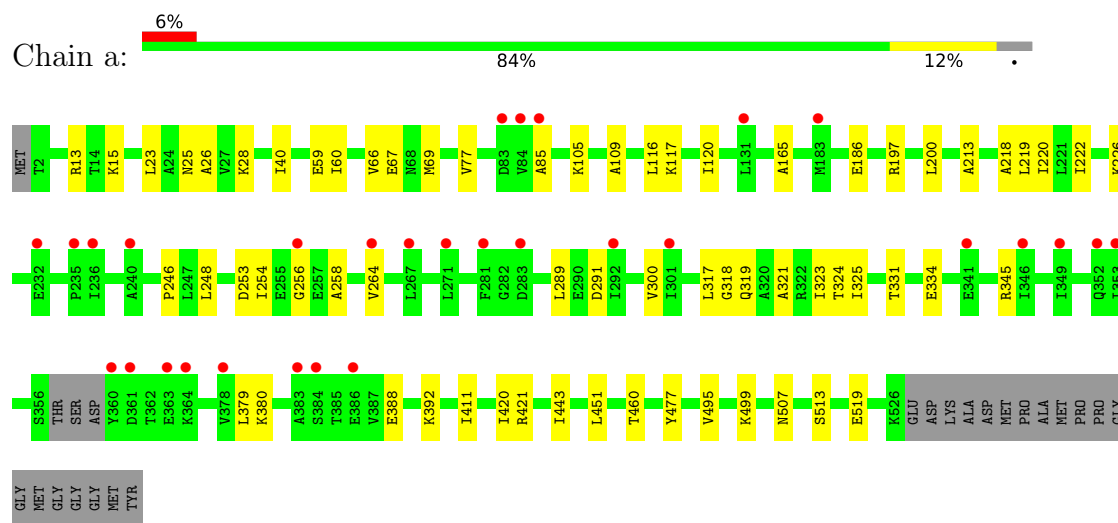
- Molecule 1: 60 kDa chaperonin



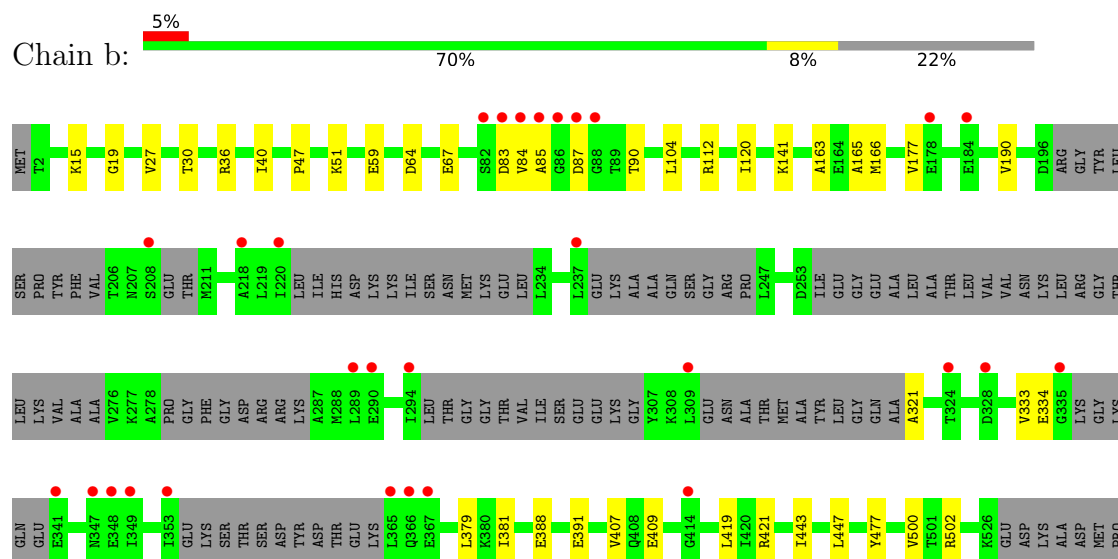
- Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin



ALA
MET
PRO
PRO
GLY
GLY
MET
GLY
GLY
GLY
MET
TYR

4 Data and refinement statistics

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 48.60 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (48.60-3.00) 95.9 (48.60-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.230 , 0.263 0.231 , 0.263	Depositor DCC
R_{free} test set	18192 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	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.*

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

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

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	0.08	0/3615	0.24	0/4880
1	B	0.08	0/3727	0.25	0/5041
1	C	0.08	0/3344	0.24	0/4527
1	D	0.08	0/3742	0.25	0/5062
1	E	0.08	0/3647	0.24	0/4933
1	F	0.08	0/3574	0.25	0/4827
1	G	0.08	0/3514	0.26	0/4756
1	H	0.08	0/3785	0.24	0/5106
1	I	0.09	0/3715	0.25	0/5024
1	J	0.08	0/3541	0.25	0/4799
1	K	0.08	0/2974	0.24	0/4025
1	L	0.07	0/3319	0.24	0/4501
1	M	0.09	0/3257	0.26	0/4407
1	N	0.08	0/3620	0.28	0/4902
1	O	0.08	0/3462	0.26	0/4684
1	P	0.08	0/3803	0.26	0/5142
1	Q	0.08	0/3600	0.26	0/4862
1	R	0.08	0/3595	0.25	0/4867
1	S	0.08	0/3697	0.27	1/5001 (0.0%)
1	T	0.09	0/3508	0.29	1/4751 (0.0%)
1	U	0.08	0/3739	0.25	0/5062
1	V	0.09	0/3591	0.27	0/4854
1	W	0.08	0/3679	0.28	1/4981 (0.0%)
1	X	0.08	0/3597	0.25	0/4865
1	Y	0.09	0/3715	0.25	0/5017
1	Z	0.08	0/3723	0.26	0/5039
1	a	0.08	0/3766	0.26	0/5099
1	b	0.08	0/2965	0.24	0/4007
All	All	0.08	0/99814	0.26	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(°)	Ideal(°)
1	S	279	PRO	N-CA-CB	7.31	110.93	103.25
1	W	279	PRO	N-CA-CB	7.18	110.78	103.25
1	T	279	PRO	N-CA-CB	6.97	110.56	103.25

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

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	43	0
1	B	3706	0	3668	29	0
1	C	3335	0	3252	33	0
1	D	3721	0	3751	41	0
1	E	3631	0	3624	38	0
1	F	3560	0	3514	34	0
1	G	3500	0	3438	39	0
1	H	3766	0	3823	44	0
1	I	3697	0	3728	41	0
1	J	3525	0	3391	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2968	0	2840	35	0
1	L	3309	0	3145	35	0
1	M	3247	0	3211	31	0
1	N	3603	0	3541	41	0
1	O	3451	0	3335	28	0
1	P	3780	0	3812	34	0
1	Q	3585	0	3577	44	0
1	R	3576	0	3541	32	0
1	S	3677	0	3683	36	0
1	T	3494	0	3435	38	0
1	U	3718	0	3723	42	0
1	V	3575	0	3506	49	0
1	W	3661	0	3601	33	0
1	X	3581	0	3504	32	0
1	Y	3695	0	3689	28	0
1	Z	3703	0	3669	43	0
1	a	3743	0	3741	37	0
1	b	2961	0	2899	26	0
2	A	5	0	0	0	0
2	B	5	0	0	0	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	1	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	955	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (955) 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:S:173:GLY:O	1:S:404:ARG:NH1	2.26	0.68
1:Z:339:GLN:HA	1:Z:342:ILE:HG12	1.76	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:C:421:ARG:NH2	1:C:473:ALA:O	2.29	0.66
1:M:120:ILE:HG23	1:M:443:ILE:HD11	1.76	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:V:69:MET:HG3	1:b:47:PRO:HG3	1.78	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:Z:386:GLU:OE1	1:a:197:ARG:NH2	2.30	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:T:166:MET:HE1	1:T:407:VAL:HG21	1.79	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:N:320:ALA:HA	1:N:335:GLY:HA2	1.80	0.63
1:Z:325:ILE:HG12	1:Z:330:THR:HG23	1.80	0.63
1:a:186:GLU:HB2	1:a:380:LYS:HE2	1.81	0.63
1:N:320:ALA:HB3	1:N:323:ILE:HD11	1.80	0.63
1:R:120:ILE:HG23	1:R:443:ILE:HD11	1.81	0.63
1:Z:173:GLY:O	1:Z:404:ARG:NH2	2.32	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:I:248:LEU:HD22	1:I:323:ILE:HG21	1.81	0.62
1:L:183:MET:HE2	1:L:384:SER:HB3	1.81	0.62
1:W:291:ASP:HB3	1:W:372:LEU:HD21	1.80	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:a:220:ILE:HB	1:a:318:GLY:HA3	1.82	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:U:193:MET:HE3	1:U:371:LYS:HD3	1.82	0.61
1:X:112:ARG:NH1	1:X:115:ASP:OD2	2.33	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:V:289:LEU:HD23	1:V:292:ILE:HD11	1.82	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:R:173:GLY:O	1:R:404:ARG:NH2	2.31	0.60
1:Z:227:ILE:O	1:Z:255:GLU:N	2.35	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	1.84	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:S:247:LEU:HB3	1:S:273:VAL:HG12	1.82	0.60
1:G:197:ARG:HE	1:G:279:PRO:HA	1.65	0.60
1:Y:248:LEU:HD11	1:Y:276:VAL:HG23	1.83	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	1.84	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: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:B:296:THR:HG23	1:B:318:GLY:HA3	1.84	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:186:GLU:OE1	1:B:188:LYS:NZ	2.36	0.58
1:A:213:ALA:HB3	1:A:325:ILE:HB	1.85	0.58
1:I:36:ARG:HD3	1:J:519:GLU:HG3	1.85	0.58
1:X:248:LEU:HD22	1:X:323:ILE:HG21	1.86	0.58
1:J:180:ALA:HB2	1:J:380:LYS:HB3	1.84	0.58
1:G:40:ILE:HD13	1:G:59:GLU:HG3	1.85	0.58
1:H:138:ILE:HG12	1:H:147:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:190:VAL:HG21	1:Q:333:VAL:HG13	1.84	0.58
1:B:120:ILE:HG23	1:B:443:ILE:HD11	1.84	0.58
1:P:294:ILE:HD12	1:P:345:ARG:HD2	1.86	0.58
1:S:325:ILE:HG12	1:S:330:THR:HG23	1.86	0.58
1:V:221:LEU:HD23	1:V:249:ILE:HG23	1.85	0.58
1:a:291:ASP:OD1	1:a:345:ARG:NH1	2.36	0.58
1:R:386:GLU:OE1	1:S:197:ARG:NH2	2.37	0.58
1:I:66:VAL:HA	1:I:69:MET:HE3	1.85	0.57
1:V:59:GLU:HG3	1:W:4:LYS:HE2	1.85	0.57
1:W:54:VAL:HG22	1:W:89:THR:HG21	1.86	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:E:193:MET:HE3	1:E:371:LYS:HD3	1.85	0.57
1:G:262:LEU:HD22	1:G:273:VAL:HG11	1.86	0.57
1:L:187:LEU:HD13	1:L:379:LEU:HD23	1.84	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:C:166:MET:HE1	1:C:407:VAL:HG21	1.86	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:K:47:PRO:HG3	1:L:69:MET:HG3	1.87	0.57
1:V:413:VAL:HG12	1:V:490:ILE:HG13	1.87	0.57
1:Y:393:LYS:NZ	1:Y:397:GLU:OE2	2.38	0.57
1:L:120:ILE:HG23	1:L:443:ILE:HD11	1.87	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:A:441:GLU:HG2	1:A:444:ARG:HH21	1.69	0.57
1:F:120:ILE:HG23	1:F:443:ILE:HD11	1.86	0.57
1:E:248:LEU:HD22	1:E:323:ILE:HD13	1.87	0.56
1:N:322:ARG:HB3	1:N:333:VAL:HB	1.87	0.56
1:X:120:ILE:HG23	1:X:443:ILE:HD11	1.86	0.56
1:F:213:ALA:HB3	1:F:325:ILE:HB	1.87	0.56
1:O:27:VAL:HG12	1:O:90:THR:HG23	1.87	0.56
1:V:247:LEU:HB3	1:V:273:VAL:HG12	1.87	0.56
1:F:194:GLN:O	1:F:371:LYS:NZ	2.28	0.56
1:G:353:ILE:HG22	1:G:354:GLU:HG3	1.88	0.56
1:I:138:ILE:HG12	1:I:147:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:82:SER:HA	1:M:86:GLY:HA2	1.86	0.56
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.87	0.56
1:T:17:LYS:HD2	1:T:104:LEU:HD12	1.87	0.56
1:W:47:PRO:HG3	1:X:69:MET:HG2	1.88	0.56
1:Z:214:GLU:HG2	1:Z:324:THR:HG22	1.86	0.56
1:Q:120:ILE:HG23	1:Q:443:ILE:HD11	1.87	0.56
1:S:214:GLU:OE1	1:S:322:ARG:NH2	2.39	0.56
1:U:109:ALA:HA	1:a:105:LYS:HG2	1.86	0.56
1:V:17:LYS:HD2	1:V:104:LEU:HD12	1.87	0.56
1:B:248:LEU:HD22	1:B:323:ILE:HG21	1.88	0.56
1:N:218:ALA:HB2	1:N:246:PRO:HG2	1.88	0.56
1:A:82:SER:HA	1:A:86:GLY:H	1.70	0.56
1:B:17:LYS:HD2	1:B:104:LEU:HD12	1.88	0.56
1:U:180:ALA:HB2	1:U:380:LYS:HB3	1.87	0.56
1:Y:381:ILE:HG12	1:Y:396:VAL:HG21	1.87	0.56
1:P:120:ILE:HG23	1:P:443:ILE:HD11	1.88	0.56
1:b:120:ILE:HG23	1:b:443:ILE:HD11	1.88	0.56
1:Z:177:VAL:HG21	1:Z:397:GLU:HG2	1.88	0.56
1:H:302:SER:H	1:H:307:TYR:HB2	1.71	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:P:47:PRO:HG3	1:Q:69:MET:HG2	1.86	0.55
1:T:120:ILE:HG23	1:T:443:ILE:HD11	1.88	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:B:109:ALA:HA	1:K:105:LYS:HG2	1.87	0.55
1:H:47:PRO:HG3	1:I:69:MET:HG2	1.88	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	1.89	0.55
1:A:392:LYS:HG2	1:A:395:ARG:HH21	1.72	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:B:77:VAL:HA	1:B:80:LYS:HE2	1.87	0.55
1:E:213:ALA:HB3	1:E:325:ILE:HB	1.88	0.55
1:V:213:ALA:HB3	1:V:325:ILE:HB	1.88	0.55
1:T:386:GLU:OE1	1:U:197:ARG:NH2	2.32	0.55
1:V:87:ASP:OD1	1:V:88:GLY:N	2.39	0.55
1:C:247:LEU:O	1:C:273:VAL:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:a:219:LEU:HD13	1:a:317:LEU:HD12	1.88	0.55
1:H:173:GLY:O	1:H:404:ARG:NH2	2.39	0.54
1:Y:120:ILE:HG23	1:Y:443:ILE:HD11	1.89	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:a:218:ALA:HB2	1:a:246:PRO:HG2	1.90	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	1.89	0.54
1:A:295:LEU:HD12	1:A:342:ILE:HD13	1.90	0.54
1:P:382:GLY:O	1:P:392:LYS:NZ	2.40	0.54
1:W:248:LEU:HD22	1:W:323:ILE:HG21	1.88	0.54
1:b:409:GLU:OE2	1:b:502:ARG:NH2	2.38	0.54
1:A:199:TYR:OH	1:A:327:LYS:NZ	2.33	0.54
1:E:109:ALA:HA	1:H:105:LYS:HG2	1.90	0.54
1:E:166:MET:HE1	1:E:407:VAL:HG21	1.90	0.54
1:F:324:THR:OG1	1:F:331:THR:OG1	2.24	0.54
1:J:120:ILE:HG23	1:J:443:ILE:HD11	1.89	0.54
1:X:69:MET:HE1	1:X:521:ALA:HB1	1.90	0.54
1:H:83:ASP:OD2	1:H:327:LYS:NZ	2.34	0.54
1:T:102:GLU:O	1:T:106:ASN:ND2	2.41	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:I:246:PRO:HB3	1:I:272:LYS:HB3	1.90	0.53
1:N:166:MET:HE1	1:N:407:VAL:HG21	1.90	0.53
1:R:166:MET:HE1	1:R:407:VAL:HG21	1.90	0.53
1:b:177:VAL:HG22	1:b:379:LEU:HD12	1.89	0.53
1:I:193:MET:HE3	1:I:371:LYS:HD3	1.89	0.53
1:L:39:LEU:HD13	1:M:73:MET:HE1	1.89	0.53
1:L:164:GLU:OE2	1:L:168:LYS:NZ	2.36	0.53
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.90	0.53
1:Q:40:ILE:HB	1:Q:48:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:16:LEU:HD13	1:U:515:LEU:HD22	1.90	0.53
1:V:112:ARG:NH1	1:V:115:ASP:OD2	2.40	0.53
1:X:180:ALA:HB2	1:X:380:LYS:HB3	1.89	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: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:P:192:GLY:HA2	1:P:295:LEU:HD21	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:Z:236:ILE:HD11	1:Z:317:LEU:HD11	1.90	0.53
1:E:345:ARG:HH21	1:E:368:ARG:HH22	1.56	0.53
1:F:102:GLU:O	1:F:106:ASN:ND2	2.40	0.53
1:H:413:VAL:HG22	1:H:490:ILE:HD11	1.90	0.53
1:L:215:LEU:HB2	1:L:323:ILE:HG23	1.89	0.53
1:N:40:ILE:HD13	1:N:59:GLU:HG3	1.89	0.53
1:S:117:LYS:HG3	1:S:513:SER:HB3	1.91	0.53
1:V:278:ALA:HB3	1:V:285:ARG:HE	1.74	0.53
1:H:33:PRO:HG2	1:H:481:ALA:HB3	1.91	0.53
1:S:193:MET:HE3	1:S:371:LYS:HD3	1.91	0.53
1:U:333:VAL:HG12	1:U:334:GLU:HG3	1.90	0.53
1:H:246:PRO:HB3	1:H:272:LYS:HB3	1.90	0.53
1:M:81:THR:OG1	1:M:507:ASN:ND2	2.38	0.53
1:N:218:ALA:HB3	1:N:323:ILE:HD13	1.91	0.53
1:a:117:LYS:HG3	1:a:513:SER:HB3	1.90	0.53
1:A:247:LEU:HB3	1:A:273:VAL:HG12	1.91	0.52
1:G:381:ILE:HG12	1:G:396:VAL:HG21	1.91	0.52
1:b:419:LEU:HD22	1:b:447:LEU:HD22	1.91	0.52
1:Y:386:GLU:OE1	1:Z:197:ARG:NH2	2.40	0.52
1:H:69:MET:HE1	1:H:521:ALA:HB1	1.91	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:K:166:MET:HE1	1:K:407:VAL:HG21	1.91	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: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:Z:25:ASN:HA	1:Z:28:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:HE1	1:A:521:ALA:HB1	1.90	0.52
1:A:200:LEU:HD23	1:A:259:LEU:HD12	1.92	0.52
1:E:216:ASP:OD1	1:E:322:ARG:NH1	2.43	0.52
1:L:180:ALA:HA	1:L:380:LYS:HE3	1.91	0.52
1:B:152:ALA:O	1:B:395:ARG:NH1	2.43	0.52
1:T:421:ARG:NH1	1:T:473:ALA:O	2.43	0.52
1:U:468:GLU:HG2	1:Z:465:VAL:HG11	1.91	0.52
1:S:33:PRO:HG2	1:S:481:ALA:HB3	1.92	0.52
1:X:197:ARG:HE	1:X:277:LYS:HB2	1.74	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:A:85:ALA:HB1	1:A:500:VAL:HG22	1.91	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:M:168:LYS:HG2	1:M:189:VAL:HG21	1.92	0.52
1:X:325:ILE:HG13	1:X:330:THR:HG23	1.93	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	2.43	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
1:E:69:MET:HE1	1:E:521:ALA:HB1	1.93	0.51
1:G:77:VAL:HA	1:G:80:LYS:HE2	1.91	0.51
1:Z:138:ILE:HG13	1:Z:143:GLU:HB3	1.92	0.51
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.93	0.51
1:M:250:ILE:HG22	1:M:276:VAL:HB	1.92	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:A:87:ASP:OD1	1:A:88:GLY:N	2.43	0.51
1:U:469:LYS:HD3	1:U:486:TYR:CZ	2.45	0.51
1:V:138:ILE:HG12	1:V:147:VAL:HG21	1.93	0.51
1:X:169:VAL:HG12	1:X:173:GLY:HA3	1.91	0.51
1:Q:385:THR:HG22	1:Q:387:VAL:H	1.75	0.51
1:F:77:VAL:HA	1:F:80:LYS:HE2	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:N:77:VAL:HG12	1:N:507:ASN:HB3	1.93	0.51
1:W:27:VAL:HG12	1:W:90:THR:HG23	1.92	0.51
1:A:381:ILE:HG12	1:A:396:VAL:HG21	1.93	0.51
1:Z:248:LEU:HD22	1:Z:323:ILE:HG21	1.92	0.51
1:N:321:ALA:HB3	1:N:334:GLU:HB3	1.93	0.50
1:U:105:LYS:HG2	1:a:109:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:V:517:THR:O	1:b:36:ARG:HB3	2.12	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:P:240:ALA:HA	1:P:314:MET:HE1	1.92	0.50
1:Q:171:LYS:O	1:Q:404:ARG:NH1	2.44	0.50
1:C:41:ASP:HB2	1:D:523:THR:HG22	1.92	0.50
1:E:58:LYS:HA	1:E:75:ARG:HH21	1.77	0.50
1:H:54:VAL:HG22	1:H:89:THR:HG21	1.93	0.50
1:H:183:MET:HE3	1:I:282:GLY:HA2	1.93	0.50
1:K:33:PRO:HG2	1:K:481:ALA:HB3	1.92	0.50
1:M:29:VAL:HG11	1:N:519:GLU:HB2	1.93	0.50
1:U:203:TYR:HB3	1:U:267:LEU:HD21	1.94	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: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:P:254:ILE:HD13	1:P:275:ALA:HB1	1.94	0.50
1:U:248:LEU:HD22	1:U:323:ILE:HG21	1.94	0.50
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:G:291:ASP:OD1	1:G:368:ARG:NH2	2.44	0.50
1:R:36:ARG:NH2	1:R:457:ASN:OD1	2.44	0.50
1:R:220:ILE:HG22	1:R:248:LEU:HB3	1.94	0.50
1:G:69:MET:HE1	1:G:521:ALA:HB1	1.94	0.50
1:H:120:ILE:HG23	1:H:443:ILE:HD11	1.94	0.50
1:R:384:SER:OG	1:R:388:GLU:OE2	2.28	0.50
1:S:85:ALA:HB1	1:S:500:VAL:HG22	1.94	0.50
1:U:411:ILE:HD13	1:U:497:PRO:HA	1.94	0.50
1:V:205:VAL:HA	1:V:213:ALA:HB2	1.94	0.50
1:b:85:ALA:HB1	1:b:500:VAL:HG22	1.94	0.50
1:I:75:ARG:O	1:I:79:SER:OG	2.26	0.50
1:L:62:LEU:HB2	1:L:68:ASN:HB2	1.93	0.50
1:M:54:VAL:HG22	1:M:89:THR:HG21	1.94	0.50
1:N:411:ILE:HD12	1:N:495:VAL:HG21	1.93	0.50
1:W:166:MET:HE1	1:W:407:VAL:HG21	1.93	0.50
1:Z:295:LEU:HD11	1:Z:372:LEU:HG	1.93	0.50
1:L:77:VAL:HA	1:L:80:LYS:HE2	1.93	0.49
1:O:149:THR:HG23	1:O:155:ASP:H	1.77	0.49
1:S:17:LYS:HD2	1:S:104:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:383:ALA:HB2	1:S:392:LYS:HD3	1.94	0.49
1:D:450:PRO:O	1:D:454:ILE:HG12	2.12	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:33:PRO:HG2	1:D:481:ALA:HB3	1.95	0.49
1:J:243:SER:O	1:J:245:ARG:N	2.46	0.49
1:J:325:ILE:HG12	1:J:330:THR:HG23	1.94	0.49
1:U:215:LEU:HB2	1:U:323:ILE:HB	1.93	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:a:213:ALA:HB3	1:a:325:ILE:HB	1.93	0.49
1:E:382:GLY:HA2	1:E:389:MET:HG2	1.93	0.49
1:W:247:LEU:HB3	1:W:273:VAL:HG23	1.93	0.49
1:Y:237:LEU:HD11	1:Y:317:LEU:HD11	1.95	0.49
1:D:69:MET:HE1	1:D:521:ALA:HB1	1.93	0.49
1:G:31:LEU:O	1:G:457:ASN:ND2	2.46	0.49
1:J:47:PRO:HG3	1:K:69:MET:HG2	1.94	0.49
1:J:333:VAL:HG12	1:J:334:GLU:HG2	1.94	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:G:165:ALA:HB2	1:G:379:LEU:HD21	1.95	0.49
1:H:102:GLU:O	1:H:106:ASN:ND2	2.43	0.49
1:L:502:ARG:NH1	1:L:506:GLU:OE1	2.46	0.49
1:W:33:PRO:HG2	1:W:481:ALA:HB3	1.95	0.49
1:X:221:LEU:HB2	1:X:247:LEU:HD11	1.95	0.49
1:B:40:ILE:HD13	1:B:59:GLU:HG3	1.94	0.49
1:D:192:GLY:HA2	1:D:295:LEU:HD21	1.94	0.49
1:H:2:THR:O	1:H:4:LYS:NZ	2.40	0.49
1:S:216:ASP:OD1	1:S:322:ARG:NH1	2.45	0.49
1:T:353:ILE:HG23	1:T:362:THR:HG23	1.95	0.49
1:b:165:ALA:HB2	1:b:379:LEU:HD21	1.94	0.49
1:H:311:ASN:O	1:H:313:THR:N	2.46	0.49
1:P:66:VAL:HA	1:P:69:MET:HE2	1.95	0.49
1:W:236:ILE:HG21	1:W:312:ALA:HB3	1.94	0.49
1:A:120:ILE:HG23	1:A:443:ILE:HD11	1.93	0.49
1:G:16:LEU:HD13	1:G:515:LEU:HD22	1.95	0.49
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.94	0.49
1:M:326:ASP:OD1	1:M:327:LYS:N	2.39	0.49
1:R:179:GLU:OE1	1:R:390:LYS:NZ	2.44	0.49
1:D:165:ALA:HB2	1:D:379:LEU:HD21	1.95	0.48
1:O:112:ARG:NH1	1:U:458:THR:O	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:179:GLU:OE2	1:Q:390:LYS:NZ	2.41	0.48
1:X:27:VAL:HG12	1:X:90:THR:HG23	1.94	0.48
1:J:36:ARG:HH12	1:K:114:ILE:HB	1.76	0.48
1:Q:175:ILE:HG12	1:Q:377:ALA:HB3	1.95	0.48
1:R:289:LEU:HD23	1:R:292:ILE:HD12	1.94	0.48
1:W:289:LEU:HD23	1:W:292:ILE:HD12	1.95	0.48
1:A:228:SER:HG	1:A:257:GLU:N	2.10	0.48
1:C:47:PRO:HG3	1:D:69:MET:HG2	1.94	0.48
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.94	0.48
1:Q:25:ASN:HA	1:Q:28:LYS:HE2	1.95	0.48
1:R:200:LEU:HD21	1:R:277:LYS:HE3	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:168:LYS:HG2	1:J:189:VAL:HG21	1.95	0.48
1:P:411:ILE:HD13	1:P:497:PRO:HA	1.96	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:D:262:LEU:HD22	1:D:273:VAL:HG11	1.94	0.48
1:J:253:ASP:OD1	1:J:254:ILE:N	2.46	0.48
1:L:66:VAL:HA	1:L:69:MET:HE2	1.96	0.48
1:N:69:MET:HE1	1:N:521:ALA:HB1	1.95	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:Z:314:MET:HG2	1:Z:317:LEU:HD12	1.96	0.48
1:B:165:ALA:HB2	1:B:379:LEU:HD21	1.95	0.48
1:G:219:LEU:O	1:G:248:LEU:N	2.28	0.48
1:R:207:ASN:HB3	1:R:210:THR:HG22	1.95	0.48
1:U:233:LEU:HD23	1:U:237:LEU:HB2	1.95	0.48
1:D:253:ASP:OD1	1:D:254:ILE:N	2.47	0.48
1:J:17:LYS:HD2	1:J:104:LEU:HD12	1.96	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
1:T:187:LEU:HD13	1:T:379:LEU:HD23	1.94	0.48
1:U:213:ALA:HB3	1:U:325:ILE:HG12	1.94	0.48
1:C:489:LEU:HB3	1:C:494:VAL:HB	1.94	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	1.95	0.48
1:E:25:ASN:HA	1:E:28:LYS:HE2	1.95	0.48
1:F:69:MET:HE1	1:F:521:ALA:HB1	1.95	0.48
1:G:166:MET:HE1	1:G:407:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:157:GLU:O	1:K:161:LEU:N	2.47	0.48
1:V:253:ASP:OD1	1:V:254:ILE:N	2.45	0.48
1:S:66:VAL:HA	1:S:69:MET:HE2	1.95	0.48
1:Z:220:ILE:HG22	1:Z:248:LEU:HB3	1.96	0.48
1:I:141:LYS:HG3	1:I:163:ALA:HB1	1.96	0.47
1:N:248:LEU:HD22	1:N:323:ILE:HG21	1.96	0.47
1:P:220:ILE:HD12	1:P:296:THR:HG21	1.95	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:P:41:ASP:HB2	1:Q:69:MET:HE2	1.96	0.47
1:K:497:PRO:HB2	1:K:500:VAL:HG23	1.96	0.47
1:L:222:ILE:HG13	1:L:250:ILE:HD12	1.97	0.47
1:M:328:ASP:OD1	1:M:329:ASN:N	2.42	0.47
1:Q:294:ILE:HD12	1:Q:345:ARG:HH11	1.79	0.47
1:X:166:MET:HE1	1:X:407:VAL:HG21	1.96	0.47
1:H:117:LYS:HG3	1:H:513:SER:HB3	1.96	0.47
1:H:132:ARG:NH2	1:H:409:GLU:OE1	2.48	0.47
1:J:117:LYS:HG3	1:J:513:SER:HB3	1.96	0.47
1:O:87:ASP:OD2	1:O:88:GLY:N	2.47	0.47
1:S:386:GLU:OE2	1:T:277:LYS:NZ	2.43	0.47
1:W:252:GLU:HG3	1:W:285:ARG:HH11	1.80	0.47
1:A:194:GLN:O	1:A:371:LYS:NZ	2.34	0.47
1:C:116:LEU:O	1:C:120:ILE:HG12	2.14	0.47
1:M:141:LYS:HZ2	1:M:167:ASP:HA	1.80	0.47
1:Q:420:ILE:HD12	1:Q:451:LEU:HD13	1.97	0.47
1:a:200:LEU:HD22	1:a:254:ILE:HB	1.97	0.47
1:A:4:LYS:NZ	1:G:59:GLU:OE1	2.46	0.47
1:I:132:ARG:HH22	1:I:409:GLU:HB3	1.79	0.47
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.96	0.47
1:L:219:LEU:O	1:L:248:LEU:N	2.47	0.47
1:P:166:MET:HE1	1:P:407:VAL:HG21	1.96	0.47
1:P:349:ILE:HG21	1:P:369:LEU:HB2	1.97	0.47
1:R:91:THR:N	2:R:602:SO4:O3	2.43	0.47
1:T:382:GLY:O	1:T:392:LYS:NZ	2.42	0.47
1:a:23:LEU:HD12	1:a:60:ILE:HD12	1.95	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:b:27:VAL:HG22	1:b:90:THR:HG23	1.95	0.47
1:C:413:VAL:HG23	1:C:489:LEU:HB2	1.96	0.47
1:G:6:ILE:HG12	1:G:522:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:25:ASN:HA	1:O:28:LYS:HE2	1.97	0.47
1:S:321:ALA:HB3	1:S:334:GLU:HB3	1.97	0.47
1:A:187:LEU:HD13	1:A:379:LEU:HD23	1.96	0.47
1:A:166:MET:HE1	1:A:407:VAL:HG21	1.96	0.46
1:I:295:LEU:HA	1:I:342:ILE:HD11	1.97	0.46
1:J:220:ILE:O	1:J:318:GLY:N	2.47	0.46
1:Q:165:ALA:HB2	1:Q:379:LEU:HD21	1.97	0.46
1:T:291:ASP:HB3	1:T:372:LEU:HD21	1.96	0.46
1:U:294:ILE:HD12	1:U:345:ARG:HD2	1.97	0.46
1:X:25:ASN:HA	1:X:28:LYS:HE2	1.97	0.46
1:X:205:VAL:HA	1:X:213:ALA:HB2	1.97	0.46
1:E:105:LYS:HG2	1:H:109:ALA:HA	1.96	0.46
1:F:296:THR:O	1:F:319:GLN:N	2.48	0.46
1:T:77:VAL:HA	1:T:80:LYS:HE2	1.96	0.46
1:U:62:LEU:HB2	1:U:68:ASN:HB2	1.97	0.46
1:A:112:ARG:HH22	1:G:484:GLU:CD	2.23	0.46
1:A:326:ASP:OD1	1:A:327:LYS:N	2.45	0.46
1:E:23:LEU:HD12	1:E:60:ILE:HD12	1.96	0.46
1:L:166:MET:HE1	1:L:407:VAL:HG21	1.97	0.46
1:N:224:ASP:O	1:N:285:ARG:NH2	2.47	0.46
1:Q:7:LEU:HD23	1:Q:12:ALA:HA	1.97	0.46
1:S:438:THR:O	1:S:442:ILE:HG12	2.16	0.46
1:T:177:VAL:HG22	1:T:379:LEU:HD12	1.98	0.46
1:U:222:ILE:HG21	1:U:300:VAL:HG22	1.98	0.46
1:V:120:ILE:HG23	1:V:443:ILE:HD11	1.97	0.46
1:X:234:LEU:O	1:X:236:ILE:N	2.44	0.46
1:a:77:VAL:HG12	1:a:507:ASN:HB3	1.97	0.46
1:a:165:ALA:HB2	1:a:379:LEU:HD21	1.97	0.46
1:b:421:ARG:NH2	1:b:477:TYR:O	2.48	0.46
1:F:419:LEU:HD22	1:F:447:LEU:HD22	1.98	0.46
1:N:117:LYS:HG3	1:N:513:SER:HB3	1.96	0.46
1:Q:31:LEU:O	1:Q:457:ASN:ND2	2.44	0.46
1:R:438:THR:O	1:R:442:ILE:HG12	2.16	0.46
1:S:389:MET:HG2	1:S:393:LYS:HG3	1.96	0.46
1:D:166:MET:HE1	1:D:407:VAL:HG21	1.98	0.46
1:F:117:LYS:HG3	1:F:513:SER:HB2	1.96	0.46
1:Z:77:VAL:HG12	1:Z:507:ASN:HB3	1.97	0.46
1:b:166:MET:HE1	1:b:407:VAL:HG11	1.97	0.46
1:B:222:ILE:HG21	1:B:300:VAL:HG22	1.98	0.46
1:Q:247:LEU:HB3	1:Q:273:VAL:HG12	1.97	0.46
1:W:25:ASN:HA	1:W:28:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:77:VAL:HA	1:Y:80:LYS:HE2	1.98	0.46
1:a:25:ASN:HA	1:a:28:LYS:HE2	1.97	0.46
1:a:324:THR:HG1	1:a:331:THR:HG1	1.62	0.46
1:F:480:ASN:HD22	1:F:494:VAL:HG21	1.81	0.46
1:F:91:THR:N	2:F:601:SO4:O3	2.46	0.46
1:O:294:ILE:HG22	1:O:342:ILE:HD13	1.98	0.46
1:S:227:ILE:HG23	1:S:228:SER:H	1.80	0.46
1:T:15:LYS:NZ	1:T:64:ASP:OD2	2.46	0.46
1:W:40:ILE:HD13	1:W:59:GLU:HG3	1.98	0.46
1:Z:116:LEU:O	1:Z:120:ILE:HG12	2.15	0.46
1:a:388:GLU:O	1:a:392:LYS:N	2.31	0.46
1:D:262:LEU:HD13	1:D:273:VAL:HG11	1.97	0.45
1:L:175:ILE:HG12	1:L:377:ALA:HB3	1.97	0.45
1:S:141:LYS:HG3	1:S:163:ALA:HB1	1.97	0.45
1:V:193:MET:HB2	1:V:371:LYS:HB3	1.97	0.45
1:X:247:LEU:HB3	1:X:273:VAL:HG12	1.97	0.45
1:Y:36:ARG:HH12	1:Z:114:ILE:HB	1.80	0.45
1:Z:33:PRO:HG2	1:Z:481:ALA:HB3	1.97	0.45
1:D:261:THR:O	1:D:265:ASN:ND2	2.31	0.45
1:D:465:VAL:HG21	1:H:468:GLU:HG3	1.98	0.45
1:E:206:THR:H	1:E:213:ALA:HA	1.82	0.45
1:K:160:GLU:HA	1:K:163:ALA:HB2	1.97	0.45
1:M:77:VAL:HG12	1:M:507:ASN:HB3	1.98	0.45
1:T:30:THR:HB	1:T:51:LYS:O	2.16	0.45
1:V:66:VAL:HA	1:V:69:MET:HE2	1.98	0.45
1:X:62:LEU:HB2	1:X:68:ASN:HB2	1.98	0.45
1:Z:261:THR:O	1:Z:265:ASN:ND2	2.50	0.45
1:I:333:VAL:HG22	1:I:376:VAL:HG11	1.98	0.45
1:J:261:THR:O	1:J:265:ASN:ND2	2.49	0.45
1:R:77:VAL:HA	1:R:80:LYS:HE2	1.97	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:W:158:ILE:HD11	1:W:392:LYS:HE3	1.98	0.45
1:B:223:HIS:O	1:B:251:ALA:HA	2.16	0.45
1:E:117:LYS:HG3	1:E:513:SER:HB3	1.99	0.45
1:K:77:VAL:HG12	1:K:507:ASN:HB3	1.97	0.45
1:Q:102:GLU:O	1:Q:106:ASN:ND2	2.45	0.45
1:G:205:VAL:HA	1:G:213:ALA:HB2	1.99	0.45
1:I:15:LYS:HE3	1:I:67:GLU:HG3	1.98	0.45
1:N:393:LYS:NZ	1:N:397:GLU:OE2	2.45	0.45
1:V:64:ASP:HB3	1:V:67:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:U:215:LEU:HB3	1:U:218:ALA:HB2	1.98	0.45
1:Y:85:ALA:HB1	1:Y:500:VAL:HG22	1.99	0.45
1:a:253:ASP:OD1	1:a:254:ILE:N	2.48	0.45
1:F:25:ASN:HA	1:F:28:LYS:HE2	1.97	0.45
1:G:222:ILE:HG21	1:G:300:VAL:HG12	1.99	0.45
1:J:443:ILE:O	1:J:447:LEU:HG	2.16	0.45
1:M:64:ASP:HB3	1:M:67:GLU:HB2	1.98	0.45
1:N:333:VAL:HG22	1:N:376:VAL:HG11	1.98	0.45
1:S:248:LEU:HD22	1:S:323:ILE:HG21	1.98	0.45
1:T:180:ALA:HB2	1:T:380:LYS:HB3	1.99	0.45
1:T:502:ARG:NH1	1:T:506:GLU:OE1	2.42	0.45
1:b:64:ASP:HB3	1:b:67:GLU:HB2	1.97	0.45
1:J:205:VAL:HA	1:J:213:ALA:HB2	1.98	0.45
1:L:161:LEU:HD11	1:L:187:LEU:HB2	1.98	0.45
1:Q:214:GLU:OE1	1:Q:322:ARG:NH1	2.50	0.45
1:Q:438:THR:O	1:Q:442:ILE:HG12	2.17	0.45
1:U:136:ARG:NH2	1:U:476:ASP:OD2	2.48	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:N:222:ILE:HD12	1:N:293:ALA:HB2	1.98	0.45
1:O:158:ILE:HG23	1:O:396:VAL:HG22	1.98	0.45
1:S:120:ILE:HG23	1:S:443:ILE:HD11	1.97	0.45
1:T:31:LEU:O	1:T:457:ASN:ND2	2.45	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: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:P:116:LEU:O	1:P:120:ILE:HG12	2.17	0.45
1:E:187:LEU:HD13	1:E:379:LEU:HD23	1.99	0.44
1:N:15:LYS:NZ	1:N:67:GLU:OE2	2.50	0.44
1:N:76:GLU:O	1:N:79:SER:OG	2.33	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:a:226:LYS:HG3	1:a:253:ASP:HB3	1.98	0.44
1:D:420:ILE:HD12	1:D:451:LEU:HD13	1.98	0.44
1:L:81:THR:HG23	1:L:503:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:U:321:ALA:HB3	1:U:334:GLU:HB2	1.98	0.44
1:V:292:ILE:HG13	1:V:293:ALA:N	2.32	0.44
1:Y:413:VAL:HG23	1:Y:489:LEU:HB2	1.98	0.44
1:A:193:MET:HE3	1:A:371:LYS:HE3	1.99	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:Q:291:ASP:HB3	1:Q:372:LEU:HD11	2.00	0.44
1:a:15:LYS:HE3	1:a:67:GLU:HG3	1.99	0.44
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:D:236:ILE:HA	1:D:239:LYS:HZ2	1.83	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: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:Q:47:PRO:HB3	1:R:69:MET:HG2	2.00	0.44
1:Q:194:GLN:HE21	1:Q:329:ASN:HB3	1.83	0.44
1:W:77:VAL:HG12	1:W:507:ASN:HB3	1.99	0.44
1:Y:38:VAL:HG22	1:Z:520:ALA:HB3	1.98	0.44
1:a:248:LEU:HD22	1:a:323:ILE:HG21	1.99	0.44
1:J:66:VAL:HA	1:J:69:MET:HE2	1.99	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:a:411:ILE:HD12	1:a:495:VAL:HG21	2.00	0.44
1:C:381:ILE:HG12	1:C:396:VAL:HG21	1.99	0.44
1:H:205:VAL:HA	1:H:213:ALA:HB2	2.00	0.44
1:H:340:GLU:HA	1:H:343:LYS:HE2	1.99	0.44
1:H:517:THR:O	1:N:36:ARG:HB3	2.18	0.44
1:L:161:LEU:HG	1:L:379:LEU:HD22	1.99	0.44
1:W:221:LEU:HD23	1:W:249:ILE:HG12	2.00	0.44
1:B:193:MET:HB2	1:B:371:LYS:HB3	1.99	0.44
1:G:105:LYS:HG2	1:M:109:ALA:HA	2.00	0.44
1:K:69:MET:HE1	1:K:521:ALA:HB1	2.00	0.44
1:R:333:VAL:HG22	1:R:376:VAL:HG11	1.99	0.44
1:T:76:GLU:O	1:T:79:SER:OG	2.33	0.44
1:V:7:LEU:HD12	1:V:66:VAL:HG21	2.00	0.44
1:D:349:ILE:HG22	1:D:369:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:59:GLU:OE1	1:L:4:LYS:NZ	2.50	0.44
1:N:30:THR:HB	1:N:51:LYS:O	2.18	0.44
1:O:218:ALA:HB2	1:O:246:PRO:HG2	2.00	0.44
1:U:77:VAL:HG12	1:U:507:ASN:HB3	1.98	0.44
1:G:208:SER:C	1:G:210:THR:H	2.26	0.43
1:G:488:ASN:HB3	1:G:491:GLU:HG2	2.00	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:Q:195:PHE:CD1	1:Q:279:PRO:HG3	2.53	0.43
1:S:192:GLY:HA2	1:S:295:LEU:HD21	1.98	0.43
1:Y:138:ILE:HG12	1:Y:147:VAL:HG21	2.00	0.43
1:a:420:ILE:HD12	1:a:451:LEU:HD13	2.00	0.43
1:D:25:ASN:HA	1:D:28:LYS:HE2	2.00	0.43
1:D:138:ILE:HG12	1:D:147:VAL:HG21	2.00	0.43
1:P:222:ILE:HG21	1:P:300:VAL:HG22	2.00	0.43
1:Z:138:ILE:HG12	1:Z:147:VAL:HG21	2.00	0.43
1:G:469:LYS:HD2	1:G:486:TYR:CZ	2.53	0.43
1:I:64:ASP:HB3	1:I:67:GLU:HB2	1.99	0.43
1:O:47:PRO:HG3	1:P:69:MET:HG3	2.01	0.43
1:S:200:LEU:HD21	1:S:277:LYS:HG2	2.01	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:83:ASP:OD1	1:b:84:VAL:N	2.51	0.43
1:b:190:VAL:HG21	1:b:333:VAL:HG13	2.01	0.43
1:D:79:SER:HA	1:D:89:THR:HG22	2.00	0.43
1:H:66:VAL:HA	1:H:69:MET:HE2	2.00	0.43
1:H:165:ALA:HB2	1:H:379:LEU:HD21	2.01	0.43
1:K:62:LEU:HB2	1:K:68:ASN:HB2	2.01	0.43
1:Y:214:GLU:OE1	1:Y:322:ARG:NH2	2.50	0.43
1:a:421:ARG:NH2	1:a:477:TYR:O	2.51	0.43
1:b:321:ALA:N	1:b:334:GLU:O	2.51	0.43
1:P:102:GLU:O	1:P:106:ASN:ND2	2.50	0.43
1:Q:219:LEU:O	1:Q:248:LEU:N	2.34	0.43
1:a:13:ARG:NH2	1:a:519:GLU:OE2	2.46	0.43
1:b:177:VAL:HG13	1:b:381:ILE:HD13	2.01	0.43
1:C:476:ASP:HB2	1:C:488:ASN:ND2	2.33	0.43
1:D:187:LEU:HD13	1:D:379:LEU:HD23	1.99	0.43
1:G:123:ALA:HB2	1:G:440:ILE:HD13	2.01	0.43
1:J:420:ILE:HD11	1:J:448:GLU:HA	2.00	0.43
1:P:438:THR:O	1:P:442:ILE:HG12	2.19	0.43
1:R:171:LYS:O	1:R:404:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:194:GLN:NE2	1:W:331:THR:OG1	2.50	0.43
1:X:222:ILE:HG23	1:X:289:LEU:HD22	2.01	0.43
1:Y:30:THR:HB	1:Y:51:LYS:O	2.18	0.43
1:a:256:GLY:C	1:a:258:ALA:H	2.26	0.43
1:E:262:LEU:HD22	1:E:273:VAL:HG11	1.99	0.43
1:H:13:ARG:HB3	1:H:104:LEU:HD21	2.00	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:R:98:ALA:HB2	1:R:449:GLU:HG2	2.01	0.43
1:U:302:SER:C	1:U:307:TYR:H	2.27	0.43
1:b:87:ASP:HB3	2:b:601:SO4:O1	2.18	0.43
1:b:321:ALA:N	1:b:333:VAL:O	2.52	0.43
1:A:222:ILE:HG21	1:A:300:VAL:HG12	2.00	0.43
1:B:420:ILE:HG21	1:B:471:LYS:HG2	2.01	0.43
1:C:77:VAL:HG12	1:C:507:ASN:HB3	2.01	0.43
1:D:221:LEU:HD23	1:D:249:ILE:HG12	2.00	0.43
1:D:254:ILE:HG22	1:D:259:LEU:HB2	1.99	0.43
1:H:519:GLU:HG3	1:N:36:ARG:CZ	2.48	0.43
1:J:166:MET:HE1	1:J:407:VAL:HG21	2.01	0.43
1:N:6:ILE:HD12	1:N:522:ILE:HG12	2.01	0.43
1:O:295:LEU:HA	1:O:342:ILE:HD11	2.01	0.43
1:Q:19:GLY:HA3	1:Q:67:GLU:O	2.19	0.43
1:R:278:ALA:HB1	1:R:289:LEU:HD21	2.00	0.43
1:U:69:MET:HE1	1:U:521:ALA:HB1	2.00	0.43
1:U:230:MET:HE3	1:U:233:LEU:HD22	2.01	0.43
1:Y:205:VAL:HA	1:Y:213:ALA:HB2	2.01	0.43
1:Z:161:LEU:HD11	1:Z:187:LEU:HB2	2.00	0.43
1:b:141:LYS:HG3	1:b:163:ALA:HB1	2.01	0.43
1:A:122:ARG:NH1	1:A:436:GLN:OE1	2.52	0.43
1:F:166:MET:HE1	1:F:407:VAL:HG21	2.00	0.43
1:F:469:LYS:HD2	1:F:486:TYR:CZ	2.54	0.43
1:K:324:THR:O	1:K:331:THR:N	2.51	0.43
1:T:489:LEU:HB3	1:T:494:VAL:HB	2.01	0.43
1:V:177:VAL:HG22	1:V:379:LEU:HD12	2.01	0.43
1:W:409:GLU:OE2	1:W:502:ARG:NH2	2.51	0.43
1:Y:36:ARG:HH22	1:Z:114:ILE:HB	1.84	0.43
1:C:30:THR:HB	1:C:51:LYS:O	2.19	0.43
1:E:36:ARG:CZ	1:F:519:GLU:HG3	2.48	0.43
1:E:82:SER:HA	1:E:86:GLY:H	1.84	0.43
1:F:476:ASP:HB2	1:F:488:ASN:ND2	2.34	0.43
1:I:68:ASN:O	1:I:72:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:ALA:HB3	1:I:254:ILE:HG12	1.99	0.43
1:I:291:ASP:HB3	1:I:372:LEU:HD11	2.01	0.43
1:J:250:ILE:HG12	1:J:276:VAL:HB	2.01	0.43
1:K:420:ILE:HD11	1:K:448:GLU:HA	2.00	0.43
1:R:320:ALA:HA	1:R:335:GLY:HA2	2.00	0.43
1:W:222:ILE:HG23	1:W:289:LEU:HD22	2.01	0.43
1:W:448:GLU:HB3	1:W:467:LEU:HD21	2.01	0.43
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:H:187:LEU:HD13	1:H:379:LEU:HD23	2.01	0.42
1:L:54:VAL:HG22	1:L:89:THR:HG21	2.00	0.42
1:T:320:ALA:HA	1:T:335:GLY:HA2	2.00	0.42
1:G:33:PRO:HG2	1:G:481:ALA:HB3	2.02	0.42
1:P:443:ILE:O	1:P:447:LEU:HG	2.19	0.42
1:R:409:GLU:OE2	1:R:502:ARG:NH2	2.49	0.42
1:V:211:MET:HE2	1:V:211:MET:HA	2.02	0.42
1:A:102:GLU:O	1:A:106:ASN:ND2	2.48	0.42
1:D:215:LEU:HB3	1:D:218:ALA:HB2	2.00	0.42
1:I:62:LEU:HB2	1:I:68:ASN:HB2	2.01	0.42
1:I:177:VAL:HG13	1:I:381:ILE:HD13	2.00	0.42
1:I:309:LEU:C	1:I:311:ASN:H	2.28	0.42
1:J:36:ARG:HD2	1:K:519:GLU:HG2	2.02	0.42
1:M:30:THR:HB	1:M:51:LYS:O	2.18	0.42
1:a:218:ALA:O	1:a:319:GLN:HA	2.19	0.42
1:a:222:ILE:HG21	1:a:300:VAL:HG22	2.02	0.42
1:H:19:GLY:HA3	1:H:67:GLU:O	2.19	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:O:41:ASP:HB3	1:P:523:THR:HA	2.00	0.42
1:D:171:LYS:HE3	1:D:407:VAL:HG12	2.02	0.42
1:G:158:ILE:HG23	1:G:396:VAL:HG22	2.01	0.42
1:G:476:ASP:HB2	1:G:488:ASN:ND2	2.34	0.42
1:H:43:LYS:HE2	1:H:43:LYS:HB2	1.90	0.42
1:I:213:ALA:HB3	1:I:325:ILE:HB	2.00	0.42
1:J:36:ARG:HB3	1:K:517:THR:O	2.20	0.42
1:N:220:ILE:N	1:N:318:GLY:O	2.42	0.42
1:P:30:THR:HB	1:P:51:LYS:O	2.20	0.42
1:W:420:ILE:HD11	1:W:448:GLU:HA	2.00	0.42
1:X:200:LEU:HB2	1:X:275:ALA:HB3	2.00	0.42
1:B:20:VAL:HG13	1:B:74:VAL:HG21	2.01	0.42
1:B:166:MET:HE1	1:B:407:VAL:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LYS:HD2	1:B:486:TYR:CZ	2.54	0.42
1:H:193:MET:HE3	1:H:371:LYS:HD3	2.01	0.42
1:H:346:ILE:HG23	1:H:369:LEU:HD11	2.01	0.42
1:K:476:ASP:HB2	1:K:488:ASN:ND2	2.35	0.42
1:L:489:LEU:HB3	1:L:494:VAL:HB	2.01	0.42
1:M:443:ILE:O	1:M:447:LEU:HG	2.20	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: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:V:217:GLU:N	1:V:321:ALA:O	2.41	0.42
1:Z:178:GLU:HG3	1:Z:322:ARG:CZ	2.49	0.42
1:E:237:LEU:O	1:E:241:ALA:N	2.53	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:V:73:MET:HE3	1:V:511:VAL:HG23	2.01	0.42
1:W:193:MET:HE3	1:W:371:LYS:HD3	2.02	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:G:443:ILE:O	1:G:447:LEU:HG	2.20	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:Z:64:ASP:HB3	1:Z:67:GLU:HB2	2.02	0.42
1:b:30:THR:HB	1:b:51:LYS:O	2.20	0.42
1:A:520:ALA:HB3	1:G:38:VAL:HG22	2.02	0.42
1:C:82:SER:HA	1:C:85:ALA:HB3	2.01	0.42
1:C:138:ILE:HD12	1:C:406:ALA:HB1	2.02	0.42
1:L:319:GLN:O	1:L:336:LYS:N	2.52	0.42
1:O:15:LYS:NZ	1:O:67:GLU:OE2	2.53	0.42
1:P:136:ARG:NH2	1:P:476:ASP:OD2	2.52	0.42
1:Q:158:ILE:HG23	1:Q:396:VAL:HG22	2.01	0.42
1:R:131:LEU:HD23	1:R:502:ARG:HB3	2.02	0.42
1:U:54:VAL:HG22	1:U:89:THR:HG21	2.02	0.42
1:V:54:VAL:HG22	1:V:89:THR:HG21	2.00	0.42
1:Y:41:ASP:HB2	1:Z:523:THR:HG22	2.01	0.42
1:E:102:GLU:O	1:E:106:ASN:ND2	2.49	0.42
1:E:116:LEU:O	1:E:120:ILE:HG12	2.20	0.42
1:F:179:GLU:HG2	1:F:393:LYS:HD2	2.01	0.42
1:J:320:ALA:HA	1:J:335:GLY:HA2	2.01	0.42
1:L:6:ILE:HG12	1:L:522:ILE:HG12	2.01	0.42
1:M:498:THR:O	1:M:502:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:W:273:VAL:HG22	1:W:274:ALA:H	1.85	0.42
1:a:460:THR:HG22	1:b:112:ARG:HD2	2.02	0.42
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:P:227:ILE:C	1:P:229:ASN:H	2.28	0.41
1:Q:18:VAL:HG12	1:Q:22:LYS:HE2	2.01	0.41
1:R:215:LEU:HB3	1:R:218:ALA:HB2	2.02	0.41
1:V:476:ASP:HB2	1:V:488:ASN:ND2	2.34	0.41
1:a:222:ILE:HG23	1:a:289:LEU:HD22	2.02	0.41
1:A:409:GLU:OE2	1:A:502:ARG:NH2	2.54	0.41
1:C:81:THR:O	1:C:85:ALA:HB2	2.20	0.41
1:F:439:GLY:HA2	1:F:442:ILE:HD12	2.01	0.41
1:M:323:ILE:HD12	1:M:332:ILE:HG12	2.02	0.41
1:X:296:THR:O	1:X:319:GLN:N	2.52	0.41
1:A:171:LYS:O	1:A:404:ARG:NH1	2.53	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:E:230:MET:HE3	1:E:234:LEU:HG	2.01	0.41
1:H:40:ILE:HD13	1:H:59:GLU:HG3	2.02	0.41
1:R:210:THR:HG23	1:R:212:GLU:H	1.85	0.41
1:Y:480:ASN:HD22	1:Y:494:VAL:HG21	1.85	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:N:180:ALA:HB2	1:N:380:LYS:HB3	2.02	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
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:G:141:LYS:HA	1:G:141:LYS:HD3	1.88	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:T:128:VAL:O	1:T:132:ARG:HG2	2.21	0.41
1:V:36:ARG:NH2	1:V:457:ASN:OD1	2.53	0.41
1:V:455:VAL:O	1:V:458:THR:OG1	2.26	0.41
1:Z:497:PRO:HB2	1:Z:500:VAL:HG23	2.02	0.41
1:B:177:VAL:HG13	1:B:381:ILE:HD13	2.01	0.41
1:H:182:GLY:C	1:H:183:MET:HE2	2.45	0.41
1:I:209:GLU:HG2	1:I:210:THR:HG23	2.03	0.41
1:K:177:VAL:HG22	1:K:379:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:GLU:O	1:L:106:ASN:ND2	2.48	0.41
1:R:217:GLU:O	1:R:245:ARG:NH1	2.53	0.41
1:V:320:ALA:HA	1:V:335:GLY:HA2	2.02	0.41
1:W:443:ILE:O	1:W:447:LEU:HG	2.20	0.41
1:A:177:VAL:HG13	1:A:381:ILE:HD13	2.02	0.41
1:C:131:LEU:HD23	1:C:502:ARG:HB3	2.03	0.41
1:J:30:THR:HB	1:J:51:LYS:O	2.21	0.41
1:K:25:ASN:HA	1:K:28:LYS:HE2	2.03	0.41
1:N:138:ILE:HG12	1:N:147:VAL:HG21	2.03	0.41
1:P:25:ASN:HA	1:P:28:LYS:HE2	2.03	0.41
1:Q:185:THR:HG23	1:Q:380:LYS:O	2.21	0.41
1:S:220:ILE:HD11	1:S:323:ILE:HD11	2.03	0.41
1:U:389:MET:HE3	1:U:389:MET:HB3	1.99	0.41
1:X:31:LEU:O	1:X:457:ASN:ND2	2.53	0.41
1:Y:69:MET:HE1	1:Y:521:ALA:HB1	2.03	0.41
1:Y:325:ILE:HG12	1:Y:330:THR:HG23	2.02	0.41
1:a:26:ALA:HB3	1:a:60:ILE:HD11	2.03	0.41
1:B:38:VAL:HG13	1:C:520:ALA:HB3	2.03	0.41
1:C:224:ASP:OD1	1:C:225:LYS:N	2.54	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:K:141:LYS:HE3	1:K:163:ALA:HB1	2.01	0.41
1:L:31:LEU:O	1:L:457:ASN:ND2	2.52	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:T:223:HIS:NE2	1:T:225:LYS:HB2	2.36	0.41
1:U:326:ASP:OD1	1:U:327:LYS:N	2.47	0.41
1:V:302:SER:OG	1:V:303:GLU:N	2.44	0.41
1:W:98:ALA:HB2	1:W:449:GLU:HG3	2.03	0.41
1:X:443:ILE:O	1:X:447:LEU:HG	2.21	0.41
1:b:443:ILE:O	1:b:447:LEU:HG	2.20	0.41
1:A:30:THR:HB	1:A:51:LYS:O	2.20	0.41
1:A:40:ILE:HD13	1:A:59:GLU:HG3	2.02	0.41
1:B:222:ILE:HG22	1:B:300:VAL:HG13	2.03	0.41
1:C:15:LYS:HE3	1:C:15:LYS:HB3	1.94	0.41
1:C:323:ILE:HD12	1:C:332:ILE:HG12	2.02	0.41
1:C:476:ASP:HB2	1:C:488:ASN:HD21	1.85	0.41
1:D:36:ARG:HB3	1:E:517:THR:O	2.21	0.41
1:E:242:GLN:H	1:E:242:GLN:HG2	1.68	0.41
1:H:30:THR:HB	1:H:51:LYS:O	2.19	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:I:325:ILE:HG13	1:I:330:THR:HG23	2.02	0.41
1:I:476:ASP:HB2	1:I:488:ASN:ND2	2.36	0.41
1:J:17:LYS:NZ	1:J:21:ASP:OD2	2.53	0.41
1:K:164:GLU:O	1:K:168:LYS:HG2	2.21	0.41
1:Q:13:ARG:NH1	5:Q:701:HOH:O	2.53	0.41
1:Q:158:ILE:HD12	1:Q:396:VAL:HG22	2.03	0.41
1:Q:325:ILE:HG22	1:Q:330:THR:HG23	2.02	0.41
1:R:224:ASP:H	1:R:301:ILE:HD11	1.84	0.41
1:V:193:MET:HE3	1:V:371:LYS:HD3	2.03	0.41
1:V:205:VAL:HG11	1:V:211:MET:HA	2.02	0.41
1:a:321:ALA:HB3	1:a:334:GLU:HB3	2.03	0.41
1:b:19:GLY:HA3	1:b:67:GLU:O	2.21	0.41
1:A:277:LYS:HG2	1:A:278:ALA:H	1.85	0.41
1:D:30:THR:HB	1:D:51:LYS:O	2.21	0.41
1:F:455:VAL:O	1:F:458:THR:OG1	2.29	0.41
1:J:411:ILE:HD13	1:J:497:PRO:HA	2.03	0.41
1:K:59:GLU:O	1:L:4:LYS:HG3	2.21	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:H:476:ASP:HB2	1:H:488:ASN:ND2	2.36	0.40
1:K:164:GLU:O	1:K:168:LYS:N	2.53	0.40
1:S:510:SER:O	1:S:514:ILE:HG12	2.20	0.40
1:Z:187:LEU:HD13	1:Z:379:LEU:HD23	2.02	0.40
1:D:476:ASP:HB2	1:D:488:ASN:ND2	2.36	0.40
1:I:227:ILE:HG23	1:I:228:SER:N	2.35	0.40
1:J:409:GLU:OE2	1:J:502:ARG:NH2	2.48	0.40
1:L:453:GLN:NE2	1:L:457:ASN:OD1	2.54	0.40
1:N:166:MET:O	1:N:170:GLY:N	2.54	0.40
1:U:253:ASP:OD1	1:U:254:ILE:N	2.49	0.40
1:W:451:LEU:HD11	1:W:470:VAL:HG11	2.03	0.40
1:X:30:THR:HB	1:X:51:LYS:O	2.20	0.40
1:X:197:ARG:HD2	1:X:197:ARG:HA	1.92	0.40
1:A:276:VAL:HG21	1:A:325:ILE:HD12	2.03	0.40
1:C:36:ARG:HD3	1:D:519:GLU:HB2	2.03	0.40
1:D:76:GLU:O	1:D:79:SER:OG	2.34	0.40
1:D:207:ASN:HB2	1:D:209:GLU:OE1	2.22	0.40
1:D:411:ILE:HD13	1:D:497:PRO:HA	2.03	0.40
1:E:46:ALA:HB2	1:F:76:GLU:HG3	2.02	0.40
1:E:480:ASN:OD1	1:E:482:ARG:HG2	2.21	0.40
1:I:220:ILE:HG13	1:I:296:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:THR:HB	1:K:51:LYS:O	2.22	0.40
1:N:66:VAL:HA	1:N:69:MET:HE2	2.02	0.40
1:T:15:LYS:NZ	1:T:67:GLU:OE2	2.54	0.40
1:V:409:GLU:OE2	1:V:502:ARG:NH2	2.52	0.40
1:b:388:GLU:HA	1:b:391:GLU:HG2	2.04	0.40
1:E:36:ARG:HB3	1:F:517:THR:O	2.20	0.40
1:J:98:ALA:HB2	1:J:449:GLU:HG3	2.03	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:K:443:ILE:O	1:K:447:LEU:HG	2.21	0.40
1:L:192:GLY:H	1:L:375:GLY:HA2	1.86	0.40
1:O:166:MET:HE2	1:O:171:LYS:HA	2.03	0.40
1:S:59:GLU:O	1:T:4:LYS:HG3	2.20	0.40
1:T:83:ASP:OD1	1:T:84:VAL:N	2.49	0.40
1:U:30:THR:HB	1:U:51:LYS:O	2.21	0.40
1:V:158:ILE:HD12	1:V:396:VAL:HG22	2.03	0.40
1:a:116:LEU:O	1:a:120:ILE:HG12	2.21	0.40
1:B:230:MET:HE3	1:B:261:THR:HB	2.03	0.40
1:F:77:VAL:HG12	1:F:507:ASN:HB3	2.04	0.40
1:F:197:ARG:HB3	1:F:277:LYS:HB2	2.03	0.40
1:I:36:ARG:HB3	1:J:517:THR:O	2.22	0.40
1:J:247:LEU:HB3	1:J:273:VAL:HG12	2.02	0.40
1:M:321:ALA:HB3	1:M:334:GLU:HB2	2.04	0.40
1:Z:161:LEU:HG	1:Z:379:LEU:HD22	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	30	65
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%)	43	76
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

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

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	360/427 (84%)	359 (100%)	1 (0%)	86	91
1	B	358/427 (84%)	358 (100%)	0	100	100
1	C	310/427 (73%)	308 (99%)	2 (1%)	78	88
1	D	367/427 (86%)	367 (100%)	0	100	100
1	E	353/427 (83%)	352 (100%)	1 (0%)	86	91
1	F	347/427 (81%)	346 (100%)	1 (0%)	86	91
1	G	331/427 (78%)	331 (100%)	0	100	100
1	H	381/427 (89%)	381 (100%)	0	100	100
1	I	369/427 (86%)	368 (100%)	1 (0%)	86	91
1	J	328/427 (77%)	326 (99%)	2 (1%)	78	88
1	K	266/427 (62%)	264 (99%)	2 (1%)	73	86
1	L	299/427 (70%)	298 (100%)	1 (0%)	86	91
1	M	307/427 (72%)	306 (100%)	1 (0%)	86	91
1	N	343/427 (80%)	343 (100%)	0	100	100
1	O	324/427 (76%)	323 (100%)	1 (0%)	86	91
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%)	345 (99%)	2 (1%)	78	88
1	S	362/427 (85%)	360 (99%)	2 (1%)	78	88
1	T	332/427 (78%)	332 (100%)	0	100	100
1	U	366/427 (86%)	363 (99%)	3 (1%)	73	86
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%)	347 (100%)	1 (0%)	86	91
1	X	340/427 (80%)	340 (100%)	0	100	100
1	Y	362/427 (85%)	361 (100%)	1 (0%)	86	91
1	Z	359/427 (84%)	358 (100%)	1 (0%)	86	91
1	a	368/427 (86%)	367 (100%)	1 (0%)	86	91
1	b	279/427 (65%)	278 (100%)	1 (0%)	84	90
All	All	9578/11956 (80%)	9553 (100%)	25 (0%)	86	91

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	VAL
1	C	169	VAL
1	C	495	VAL
1	E	169	VAL
1	F	169	VAL
1	I	443	ILE
1	J	76	GLU
1	J	183	MET
1	K	169	VAL
1	K	461	THR
1	L	323	ILE
1	M	169	VAL
1	O	443	ILE
1	R	36	ARG
1	R	301	ILE
1	S	271	LEU
1	S	476	ASP
1	U	50	THR
1	U	227	ILE
1	U	259	LEU
1	W	476	ASP
1	Y	189	VAL
1	Z	220	ILE
1	a	264	VAL
1	b	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	194	GLN
1	B	72	GLN
1	B	194	GLN
1	C	223	HIS
1	D	153	ASN
1	D	194	GLN
1	F	223	HIS
1	H	37	ASN
1	H	311	ASN
1	H	507	ASN
1	J	207	ASN
1	K	347	ASN
1	K	488	ASN
1	M	153	ASN
1	O	488	ASN
1	P	311	ASN
1	Q	37	ASN
1	Q	194	GLN
1	R	153	ASN
1	R	408	GLN
1	T	72	GLN
1	U	194	GLN
1	U	319	GLN
1	V	408	GLN
1	W	68	ASN
1	W	72	GLN
1	W	194	GLN
1	X	329	ASN
1	Y	194	GLN
1	a	265	ASN
1	b	401	HIS

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 [i](#)

There are no oligosaccharides 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	T	602	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	M	602	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	N	601	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	V	602	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	G	601	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	R	602	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	601	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	L	601	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	P	601	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	b	601	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	B	601	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	K	601	-	4,4,4	0.22	0	6,6,6	0.07	0
2	SO4	Z	601	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	J	601	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	E	601	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	D	601	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	a	601	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	Y	601	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	U	601	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	F	601	-	4,4,4	0.25	0	6,6,6	0.05	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	R	602	SO4	1	0
2	b	601	SO4	1	0
2	F	601	SO4	1	0

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	499/545 (91%)	0.32	20 (4%) 42 23	18, 51, 104, 115	0
1	B	519/545 (95%)	0.23	32 (6%) 26 14	14, 44, 104, 121	0
1	C	478/545 (87%)	0.38	38 (7%) 18 10	18, 52, 103, 127	0
1	D	517/545 (94%)	0.35	26 (5%) 34 18	18, 58, 110, 129	0
1	E	509/545 (93%)	0.44	35 (6%) 23 12	20, 66, 110, 123	0
1	F	497/545 (91%)	0.34	24 (4%) 35 19	16, 46, 102, 122	0
1	G	499/545 (91%)	0.51	40 (8%) 18 9	19, 59, 113, 125	0
1	H	515/545 (94%)	0.27	10 (1%) 66 43	18, 60, 102, 111	0
1	I	512/545 (93%)	0.16	18 (3%) 47 27	17, 52, 97, 116	0
1	J	507/545 (93%)	0.46	36 (7%) 22 11	18, 63, 116, 133	0
1	K	433/545 (79%)	0.48	40 (9%) 14 8	20, 54, 121, 138	0
1	L	484/545 (88%)	0.56	52 (10%) 11 6	21, 53, 125, 136	0
1	M	463/545 (84%)	0.40	25 (5%) 31 16	24, 55, 108, 129	0
1	N	511/545 (93%)	0.54	38 (7%) 20 10	21, 65, 112, 128	0
1	O	492/545 (90%)	0.42	44 (8%) 15 8	20, 50, 122, 132	0
1	P	522/545 (95%)	0.11	8 (1%) 72 49	15, 49, 92, 116	0
1	Q	502/545 (92%)	0.22	24 (4%) 35 19	11, 44, 110, 134	0
1	R	502/545 (92%)	0.23	40 (7%) 18 9	11, 37, 106, 125	0
1	S	512/545 (93%)	0.26	15 (2%) 53 31	15, 61, 100, 118	0
1	T	497/545 (91%)	0.41	19 (3%) 44 24	23, 62, 98, 111	0
1	U	518/545 (95%)	0.50	24 (4%) 37 20	24, 74, 106, 124	0
1	V	500/545 (91%)	0.44	44 (8%) 15 8	15, 49, 119, 139	0
1	W	517/545 (94%)	0.42	48 (9%) 14 7	14, 55, 119, 127	0
1	X	504/545 (92%)	0.50	42 (8%) 17 9	15, 61, 124, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	512/545 (93%)	0.39	33 (6%) 25 13	21, 58, 110, 139	0
1	Z	518/545 (95%)	0.55	33 (6%) 25 13	25, 75, 113, 124	0
1	a	522/545 (95%)	0.61	30 (5%) 29 15	27, 74, 111, 126	0
1	b	423/545 (77%)	0.43	29 (6%) 23 12	19, 49, 119, 136	0
All	All	13984/15260 (91%)	0.39	867 (6%) 26 14	11, 56, 113, 144	0

All (867) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	335	GLY	5.1
1	F	253	ASP	4.9
1	G	376	VAL	4.7
1	N	253	ASP	4.7
1	O	278	ALA	4.6
1	T	281	PHE	4.6
1	Y	270	THR	4.6
1	a	384	SER	4.5
1	O	309	LEU	4.5
1	O	83	ASP	4.4
1	a	85	ALA	4.4
1	L	194	GLN	4.4
1	F	307	TYR	4.4
1	L	285	ARG	4.3
1	R	251	ALA	4.3
1	V	293	ALA	4.2
1	L	85	ALA	4.1
1	J	309	LEU	4.1
1	R	293	ALA	4.1
1	R	253	ASP	4.1
1	S	83	ASP	4.1
1	Z	381	ILE	4.1
1	X	278	ALA	4.1
1	X	233	LEU	4.1
1	Y	251	ALA	4.0
1	R	273	VAL	4.0
1	J	83	ASP	4.0
1	T	258	ALA	4.0
1	C	219	LEU	4.0
1	E	236	ILE	3.9
1	L	288	MET	3.9
1	M	278	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	Z	85	ALA	3.9
1	A	291	ASP	3.9
1	F	226	LYS	3.9
1	K	84	VAL	3.8
1	F	224	ASP	3.8
1	N	313	THR	3.8
1	J	82	SER	3.8
1	W	198	GLY	3.8
1	D	243	SER	3.8
1	V	346	ILE	3.8
1	X	373	SER	3.7
1	T	196	ASP	3.7
1	E	374	GLY	3.7
1	T	310	GLU	3.7
1	G	319	GLN	3.7
1	Y	358	SER	3.7
1	F	275	ALA	3.7
1	A	253	ASP	3.7
1	O	235	PRO	3.7
1	E	359	ASP	3.7
1	V	260	ALA	3.7
1	Q	309	LEU	3.7
1	U	87	ASP	3.6
1	I	82	SER	3.6
1	a	281	PHE	3.6
1	Q	260	ALA	3.6
1	R	228	SER	3.6
1	W	195	PHE	3.5
1	C	297	GLY	3.5
1	R	347	ASN	3.5
1	V	259	LEU	3.5
1	Z	360	TYR	3.5
1	E	358	SER	3.5
1	N	223	HIS	3.5
1	B	253	ASP	3.5
1	K	85	ALA	3.5
1	H	309	LEU	3.5
1	O	87	ASP	3.5
1	X	359	ASP	3.5
1	S	228	SER	3.5
1	U	254	ILE	3.5
1	V	389	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	b	220	ILE	3.4
1	Y	210	THR	3.4
1	L	220	ILE	3.4
1	N	222	ILE	3.4
1	R	361	ASP	3.4
1	L	290	GLU	3.4
1	W	200	LEU	3.4
1	W	309	LEU	3.4
1	U	243	SER	3.4
1	L	204	PHE	3.4
1	Z	203	TYR	3.4
1	A	302	SER	3.4
1	U	384	SER	3.4
1	G	363	GLU	3.4
1	D	294	ILE	3.4
1	M	359	ASP	3.3
1	G	269	GLY	3.3
1	a	349	ILE	3.3
1	A	309	LEU	3.3
1	X	237	LEU	3.3
1	a	84	VAL	3.3
1	W	361	ASP	3.3
1	b	87	ASP	3.3
1	Y	309	LEU	3.3
1	Z	211	MET	3.3
1	D	291	ASP	3.3
1	a	341	GLU	3.3
1	a	383	ALA	3.3
1	N	276	VAL	3.3
1	I	229	ASN	3.3
1	U	359	ASP	3.2
1	E	232	GLU	3.2
1	b	414	GLY	3.2
1	I	228	SER	3.2
1	W	271	LEU	3.2
1	J	213	ALA	3.2
1	E	361	ASP	3.2
1	L	328	ASP	3.2
1	K	325	ILE	3.2
1	X	222	ILE	3.2
1	S	293	ALA	3.2
1	V	320	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	a	364	LYS	3.2
1	C	223	HIS	3.2
1	L	228	SER	3.2
1	E	332	ILE	3.2
1	N	326	ASP	3.2
1	R	275	ALA	3.2
1	T	85	ALA	3.2
1	V	233	LEU	3.2
1	Y	232	GLU	3.2
1	b	347	ASN	3.2
1	L	223	HIS	3.2
1	V	294	ILE	3.2
1	C	365	LEU	3.1
1	J	247	LEU	3.1
1	G	294	ILE	3.1
1	A	278	ALA	3.1
1	Y	180	ALA	3.1
1	N	291	ASP	3.1
1	L	301	ILE	3.1
1	U	275	ALA	3.1
1	L	201	SER	3.1
1	L	374	GLY	3.1
1	U	240	ALA	3.1
1	F	268	ARG	3.1
1	S	235	PRO	3.1
1	b	349	ILE	3.1
1	K	339	GLN	3.1
1	N	259	LEU	3.1
1	Q	242	GLN	3.1
1	Q	282	GLY	3.1
1	D	273	VAL	3.1
1	Q	228	SER	3.1
1	E	349	ILE	3.1
1	J	272	LYS	3.0
1	A	209	GLU	3.0
1	V	230	MET	3.0
1	K	278	ALA	3.0
1	N	312	ALA	3.0
1	W	260	ALA	3.0
1	Z	84	VAL	3.0
1	a	378	VAL	3.0
1	G	209	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	R	294	ILE	3.0
1	W	227	ILE	3.0
1	Y	235	PRO	3.0
1	C	291	ASP	3.0
1	O	196	ASP	3.0
1	b	309	LEU	3.0
1	K	180	ALA	3.0
1	F	223	HIS	3.0
1	J	231	LYS	3.0
1	E	257	GLU	3.0
1	L	250	ILE	3.0
1	V	214	GLU	3.0
1	C	243	SER	3.0
1	W	203	TYR	3.0
1	L	291	ASP	3.0
1	L	88	GLY	3.0
1	R	299	THR	3.0
1	Y	261	THR	3.0
1	M	367	GLU	3.0
1	B	312	ALA	3.0
1	I	243	SER	3.0
1	A	360	TYR	3.0
1	H	181	LYS	3.0
1	Q	253	ASP	3.0
1	V	359	ASP	3.0
1	G	313	THR	3.0
1	T	247	LEU	2.9
1	E	223	HIS	2.9
1	W	276	VAL	2.9
1	K	342	ILE	2.9
1	R	236	ILE	2.9
1	A	207	ASN	2.9
1	Q	197	ARG	2.9
1	A	84	VAL	2.9
1	Q	254	ILE	2.9
1	K	185	THR	2.9
1	W	277	LYS	2.9
1	D	238	GLU	2.9
1	G	218	ALA	2.9
1	X	204	PHE	2.9
1	B	229	ASN	2.9
1	Q	279	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	291	ASP	2.9
1	a	83	ASP	2.9
1	B	257	GLU	2.9
1	L	212	GLU	2.9
1	O	193	MET	2.9
1	Y	295	LEU	2.9
1	a	346	ILE	2.9
1	L	303	GLU	2.8
1	L	341	GLU	2.8
1	N	363	GLU	2.8
1	B	198	GLY	2.8
1	J	200	LEU	2.8
1	L	200	LEU	2.8
1	L	262	LEU	2.8
1	N	281	PHE	2.8
1	N	349	ILE	2.8
1	V	292	ILE	2.8
1	W	302	SER	2.8
1	C	278	ALA	2.8
1	L	274	ALA	2.8
1	N	362	THR	2.8
1	Q	83	ASP	2.8
1	W	308	LYS	2.8
1	R	222	ILE	2.8
1	V	349	ILE	2.8
1	X	228	SER	2.8
1	b	178	GLU	2.8
1	O	233	LEU	2.8
1	Y	237	LEU	2.8
1	A	236	ILE	2.8
1	O	292	ILE	2.8
1	W	306	GLY	2.8
1	W	278	ALA	2.8
1	Y	168	LYS	2.8
1	A	219	LEU	2.8
1	O	221	LEU	2.8
1	V	261	THR	2.8
1	J	288	MET	2.8
1	N	227	ILE	2.8
1	V	326	ASP	2.8
1	W	224	ASP	2.8
1	Y	182	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	W	229	ASN	2.8
1	V	189	VAL	2.8
1	J	369	LEU	2.8
1	K	219	LEU	2.8
1	K	372	LEU	2.8
1	M	250	ILE	2.8
1	M	301	ILE	2.8
1	Y	381	ILE	2.8
1	S	182	GLY	2.7
1	J	258	ALA	2.7
1	L	260	ALA	2.7
1	V	84	VAL	2.7
1	D	233	LEU	2.7
1	G	219	LEU	2.7
1	K	183	MET	2.7
1	N	230	MET	2.7
1	V	354	GLU	2.7
1	b	290	GLU	2.7
1	G	256	GLY	2.7
1	b	83	ASP	2.7
1	N	316	TYR	2.7
1	V	203	TYR	2.7
1	V	347	ASN	2.7
1	B	218	ALA	2.7
1	E	241	ALA	2.7
1	E	278	ALA	2.7
1	A	235	PRO	2.7
1	W	279	PRO	2.7
1	J	227	ILE	2.7
1	N	354	GLU	2.7
1	G	296	THR	2.7
1	I	361	ASP	2.7
1	M	224	ASP	2.7
1	L	203	TYR	2.7
1	F	251	ALA	2.7
1	M	85	ALA	2.7
1	R	227	ILE	2.7
1	Z	337	GLY	2.7
1	a	232	GLU	2.7
1	B	308	LYS	2.7
1	K	362	THR	2.7
1	L	278	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	Q	271	LEU	2.7
1	Z	387	VAL	2.7
1	R	265	ASN	2.7
1	S	311	ASN	2.7
1	N	294	ILE	2.7
1	O	239	LYS	2.7
1	P	255	GLU	2.7
1	S	257	GLU	2.7
1	T	182	GLY	2.7
1	X	282	GLY	2.7
1	E	362	THR	2.7
1	B	258	ALA	2.7
1	K	376	VAL	2.7
1	K	378	VAL	2.7
1	R	237	LEU	2.7
1	V	267	LEU	2.7
1	b	237	LEU	2.7
1	B	361	ASP	2.7
1	C	250	ILE	2.6
1	W	314	MET	2.6
1	D	232	GLU	2.6
1	G	375	GLY	2.6
1	Z	354	GLU	2.6
1	D	356	SER	2.6
1	J	248	LEU	2.6
1	N	365	LEU	2.6
1	X	169	VAL	2.6
1	M	83	ASP	2.6
1	V	291	ASP	2.6
1	D	230	MET	2.6
1	H	182	GLY	2.6
1	Y	238	GLU	2.6
1	N	84	VAL	2.6
1	R	219	LEU	2.6
1	O	373	SER	2.6
1	U	316	TYR	2.6
1	X	381	ILE	2.6
1	Y	236	ILE	2.6
1	B	232	GLU	2.6
1	X	184	GLU	2.6
1	Z	232	GLU	2.6
1	O	234	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	W	259	LEU	2.6
1	C	251	ALA	2.6
1	V	251	ALA	2.6
1	G	285	ARG	2.6
1	R	360	TYR	2.6
1	U	279	PRO	2.6
1	U	281	PHE	2.6
1	A	335	GLY	2.6
1	D	310	GLU	2.6
1	C	284	ARG	2.6
1	A	220	ILE	2.6
1	J	294	ILE	2.6
1	Y	230	MET	2.6
1	V	302	SER	2.6
1	C	311	ASN	2.6
1	F	229	ASN	2.6
1	R	341	GLU	2.6
1	N	293	ALA	2.6
1	O	293	ALA	2.6
1	C	299	THR	2.6
1	M	325	ILE	2.5
1	R	349	ILE	2.5
1	V	254	ILE	2.5
1	W	250	ILE	2.5
1	B	223	HIS	2.5
1	O	203	TYR	2.5
1	W	337	GLY	2.5
1	G	365	LEU	2.5
1	J	365	LEU	2.5
1	I	268	ARG	2.5
1	N	283	ASP	2.5
1	T	184	GLU	2.5
1	V	168	LYS	2.5
1	Z	311	ASN	2.5
1	K	320	ALA	2.5
1	D	270	THR	2.5
1	L	332	ILE	2.5
1	P	307	TYR	2.5
1	a	360	TYR	2.5
1	F	228	SER	2.5
1	G	369	LEU	2.5
1	X	181	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	300	VAL	2.5
1	F	340	GLU	2.5
1	R	87	ASP	2.5
1	R	232	GLU	2.5
1	U	311	ASN	2.5
1	X	386	GLU	2.5
1	Y	265	ASN	2.5
1	a	361	ASP	2.5
1	K	323	ILE	2.5
1	X	299	THR	2.5
1	Z	314	MET	2.5
1	K	199	TYR	2.5
1	L	360	TYR	2.5
1	F	271	LEU	2.5
1	L	355	LYS	2.5
1	R	286	LYS	2.5
1	X	242	GLN	2.5
1	J	276	VAL	2.5
1	F	240	ALA	2.5
1	G	320	ALA	2.5
1	b	348	GLU	2.5
1	F	291	ASP	2.5
1	T	224	ASP	2.5
1	Y	254	ILE	2.5
1	C	324	THR	2.5
1	G	204	PHE	2.5
1	E	226	LYS	2.5
1	K	364	LYS	2.5
1	V	289	LEU	2.5
1	C	273	VAL	2.5
1	B	251	ALA	2.5
1	C	201	SER	2.5
1	R	315	ALA	2.5
1	Y	240	ALA	2.5
1	D	236	ILE	2.5
1	J	363	GLU	2.5
1	K	184	GLU	2.5
1	D	311	ASN	2.5
1	K	83	ASP	2.5
1	H	313	THR	2.5
1	J	271	LEU	2.5
1	O	271	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	X	271	LEU	2.5
1	X	295	LEU	2.5
1	Y	233	LEU	2.5
1	C	360	TYR	2.5
1	L	205	VAL	2.5
1	A	242	GLN	2.5
1	X	319	GLN	2.5
1	K	275	ALA	2.4
1	B	228	SER	2.4
1	L	334	GLU	2.4
1	W	252	GLU	2.4
1	Z	310	GLU	2.4
1	G	284	ARG	2.4
1	O	237	LEU	2.4
1	T	331	THR	2.4
1	Y	283	ASP	2.4
1	D	271	LEU	2.4
1	O	223	HIS	2.4
1	R	316	TYR	2.4
1	B	300	VAL	2.4
1	O	88	GLY	2.4
1	T	273	VAL	2.4
1	W	335	GLY	2.4
1	U	242	GLN	2.4
1	V	85	ALA	2.4
1	I	227	ILE	2.4
1	X	301	ILE	2.4
1	O	82	SER	2.4
1	S	243	SER	2.4
1	R	281	PHE	2.4
1	M	345	ARG	2.4
1	Z	355	LYS	2.4
1	M	229	ASN	2.4
1	O	347	ASN	2.4
1	Q	299	THR	2.4
1	X	253	ASP	2.4
1	K	335	GLY	2.4
1	V	88	GLY	2.4
1	N	241	ALA	2.4
1	O	294	ILE	2.4
1	R	301	ILE	2.4
1	X	251	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	b	85	ALA	2.4
1	D	305	LYS	2.4
1	b	184	GLU	2.4
1	J	243	SER	2.4
1	C	221	LEU	2.4
1	D	309	LEU	2.4
1	L	259	LEU	2.4
1	T	259	LEU	2.4
1	B	270	THR	2.4
1	M	154	ASN	2.4
1	E	291	ASP	2.4
1	I	83	ASP	2.4
1	M	177	VAL	2.4
1	M	326	ASP	2.4
1	B	307	TYR	2.4
1	O	360	TYR	2.4
1	K	163	ALA	2.4
1	a	353	ILE	2.4
1	K	288	MET	2.4
1	Y	314	MET	2.4
1	C	285	ARG	2.4
1	O	289	LEU	2.4
1	U	309	LEU	2.4
1	a	267	LEU	2.4
1	S	333	VAL	2.4
1	a	235	PRO	2.4
1	E	196	ASP	2.4
1	G	328	ASP	2.4
1	H	359	ASP	2.4
1	V	374	GLY	2.4
1	G	85	ALA	2.4
1	U	227	ILE	2.4
1	W	251	ALA	2.4
1	X	220	ILE	2.4
1	X	342	ILE	2.4
1	N	319	GLN	2.4
1	W	319	GLN	2.4
1	G	247	LEU	2.4
1	J	221	LEU	2.4
1	R	317	LEU	2.4
1	Y	252	GLU	2.4
1	Z	255	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	182	GLY	2.3
1	b	324	THR	2.3
1	F	249	ILE	2.3
1	C	361	ASP	2.3
1	D	83	ASP	2.3
1	G	253	ASP	2.3
1	N	360	TYR	2.3
1	O	346	ILE	2.3
1	V	328	ASP	2.3
1	C	319	GLN	2.3
1	Q	281	PHE	2.3
1	V	295	LEU	2.3
1	B	246	PRO	2.3
1	E	356	SER	2.3
1	S	279	PRO	2.3
1	D	268	ARG	2.3
1	N	458	THR	2.3
1	P	176	THR	2.3
1	Q	277	LYS	2.3
1	b	88	GLY	2.3
1	E	85	ALA	2.3
1	G	353	ILE	2.3
1	W	294	ILE	2.3
1	W	301	ILE	2.3
1	E	224	ASP	2.3
1	E	326	ASP	2.3
1	W	359	ASP	2.3
1	Q	200	LEU	2.3
1	a	131	LEU	2.3
1	a	271	LEU	2.3
1	R	242	GLN	2.3
1	D	184	GLU	2.3
1	N	257	GLU	2.3
1	O	354	GLU	2.3
1	W	255	GLU	2.3
1	H	231	LYS	2.3
1	C	325	ILE	2.3
1	D	337	GLY	2.3
1	L	213	ALA	2.3
1	N	228	SER	2.3
1	b	86	GLY	2.3
1	a	240	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	223	HIS	2.3
1	B	309	LEU	2.3
1	N	234	LEU	2.3
1	X	200	LEU	2.3
1	S	303	GLU	2.3
1	O	345	ARG	2.3
1	B	236	ILE	2.3
1	C	282	GLY	2.3
1	G	220	ILE	2.3
1	O	342	ILE	2.3
1	C	275	ALA	2.3
1	D	312	ALA	2.3
1	O	258	ALA	2.3
1	R	218	ALA	2.3
1	X	275	ALA	2.3
1	U	185	THR	2.3
1	U	330	THR	2.3
1	Y	324	THR	2.3
1	W	295	LEU	2.3
1	K	204	PHE	2.3
1	V	265	ASN	2.3
1	Z	229	ASN	2.3
1	C	224	ASP	2.3
1	a	283	ASP	2.3
1	G	264	VAL	2.3
1	G	268	ARG	2.3
1	I	84	VAL	2.3
1	J	212	GLU	2.3
1	J	284	ARG	2.3
1	K	197	ARG	2.3
1	L	178	GLU	2.3
1	L	300	VAL	2.3
1	N	300	VAL	2.3
1	O	238	GLU	2.3
1	S	178	GLU	2.3
1	a	264	VAL	2.3
1	Z	342	ILE	2.3
1	B	182	GLY	2.3
1	V	193	MET	2.3
1	Z	288	MET	2.3
1	A	270	THR	2.3
1	J	262	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	319	GLN	2.3
1	J	242	GLN	2.3
1	R	345	ARG	2.3
1	Q	361	ASP	2.3
1	W	273	VAL	2.3
1	Q	294	ILE	2.2
1	X	292	ILE	2.2
1	Y	222	ILE	2.2
1	a	236	ILE	2.2
1	L	246	PRO	2.2
1	E	230	MET	2.2
1	F	183	MET	2.2
1	H	183	MET	2.2
1	O	344	ALA	2.2
1	W	315	ALA	2.2
1	Z	240	ALA	2.2
1	b	218	ALA	2.2
1	O	248	LEU	2.2
1	B	243	SER	2.2
1	G	231	LYS	2.2
1	M	82	SER	2.2
1	b	366	GLN	2.2
1	C	217	GLU	2.2
1	K	160	GLU	2.2
1	K	214	GLU	2.2
1	L	354	GLU	2.2
1	M	179	GLU	2.2
1	P	304	GLU	2.2
1	U	61	GLU	2.2
1	b	341	GLU	2.2
1	F	294	ILE	2.2
1	K	220	ILE	2.2
1	C	85	ALA	2.2
1	J	215	LEU	2.2
1	L	275	ALA	2.2
1	W	244	GLY	2.2
1	Z	215	LEU	2.2
1	C	204	PHE	2.2
1	I	204	PHE	2.2
1	T	364	LYS	2.2
1	X	273	VAL	2.2
1	L	352	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	339	GLN	2.2
1	V	339	GLN	2.2
1	B	311	ASN	2.2
1	K	207	ASN	2.2
1	T	265	ASN	2.2
1	J	232	GLU	2.2
1	M	310	GLU	2.2
1	N	301	ILE	2.2
1	P	303	GLU	2.2
1	R	252	GLU	2.2
1	X	257	GLU	2.2
1	L	224	ASP	2.2
1	E	382	GLY	2.2
1	M	88	GLY	2.2
1	M	344	ALA	2.2
1	O	166	MET	2.2
1	V	361	ASP	2.2
1	W	370	ALA	2.2
1	Z	183	MET	2.2
1	a	183	MET	2.2
1	D	338	LYS	2.2
1	M	350	LYS	2.2
1	M	285	ARG	2.2
1	A	300	VAL	2.2
1	E	273	VAL	2.2
1	C	384	SER	2.2
1	W	228	SER	2.2
1	b	208	SER	2.2
1	N	242	GLN	2.2
1	T	325	ILE	2.2
1	D	255	GLU	2.2
1	F	191	GLU	2.2
1	I	255	GLU	2.2
1	M	441	GLU	2.2
1	P	229	ASN	2.2
1	N	314	MET	2.2
1	T	279	PRO	2.2
1	b	335	GLY	2.2
1	C	327	LYS	2.2
1	L	277	LYS	2.2
1	O	291	ASP	2.2
1	C	401	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	276	VAL	2.2
1	G	228	SER	2.2
1	R	319	GLN	2.2
1	W	254	ILE	2.2
1	Z	301	ILE	2.2
1	b	353	ILE	2.2
1	R	295	LEU	2.2
1	B	310	GLU	2.2
1	I	311	ASN	2.2
1	U	241	ALA	2.2
1	W	85	ALA	2.2
1	a	363	GLU	2.2
1	a	386	GLU	2.2
1	I	244	GLY	2.2
1	R	170	GLY	2.2
1	W	196	ASP	2.2
1	Z	87	ASP	2.2
1	J	261	THR	2.1
1	Q	84	VAL	2.1
1	X	300	VAL	2.1
1	a	301	ILE	2.1
1	D	267	LEU	2.1
1	E	193	MET	2.1
1	M	230	MET	2.1
1	N	327	LYS	2.1
1	E	354	GLU	2.1
1	F	310	GLU	2.1
1	L	251	ALA	2.1
1	L	383	ALA	2.1
1	Q	208	SER	2.1
1	O	232	GLU	2.1
1	O	252	GLU	2.1
1	K	382	GLY	2.1
1	S	244	GLY	2.1
1	P	207	ASN	2.1
1	D	283	ASP	2.1
1	E	87	ASP	2.1
1	J	361	ASP	2.1
1	O	283	ASP	2.1
1	V	83	ASP	2.1
1	G	455	VAL	2.1
1	J	273	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	362	THR	2.1
1	I	331	THR	2.1
1	R	296	THR	2.1
1	W	210	THR	2.1
1	W	362	THR	2.1
1	E	353	ILE	2.1
1	G	332	ILE	2.1
1	J	203	TYR	2.1
1	J	307	TYR	2.1
1	M	222	ILE	2.1
1	O	227	ILE	2.1
1	X	332	ILE	2.1
1	C	308	LYS	2.1
1	F	308	LYS	2.1
1	G	272	LYS	2.1
1	S	309	LEU	2.1
1	V	200	LEU	2.1
1	V	237	LEU	2.1
1	Q	183	MET	2.1
1	Q	211	MET	2.1
1	U	314	MET	2.1
1	C	245	ARG	2.1
1	I	312	ALA	2.1
1	W	320	ALA	2.1
1	A	228	SER	2.1
1	B	217	GLU	2.1
1	D	182	GLY	2.1
1	G	217	GLU	2.1
1	J	279	PRO	2.1
1	J	474	GLU	2.1
1	K	86	GLY	2.1
1	K	373	SER	2.1
1	U	139	SER	2.1
1	X	208	SER	2.1
1	X	290	GLU	2.1
1	G	216	ASP	2.1
1	G	276	VAL	2.1
1	N	224	ASP	2.1
1	B	222	ILE	2.1
1	G	206	THR	2.1
1	J	210	THR	2.1
1	L	206	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	294	ILE	2.1
1	Q	355	LYS	2.1
1	U	270	THR	2.1
1	U	349	ILE	2.1
1	Y	234	LEU	2.1
1	R	240	ALA	2.1
1	a	352	GLN	2.1
1	G	281	PHE	2.1
1	K	82	SER	2.1
1	K	228	SER	2.1
1	G	333	VAL	2.1
1	C	87	ASP	2.1
1	W	272	LYS	2.1
1	W	267	LEU	2.1
1	Y	155	ASP	2.1
1	Y	181	LYS	2.1
1	E	221	LEU	2.1
1	H	301	ILE	2.1
1	P	200	LEU	2.1
1	Z	227	ILE	2.1
1	N	368	ARG	2.1
1	A	211	MET	2.1
1	R	282	GLY	2.1
1	T	244	GLY	2.1
1	X	256	GLY	2.1
1	a	256	GLY	2.1
1	N	279	PRO	2.1
1	T	179	GLU	2.1
1	W	354	GLU	2.1
1	b	82	SER	2.1
1	F	264	VAL	2.1
1	K	190	VAL	2.1
1	B	265	ASN	2.1
1	B	292	ILE	2.1
1	B	365	LEU	2.1
1	K	368	ARG	2.1
1	O	365	LEU	2.1
1	X	309	LEU	2.1
1	b	289	LEU	2.1
1	b	294	ILE	2.1
1	B	299	THR	2.1
1	W	307	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	Z	81	THR	2.1
1	L	320	ALA	2.1
1	Q	241	ALA	2.1
1	Y	241	ALA	2.1
1	L	198	GLY	2.1
1	Z	88	GLY	2.1
1	B	303	GLU	2.1
1	G	235	PRO	2.1
1	I	61	GLU	2.1
1	L	214	GLU	2.1
1	N	44	PHE	2.1
1	V	204	PHE	2.1
1	I	308	LYS	2.0
1	K	205	VAL	2.0
1	B	200	LEU	2.0
1	E	259	LEU	2.0
1	F	219	LEU	2.0
1	K	227	ILE	2.0
1	L	207	ASN	2.0
1	O	285	ARG	2.0
1	V	329	ASN	2.0
1	Y	301	ILE	2.0
1	Z	353	ILE	2.0
1	X	223	HIS	2.0
1	E	83	ASP	2.0
1	I	253	ASP	2.0
1	M	330	THR	2.0
1	U	258	ALA	2.0
1	W	316	TYR	2.0
1	X	83	ASP	2.0
1	Z	383	ALA	2.0
1	Z	398	ASP	2.0
1	b	328	ASP	2.0
1	V	198	GLY	2.0
1	V	282	GLY	2.0
1	B	272	LYS	2.0
1	C	252	GLU	2.0
1	C	336	LYS	2.0
1	G	226	LYS	2.0
1	R	338	LYS	2.0
1	W	304	GLU	2.0
1	X	272	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	X	371	LYS	2.0
1	Y	272	LYS	2.0
1	Z	61	GLU	2.0
1	b	367	GLU	2.0
1	b	84	VAL	2.0
1	L	345	ARG	2.0
1	O	259	LEU	2.0
1	X	197	ARG	2.0
1	X	221	LEU	2.0
1	Z	295	LEU	2.0
1	J	254	ILE	2.0
1	L	222	ILE	2.0
1	Q	346	ILE	2.0
1	R	342	ILE	2.0
1	S	381	ILE	2.0
1	a	292	ILE	2.0
1	E	288	MET	2.0
1	G	329	ASN	2.0
1	E	206	THR	2.0
1	F	241	ALA	2.0
1	T	330	THR	2.0
1	U	312	ALA	2.0
1	Z	241	ALA	2.0
1	C	462	ASP	2.0
1	K	224	ASP	2.0
1	L	326	ASP	2.0
1	Y	392	LYS	2.0
1	A	290	GLU	2.0
1	C	157	GLU	2.0
1	E	367	GLU	2.0
1	F	248	LEU	2.0
1	Z	372	LEU	2.0
1	b	365	LEU	2.0
1	E	254	ILE	2.0
1	H	236	ILE	2.0
1	O	220	ILE	2.0
1	O	349	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	Q	601	1/1	0.52	0.35	67,67,67,67	0
4	MG	S	601	1/1	0.56	0.15	54,54,54,54	0
2	SO4	Z	601	5/5	0.59	0.25	49,51,72,74	5
2	SO4	T	602	5/5	0.61	0.23	37,47,50,59	5
2	SO4	M	602	5/5	0.66	0.19	54,55,71,77	5
2	SO4	P	601	5/5	0.66	0.23	29,35,57,64	5
4	MG	V	601	1/1	0.67	0.28	61,61,61,61	0
2	SO4	U	601	5/5	0.68	0.22	55,62,75,80	5
2	SO4	K	601	5/5	0.69	0.32	42,55,61,61	5
4	MG	M	601	1/1	0.70	0.16	53,53,53,53	0
2	SO4	L	601	5/5	0.70	0.18	38,55,60,64	5
2	SO4	C	601	5/5	0.70	0.17	41,46,67,74	5
4	MG	H	601	1/1	0.70	0.15	51,51,51,51	0
4	MG	T	601	1/1	0.71	0.24	58,58,58,58	0
2	SO4	A	601	5/5	0.71	0.22	37,61,63,70	5
2	SO4	b	601	5/5	0.72	0.36	62,84,95,96	0
2	SO4	E	601	5/5	0.74	0.22	43,47,62,63	5
2	SO4	G	601	5/5	0.74	0.20	36,48,56,57	5
2	SO4	B	601	5/5	0.75	0.25	24,30,35,36	5
2	SO4	V	602	5/5	0.75	0.22	34,35,45,48	5
3	CA	G	602	1/1	0.76	0.09	76,76,76,76	0
2	SO4	N	601	5/5	0.77	0.16	41,47,51,54	5
2	SO4	Y	601	5/5	0.77	0.14	34,41,58,58	5
4	MG	R	601	1/1	0.77	0.10	34,34,34,34	0
3	CA	M	603	1/1	0.79	0.12	78,78,78,78	0
3	CA	O	601	1/1	0.79	0.09	73,73,73,73	0
2	SO4	J	601	5/5	0.79	0.20	33,42,51,52	5
3	CA	B	602	1/1	0.80	0.10	77,77,77,77	0
2	SO4	a	601	5/5	0.81	0.16	50,53,63,69	5
3	CA	Z	602	1/1	0.82	0.10	92,92,92,92	0
2	SO4	D	601	5/5	0.83	0.16	33,44,50,50	5
3	CA	Y	602	1/1	0.84	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	F	601	5/5	0.84	0.18	25,34,38,38	5
3	CA	A	602	1/1	0.84	0.08	72,72,72,72	0
3	CA	K	602	1/1	0.86	0.08	82,82,82,82	0
3	CA	F	602	1/1	0.86	0.08	77,77,77,77	0
3	CA	P	602	1/1	0.88	0.09	71,71,71,71	0
3	CA	J	602	1/1	0.89	0.16	72,72,72,72	0
2	SO4	R	602	5/5	0.89	0.17	23,33,34,34	5
3	CA	R	603	1/1	0.90	0.06	64,64,64,64	0
3	CA	Q	602	1/1	0.90	0.11	78,78,78,78	0
3	CA	a	602	1/1	0.91	0.08	78,78,78,78	0
3	CA	I	601	1/1	0.91	0.07	79,79,79,79	0
3	CA	T	603	1/1	0.92	0.10	69,69,69,69	0
3	CA	U	602	1/1	0.94	0.07	62,62,62,62	0
3	CA	V	603	1/1	0.94	0.06	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.