



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:35 PM GMT

PDB ID : 1PCQ  
Title : Crystal structure of groEL-groES  
Authors : Chaudhry, C.; Farr, G.W.; Todd, M.J.; Rye, H.S.; Brunger, A.T.; Adams, P.D.; Horwich, A.L.; Sigler, P.B.  
Deposited on : 2003-05-16  
Resolution : 2.81 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

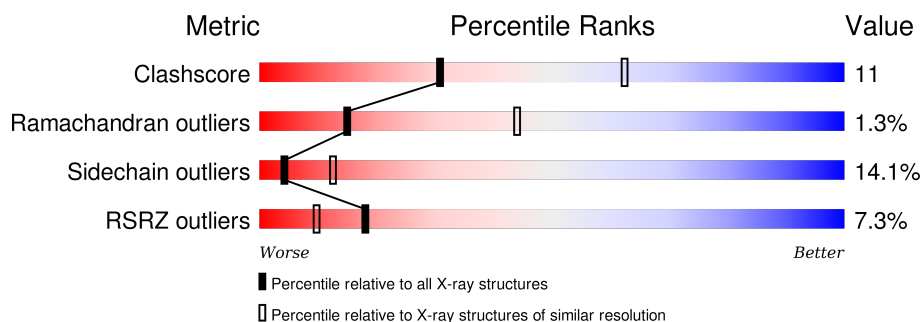
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	524	<div> <div>8%</div> <div>71% 23% 5%</div> </div>
1	B	524	<div> <div>10%</div> <div>73% 22% .</div> </div>
1	C	524	<div> <div>7%</div> <div>71% 23% 5%</div> </div>
1	D	524	<div> <div>9%</div> <div>70% 25% 5%</div> </div>
1	E	524	<div> <div>11%</div> <div>73% 23% .</div> </div>
1	F	524	<div> <div>14%</div> <div>74% 21% 5%</div> </div>
1	G	524	<div> <div>10%</div> <div>72% 23% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	524	
1	I	524	
1	J	524	
1	K	524	
1	L	524	
1	M	524	
1	N	524	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59304 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	I	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	J	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	K	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	L	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	M	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	N	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			

- Molecule 2 is a protein called groES protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	P	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	Q	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	R	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	S	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	T	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	U	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

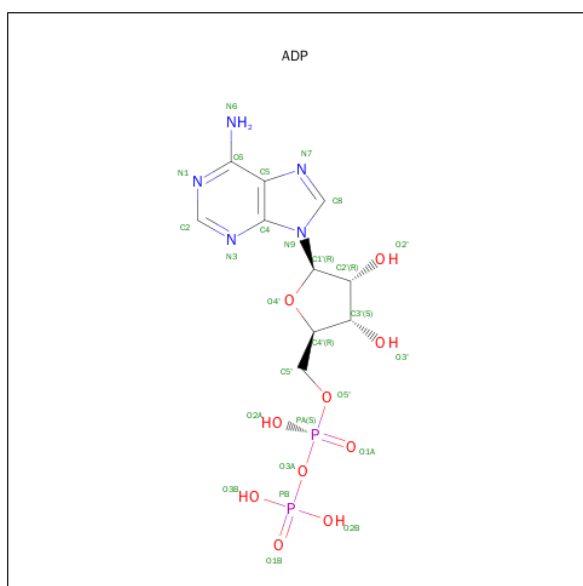
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		

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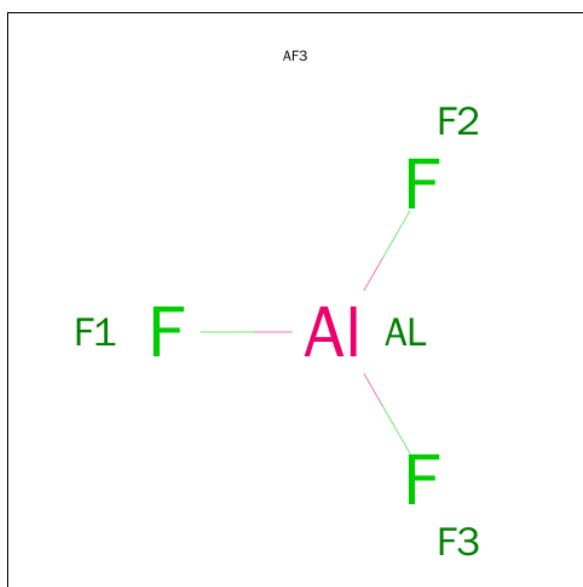
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula:  $AlF_3$ ).

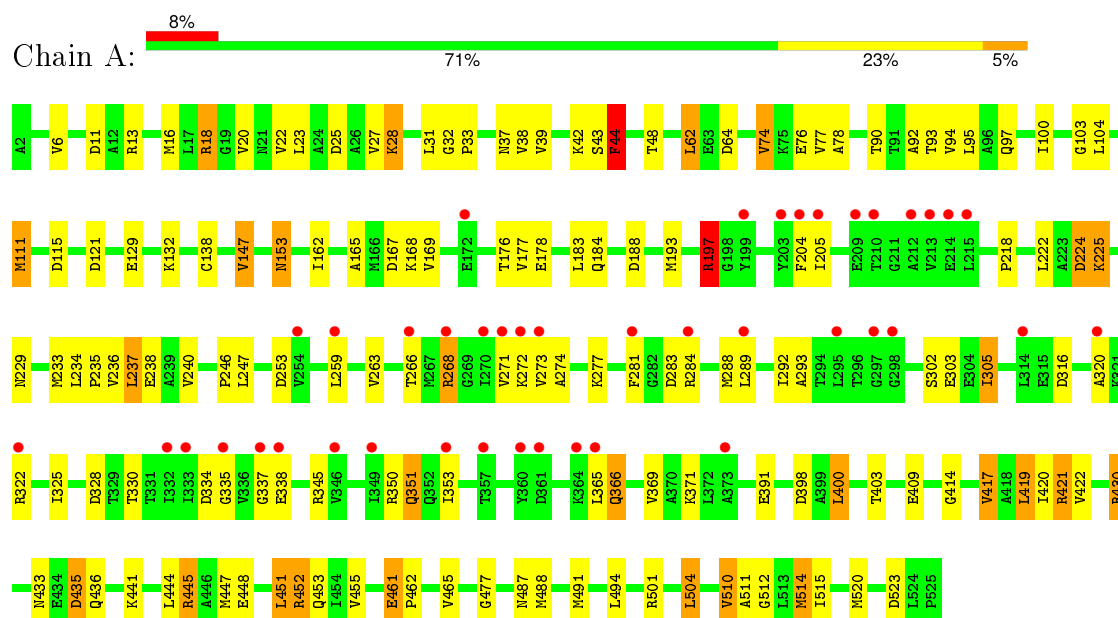


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Al	F	0	0
			4	1	3		
6	B	1	Total	Al	F	0	0
			4	1	3		
6	C	1	Total	Al	F	0	0
			4	1	3		
6	D	1	Total	Al	F	0	0
			4	1	3		
6	E	1	Total	Al	F	0	0
			4	1	3		
6	F	1	Total	Al	F	0	0
			4	1	3		
6	G	1	Total	Al	F	0	0
			4	1	3		

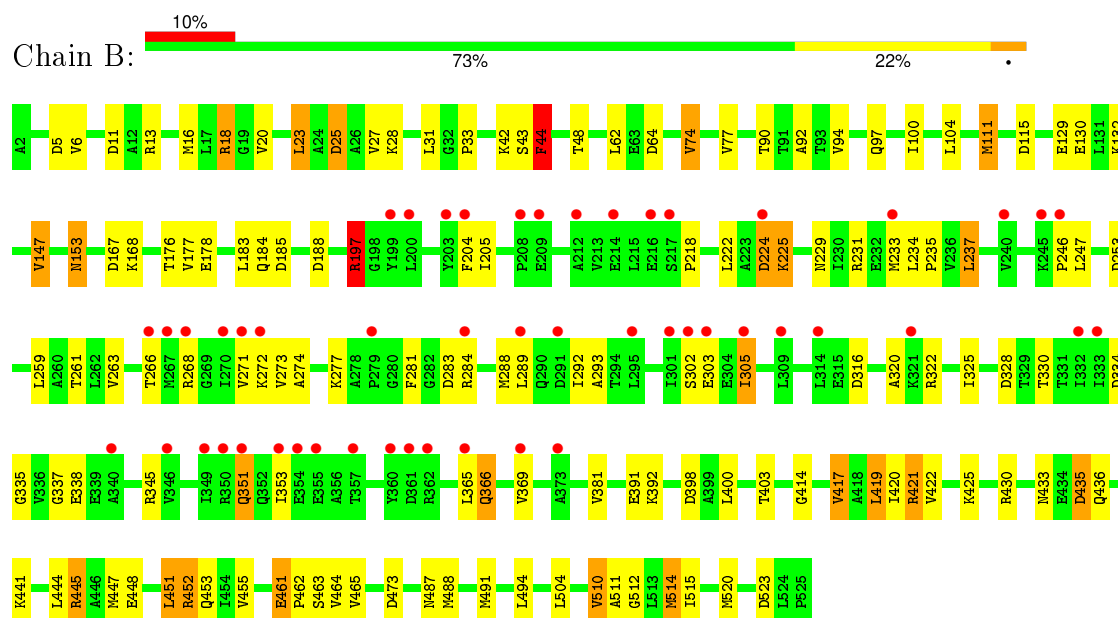
### 3 Residue-property plots

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

#### • Molecule 1: groEL protein

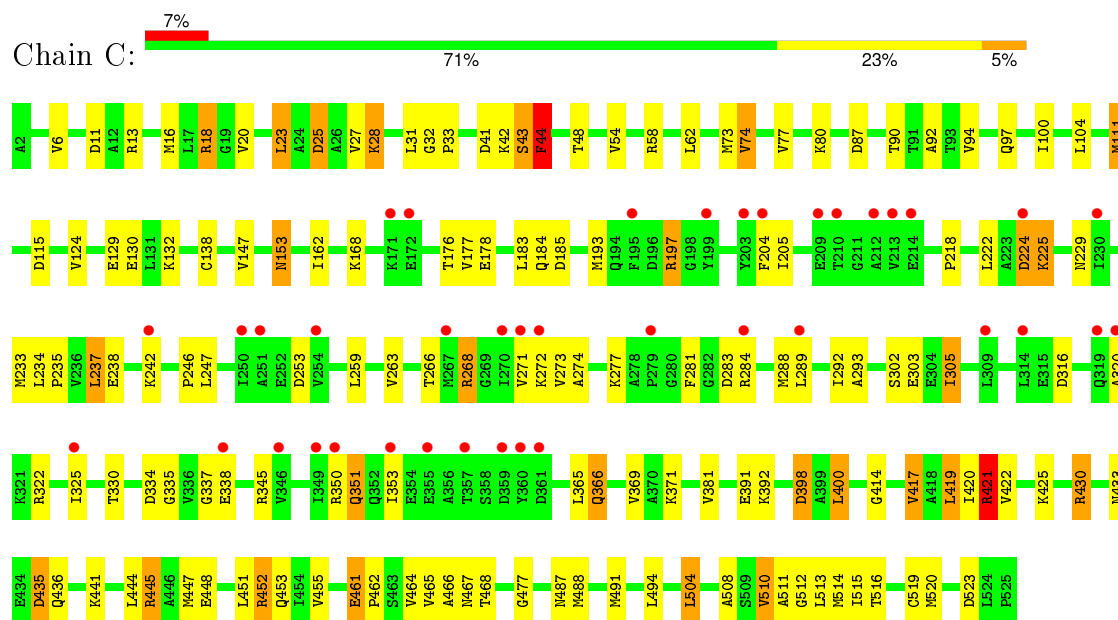


#### • Molecule 1: groEL protein

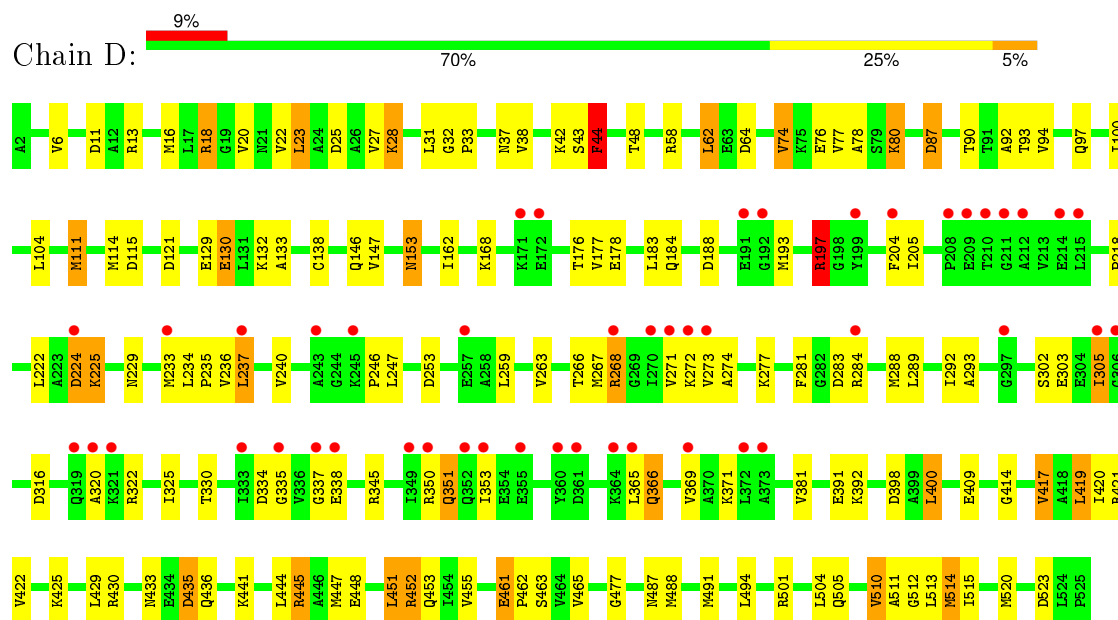




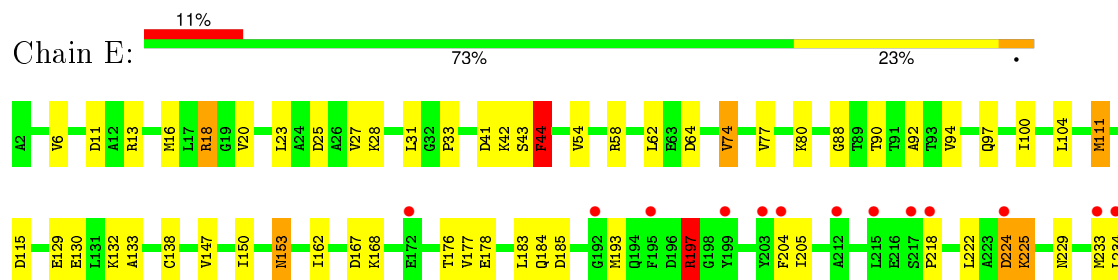
- Molecule 1: groEL protein

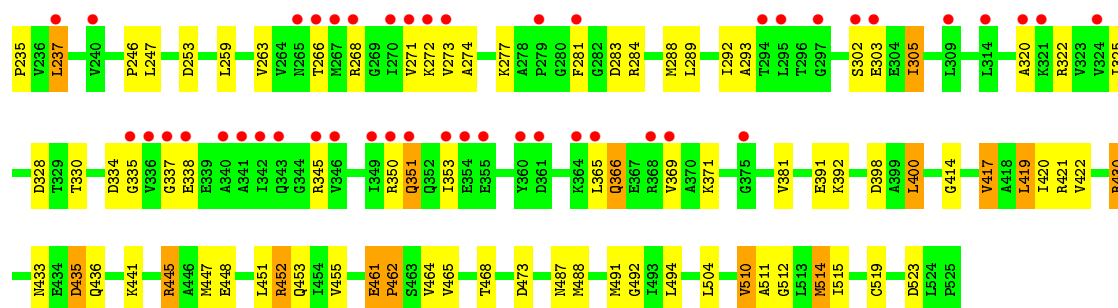


- Molecule 1: groEL protein

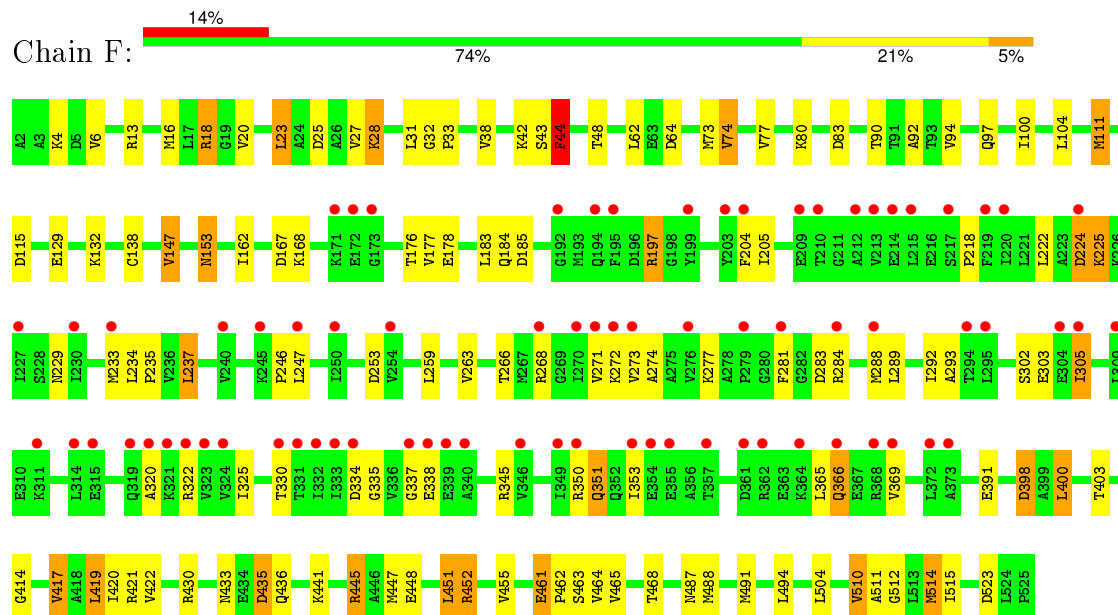


- Molecule 1: groEL protein

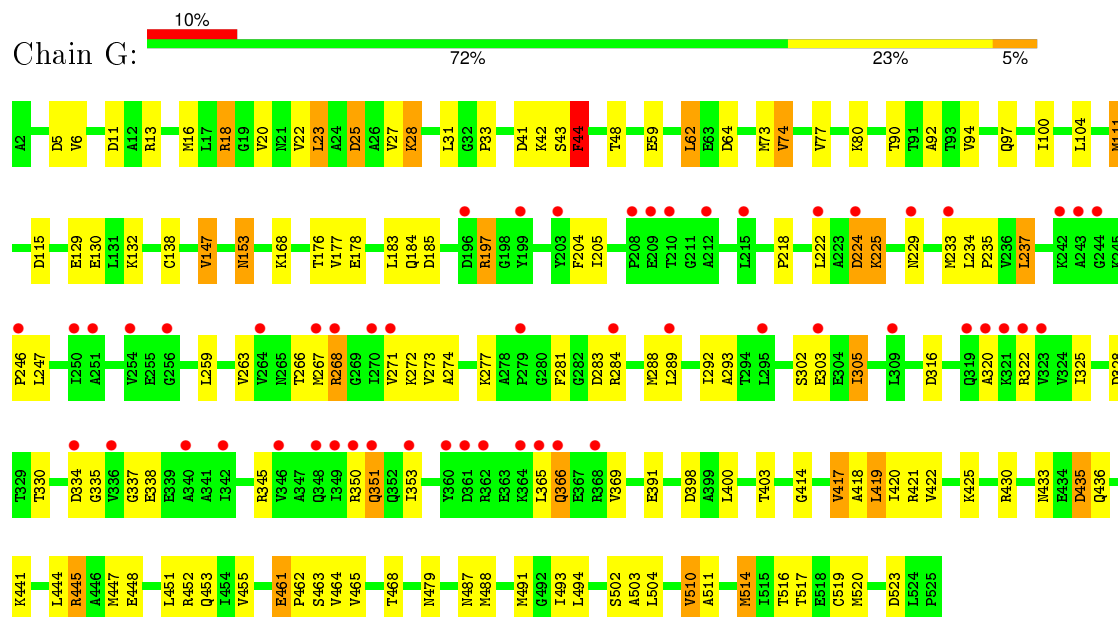




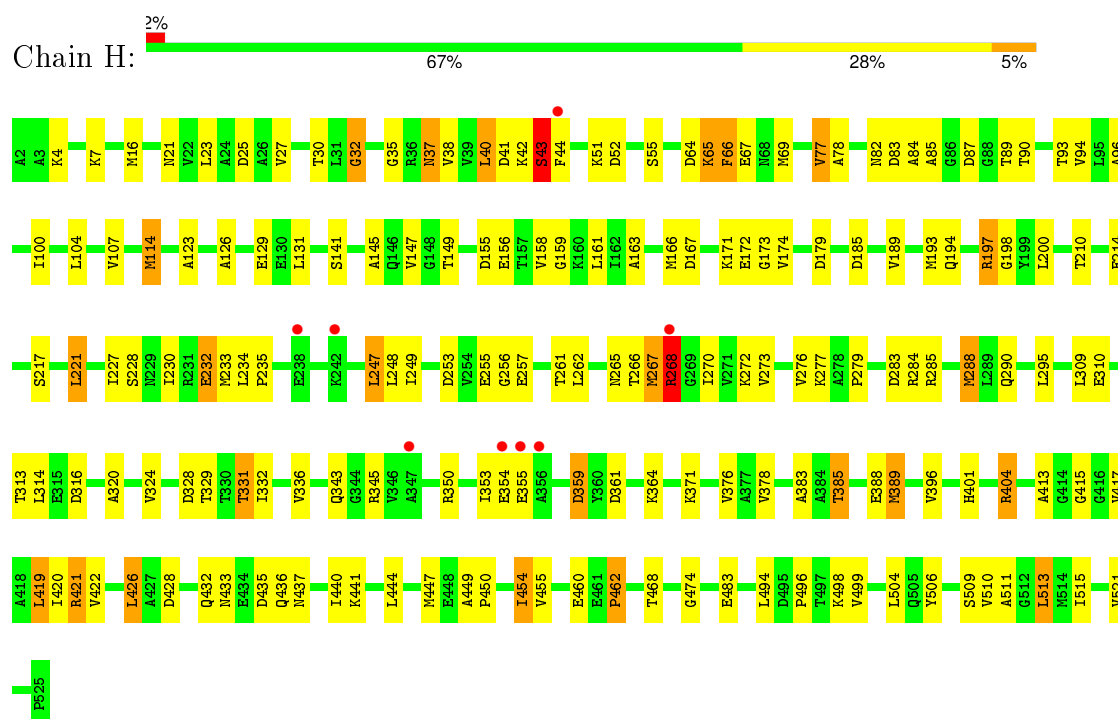
- Molecule 1: groEL protein



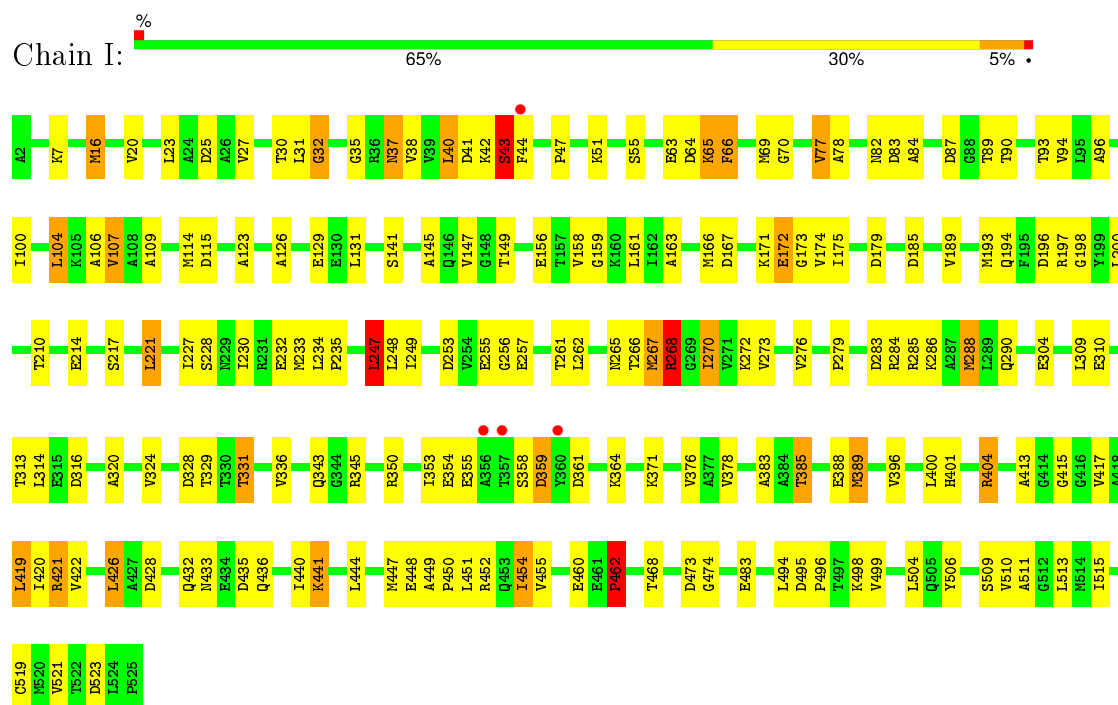
- Molecule 1: groEL protein



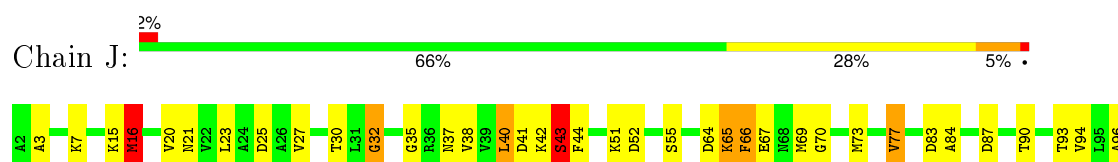
- Molecule 1: groEL protein

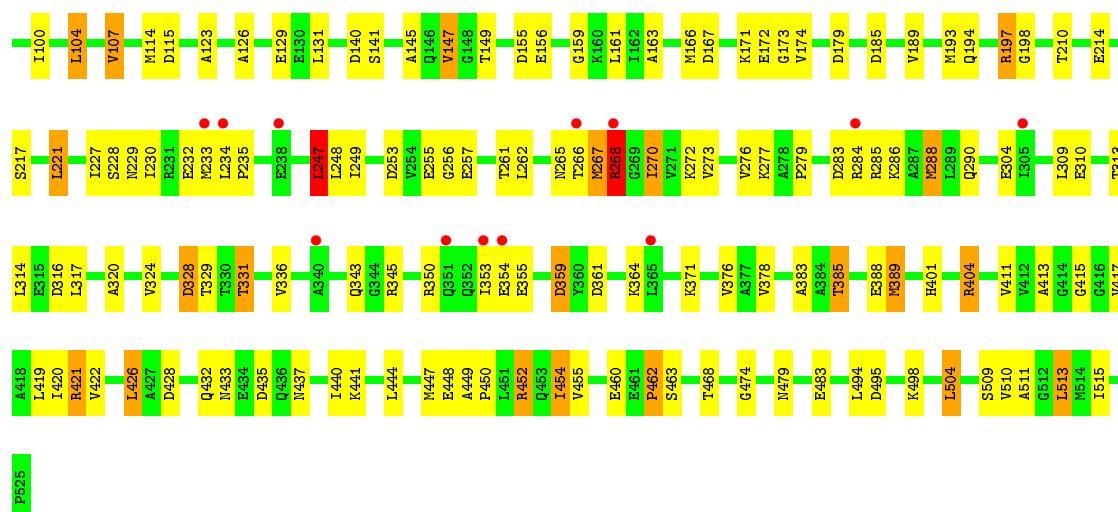


- Molecule 1: groEL protein

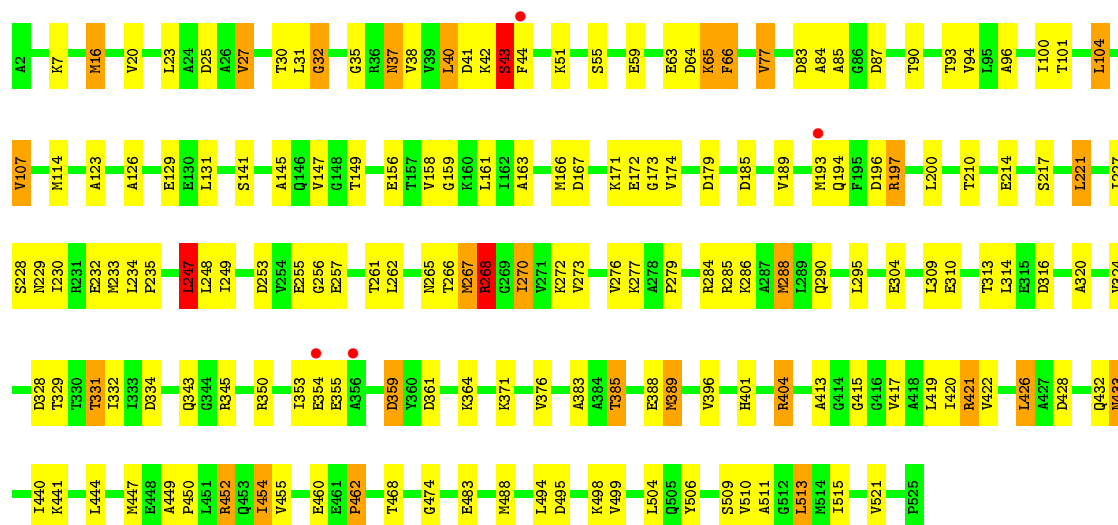


- Molecule 1: groEL protein

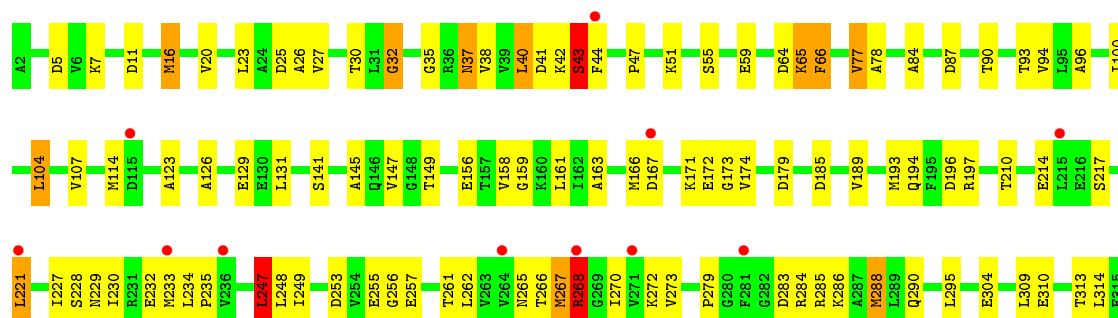


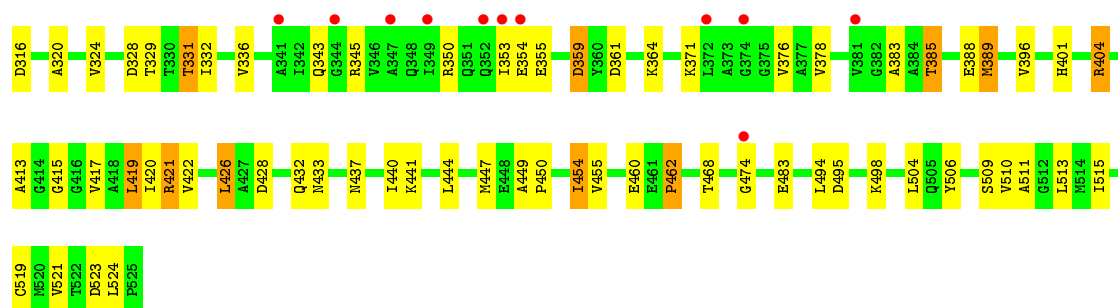


- Molecule 1: groEL protein

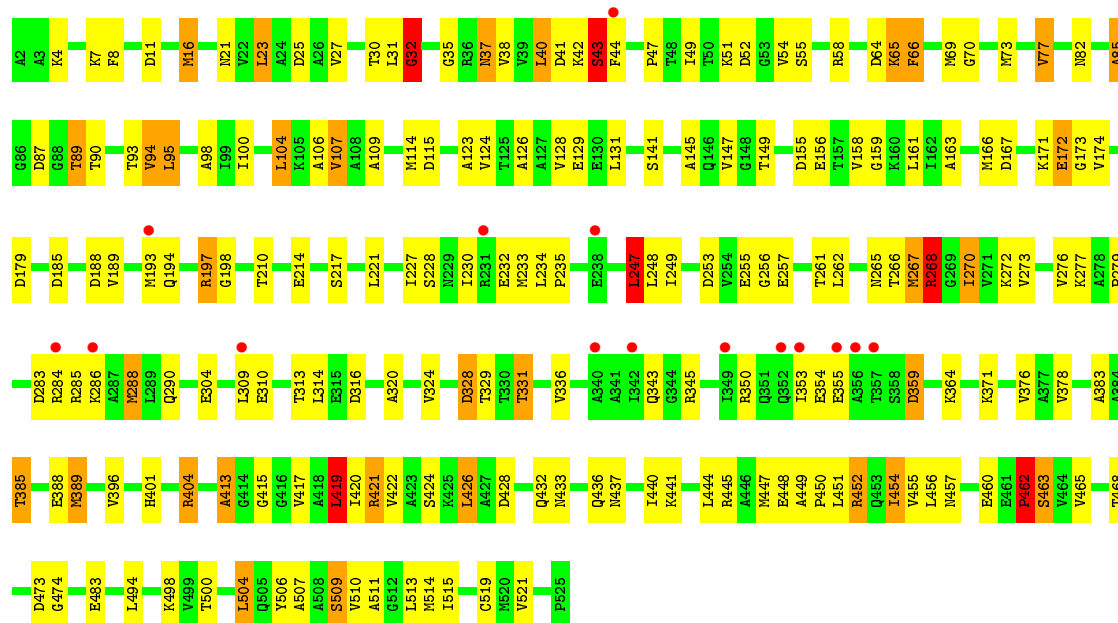


- Molecule 1: groEL protein

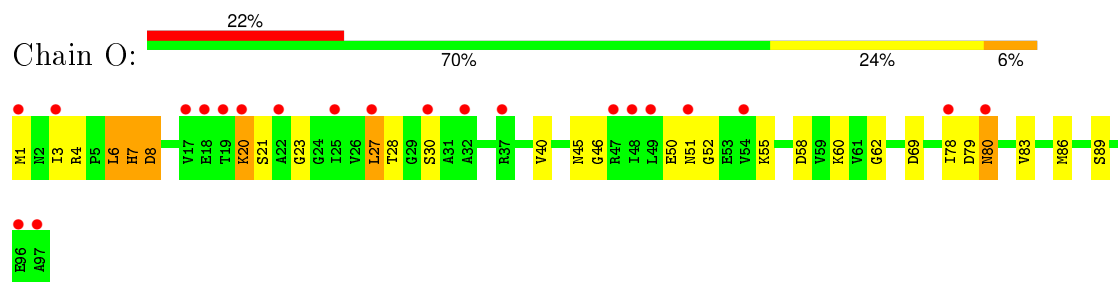




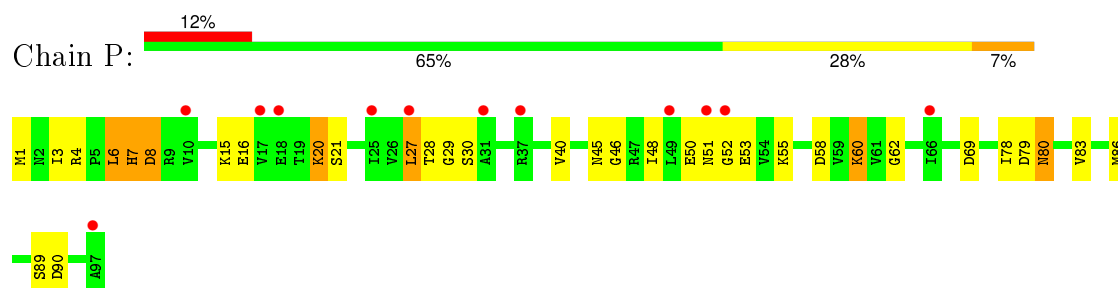
• Molecule 1: groEL protein



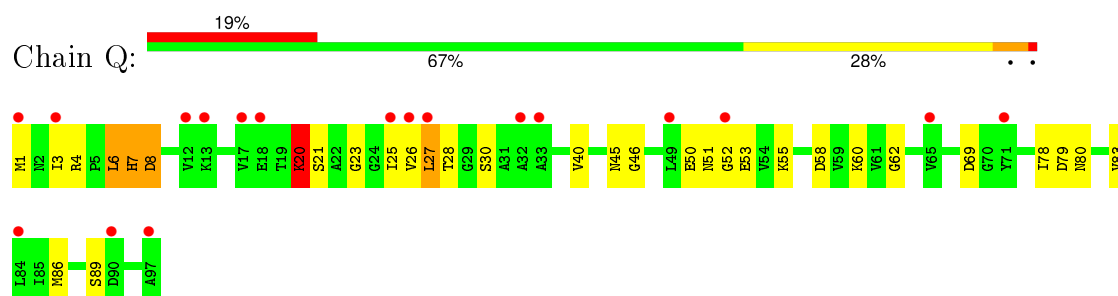
- Molecule 2: groES protein



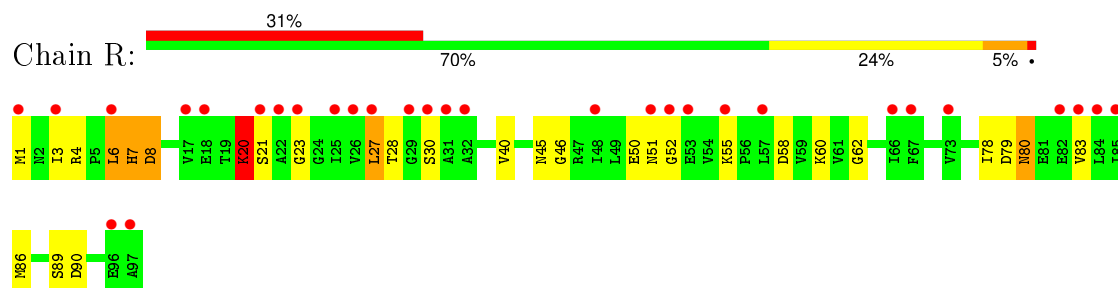
- Molecule 2: groES protein



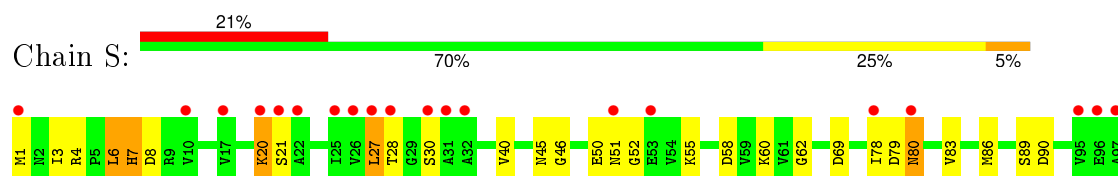
- Molecule 2: groES protein



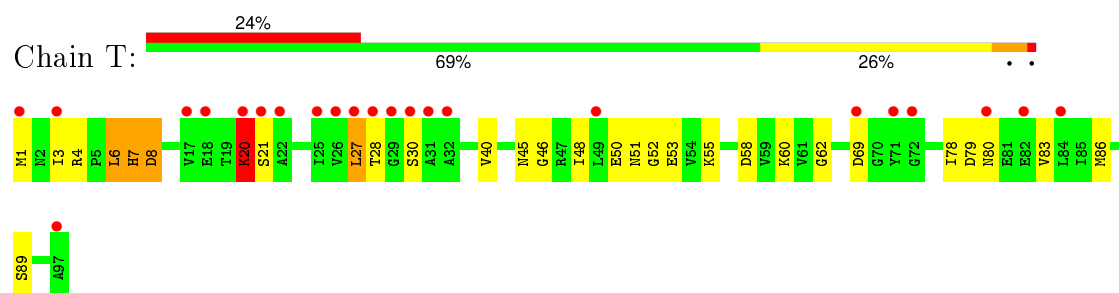
- Molecule 2: groES protein



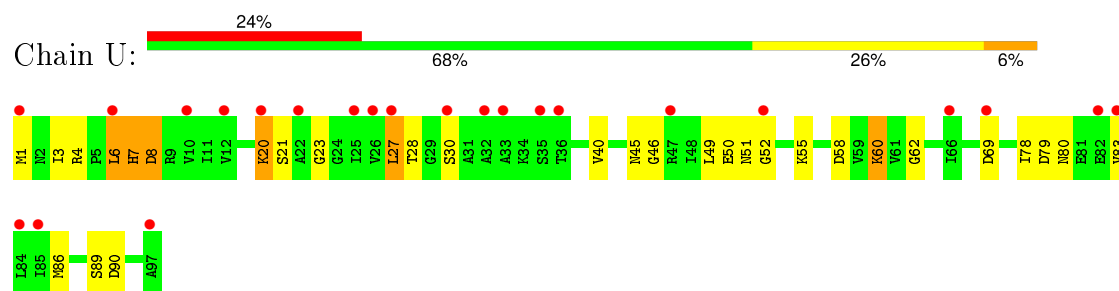
- Molecule 2: groES protein



- Molecule 2: groES protein



- Molecule 2: groES protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.55Å 266.86Å 187.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.81 49.44 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.39-2.81) 60.7 (49.44-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.262 , 0.278 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.958	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 70.2	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	6 of 345474 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	59304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ADP, AF3

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	0.70	1/3883 (0.0%)	0.93	19/5243 (0.4%)
1	B	0.61	0/3883	0.96	23/5243 (0.4%)
1	C	0.66	0/3883	0.91	19/5243 (0.4%)
1	D	0.68	1/3883 (0.0%)	0.92	19/5243 (0.4%)
1	E	0.54	0/3883	0.86	17/5243 (0.3%)
1	F	0.54	0/3883	0.87	17/5243 (0.3%)
1	G	0.62	0/3883	0.92	20/5243 (0.4%)
1	H	0.60	0/3884	0.83	15/5243 (0.3%)
1	I	0.64	0/3884	0.87	19/5243 (0.4%)
1	J	0.60	1/3884 (0.0%)	0.85	20/5243 (0.4%)
1	K	0.52	0/3884	0.86	16/5243 (0.3%)
1	L	0.49	0/3884	0.81	17/5243 (0.3%)
1	M	0.83	4/3884 (0.1%)	0.99	24/5243 (0.5%)
1	N	0.60	0/3884	0.85	16/5243 (0.3%)
2	O	0.35	0/732	0.69	4/983 (0.4%)
2	P	0.35	0/732	0.69	5/983 (0.5%)
2	Q	0.34	0/732	0.69	4/983 (0.4%)
2	R	0.34	0/732	0.69	4/983 (0.4%)
2	S	0.35	0/732	0.69	4/983 (0.4%)
2	T	0.35	0/732	0.69	4/983 (0.4%)
2	U	0.35	0/732	0.69	5/983 (0.5%)
All	All	0.60	7/59493 (0.0%)	0.87	291/80283 (0.4%)

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	M	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	95	LEU	CG-CD1	7.61	1.80	1.51
1	D	130	GLU	CD-OE1	5.75	1.31	1.25
1	M	94	VAL	C-O	5.54	1.33	1.23
1	M	85	ALA	CA-CB	5.50	1.64	1.52
1	A	76	GLU	CD-OE1	5.26	1.31	1.25
1	J	16	MET	SD-CE	5.08	2.06	1.77
1	M	419	LEU	CG-CD2	5.04	1.70	1.51

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	NE-CZ-NH1	-19.61	110.50	120.30
1	B	231	ARG	NE-CZ-NH2	18.76	129.68	120.30
1	K	268	ARG	NE-CZ-NH2	-14.05	113.28	120.30
1	M	268	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	K	268	ARG	NE-CZ-NH1	13.45	127.03	120.30
1	M	268	ARG	NE-CZ-NH1	13.08	126.84	120.30
1	G	197	ARG	NE-CZ-NH1	-11.84	114.38	120.30
1	G	268	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	A	268	ARG	NE-CZ-NH2	-11.69	114.45	120.30
1	D	268	ARG	NE-CZ-NH1	11.55	126.08	120.30
1	D	268	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	G	268	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	A	268	ARG	NE-CZ-NH1	11.44	126.02	120.30
1	C	197	ARG	NE-CZ-NH1	-11.37	114.62	120.30
1	F	197	ARG	NE-CZ-NH1	-11.35	114.63	120.30
1	G	197	ARG	NE-CZ-NH2	11.21	125.90	120.30
1	F	197	ARG	NE-CZ-NH2	10.85	125.72	120.30
1	C	197	ARG	NE-CZ-NH2	10.75	125.68	120.30
1	C	268	ARG	NE-CZ-NH1	-9.40	115.60	120.30
1	B	231	ARG	CD-NE-CZ	9.39	136.74	123.60
1	M	25	ASP	CB-CG-OD2	9.37	126.73	118.30
1	F	268	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	C	268	ARG	NE-CZ-NH2	9.27	124.94	120.30
1	E	268	ARG	NE-CZ-NH2	9.20	124.90	120.30
1	F	268	ARG	NE-CZ-NH2	9.18	124.89	120.30
1	E	268	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	B	268	ARG	NE-CZ-NH2	9.15	124.88	120.30
1	N	25	ASP	CB-CG-OD2	9.08	126.47	118.30
1	B	268	ARG	NE-CZ-NH1	-9.08	115.76	120.30
1	K	25	ASP	CB-CG-OD2	8.82	126.24	118.30
1	A	523	ASP	CB-CG-OD2	8.82	126.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	197	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	197	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	B	197	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	D	197	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	B	197	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	E	197	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	M	428	ASP	CB-CG-OD2	8.07	125.57	118.30
1	J	25	ASP	CB-CG-OD2	8.04	125.53	118.30
1	C	25	ASP	CB-CG-OD2	7.79	125.31	118.30
1	J	428	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	197	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	D	197	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	I	428	ASP	CB-CG-OD2	7.62	125.16	118.30
1	L	25	ASP	CB-CG-OD2	7.28	124.85	118.30
1	G	523	ASP	CB-CG-OD2	7.27	124.85	118.30
1	L	428	ASP	CB-CG-OD2	7.25	124.82	118.30
1	D	523	ASP	CB-CG-OD2	7.14	124.72	118.30
1	A	11	ASP	CB-CG-OD2	7.14	124.72	118.30
1	H	428	ASP	CB-CG-OD2	7.13	124.72	118.30
1	N	428	ASP	CB-CG-OD2	7.10	124.69	118.30
1	I	268	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	I	268	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	G	115	ASP	CB-CG-OD2	7.05	124.64	118.30
1	H	25	ASP	CB-CG-OD2	6.92	124.53	118.30
1	I	25	ASP	CB-CG-OD2	6.86	124.47	118.30
1	E	115	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	115	ASP	CB-CG-OD2	6.81	124.43	118.30
1	I	473	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	523	ASP	CB-CG-OD2	6.79	124.41	118.30
1	K	428	ASP	CB-CG-OD2	6.77	124.39	118.30
1	M	115	ASP	CB-CG-OD2	6.74	124.36	118.30
1	F	523	ASP	CB-CG-OD2	6.73	124.36	118.30
1	F	115	ASP	CB-CG-OD2	6.68	124.31	118.30
1	N	268	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	G	11	ASP	CB-CG-OD2	6.67	124.30	118.30
1	H	268	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	E	64	ASP	CB-CG-OD2	6.65	124.29	118.30
1	A	64	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	435	ASP	CB-CG-OD2	6.64	124.27	118.30
1	D	115	ASP	CB-CG-OD2	6.62	124.26	118.30
1	L	268	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	M	41	ASP	CB-CG-OD2	6.58	124.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	268	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	J	268	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	F	64	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	121	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	523	ASP	CB-CG-OD2	6.55	124.20	118.30
1	H	268	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	L	268	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	H	41	ASP	CB-CG-OD2	6.52	124.16	118.30
1	A	435	ASP	CB-CG-OD2	6.47	124.12	118.30
1	G	435	ASP	CB-CG-OD2	6.43	124.09	118.30
1	D	334	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	334	ASP	CB-CG-OD2	6.38	124.05	118.30
1	D	121	ASP	CB-CG-OD1	6.38	124.04	118.30
1	G	334	ASP	CB-CG-OD2	6.38	124.04	118.30
1	M	11	ASP	CB-CG-OD2	6.38	124.04	118.30
1	D	11	ASP	CB-CG-OD2	6.37	124.03	118.30
1	J	268	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	B	115	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	11	ASP	CB-CG-OD2	6.32	123.99	118.30
1	E	523	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	334	ASP	CB-CG-OD2	6.29	123.96	118.30
1	F	334	ASP	CB-CG-OD2	6.21	123.89	118.30
1	M	473	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	334	ASP	CB-CG-OD2	6.20	123.88	118.30
1	I	435	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	473	ASP	CB-CG-OD2	6.13	123.81	118.30
1	M	445	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	E	41	ASP	CB-CG-OD2	6.08	123.77	118.30
1	E	334	ASP	CB-CG-OD2	6.08	123.77	118.30
1	D	283	ASP	CB-CG-OD2	6.07	123.76	118.30
1	I	83	ASP	CB-CG-OD2	6.00	123.69	118.30
1	F	435	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	283	ASP	CB-CG-OD2	5.92	123.62	118.30
1	E	11	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	283	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	435	ASP	CB-CG-OD2	5.91	123.62	118.30
1	K	83	ASP	CB-CG-OD2	5.91	123.61	118.30
1	H	83	ASP	CB-CG-OD2	5.87	123.59	118.30
1	C	41	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	435	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	283	ASP	CB-CG-OD2	5.85	123.57	118.30
1	E	283	ASP	CB-CG-OD2	5.85	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ASP	CB-CG-OD2	5.82	123.53	118.30
1	C	398	ASP	CB-CG-OD1	5.80	123.52	118.30
1	F	283	ASP	CB-CG-OD2	5.80	123.52	118.30
1	L	179	ASP	CB-CG-OD2	5.79	123.51	118.30
1	E	435	ASP	CB-CG-OD2	5.75	123.48	118.30
1	M	253	ASP	CB-CG-OD2	5.74	123.47	118.30
1	M	268	ARG	CD-NE-CZ	5.74	131.63	123.60
1	M	52	ASP	CB-CG-OD2	5.74	123.46	118.30
1	M	456	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	M	462	PRO	N-CD-CG	-5.71	94.63	103.20
1	M	179	ASP	CB-CG-OD2	5.70	123.43	118.30
1	L	196	ASP	CB-CG-OD2	5.69	123.42	118.30
1	G	283	ASP	CB-CG-OD2	5.68	123.42	118.30
1	G	268	ARG	CD-NE-CZ	5.68	131.55	123.60
1	D	114	MET	CG-SD-CE	-5.67	91.12	100.20
1	D	188	ASP	CB-CG-OD2	5.66	123.39	118.30
1	F	167	ASP	CB-CG-OD2	5.66	123.39	118.30
1	I	115	ASP	CB-CG-OD2	5.66	123.39	118.30
1	G	41	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	268	ARG	CD-NE-CZ	5.63	131.49	123.60
1	K	268	ARG	CD-NE-CZ	5.62	131.47	123.60
1	B	5	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	268	ARG	CD-NE-CZ	5.61	131.45	123.60
1	N	115	ASP	CB-CG-OD2	5.59	123.33	118.30
1	E	224	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	188	ASP	CB-CG-OD2	5.58	123.32	118.30
1	I	253	ASP	CB-CG-OD2	5.58	123.32	118.30
1	N	179	ASP	CB-CG-OD2	5.57	123.31	118.30
1	J	253	ASP	CB-CG-OD2	5.56	123.30	118.30
2	P	8	ASP	CB-CG-OD2	5.49	123.24	118.30
1	F	224	ASP	CB-CG-OD2	5.47	123.22	118.30
1	K	179	ASP	CB-CG-OD2	5.46	123.21	118.30
2	Q	58	ASP	CB-CG-OD2	5.44	123.20	118.30
1	D	316	ASP	CB-CG-OD2	5.43	123.19	118.30
1	N	188	ASP	CB-CG-OD2	5.42	123.18	118.30
1	I	359	ASP	CB-CG-OD2	5.41	123.17	118.30
1	J	316	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	25	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	188	ASP	CB-CG-OD2	5.39	123.15	118.30
1	N	435	ASP	CB-CG-OD2	5.38	123.15	118.30
1	J	52	ASP	CB-CG-OD2	5.38	123.14	118.30
1	M	328	ASP	CB-CG-OD2	5.38	123.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	253	ASP	CB-CG-OD2	5.38	123.14	118.30
1	N	247	LEU	CA-CB-CG	5.38	127.66	115.30
1	B	328	ASP	CB-CG-OD2	5.37	123.13	118.30
1	G	5	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	224	ASP	CB-CG-OD2	5.37	123.13	118.30
1	F	83	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	224	ASP	CB-CG-OD2	5.35	123.12	118.30
1	J	435	ASP	CB-CG-OD2	5.35	123.12	118.30
1	M	188	ASP	CB-CG-OD2	5.35	123.11	118.30
1	I	523	ASP	CB-CG-OD2	5.34	123.11	118.30
1	L	523	ASP	CB-CG-OD2	5.34	123.11	118.30
1	G	25	ASP	CB-CG-OD2	5.34	123.11	118.30
1	J	140	ASP	CB-CG-OD2	5.34	123.10	118.30
1	I	179	ASP	CB-CG-OD2	5.33	123.10	118.30
1	F	23	LEU	CA-CB-CG	5.33	127.56	115.30
1	L	359	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	64	ASP	CB-CG-OD2	5.31	123.08	118.30
1	J	41	ASP	CB-CG-OD2	5.31	123.08	118.30
2	S	90	ASP	CB-CG-OD2	5.28	123.06	118.30
1	J	247	LEU	CA-CB-CG	5.28	127.45	115.30
1	N	52	ASP	CB-CG-OD2	5.28	123.05	118.30
1	H	435	ASP	CB-CG-OD2	5.28	123.05	118.30
2	R	8	ASP	CB-CG-OD2	5.28	123.05	118.30
1	N	328	ASP	CB-CG-OD2	5.27	123.05	118.30
2	O	79	ASP	CB-CG-OD2	5.27	123.05	118.30
2	P	90	ASP	CB-CG-OD2	5.27	123.05	118.30
1	L	11	ASP	CB-CG-OD2	5.27	123.04	118.30
1	M	23	LEU	CB-CG-CD1	-5.27	102.05	111.00
1	B	167	ASP	CB-CG-OD2	5.25	123.03	118.30
2	Q	69	ASP	CB-CG-OD2	5.25	123.03	118.30
2	P	79	ASP	CB-CG-OD2	5.25	123.02	118.30
1	G	224	ASP	CB-CG-OD2	5.24	123.02	118.30
1	G	64	ASP	CB-CG-OD2	5.24	123.02	118.30
1	I	247	LEU	CA-CB-CG	5.24	127.35	115.30
1	K	253	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	328	ASP	CB-CG-OD2	5.23	123.01	118.30
1	J	179	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	224	ASP	CB-CG-OD2	5.23	123.00	118.30
1	C	23	LEU	CA-CB-CG	5.22	127.32	115.30
1	K	361	ASP	CB-CG-OD2	5.22	123.00	118.30
1	J	115	ASP	CB-CG-OD2	5.22	123.00	118.30
1	I	495	ASP	CB-CG-OD2	5.22	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	316	ASP	CB-CG-OD2	5.22	123.00	118.30
1	I	41	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	421	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	H	179	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	167	ASP	CB-CG-OD2	5.20	122.98	118.30
2	T	8	ASP	CB-CG-OD2	5.20	122.98	118.30
1	L	41	ASP	CB-CG-OD2	5.19	122.97	118.30
2	U	58	ASP	CB-CG-OD2	5.19	122.97	118.30
1	N	83	ASP	CB-CG-OD2	5.19	122.97	118.30
2	Q	8	ASP	CB-CG-OD2	5.19	122.97	118.30
1	N	155	ASP	CB-CG-OD2	5.19	122.97	118.30
1	N	283	ASP	CB-CG-OD2	5.19	122.97	118.30
2	R	58	ASP	CB-CG-OD2	5.18	122.97	118.30
2	S	58	ASP	CB-CG-OD2	5.18	122.97	118.30
1	F	253	ASP	CB-CG-OD2	5.18	122.96	118.30
1	J	361	ASP	CB-CG-OD2	5.18	122.96	118.30
2	R	90	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	224	ASP	CB-CG-OD2	5.17	122.95	118.30
1	H	361	ASP	CB-CG-OD2	5.17	122.95	118.30
1	M	359	ASP	CB-CG-OD2	5.17	122.95	118.30
1	F	197	ARG	CD-NE-CZ	5.17	130.84	123.60
1	K	247	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	316	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	115	ASP	CB-CG-OD2	5.17	122.95	118.30
1	H	283	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	197	ARG	CD-NE-CZ	5.16	130.83	123.60
1	J	155	ASP	CB-CG-OD2	5.16	122.94	118.30
1	G	23	LEU	CA-CB-CG	5.16	127.17	115.30
1	G	197	ARG	CD-NE-CZ	5.16	130.82	123.60
2	O	69	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	11	ASP	CB-CG-OD2	5.15	122.93	118.30
1	L	361	ASP	CB-CG-OD2	5.15	122.93	118.30
2	S	79	ASP	CB-CG-OD2	5.14	122.93	118.30
2	U	79	ASP	CB-CG-OD2	5.14	122.93	118.30
1	H	52	ASP	CB-CG-OD2	5.14	122.93	118.30
1	G	316	ASP	CB-CG-OD2	5.14	122.93	118.30
1	K	334	ASP	CB-CG-OD2	5.14	122.92	118.30
1	L	5	ASP	CB-CG-OD2	5.14	122.92	118.30
1	H	359	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	253	ASP	CB-CG-OD2	5.13	122.92	118.30
2	P	58	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	253	ASP	CB-CG-OD2	5.12	122.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	155	ASP	CB-CG-OD2	5.12	122.91	118.30
1	L	247	LEU	CA-CB-CG	5.12	127.08	115.30
2	Q	79	ASP	CB-CG-OD2	5.12	122.91	118.30
2	R	79	ASP	CB-CG-OD2	5.12	122.91	118.30
2	U	8	ASP	CB-CG-OD2	5.12	122.91	118.30
1	L	253	ASP	CB-CG-OD2	5.11	122.90	118.30
1	F	398	ASP	CB-CG-OD1	5.11	122.90	118.30
2	T	58	ASP	CB-CG-OD2	5.11	122.90	118.30
1	I	196	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	316	ASP	CB-CG-OD2	5.10	122.89	118.30
1	J	83	ASP	CB-CG-OD2	5.10	122.89	118.30
1	K	359	ASP	CB-CG-OD2	5.10	122.89	118.30
2	S	69	ASP	CB-CG-OD2	5.10	122.89	118.30
1	J	283	ASP	CB-CG-OD2	5.09	122.89	118.30
1	K	316	ASP	CB-CG-OD2	5.09	122.88	118.30
1	L	495	ASP	CB-CG-OD2	5.09	122.88	118.30
1	N	359	ASP	CB-CG-OD2	5.09	122.88	118.30
2	O	8	ASP	CB-CG-OD2	5.09	122.88	118.30
2	T	79	ASP	CB-CG-OD2	5.09	122.88	118.30
1	L	316	ASP	CB-CG-OD2	5.09	122.88	118.30
1	K	41	ASP	CB-CG-OD2	5.08	122.88	118.30
2	O	58	ASP	CB-CG-OD2	5.08	122.88	118.30
1	E	473	ASP	CB-CG-OD2	5.08	122.87	118.30
1	M	316	ASP	CB-CG-OD2	5.08	122.87	118.30
2	U	90	ASP	CB-CG-OD2	5.08	122.87	118.30
1	J	495	ASP	CB-CG-OD2	5.07	122.86	118.30
2	T	69	ASP	CB-CG-OD2	5.07	122.86	118.30
2	U	69	ASP	CB-CG-OD2	5.06	122.86	118.30
1	M	95	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	I	316	ASP	CB-CG-OD2	5.05	122.85	118.30
1	M	247	LEU	CA-CB-CG	5.05	126.92	115.30
1	I	283	ASP	CB-CG-OD2	5.05	122.85	118.30
1	J	328	ASP	CB-CG-OD2	5.05	122.85	118.30
1	I	462	PRO	N-CD-CG	-5.05	95.63	103.20
1	M	283	ASP	CB-CG-OD2	5.05	122.84	118.30
1	K	495	ASP	CB-CG-OD2	5.05	122.84	118.30
1	G	328	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	316	ASP	CB-CG-OD2	5.04	122.83	118.30
1	M	155	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	253	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	328	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	87	ASP	CB-CG-OD2	5.03	122.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	283	ASP	CB-CG-OD2	5.03	122.82	118.30
1	K	196	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	253	ASP	CB-CG-OD2	5.02	122.82	118.30
1	H	253	ASP	CB-CG-OD2	5.02	122.81	118.30
1	A	167	ASP	CB-CG-OD2	5.01	122.81	118.30
2	P	69	ASP	CB-CG-OD2	5.00	122.80	118.30
1	D	253	ASP	CB-CG-OD2	5.00	122.80	118.30
1	J	359	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	32	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3976	91	0
1	B	3855	0	3976	75	0
1	C	3855	0	3976	95	0
1	D	3855	0	3976	90	0
1	E	3855	0	3976	75	0
1	F	3855	0	3976	72	0
1	G	3855	0	3976	83	0
1	H	3856	0	3976	92	0
1	I	3856	0	3976	97	0
1	J	3856	0	3976	98	0
1	K	3856	0	3976	92	0
1	L	3856	0	3976	81	0
1	M	3856	0	3976	129	0
1	N	3856	0	3976	102	0
2	O	728	0	762	13	0
2	P	728	0	762	19	0
2	Q	728	0	762	16	0
2	R	728	0	762	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	728	0	762	11	0
2	T	728	0	762	13	0
2	U	728	0	762	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	27	0	12	4	0
5	B	27	0	12	1	0
5	C	27	0	12	5	0
5	D	27	0	12	2	0
5	E	27	0	12	1	0
5	F	27	0	12	3	0
5	G	27	0	12	1	0
6	A	4	0	0	1	0
6	B	4	0	0	0	0
6	C	4	0	0	1	0
6	D	4	0	0	0	0
6	E	4	0	0	0	0
6	F	4	0	0	0	0
6	G	4	0	0	1	0
All	All	59304	0	61082	1315	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 11.

All (1315) 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:M:95:LEU:CG	1:M:95:LEU:CD1	1.80	1.60
1:F:73:MET:CE	1:F:73:MET:SD	2.01	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:MET:CE	1:H:114:MET:SD	2.02	1.48
1:G:73:MET:SD	1:G:73:MET:CE	2.01	1.48
1:N:16:MET:SD	1:N:16:MET:CE	2.01	1.47
1:M:16:MET:SD	1:M:16:MET:CE	2.03	1.46
1:M:447:MET:CE	1:M:447:MET:SD	2.04	1.45
1:C:73:MET:SD	1:C:73:MET:CE	2.01	1.45
1:J:16:MET:CE	1:J:16:MET:SD	2.06	1.40
1:D:18:ARG:CB	1:D:18:ARG:HH11	1.49	1.25
1:C:18:ARG:CB	1:C:18:ARG:HH11	1.48	1.24
1:B:18:ARG:CB	1:B:18:ARG:HH11	1.51	1.22
1:C:18:ARG:NH1	1:C:18:ARG:HB3	1.54	1.22
1:A:18:ARG:CB	1:A:18:ARG:HH11	1.55	1.16
1:D:18:ARG:HB3	1:D:18:ARG:NH1	1.59	1.16
1:G:18:ARG:CB	1:G:18:ARG:HH11	1.58	1.16
1:E:18:ARG:HH11	1:E:18:ARG:CB	1.57	1.15
1:B:18:ARG:HB3	1:B:18:ARG:NH1	1.60	1.15
1:F:18:ARG:HH11	1:F:18:ARG:CB	1.59	1.13
1:A:197:ARG:HD3	1:A:277:LYS:HB2	1.30	1.13
1:E:197:ARG:HD3	1:E:277:LYS:HB2	1.28	1.13
1:B:197:ARG:HD3	1:B:277:LYS:HB2	1.29	1.12
1:E:18:ARG:NH1	1:E:18:ARG:HB3	1.67	1.09
1:G:18:ARG:NH1	1:G:18:ARG:HB3	1.65	1.08
1:D:197:ARG:HD3	1:D:277:LYS:HB2	1.31	1.08
1:A:18:ARG:HB3	1:A:18:ARG:NH1	1.68	1.08
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.32	1.07
1:F:204:PHE:HE2	1:F:266:THR:HG21	1.20	1.07
1:F:18:ARG:NH1	1:F:18:ARG:HB3	1.70	1.06
1:F:18:ARG:HB3	1:F:18:ARG:HH11	0.89	1.05
1:E:204:PHE:HE2	1:E:266:THR:HG21	1.22	1.05
1:C:204:PHE:HE2	1:C:266:THR:HG21	1.19	1.05
1:C:197:ARG:HD2	1:C:277:LYS:HB2	1.38	1.04
1:G:204:PHE:HE2	1:G:266:THR:HG21	1.21	1.04
1:A:18:ARG:HB3	1:A:18:ARG:HH11	0.89	1.03
1:D:204:PHE:HE2	1:D:266:THR:HG21	1.19	1.03
1:F:197:ARG:HD2	1:F:277:LYS:HB2	1.37	1.03
1:A:204:PHE:HE2	1:A:266:THR:HG21	1.20	1.02
1:B:204:PHE:HE2	1:B:266:THR:HG21	1.20	1.02
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.42	1.01
1:E:18:ARG:HH11	1:E:18:ARG:HB3	0.85	1.01
1:G:197:ARG:HD2	1:G:277:LYS:HB2	1.39	1.01
1:G:18:ARG:HH11	1:G:18:ARG:HB3	0.82	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:GLU:HG2	2:Q:51:ASN:HB2	1.45	0.98
1:C:204:PHE:CE2	1:C:266:THR:HG21	2.01	0.96
1:B:18:ARG:HH11	1:B:18:ARG:HB3	0.79	0.95
2:Q:50:GLU:HG2	2:R:51:ASN:HB2	1.48	0.95
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.47	0.95
1:D:204:PHE:CE2	1:D:266:THR:HG21	2.01	0.94
1:D:18:ARG:HH11	1:D:18:ARG:HB3	0.79	0.94
1:B:204:PHE:CE2	1:B:266:THR:HG21	2.01	0.94
1:E:204:PHE:CE2	1:E:266:THR:HG21	2.03	0.94
1:F:204:PHE:CE2	1:F:266:THR:HG21	2.02	0.94
1:A:204:PHE:CE2	1:A:266:THR:HG21	2.01	0.94
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.50	0.94
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.47	0.93
1:G:204:PHE:CE2	1:G:266:THR:HG21	2.02	0.92
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.49	0.92
2:T:50:GLU:HG2	2:U:51:ASN:HB2	1.52	0.90
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.51	0.90
2:S:50:GLU:HG2	2:T:51:ASN:HB2	1.54	0.90
1:K:65:LYS:O	1:K:66:PHE:HB2	1.70	0.89
1:N:65:LYS:O	1:N:66:PHE:HB2	1.73	0.88
1:C:18:ARG:HB3	1:C:18:ARG:HH11	0.74	0.88
1:M:90:THR:O	1:M:94:VAL:HG23	1.74	0.86
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.58	0.85
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.58	0.85
2:O:50:GLU:HG2	2:P:51:ASN:HB2	1.59	0.85
1:J:123:ALA:HB2	1:J:440:ILE:HG23	1.57	0.85
1:M:65:LYS:O	1:M:66:PHE:HB2	1.76	0.84
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.55	0.84
1:B:197:ARG:HD3	1:B:277:LYS:CB	2.08	0.84
1:C:90:THR:O	1:C:94:VAL:HG23	1.78	0.84
1:G:90:THR:O	1:G:94:VAL:HG23	1.77	0.84
1:A:90:THR:O	1:A:94:VAL:HG23	1.77	0.83
1:I:65:LYS:O	1:I:66:PHE:HB2	1.77	0.83
1:M:511:ALA:O	1:M:515:ILE:HD12	1.79	0.83
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.58	0.83
1:D:197:ARG:HD3	1:D:277:LYS:CB	2.10	0.82
1:H:123:ALA:HB2	1:H:440:ILE:HG23	1.60	0.82
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.45	0.82
1:E:197:ARG:HD3	1:E:277:LYS:CB	2.08	0.81
2:R:50:GLU:HG2	2:S:51:ASN:HB2	1.62	0.81
1:D:90:THR:O	1:D:94:VAL:HG23	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:51:ASN:HB2	2:U:50:GLU:HG2	1.62	0.80
1:M:95:LEU:CD1	1:M:95:LEU:CB	2.59	0.80
1:H:65:LYS:O	1:H:66:PHE:HB2	1.78	0.80
1:A:197:ARG:HD3	1:A:277:LYS:CB	2.09	0.80
1:E:430:ARG:HH11	1:E:430:ARG:HG2	1.45	0.80
1:L:65:LYS:O	1:L:66:PHE:HB2	1.80	0.79
1:A:414:GLY:O	1:A:417:VAL:HG12	1.81	0.79
1:L:123:ALA:HB2	1:L:440:ILE:HG23	1.63	0.79
1:B:90:THR:O	1:B:94:VAL:HG23	1.82	0.79
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.48	0.78
1:J:65:LYS:O	1:J:66:PHE:HB2	1.82	0.78
1:C:510:VAL:HG12	1:C:514:MET:CE	2.13	0.78
1:F:90:THR:O	1:F:94:VAL:HG23	1.83	0.77
1:C:414:GLY:O	1:C:417:VAL:HG12	1.84	0.77
1:G:414:GLY:O	1:G:417:VAL:HG12	1.85	0.77
1:J:90:THR:O	1:J:94:VAL:HG23	1.84	0.76
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.51	0.76
1:M:95:LEU:O	1:M:98:ALA:HB3	1.86	0.76
1:J:444:LEU:HA	1:J:447:MET:HE3	1.68	0.76
1:F:414:GLY:O	1:F:417:VAL:HG12	1.85	0.75
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.68	0.75
1:L:444:LEU:HA	1:L:447:MET:HE3	1.67	0.75
1:M:444:LEU:HD23	1:M:447:MET:CE	2.17	0.75
1:D:452:ARG:HH11	1:D:452:ARG:HG2	1.52	0.74
1:M:444:LEU:HA	1:M:447:MET:HE3	1.69	0.74
1:F:430:ARG:HH11	1:F:430:ARG:HG2	1.51	0.74
1:D:430:ARG:HH11	1:D:430:ARG:HG2	1.52	0.74
1:I:166:MET:HE2	1:I:171:LYS:HA	1.69	0.74
1:H:90:THR:O	1:H:94:VAL:HG23	1.88	0.74
1:M:421:ARG:HD2	1:M:474:GLY:O	1.89	0.73
1:B:414:GLY:O	1:B:417:VAL:HG12	1.88	0.72
1:N:444:LEU:HA	1:N:447:MET:HE3	1.70	0.72
1:L:126:ALA:HB1	1:L:426:LEU:HD22	1.71	0.72
1:A:18:ARG:CB	1:A:18:ARG:NH1	2.41	0.71
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.54	0.71
1:L:90:THR:O	1:L:94:VAL:HG23	1.89	0.71
1:M:444:LEU:HD23	1:M:447:MET:HE1	1.70	0.71
1:N:65:LYS:O	1:N:66:PHE:CB	2.38	0.71
1:E:414:GLY:O	1:E:417:VAL:HG12	1.90	0.71
1:D:18:ARG:CG	1:D:18:ARG:HH11	2.03	0.71
1:H:444:LEU:HD23	1:H:447:MET:HE3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:GLY:O	1:D:417:VAL:HG12	1.91	0.71
1:D:461:GLU:OE2	1:J:452:ARG:NH2	2.24	0.70
1:N:126:ALA:HB1	1:N:426:LEU:HD22	1.74	0.70
1:H:421:ARG:HD2	1:H:474:GLY:O	1.91	0.70
1:C:452:ARG:HG2	1:C:452:ARG:HH11	1.56	0.70
1:J:511:ALA:O	1:J:515:ILE:HD12	1.91	0.70
1:K:511:ALA:O	1:K:515:ILE:HD12	1.91	0.70
1:J:126:ALA:HB1	1:J:426:LEU:HD22	1.74	0.70
1:I:421:ARG:HD2	1:I:474:GLY:O	1.92	0.69
1:C:18:ARG:NH1	1:C:18:ARG:CB	2.33	0.69
1:E:90:THR:O	1:E:94:VAL:HG23	1.91	0.69
1:C:18:ARG:CG	1:C:18:ARG:HH11	2.06	0.69
1:C:417:VAL:HG11	1:C:488:MET:HG3	1.73	0.69
1:B:18:ARG:CG	1:B:18:ARG:HH11	2.06	0.69
1:L:166:MET:HE2	1:L:171:LYS:HA	1.75	0.69
1:A:414:GLY:O	1:A:417:VAL:CG1	2.41	0.69
1:L:511:ALA:O	1:L:515:ILE:HD12	1.93	0.69
1:D:452:ARG:NH1	1:D:452:ARG:HG2	2.05	0.68
1:M:65:LYS:O	1:M:66:PHE:CB	2.42	0.68
1:L:40:LEU:HD12	1:M:521:VAL:HB	1.76	0.68
1:A:18:ARG:CG	1:A:18:ARG:HH11	2.06	0.68
1:K:65:LYS:O	1:K:66:PHE:CB	2.38	0.68
1:J:421:ARG:HD2	1:J:474:GLY:O	1.93	0.68
1:I:65:LYS:O	1:I:66:PHE:CB	2.42	0.68
1:N:421:ARG:HD2	1:N:474:GLY:O	1.94	0.68
1:K:421:ARG:HD2	1:K:474:GLY:O	1.94	0.67
1:A:417:VAL:HG11	1:A:488:MET:HG3	1.77	0.67
1:N:166:MET:HE2	1:N:171:LYS:HA	1.75	0.67
1:B:417:VAL:HG11	1:B:488:MET:HG3	1.77	0.67
1:M:126:ALA:HB1	1:M:426:LEU:HD22	1.77	0.67
1:I:511:ALA:O	1:I:515:ILE:HD12	1.94	0.67
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.77	0.66
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.78	0.66
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.77	0.66
1:N:511:ALA:O	1:N:515:ILE:HD12	1.95	0.66
1:H:126:ALA:HB1	1:H:426:LEU:HD22	1.77	0.66
1:G:417:VAL:HG11	1:G:488:MET:HG3	1.78	0.66
1:A:452:ARG:NH1	1:A:452:ARG:HG2	2.11	0.66
1:C:44:PHE:CD1	1:C:44:PHE:N	2.64	0.66
1:M:494:LEU:HD12	1:M:494:LEU:O	1.95	0.66
1:J:166:MET:HE3	1:J:171:LYS:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:444:LEU:HA	1:I:447:MET:HE3	1.75	0.66
1:A:74:VAL:O	1:A:77:VAL:HG13	1.95	0.66
1:K:90:THR:O	1:K:94:VAL:HG23	1.95	0.66
1:D:18:ARG:CB	1:D:18:ARG:NH1	2.35	0.66
1:B:44:PHE:CD1	1:B:44:PHE:N	2.64	0.65
1:F:417:VAL:HG11	1:F:488:MET:HG3	1.77	0.65
1:F:44:PHE:N	1:F:44:PHE:CD1	2.64	0.65
1:I:444:LEU:HD23	1:I:447:MET:CE	2.27	0.64
1:H:65:LYS:O	1:H:66:PHE:CB	2.45	0.64
1:A:448:GLU:HB3	1:A:452:ARG:HD2	1.79	0.64
1:M:166:MET:HE3	1:M:171:LYS:HA	1.77	0.64
1:C:510:VAL:HG12	1:C:514:MET:HE1	1.80	0.64
1:C:414:GLY:O	1:C:417:VAL:CG1	2.46	0.64
1:M:30:THR:HB	1:M:51:LYS:O	1.97	0.64
1:K:126:ALA:HB1	1:K:426:LEU:HD22	1.80	0.64
1:A:452:ARG:HH11	1:A:452:ARG:HG2	1.63	0.64
1:N:90:THR:O	1:N:94:VAL:HG23	1.97	0.64
1:A:44:PHE:CD1	1:A:44:PHE:N	2.66	0.64
1:D:74:VAL:O	1:D:77:VAL:HG13	1.98	0.64
1:G:414:GLY:O	1:G:417:VAL:CG1	2.46	0.64
1:B:74:VAL:O	1:B:77:VAL:HG13	1.97	0.64
1:A:25:ASP:HA	1:A:28:LYS:HE2	1.80	0.64
1:F:18:ARG:CG	1:F:18:ARG:HH11	2.11	0.63
1:L:65:LYS:O	1:L:66:PHE:CB	2.46	0.63
1:A:477:GLY:HA3	1:A:488:MET:SD	2.39	0.63
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.80	0.63
1:M:415:GLY:H	1:M:417:VAL:HG23	1.63	0.63
1:D:417:VAL:HG11	1:D:488:MET:HG3	1.79	0.63
1:B:18:ARG:CB	1:B:18:ARG:NH1	2.37	0.63
1:E:417:VAL:HG11	1:E:488:MET:HG3	1.80	0.63
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.81	0.63
1:B:325:ILE:HG12	1:B:330:THR:HG23	1.81	0.63
1:L:421:ARG:HD2	1:L:474:GLY:O	1.98	0.63
1:G:510:VAL:HG12	1:G:514:MET:CE	2.29	0.62
1:H:166:MET:HE2	1:H:171:LYS:HA	1.80	0.62
1:K:166:MET:HE3	1:K:171:LYS:HA	1.81	0.62
1:M:32:GLY:HA2	1:M:454:ILE:HG23	1.80	0.62
1:F:74:VAL:O	1:F:77:VAL:HG13	1.99	0.62
1:M:385:THR:HG23	1:M:388:GLU:HB2	1.81	0.62
1:I:494:LEU:O	1:I:494:LEU:HD12	2.00	0.62
1:E:18:ARG:CG	1:E:18:ARG:HH11	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.81	0.62
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.65	0.62
1:M:383:ALA:HB3	1:M:389:MET:HB2	1.81	0.62
2:P:50:GLU:CG	2:Q:51:ASN:HB2	2.27	0.62
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.81	0.62
1:F:414:GLY:O	1:F:417:VAL:CG1	2.48	0.62
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.82	0.62
1:G:44:PHE:N	1:G:44:PHE:CD1	2.65	0.62
1:K:84:ALA:O	1:K:498:LYS:HE2	2.00	0.62
1:H:494:LEU:O	1:H:494:LEU:HD12	1.99	0.62
2:P:50:GLU:HG2	2:Q:51:ASN:CB	2.27	0.62
1:E:452:ARG:HG2	1:E:452:ARG:HH11	1.65	0.62
1:B:16:MET:HG3	1:B:520:MET:HE3	1.81	0.62
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.81	0.62
1:G:74:VAL:O	1:G:77:VAL:HG13	1.98	0.62
1:D:16:MET:O	1:D:20:VAL:HG23	2.00	0.62
1:M:444:LEU:HA	1:M:447:MET:CE	2.29	0.61
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.82	0.61
1:J:444:LEU:HD23	1:J:447:MET:CE	2.30	0.61
1:M:279:PRO:O	1:M:285:ARG:HB3	2.01	0.61
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.81	0.61
1:D:510:VAL:HG12	1:D:514:MET:CE	2.30	0.61
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.81	0.61
1:M:47:PRO:HG2	1:N:73:MET:HG3	1.82	0.61
1:C:430:ARG:NH1	1:C:430:ARG:HG2	2.13	0.61
1:H:511:ALA:O	1:H:515:ILE:HD12	1.99	0.61
1:A:325:ILE:HG12	1:A:330:THR:HG23	1.83	0.61
1:B:510:VAL:HG12	1:B:514:MET:CE	2.31	0.61
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.83	0.61
1:K:444:LEU:HA	1:K:447:MET:HE3	1.82	0.61
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.81	0.61
1:C:452:ARG:HG2	1:C:452:ARG:NH1	2.14	0.60
1:E:44:PHE:N	1:E:44:PHE:CD1	2.67	0.60
1:E:74:VAL:O	1:E:77:VAL:HG13	2.01	0.60
1:L:444:LEU:HD23	1:L:447:MET:HE3	1.82	0.60
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.82	0.60
1:E:18:ARG:NH1	1:E:18:ARG:CB	2.42	0.60
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.83	0.60
1:B:414:GLY:O	1:B:417:VAL:CG1	2.49	0.60
1:L:383:ALA:HB3	1:L:389:MET:HB2	1.83	0.60
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:GLU:HB3	1:D:452:ARG:HD2	1.84	0.60
1:I:279:PRO:O	1:I:285:ARG:HB3	2.01	0.60
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.83	0.60
1:C:16:MET:HG3	1:C:520:MET:HE3	1.83	0.60
1:F:510:VAL:HG12	1:F:514:MET:CE	2.31	0.60
1:E:414:GLY:O	1:E:417:VAL:CG1	2.50	0.60
1:J:261:THR:O	1:J:265:ASN:HB2	2.02	0.60
1:I:90:THR:O	1:I:94:VAL:HG23	2.01	0.60
2:T:40:VAL:HB	2:T:62:GLY:H	1.67	0.60
2:P:7:HIS:O	2:P:8:ASP:HB3	2.02	0.59
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.84	0.59
1:F:325:ILE:HG12	1:F:330:THR:HG23	1.83	0.59
1:C:238:GLU:OE2	2:Q:26:VAL:HG23	2.02	0.59
1:C:441:LYS:HB3	1:C:445:ARG:HH21	1.67	0.59
1:E:452:ARG:NH1	1:E:452:ARG:HG2	2.17	0.59
1:I:84:ALA:O	1:I:498:LYS:HE2	2.02	0.59
1:A:510:VAL:HG12	1:A:514:MET:CE	2.32	0.59
1:J:444:LEU:HD23	1:J:447:MET:HE3	1.85	0.59
2:Q:40:VAL:HB	2:Q:62:GLY:H	1.67	0.59
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.84	0.59
1:N:30:THR:HB	1:N:51:LYS:O	2.03	0.59
1:C:448:GLU:HB3	1:C:452:ARG:HD2	1.85	0.59
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.84	0.59
1:D:325:ILE:HG12	1:D:330:THR:HG23	1.84	0.59
1:F:18:ARG:NH1	1:F:18:ARG:CB	2.45	0.59
1:F:452:ARG:HG2	1:F:452:ARG:HH11	1.68	0.59
2:R:7:HIS:O	2:R:8:ASP:HB3	2.02	0.59
2:U:40:VAL:HB	2:U:62:GLY:H	1.66	0.59
1:I:385:THR:HG23	1:I:388:GLU:HB2	1.84	0.59
1:G:18:ARG:NH1	1:G:18:ARG:CB	2.43	0.59
1:A:430:ARG:NH1	1:A:430:ARG:HG2	2.17	0.58
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.85	0.58
2:U:7:HIS:O	2:U:8:ASP:HB3	2.02	0.58
1:J:279:PRO:O	1:J:285:ARG:HB3	2.03	0.58
1:M:261:THR:O	1:M:265:ASN:HB2	2.02	0.58
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.85	0.58
1:H:279:PRO:O	1:H:285:ARG:HB3	2.02	0.58
1:I:261:THR:O	1:I:265:ASN:HB2	2.02	0.58
1:J:494:LEU:HD12	1:J:494:LEU:O	2.04	0.58
2:Q:7:HIS:O	2:Q:8:ASP:HB3	2.04	0.58
1:J:65:LYS:O	1:J:66:PHE:CB	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:444:LEU:HD23	1:N:447:MET:CE	2.33	0.58
1:L:261:THR:O	1:L:265:ASN:HB2	2.04	0.58
1:G:448:GLU:HB3	1:G:452:ARG:HD2	1.86	0.58
1:F:77:VAL:HG23	1:F:92:ALA:HB1	1.86	0.58
1:H:261:THR:O	1:H:265:ASN:HB2	2.04	0.58
1:E:224:ASP:HB3	1:E:302:SER:HA	1.86	0.58
1:H:385:THR:HG23	1:H:388:GLU:HB2	1.86	0.58
1:F:448:GLU:HB3	1:F:452:ARG:HD2	1.86	0.58
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.86	0.58
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.86	0.58
1:N:385:THR:HG23	1:N:388:GLU:HB2	1.86	0.58
1:B:224:ASP:HB3	1:B:302:SER:HA	1.85	0.58
1:C:25:ASP:HA	1:C:28:LYS:HE2	1.85	0.58
1:E:448:GLU:HB3	1:E:452:ARG:HD2	1.86	0.57
2:O:40:VAL:HB	2:O:62:GLY:H	1.69	0.57
1:N:444:LEU:HD23	1:N:447:MET:HE3	1.85	0.57
1:L:279:PRO:O	1:L:285:ARG:HB3	2.04	0.57
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.86	0.57
1:G:224:ASP:HB3	1:G:302:SER:HA	1.86	0.57
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.87	0.57
1:C:455:VAL:HG21	1:C:465:VAL:HG11	1.85	0.57
1:G:42:LYS:HG2	1:G:44:PHE:CE2	2.40	0.57
1:G:33:PRO:HA	1:G:153:ASN:HD21	1.69	0.57
1:I:455:VAL:HG11	1:I:462:PRO:HA	1.86	0.57
1:L:145:ALA:O	1:L:149:THR:HG23	2.05	0.57
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.87	0.57
1:B:448:GLU:HB3	1:B:452:ARG:HD2	1.86	0.57
1:J:149:THR:CG2	1:J:156:GLU:HA	2.34	0.57
1:N:279:PRO:O	1:N:285:ARG:HB3	2.04	0.57
1:C:74:VAL:O	1:C:77:VAL:HG13	2.04	0.57
1:H:444:LEU:HD23	1:H:447:MET:CE	2.34	0.57
1:B:452:ARG:HG2	1:B:452:ARG:HH11	1.70	0.57
1:L:163:ALA:O	1:L:167:ASP:HB2	2.05	0.57
1:M:40:LEU:HD12	1:N:521:VAL:HB	1.86	0.57
1:F:224:ASP:HB3	1:F:302:SER:HA	1.86	0.57
1:E:16:MET:O	1:E:20:VAL:HG23	2.04	0.57
1:C:18:ARG:NH1	1:C:18:ARG:CG	2.67	0.57
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.85	0.57
1:C:16:MET:O	1:C:20:VAL:HG23	2.04	0.57
1:L:444:LEU:HD23	1:L:447:MET:CE	2.35	0.57
1:J:149:THR:HG21	1:J:156:GLU:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:279:PRO:O	1:K:285:ARG:HB3	2.05	0.57
1:B:430:ARG:HG2	1:B:430:ARG:NH1	2.20	0.57
1:C:224:ASP:HB3	1:C:302:SER:HA	1.86	0.57
1:G:25:ASP:HA	1:G:28:LYS:HE2	1.87	0.57
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.86	0.57
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.87	0.57
1:K:40:LEU:HD12	1:L:521:VAL:HB	1.86	0.57
1:H:521:VAL:HB	1:N:40:LEU:HD12	1.86	0.57
1:L:494:LEU:HD12	1:L:494:LEU:O	2.04	0.57
1:M:149:THR:HG21	1:M:156:GLU:HA	1.87	0.56
2:R:40:VAL:HB	2:R:62:GLY:H	1.69	0.56
2:S:40:VAL:HB	2:S:62:GLY:H	1.69	0.56
1:B:261:THR:HG22	2:P:29:GLY:HA3	1.85	0.56
2:O:7:HIS:O	2:O:8:ASP:HB3	2.05	0.56
1:D:430:ARG:NH1	1:D:430:ARG:HG2	2.20	0.56
1:B:33:PRO:HA	1:B:153:ASN:HD21	1.70	0.56
1:M:421:ARG:O	1:M:424:SER:OG	2.19	0.56
1:I:444:LEU:HD23	1:I:447:MET:HE3	1.86	0.56
1:A:16:MET:HG3	1:A:520:MET:HE1	1.87	0.56
1:L:455:VAL:HG11	1:L:462:PRO:HA	1.86	0.56
1:N:261:THR:O	1:N:265:ASN:HB2	2.05	0.56
1:A:224:ASP:HB3	1:A:302:SER:HA	1.86	0.56
2:T:7:HIS:O	2:T:8:ASP:HB3	2.04	0.56
1:A:16:MET:O	1:A:20:VAL:HG23	2.06	0.56
1:B:452:ARG:HG2	1:B:452:ARG:NH1	2.19	0.56
2:S:7:HIS:O	2:S:8:ASP:HB3	2.04	0.56
1:F:44:PHE:HD1	1:F:44:PHE:H	1.52	0.56
1:J:145:ALA:O	1:J:149:THR:HG23	2.06	0.56
2:R:23:GLY:H	2:S:80:ASN:HD21	1.52	0.56
1:C:516:THR:OG1	1:D:37:ASN:ND2	2.39	0.56
1:E:204:PHE:HE1	1:E:274:ALA:HB2	1.70	0.56
1:J:64:ASP:OD1	1:J:65:LYS:O	2.24	0.56
1:M:145:ALA:O	1:M:149:THR:HG23	2.06	0.56
1:N:494:LEU:HD12	1:N:494:LEU:O	2.05	0.56
1:A:204:PHE:HE1	1:A:274:ALA:HB2	1.71	0.56
1:K:261:THR:O	1:K:265:ASN:HB2	2.05	0.56
2:P:40:VAL:HB	2:P:62:GLY:H	1.70	0.56
1:M:455:VAL:HG11	1:M:462:PRO:HA	1.86	0.56
1:F:430:ARG:HG2	1:F:430:ARG:NH1	2.18	0.56
1:E:510:VAL:HG12	1:E:514:MET:CE	2.36	0.56
1:N:149:THR:HG21	1:N:156:GLU:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ASP:HB3	1:D:302:SER:HA	1.88	0.56
1:I:149:THR:CG2	1:I:156:GLU:HA	2.36	0.56
1:E:433:ASN:OD1	1:E:436:GLN:HG3	2.05	0.56
1:F:204:PHE:HE1	1:F:274:ALA:HB2	1.71	0.55
1:I:149:THR:HG21	1:I:156:GLU:HA	1.88	0.55
1:D:414:GLY:O	1:D:417:VAL:CG1	2.55	0.55
2:U:7:HIS:HB2	2:U:46:GLY:O	2.07	0.55
2:T:7:HIS:HB2	2:T:46:GLY:O	2.06	0.55
1:G:441:LYS:HB3	1:G:445:ARG:HH21	1.71	0.55
1:C:204:PHE:HE1	1:C:274:ALA:HB2	1.71	0.55
1:M:149:THR:CG2	1:M:156:GLU:HA	2.37	0.55
1:N:149:THR:CG2	1:N:156:GLU:HA	2.36	0.55
1:G:100:ILE:HG13	1:G:511:ALA:HB1	1.87	0.55
1:K:444:LEU:HD23	1:K:447:MET:HE3	1.87	0.55
1:A:510:VAL:HG12	1:A:514:MET:HE1	1.88	0.55
1:H:163:ALA:O	1:H:167:ASP:HB2	2.06	0.55
2:O:80:ASN:HD21	2:U:23:GLY:H	1.54	0.55
1:M:131:LEU:HD12	1:M:422:VAL:HG11	1.87	0.55
1:H:444:LEU:HA	1:H:447:MET:HE3	1.87	0.55
1:L:149:THR:CG2	1:L:156:GLU:HA	2.37	0.55
1:F:111:MET:HG3	1:F:435:ASP:OD1	2.06	0.55
1:H:383:ALA:HB3	1:H:389:MET:HB2	1.86	0.55
1:I:415:GLY:H	1:I:417:VAL:HG23	1.71	0.55
1:N:234:LEU:N	1:N:235:PRO:HD2	2.21	0.55
1:N:145:ALA:O	1:N:149:THR:HG23	2.06	0.55
1:N:163:ALA:O	1:N:167:ASP:HB2	2.06	0.55
1:F:452:ARG:NH1	1:F:452:ARG:HG2	2.19	0.55
1:J:163:ALA:O	1:J:167:ASP:HB2	2.07	0.55
1:L:47:PRO:HG2	1:M:73:MET:HG3	1.87	0.55
1:A:419:LEU:HG	1:A:447:MET:HG2	1.89	0.55
1:A:77:VAL:HG23	1:A:92:ALA:HB1	1.89	0.55
1:I:234:LEU:N	1:I:235:PRO:HD2	2.22	0.55
1:M:234:LEU:N	1:M:235:PRO:HD2	2.22	0.55
1:G:510:VAL:HG12	1:G:514:MET:HE1	1.89	0.54
1:J:234:LEU:N	1:J:235:PRO:HD2	2.22	0.54
1:N:35:GLY:O	1:N:51:LYS:HE3	2.08	0.54
1:D:441:LYS:HB3	1:D:445:ARG:HH21	1.72	0.54
1:A:461:GLU:OE2	1:N:452:ARG:NH2	2.38	0.54
1:D:204:PHE:HE1	1:D:274:ALA:HB2	1.72	0.54
1:G:430:ARG:HG2	1:G:430:ARG:NH1	2.18	0.54
1:L:149:THR:HG21	1:L:156:GLU:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:ALA:O	1:I:149:THR:HG23	2.07	0.54
1:D:44:PHE:N	1:D:44:PHE:CD1	2.68	0.54
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.88	0.54
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.88	0.54
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.42	0.54
2:P:7:HIS:HB2	2:P:46:GLY:O	2.07	0.54
1:L:234:LEU:N	1:L:235:PRO:HD2	2.22	0.54
2:Q:7:HIS:HB2	2:Q:46:GLY:O	2.08	0.54
1:H:149:THR:HG21	1:H:156:GLU:HA	1.90	0.54
1:H:149:THR:CG2	1:H:156:GLU:HA	2.37	0.54
1:M:27:VAL:HG11	1:M:93:THR:HG21	1.90	0.54
1:K:149:THR:CG2	1:K:156:GLU:HA	2.37	0.54
1:G:204:PHE:HE1	1:G:274:ALA:HB2	1.72	0.54
1:B:204:PHE:HE1	1:B:274:ALA:HB2	1.72	0.54
1:G:44:PHE:H	1:G:44:PHE:HD1	1.52	0.54
1:M:163:ALA:O	1:M:167:ASP:HB2	2.08	0.54
1:A:433:ASN:OD1	1:A:436:GLN:HG3	2.08	0.54
1:H:35:GLY:O	1:H:51:LYS:HE3	2.06	0.54
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.90	0.54
1:K:145:ALA:O	1:K:149:THR:HG23	2.08	0.54
1:N:415:GLY:H	1:N:417:VAL:HG23	1.73	0.54
1:H:267:MET:O	1:H:268:ARG:HB2	2.08	0.54
1:B:16:MET:O	1:B:20:VAL:HG23	2.07	0.54
1:E:77:VAL:HG23	1:E:92:ALA:HB1	1.90	0.54
1:A:111:MET:HG3	1:A:435:ASP:OD1	2.08	0.54
1:K:234:LEU:N	1:K:235:PRO:HD2	2.22	0.54
1:E:33:PRO:HA	1:E:153:ASN:HD21	1.73	0.54
1:L:385:THR:HG23	1:L:388:GLU:HB2	1.88	0.54
1:K:494:LEU:O	1:K:494:LEU:HD12	2.07	0.54
1:J:385:THR:HG23	1:J:388:GLU:HB2	1.89	0.54
1:A:441:LYS:HB3	1:A:445:ARG:HH21	1.73	0.54
1:K:163:ALA:O	1:K:167:ASP:HB2	2.08	0.54
1:H:174:VAL:HB	1:H:376:VAL:HG22	1.90	0.54
1:K:444:LEU:HD23	1:K:447:MET:CE	2.38	0.54
2:O:7:HIS:HB2	2:O:46:GLY:O	2.07	0.54
1:E:441:LYS:HB3	1:E:445:ARG:HH21	1.73	0.54
1:I:30:THR:HB	1:I:51:LYS:O	2.08	0.54
1:H:145:ALA:O	1:H:149:THR:HG23	2.07	0.53
5:A:600:ADP:PB	6:A:602:AF3:F1	2.56	0.53
1:N:413:ALA:HB1	1:N:417:VAL:HB	1.90	0.53
1:E:455:VAL:HG21	1:E:465:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LYS:HG2	2:Q:25:ILE:HD12	1.90	0.53
1:N:16:MET:HB2	1:N:16:MET:CE	2.38	0.53
1:H:84:ALA:O	1:H:498:LYS:HE2	2.08	0.53
1:C:44:PHE:HD1	1:C:44:PHE:H	1.54	0.53
1:L:84:ALA:O	1:L:498:LYS:HE2	2.09	0.53
2:S:7:HIS:HB2	2:S:46:GLY:O	2.08	0.53
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.90	0.53
1:B:77:VAL:HG23	1:B:92:ALA:HB1	1.91	0.53
1:K:267:MET:O	1:K:268:ARG:HB2	2.09	0.53
1:A:42:LYS:HG2	1:A:44:PHE:CE2	2.43	0.53
2:R:7:HIS:HB2	2:R:46:GLY:O	2.08	0.53
1:D:42:LYS:HG2	1:D:44:PHE:CE2	2.44	0.53
1:H:30:THR:HB	1:H:51:LYS:O	2.09	0.53
1:K:16:MET:O	1:K:20:VAL:HG12	2.09	0.53
1:L:350:ARG:HA	1:L:353:ILE:HD12	1.91	0.53
1:J:350:ARG:HA	1:J:353:ILE:HD12	1.91	0.53
1:M:16:MET:CE	1:M:16:MET:HB2	2.39	0.53
1:K:149:THR:HG21	1:K:156:GLU:HA	1.90	0.53
1:N:267:MET:O	1:N:268:ARG:HB2	2.09	0.53
1:E:44:PHE:H	1:E:44:PHE:HD1	1.55	0.52
1:I:174:VAL:HB	1:I:376:VAL:HG22	1.90	0.52
1:I:350:ARG:HA	1:I:353:ILE:HD12	1.91	0.52
1:M:16:MET:HG2	1:M:70:GLY:HA2	1.92	0.52
1:F:197:ARG:CD	1:F:277:LYS:HB2	2.26	0.52
1:K:385:THR:HG23	1:K:388:GLU:HB2	1.90	0.52
1:M:267:MET:O	1:M:268:ARG:HB2	2.08	0.52
1:M:123:ALA:HB2	1:M:440:ILE:CG2	2.31	0.52
1:D:100:ILE:HG13	1:D:511:ALA:HB1	1.90	0.52
1:J:415:GLY:H	1:J:417:VAL:HG23	1.73	0.52
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.92	0.52
1:I:267:MET:O	1:I:268:ARG:HB2	2.09	0.52
1:B:44:PHE:HD1	1:B:44:PHE:H	1.51	0.52
1:D:77:VAL:HG23	1:D:92:ALA:HB1	1.91	0.52
1:M:413:ALA:HB1	1:M:417:VAL:HB	1.90	0.52
1:D:510:VAL:HG12	1:D:514:MET:HE1	1.91	0.52
1:G:452:ARG:NH1	1:G:452:ARG:HG2	2.24	0.52
1:I:221:LEU:HD12	1:I:249:ILE:HG23	1.91	0.52
1:G:455:VAL:HG21	1:G:465:VAL:HG11	1.92	0.52
1:I:163:ALA:O	1:I:167:ASP:HB2	2.10	0.52
1:H:64:ASP:OD1	1:H:65:LYS:O	2.26	0.52
1:H:234:LEU:N	1:H:235:PRO:HD2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HG13	1:B:511:ALA:HB1	1.92	0.52
1:L:193:MET:HG3	1:L:371:LYS:HB3	1.91	0.52
1:J:30:THR:HB	1:J:51:LYS:O	2.09	0.52
1:E:430:ARG:NH1	1:E:430:ARG:HG2	2.14	0.52
1:M:73:MET:HE1	1:M:514:MET:HG2	1.91	0.52
1:K:350:ARG:HA	1:K:353:ILE:HD12	1.91	0.52
1:A:37:ASN:ND2	1:G:516:THR:OG1	2.43	0.52
1:L:267:MET:O	1:L:268:ARG:HB2	2.10	0.52
1:D:111:MET:HG3	1:D:435:ASP:OD1	2.10	0.52
1:A:39:VAL:HG23	1:G:517:THR:HG23	1.92	0.52
1:L:30:THR:HB	1:L:51:LYS:O	2.10	0.52
1:I:35:GLY:O	1:I:51:LYS:HE3	2.09	0.52
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.13	0.52
1:L:126:ALA:CB	1:L:426:LEU:HD22	2.39	0.51
1:M:126:ALA:CB	1:M:426:LEU:HD22	2.40	0.51
1:J:404:ARG:NH1	1:J:404:ARG:HG2	2.24	0.51
1:J:194:GLN:HB2	1:J:331:THR:HB	1.92	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.11	0.51
1:F:510:VAL:HG12	1:F:514:MET:HE1	1.92	0.51
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.92	0.51
1:N:16:MET:CB	1:N:16:MET:CE	2.88	0.51
1:G:111:MET:HG3	1:G:435:ASP:OD1	2.11	0.51
1:H:193:MET:HG3	1:H:371:LYS:HB3	1.91	0.51
1:A:455:VAL:HG21	1:A:465:VAL:HG11	1.92	0.51
1:N:32:GLY:HA2	1:N:454:ILE:HG23	1.91	0.51
1:H:32:GLY:HA2	1:H:454:ILE:HG23	1.92	0.51
1:N:126:ALA:CB	1:N:426:LEU:HD22	2.39	0.51
1:J:455:VAL:HG11	1:J:462:PRO:HA	1.91	0.51
1:I:444:LEU:HA	1:I:447:MET:CE	2.41	0.51
1:J:35:GLY:O	1:J:51:LYS:HE3	2.11	0.51
1:J:290:GLN:HB3	1:J:345:ARG:HH21	1.75	0.51
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.92	0.51
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.66	0.51
1:G:16:MET:O	1:G:20:VAL:HG23	2.11	0.51
1:I:158:VAL:HG13	1:I:396:VAL:HG22	1.91	0.51
1:K:270:ILE:HG23	1:L:229:ASN:HD21	1.76	0.51
1:H:96:ALA:O	1:H:100:ILE:HG13	2.09	0.51
1:H:350:ARG:HA	1:H:353:ILE:HD12	1.91	0.51
1:M:290:GLN:HB3	1:M:345:ARG:HH21	1.76	0.51
1:J:270:ILE:HG23	1:K:229:ASN:HD21	1.76	0.51
1:H:4:LYS:HE2	1:N:59:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:84:ALA:O	1:N:498:LYS:HE2	2.11	0.51
1:C:510:VAL:HG12	1:C:514:MET:HE3	1.92	0.51
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.93	0.51
1:N:173:GLY:O	1:N:404:ARG:NH2	2.43	0.51
1:M:350:ARG:HA	1:M:353:ILE:HD12	1.91	0.51
1:E:487:ASN:O	1:E:491:MET:HG3	2.10	0.51
1:E:461:GLU:OE2	1:K:452:ARG:NH2	2.44	0.51
1:N:174:VAL:HB	1:N:376:VAL:HG22	1.91	0.51
1:L:214:GLU:HG2	1:L:324:VAL:HG12	1.93	0.51
1:N:194:GLN:HB2	1:N:331:THR:HB	1.92	0.51
2:T:50:GLU:CG	2:U:51:ASN:HB2	2.33	0.50
1:J:313:THR:HG22	1:J:314:LEU:H	1.77	0.50
1:J:267:MET:O	1:J:268:ARG:HB2	2.10	0.50
1:D:455:VAL:HG21	1:D:465:VAL:HG11	1.92	0.50
1:B:338:GLU:H	1:B:338:GLU:CD	2.15	0.50
1:M:16:MET:CE	1:M:16:MET:CB	2.89	0.50
1:C:111:MET:HG3	1:C:435:ASP:OD1	2.12	0.50
1:D:130:GLU:OE1	1:D:425:LYS:HD2	2.11	0.50
1:K:194:GLN:HB2	1:K:331:THR:HB	1.94	0.50
1:G:18:ARG:CG	1:G:18:ARG:HH11	2.19	0.50
1:H:66:PHE:HA	1:H:69:MET:HE3	1.93	0.50
1:H:126:ALA:CB	1:H:426:LEU:HD22	2.42	0.50
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.93	0.50
1:F:16:MET:O	1:F:20:VAL:HG23	2.11	0.50
1:H:194:GLN:HB2	1:H:331:THR:HB	1.94	0.50
1:M:270:ILE:HG23	1:N:229:ASN:HD21	1.77	0.50
1:C:100:ILE:HG13	1:C:511:ALA:HB1	1.94	0.50
1:H:214:GLU:HG2	1:H:324:VAL:HG12	1.94	0.50
1:H:455:VAL:HG11	1:H:462:PRO:HA	1.93	0.50
1:K:64:ASP:OD1	1:K:65:LYS:O	2.29	0.50
2:O:6:LEU:O	2:O:7:HIS:O	2.29	0.50
1:G:433:ASN:OD1	1:G:436:GLN:HG3	2.12	0.50
1:N:290:GLN:HB3	1:N:345:ARG:HH21	1.77	0.50
1:F:289:LEU:HA	1:F:292:ILE:HD12	1.94	0.50
1:J:32:GLY:HA2	1:J:454:ILE:HG23	1.94	0.50
1:C:444:LEU:O	1:C:447:MET:HB2	2.12	0.50
1:L:290:GLN:HB3	1:L:345:ARG:HH21	1.76	0.50
1:L:194:GLN:HB2	1:L:331:THR:HB	1.93	0.50
1:C:42:LYS:HG2	1:C:44:PHE:CE2	2.46	0.50
1:C:338:GLU:H	1:C:338:GLU:CD	2.15	0.50
1:L:37:ASN:H	1:L:37:ASN:ND2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:437:ASN:HA	1:M:440:ILE:HD12	1.94	0.50
1:I:47:PRO:HG2	1:J:73:MET:HG3	1.94	0.49
1:N:350:ARG:HA	1:N:353:ILE:HD12	1.93	0.49
1:K:214:GLU:HG2	1:K:324:VAL:HG12	1.94	0.49
1:I:32:GLY:HA2	1:I:454:ILE:HG23	1.94	0.49
1:M:421:ARG:CD	1:M:474:GLY:O	2.59	0.49
1:K:126:ALA:CB	1:K:426:LEU:HD22	2.42	0.49
1:A:44:PHE:H	1:A:44:PHE:HD1	1.55	0.49
1:J:173:GLY:O	1:J:404:ARG:NH2	2.45	0.49
1:H:221:LEU:HD12	1:H:249:ILE:HG23	1.94	0.49
1:I:194:GLN:HB2	1:I:331:THR:HB	1.94	0.49
1:D:512:GLY:O	1:D:515:ILE:HG13	2.12	0.49
1:G:452:ARG:HH11	1:G:452:ARG:HG2	1.76	0.49
1:K:32:GLY:HA2	1:K:454:ILE:HG23	1.94	0.49
1:I:131:LEU:HD12	1:I:422:VAL:HG11	1.93	0.49
1:K:174:VAL:HB	1:K:376:VAL:HG22	1.93	0.49
1:M:174:VAL:HB	1:M:376:VAL:HG22	1.94	0.49
1:B:441:LYS:HB3	1:B:445:ARG:HH21	1.77	0.49
1:I:173:GLY:O	1:I:404:ARG:NH2	2.46	0.49
1:L:221:LEU:HD12	1:L:249:ILE:HG23	1.94	0.49
1:E:100:ILE:HG13	1:E:511:ALA:HB1	1.93	0.49
2:T:6:LEU:O	2:T:7:HIS:O	2.31	0.49
1:L:228:SER:O	1:L:257:GLU:HB3	2.12	0.49
1:I:290:GLN:HB3	1:I:345:ARG:HH21	1.77	0.49
2:S:6:LEU:O	2:S:7:HIS:O	2.31	0.49
2:Q:23:GLY:H	2:R:80:ASN:HD21	1.59	0.49
1:F:487:ASN:O	1:F:491:MET:HG3	2.12	0.49
1:G:338:GLU:H	1:G:338:GLU:CD	2.16	0.49
1:N:214:GLU:HG2	1:N:324:VAL:HG12	1.95	0.49
1:F:419:LEU:HG	1:F:447:MET:HG2	1.94	0.49
1:G:289:LEU:HA	1:G:292:ILE:HD12	1.95	0.49
1:J:16:MET:O	1:J:20:VAL:HG12	2.12	0.49
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.94	0.49
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.95	0.49
1:K:290:GLN:HB3	1:K:345:ARG:HH21	1.78	0.49
1:D:237:LEU:HD21	1:D:271:VAL:HG21	1.94	0.49
2:T:50:GLU:HG2	2:U:51:ASN:CB	2.33	0.49
1:M:452:ARG:HG2	1:M:452:ARG:HH11	1.78	0.49
1:A:461:GLU:OE1	1:N:463:SER:HB3	2.13	0.49
1:H:290:GLN:HB3	1:H:345:ARG:HH21	1.78	0.49
1:C:351:GLN:O	1:C:351:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.95	0.49
1:K:455:VAL:HG11	1:K:462:PRO:HA	1.94	0.49
1:K:193:MET:HG3	1:K:371:LYS:HB3	1.93	0.49
1:H:413:ALA:HB1	1:H:417:VAL:HB	1.95	0.49
1:G:464:VAL:O	1:G:468:THR:HG23	2.13	0.49
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.93	0.49
1:B:455:VAL:HG21	1:B:465:VAL:HG11	1.94	0.49
1:D:338:GLU:H	1:D:338:GLU:CD	2.16	0.49
1:D:87:ASP:OD1	5:D:900:ADP:O1B	2.30	0.49
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.94	0.49
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.95	0.48
1:J:193:MET:HG3	1:J:371:LYS:HB3	1.94	0.48
1:K:30:THR:HB	1:K:51:LYS:O	2.13	0.48
1:B:433:ASN:OD1	1:B:436:GLN:HG3	2.13	0.48
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.95	0.48
1:B:237:LEU:HD21	1:B:271:VAL:HG21	1.94	0.48
1:A:338:GLU:H	1:A:338:GLU:CD	2.17	0.48
1:A:451:LEU:O	1:A:451:LEU:HD22	2.12	0.48
1:H:37:ASN:ND2	1:H:37:ASN:H	2.10	0.48
1:G:266:THR:HG23	1:G:272:LYS:HA	1.95	0.48
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.96	0.48
1:M:194:GLN:HB2	1:M:331:THR:HB	1.94	0.48
1:A:95:LEU:HD13	1:A:504:LEU:HD23	1.95	0.48
1:F:25:ASP:HA	1:F:28:LYS:HE2	1.95	0.48
1:M:313:THR:HG22	1:M:314:LEU:H	1.77	0.48
1:J:174:VAL:HB	1:J:376:VAL:HG22	1.95	0.48
1:E:419:LEU:HG	1:E:447:MET:HG2	1.96	0.48
1:F:33:PRO:HA	1:F:153:ASN:HD21	1.78	0.48
1:B:419:LEU:HG	1:B:447:MET:HG2	1.94	0.48
1:M:404:ARG:NH1	1:M:404:ARG:HG2	2.27	0.48
1:K:96:ALA:O	1:K:100:ILE:HG13	2.13	0.48
1:M:221:LEU:HD12	1:M:249:ILE:HG23	1.94	0.48
1:F:338:GLU:CD	1:F:338:GLU:H	2.16	0.48
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.96	0.48
2:R:6:LEU:O	2:R:7:HIS:O	2.31	0.48
1:E:237:LEU:HD21	1:E:271:VAL:HG21	1.94	0.48
1:H:173:GLY:O	1:H:404:ARG:NH2	2.47	0.48
1:D:451:LEU:HD22	1:D:451:LEU:O	2.13	0.48
1:F:266:THR:HG23	1:F:272:LYS:HA	1.96	0.48
1:M:415:GLY:N	1:M:417:VAL:HG23	2.27	0.48
2:Q:6:LEU:O	2:Q:7:HIS:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:CD1	5:A:600:ADP:H5'2	2.44	0.48
1:E:111:MET:HG3	1:E:435:ASP:OD1	2.13	0.48
1:K:228:SER:O	1:K:257:GLU:HB3	2.13	0.48
1:C:365:LEU:O	1:C:369:VAL:HG13	2.14	0.48
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.94	0.48
1:F:455:VAL:HG21	1:F:465:VAL:HG11	1.96	0.48
1:C:237:LEU:HD21	1:C:271:VAL:HG21	1.95	0.48
1:B:487:ASN:O	1:B:491:MET:HG3	2.14	0.48
1:G:487:ASN:O	1:G:491:MET:HG3	2.13	0.48
1:D:266:THR:HG23	1:D:272:LYS:HA	1.96	0.48
1:A:365:LEU:O	1:A:369:VAL:HG13	2.14	0.48
1:H:227:ILE:HD12	1:H:309:LEU:HD11	1.96	0.48
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.96	0.48
1:G:237:LEU:HD21	1:G:271:VAL:HG21	1.95	0.48
1:D:433:ASN:OD1	1:D:436:GLN:HG3	2.13	0.48
1:B:289:LEU:HA	1:B:292:ILE:HD12	1.96	0.48
1:E:338:GLU:CD	1:E:338:GLU:H	2.17	0.48
1:H:437:ASN:HA	1:H:440:ILE:HD12	1.95	0.48
1:C:16:MET:CG	1:C:520:MET:HE3	2.43	0.48
1:G:351:GLN:HG2	1:G:351:GLN:O	2.14	0.48
1:J:16:MET:CE	1:J:16:MET:CB	2.92	0.48
1:J:16:MET:CE	1:J:16:MET:HB2	2.44	0.48
2:U:6:LEU:O	2:U:7:HIS:O	2.32	0.48
1:M:404:ARG:HH11	1:M:404:ARG:CG	2.27	0.48
1:F:455:VAL:HG11	1:F:462:PRO:HA	1.96	0.48
1:D:289:LEU:HA	1:D:292:ILE:HD12	1.96	0.48
1:H:228:SER:O	1:H:257:GLU:HB3	2.14	0.48
1:B:25:ASP:HA	1:B:28:LYS:HE2	1.94	0.48
1:I:16:MET:O	1:I:20:VAL:HG12	2.14	0.48
2:O:23:GLY:H	2:P:80:ASN:HD21	1.62	0.48
1:F:18:ARG:CG	1:F:18:ARG:NH1	2.73	0.47
1:H:415:GLY:H	1:H:417:VAL:HG23	1.77	0.47
1:C:218:PRO:HB3	1:C:246:PRO:HB2	1.97	0.47
1:C:77:VAL:HG23	1:C:92:ALA:HB1	1.96	0.47
1:A:237:LEU:HD21	1:A:271:VAL:HG21	1.95	0.47
1:L:173:GLY:O	1:L:404:ARG:NH2	2.47	0.47
1:N:96:ALA:O	1:N:100:ILE:HG13	2.13	0.47
1:I:227:ILE:HD12	1:I:309:LEU:HD11	1.95	0.47
1:E:289:LEU:HA	1:E:292:ILE:HD12	1.96	0.47
1:I:313:THR:HG22	1:I:314:LEU:H	1.78	0.47
1:J:221:LEU:HD12	1:J:249:ILE:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:173:GLY:O	1:K:404:ARG:NH2	2.48	0.47
1:J:228:SER:O	1:J:257:GLU:HB3	2.15	0.47
1:L:313:THR:HG22	1:L:314:LEU:H	1.78	0.47
1:C:197:ARG:CD	1:C:277:LYS:HB2	2.27	0.47
1:B:266:THR:HG23	1:B:272:LYS:HA	1.96	0.47
1:N:221:LEU:HD12	1:N:249:ILE:HG23	1.95	0.47
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.97	0.47
1:E:266:THR:HG23	1:E:272:LYS:HA	1.96	0.47
1:A:266:THR:HG23	1:A:272:LYS:HA	1.97	0.47
1:C:455:VAL:HG11	1:C:462:PRO:HA	1.95	0.47
1:B:365:LEU:O	1:B:369:VAL:HG13	2.15	0.47
1:J:449:ALA:N	1:J:450:PRO:CD	2.77	0.47
1:A:100:ILE:HG13	1:A:511:ALA:HB1	1.97	0.47
1:B:18:ARG:CG	1:B:18:ARG:NH1	2.68	0.47
1:C:266:THR:HG23	1:C:272:LYS:HA	1.97	0.47
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.95	0.47
1:M:214:GLU:HG2	1:M:324:VAL:HG12	1.96	0.47
1:H:217:SER:HA	1:H:320:ALA:O	2.15	0.47
1:J:214:GLU:HG2	1:J:324:VAL:HG12	1.96	0.47
1:A:289:LEU:HA	1:A:292:ILE:HD12	1.97	0.47
1:F:218:PRO:HB3	1:F:246:PRO:HB2	1.96	0.47
1:I:126:ALA:CB	1:I:426:LEU:HD22	2.43	0.47
1:N:455:VAL:HG11	1:N:462:PRO:HA	1.96	0.47
1:N:313:THR:HG22	1:N:314:LEU:H	1.80	0.47
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.97	0.47
1:B:512:GLY:O	1:B:515:ILE:HG13	2.15	0.47
1:F:351:GLN:HG2	1:F:351:GLN:O	2.13	0.47
1:B:218:PRO:HB3	1:B:246:PRO:HB2	1.97	0.47
1:M:64:ASP:OD1	1:M:65:LYS:O	2.33	0.47
1:F:365:LEU:O	1:F:369:VAL:HG13	2.14	0.47
1:K:268:ARG:HD2	1:K:268:ARG:HA	1.35	0.47
1:L:32:GLY:HA2	1:L:454:ILE:HG23	1.95	0.47
1:C:31:LEU:CD1	5:C:800:ADP:H5'2	2.45	0.47
1:A:351:GLN:HG2	1:A:351:GLN:O	2.15	0.47
1:L:415:GLY:H	1:L:417:VAL:HG23	1.79	0.47
1:L:174:VAL:HB	1:L:376:VAL:HG22	1.95	0.47
1:K:221:LEU:HD12	1:K:249:ILE:HG23	1.96	0.47
1:I:217:SER:HA	1:I:320:ALA:O	2.15	0.47
1:G:365:LEU:O	1:G:369:VAL:HG13	2.15	0.47
1:D:365:LEU:O	1:D:369:VAL:HG13	2.15	0.47
1:A:218:PRO:HB3	1:A:246:PRO:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG22	1:G:519:CYS:HB3	1.97	0.47
1:E:42:LYS:HG2	1:E:44:PHE:CE2	2.50	0.47
1:C:487:ASN:O	1:C:491:MET:HG3	2.15	0.47
1:N:228:SER:O	1:N:257:GLU:HB3	2.15	0.47
1:K:313:THR:HG22	1:K:314:LEU:HD12	1.97	0.47
1:L:59:GLU:HG3	1:M:4:LYS:HE2	1.96	0.47
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.96	0.47
1:E:351:GLN:HG2	1:E:351:GLN:O	2.14	0.47
1:I:107:VAL:HG11	1:I:515:ILE:HG23	1.97	0.46
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.96	0.46
1:J:404:ARG:CG	1:J:404:ARG:HH11	2.27	0.46
1:F:237:LEU:HD21	1:F:271:VAL:HG21	1.96	0.46
1:H:40:LEU:HD12	1:I:521:VAL:HB	1.96	0.46
1:L:227:ILE:HD12	1:L:309:LEU:HD11	1.96	0.46
1:H:43:SER:HB2	1:H:44:PHE:CD1	2.50	0.46
1:M:95:LEU:HB2	1:M:95:LEU:CD1	2.45	0.46
2:P:6:LEU:O	2:P:7:HIS:O	2.32	0.46
1:B:147:VAL:HG22	1:B:403:THR:HG22	1.97	0.46
1:K:227:ILE:HD12	1:K:309:LEU:HD11	1.96	0.46
1:M:95:LEU:O	1:M:98:ALA:CB	2.62	0.46
1:M:419:LEU:HD22	1:M:500:THR:CG2	2.45	0.46
1:M:106:ALA:O	1:M:109:ALA:HB3	2.16	0.46
1:D:162:ILE:HG12	1:D:400:LEU:HD23	1.98	0.46
1:D:351:GLN:HG2	1:D:351:GLN:O	2.15	0.46
1:B:351:GLN:O	1:B:351:GLN:HG2	2.15	0.46
1:F:512:GLY:O	1:F:515:ILE:HG13	2.15	0.46
1:E:218:PRO:HB3	1:E:246:PRO:HB2	1.97	0.46
1:E:464:VAL:O	1:E:468:THR:HG23	2.14	0.46
1:K:313:THR:HG22	1:K:314:LEU:H	1.79	0.46
1:N:217:SER:HA	1:N:320:ALA:O	2.16	0.46
1:M:227:ILE:HD12	1:M:309:LEU:HD11	1.97	0.46
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.72	0.46
1:J:448:GLU:O	1:J:452:ARG:HD2	2.15	0.46
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.96	0.46
1:K:43:SER:HB2	1:K:44:PHE:CD1	2.50	0.46
1:J:217:SER:HA	1:J:320:ALA:O	2.15	0.46
1:E:88:GLY:HA2	5:E:1000:ADP:O2B	2.16	0.46
1:D:218:PRO:HB3	1:D:246:PRO:HB2	1.98	0.46
1:F:222:LEU:HD12	1:F:293:ALA:HB2	1.98	0.46
1:N:104:LEU:HD12	1:N:104:LEU:HA	1.77	0.46
1:C:33:PRO:HA	1:C:153:ASN:ND2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:365:LEU:O	1:E:369:VAL:HG13	2.15	0.46
1:N:149:THR:HG23	1:N:159:GLY:HA3	1.98	0.46
1:C:289:LEU:HA	1:C:292:ILE:HD12	1.97	0.46
1:H:161:LEU:HD21	1:H:185:ASP:HB3	1.98	0.46
1:E:162:ILE:HG12	1:E:400:LEU:HD23	1.98	0.46
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.50	0.46
1:C:366:GLN:O	1:C:369:VAL:HG22	2.16	0.46
1:M:173:GLY:O	1:M:404:ARG:NH2	2.48	0.46
1:H:313:THR:HG22	1:H:314:LEU:H	1.80	0.46
1:K:161:LEU:HD21	1:K:185:ASP:HB3	1.97	0.46
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.97	0.46
1:N:16:MET:O	1:N:20:VAL:HG12	2.15	0.46
1:G:218:PRO:HB3	1:G:246:PRO:HB2	1.98	0.46
1:K:37:ASN:ND2	1:K:37:ASN:H	2.13	0.46
1:C:477:GLY:HA3	1:C:488:MET:SD	2.56	0.46
1:B:261:THR:HG22	2:P:29:GLY:CA	2.45	0.46
1:J:437:ASN:HA	1:J:440:ILE:HD12	1.98	0.46
1:I:421:ARG:CD	1:I:474:GLY:O	2.63	0.46
1:I:404:ARG:HG2	1:I:404:ARG:NH1	2.31	0.46
1:K:35:GLY:O	1:K:51:LYS:HE3	2.15	0.46
1:C:31:LEU:HD12	5:C:800:ADP:H5'2	1.98	0.46
1:A:409:GLU:CD	1:A:501:ARG:HH21	2.18	0.46
1:G:222:LEU:HD12	1:G:293:ALA:HB2	1.98	0.46
1:I:77:VAL:HG13	1:I:506:TYR:HB3	1.97	0.45
1:G:197:ARG:CD	1:G:277:LYS:HB2	2.28	0.45
1:C:31:LEU:HD23	1:C:453:GLN:HB3	1.97	0.45
1:M:161:LEU:HD21	1:M:185:ASP:HB3	1.99	0.45
1:N:227:ILE:HD12	1:N:309:LEU:HD11	1.98	0.45
1:G:31:LEU:HD23	1:G:453:GLN:HB3	1.97	0.45
1:C:512:GLY:O	1:C:515:ILE:HG13	2.16	0.45
1:K:217:SER:HA	1:K:320:ALA:O	2.16	0.45
1:L:158:VAL:HG13	1:L:396:VAL:HG22	1.98	0.45
1:J:104:LEU:HA	1:J:104:LEU:HD12	1.72	0.45
2:U:7:HIS:HB3	2:U:45:ASN:HD22	1.81	0.45
1:L:38:VAL:HG22	1:M:519:CYS:HB3	1.98	0.45
1:J:84:ALA:O	1:J:498:LYS:HE2	2.16	0.45
1:M:43:SER:HB2	1:M:44:PHE:CD1	2.52	0.45
1:M:66:PHE:HA	1:M:69:MET:HE3	1.97	0.45
1:L:64:ASP:OD1	1:L:65:LYS:O	2.35	0.45
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.99	0.45
1:B:366:GLN:O	1:B:369:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:MET:HB3	1:E:237:LEU:HD12	1.98	0.45
1:I:214:GLU:HG2	1:I:324:VAL:HG12	1.98	0.45
1:L:43:SER:HB2	1:L:44:PHE:CD1	2.51	0.45
1:K:415:GLY:H	1:K:417:VAL:HG23	1.81	0.45
1:I:419:LEU:HA	1:I:419:LEU:HD13	1.78	0.45
1:M:444:LEU:CD2	1:M:447:MET:HE1	2.44	0.45
1:N:107:VAL:HG11	1:N:515:ILE:HG23	1.98	0.45
1:A:320:ALA:HA	1:A:335:GLY:HA2	1.99	0.45
2:O:20:LYS:HB3	2:O:27:LEU:HG	1.97	0.45
1:D:461:GLU:OE1	1:J:463:SER:HB3	2.17	0.45
1:M:448:GLU:O	1:M:452:ARG:HD2	2.16	0.45
1:A:366:GLN:O	1:A:369:VAL:HG22	2.16	0.45
1:D:366:GLN:O	1:D:369:VAL:HG22	2.17	0.45
1:H:149:THR:HG23	1:H:159:GLY:HA3	1.99	0.45
1:L:16:MET:O	1:L:20:VAL:HG12	2.16	0.45
1:L:161:LEU:HD21	1:L:185:ASP:HB3	1.98	0.45
1:M:228:SER:O	1:M:257:GLU:HB3	2.16	0.45
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.98	0.45
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.82	0.45
1:E:455:VAL:HG11	1:E:462:PRO:HA	1.98	0.45
1:H:131:LEU:HD12	1:H:422:VAL:HG11	1.98	0.45
1:D:222:LEU:HD12	1:D:293:ALA:HB2	1.99	0.45
1:E:54:VAL:O	1:E:58:ARG:HG3	2.17	0.45
1:N:64:ASP:OD1	1:N:65:LYS:O	2.34	0.45
1:M:35:GLY:O	1:M:51:LYS:HE3	2.17	0.45
1:I:404:ARG:HH11	1:I:404:ARG:CG	2.30	0.45
1:E:31:LEU:HD23	1:E:453:GLN:HB3	1.99	0.45
1:D:381:VAL:CG1	1:D:392:LYS:HG2	2.47	0.45
1:F:461:GLU:HB2	1:F:464:VAL:HB	1.99	0.45
1:M:266:THR:HG22	1:M:273:VAL:H	1.82	0.45
1:M:217:SER:HA	1:M:320:ALA:O	2.17	0.45
1:L:217:SER:HA	1:L:320:ALA:O	2.17	0.45
1:D:513:LEU:HD23	1:D:513:LEU:HA	1.76	0.45
2:O:50:GLU:CG	2:P:51:ASN:HB2	2.37	0.45
1:J:107:VAL:HG11	1:J:515:ILE:HG23	1.99	0.45
1:I:149:THR:HG23	1:I:159:GLY:HA3	1.99	0.45
1:M:131:LEU:CD1	1:M:422:VAL:HG11	2.46	0.45
1:L:313:THR:HG22	1:L:314:LEU:HD12	1.98	0.45
1:A:22:VAL:HG11	1:A:62:LEU:HD11	1.99	0.45
2:P:20:LYS:HB3	2:P:27:LEU:HG	1.99	0.45
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MET:CG	1:B:520:MET:HE3	2.46	0.45
1:G:455:VAL:HG11	1:G:462:PRO:HA	1.98	0.45
1:L:37:ASN:ND2	1:L:37:ASN:N	2.65	0.45
1:D:32:GLY:HA2	5:D:900:ADP:H5'1	1.99	0.45
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.98	0.45
1:A:225:LYS:H	1:A:225:LYS:HG3	1.66	0.45
1:F:4:LYS:HG3	1:G:59:GLU:O	2.17	0.45
1:E:222:LEU:HD12	1:E:293:ALA:HB2	1.99	0.45
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.99	0.44
1:J:126:ALA:CB	1:J:426:LEU:HD22	2.43	0.44
1:F:366:GLN:O	1:F:369:VAL:HG22	2.17	0.44
2:T:20:LYS:HB3	2:T:27:LEU:HG	1.98	0.44
1:N:43:SER:HB2	1:N:44:PHE:CD1	2.52	0.44
1:H:77:VAL:HG13	1:H:506:TYR:HB3	1.99	0.44
1:D:77:VAL:HG12	1:D:510:VAL:HG21	1.98	0.44
1:G:77:VAL:HG12	1:G:510:VAL:HG21	1.99	0.44
1:J:313:THR:HG22	1:J:314:LEU:HD12	1.99	0.44
1:K:100:ILE:O	1:K:104:LEU:HB2	2.17	0.44
1:L:26:ALA:HA	1:M:8:PHE:HE2	1.82	0.44
1:B:320:ALA:HA	1:B:335:GLY:HA2	1.98	0.44
1:J:247:LEU:HB3	1:J:273:VAL:HG12	1.99	0.44
1:A:421:ARG:HA	1:A:421:ARG:HD3	1.78	0.44
1:M:107:VAL:HG11	1:M:515:ILE:HG23	1.99	0.44
1:L:437:ASN:HA	1:L:440:ILE:HD12	1.99	0.44
2:P:7:HIS:HB3	2:P:45:ASN:HD22	1.83	0.44
1:C:32:GLY:HA2	5:C:800:ADP:H5'1	1.98	0.44
1:A:225:LYS:HG2	1:A:303:GLU:HB2	1.99	0.44
2:Q:20:LYS:HB3	2:Q:27:LEU:HG	1.99	0.44
1:N:158:VAL:HG13	1:N:396:VAL:HG22	1.99	0.44
1:M:54:VAL:HG12	1:M:58:ARG:HH22	1.82	0.44
1:J:513:LEU:HD12	1:J:513:LEU:HA	1.82	0.44
1:J:444:LEU:HA	1:J:447:MET:CE	2.45	0.44
1:F:233:MET:HB3	1:F:237:LEU:HD12	1.98	0.44
1:H:158:VAL:HG13	1:H:396:VAL:HG22	1.99	0.44
1:J:161:LEU:HD21	1:J:185:ASP:HB3	1.98	0.44
1:G:417:VAL:O	1:G:418:ALA:C	2.56	0.44
1:L:444:LEU:HA	1:L:447:MET:CE	2.45	0.44
1:M:149:THR:HG23	1:M:159:GLY:HA3	1.99	0.44
1:I:313:THR:HG22	1:I:314:LEU:HD12	1.98	0.44
1:H:43:SER:HB2	1:H:44:PHE:HD1	1.82	0.44
1:F:259:LEU:O	1:F:263:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:227:ILE:HD12	1:J:309:LEU:HD11	1.98	0.44
1:K:27:VAL:HG11	1:K:93:THR:HG21	2.00	0.44
1:G:18:ARG:NH1	1:G:18:ARG:CG	2.79	0.44
2:O:7:HIS:HB3	2:O:45:ASN:HD22	1.82	0.44
1:H:32:GLY:HA2	1:H:454:ILE:HD13	1.99	0.44
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.99	0.44
1:D:225:LYS:HG2	1:D:303:GLU:HB2	1.98	0.44
2:U:20:LYS:HB3	2:U:27:LEU:HG	1.99	0.44
1:K:262:LEU:HD22	1:K:273:VAL:HG21	2.00	0.44
1:G:225:LYS:H	1:G:225:LYS:HG3	1.66	0.44
1:F:100:ILE:HG13	1:F:511:ALA:HB1	1.99	0.44
1:G:366:GLN:O	1:G:369:VAL:HG22	2.17	0.44
1:A:444:LEU:O	1:A:447:MET:HB2	2.17	0.44
5:C:800:ADP:O3B	6:C:802:AF3:F3	2.25	0.44
1:C:87:ASP:OD1	5:C:800:ADP:O1B	2.35	0.44
1:I:496:PRO:HB2	1:I:499:VAL:HG13	2.00	0.44
1:I:43:SER:HB2	1:I:44:PHE:CD1	2.52	0.44
1:L:419:LEU:HA	1:L:419:LEU:HD13	1.80	0.44
1:J:66:PHE:O	1:J:67:GLU:C	2.56	0.44
1:F:77:VAL:HG12	1:F:510:VAL:HG21	1.98	0.44
1:I:82:ASN:HB2	1:I:89:THR:OG1	2.18	0.44
1:E:259:LEU:O	1:E:263:VAL:HG23	2.18	0.44
1:G:77:VAL:HG23	1:G:92:ALA:HB1	2.00	0.44
2:Q:7:HIS:HB3	2:Q:45:ASN:HD22	1.83	0.44
1:C:268:ARG:HD2	2:Q:27:LEU:HD13	2.00	0.44
1:N:286:LYS:NZ	1:N:304:GLU:OE1	2.51	0.44
1:A:162:ILE:HG12	1:A:400:LEU:HD23	2.00	0.44
1:N:161:LEU:HD21	1:N:185:ASP:HB3	2.00	0.44
1:N:16:MET:HG2	1:N:70:GLY:HA2	1.98	0.43
1:J:149:THR:HG23	1:J:159:GLY:HA3	2.00	0.43
1:N:448:GLU:O	1:N:452:ARG:HD2	2.18	0.43
1:M:313:THR:HG22	1:M:314:LEU:HD12	1.99	0.43
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.33	0.43
1:C:233:MET:HB3	1:C:237:LEU:HD12	1.99	0.43
1:M:44:PHE:CD1	1:M:44:PHE:N	2.86	0.43
1:G:225:LYS:HG2	1:G:303:GLU:HB2	1.99	0.43
1:A:234:LEU:HB2	1:A:235:PRO:HD3	2.00	0.43
1:N:131:LEU:HD12	1:N:422:VAL:HG11	1.99	0.43
1:G:320:ALA:HA	1:G:335:GLY:HA2	2.00	0.43
2:R:20:LYS:HB3	2:R:27:LEU:HG	1.98	0.43
1:K:65:LYS:HG3	1:K:65:LYS:H	1.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:PHE:H	1:I:69:MET:HG3	1.83	0.43
1:H:107:VAL:HG11	1:H:515:ILE:HG23	2.00	0.43
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.33	0.43
1:N:43:SER:HB2	1:N:44:PHE:HD1	1.84	0.43
1:G:22:VAL:HG11	1:G:62:LEU:HD11	2.00	0.43
1:M:38:VAL:HG22	1:N:519:CYS:HB3	1.99	0.43
1:F:234:LEU:HB2	1:F:235:PRO:HD3	2.00	0.43
1:B:31:LEU:CD1	5:B:700:ADP:H5'2	2.48	0.43
2:S:78:ILE:HD13	2:S:83:VAL:HG21	2.00	0.43
1:N:16:MET:CG	1:N:16:MET:CE	2.92	0.43
1:A:31:LEU:HD12	5:A:600:ADP:H5'2	2.00	0.43
1:K:413:ALA:HB1	1:K:417:VAL:HB	1.99	0.43
1:C:54:VAL:O	1:C:58:ARG:HG3	2.18	0.43
1:M:506:TYR:O	1:M:507:ALA:C	2.57	0.43
1:I:228:SER:O	1:I:257:GLU:HB3	2.17	0.43
1:C:222:LEU:HD12	1:C:293:ALA:HB2	1.99	0.43
1:N:262:LEU:HD22	1:N:273:VAL:HG21	2.01	0.43
1:K:131:LEU:HD12	1:K:422:VAL:HG11	2.00	0.43
1:J:66:PHE:HA	1:J:69:MET:HE3	1.99	0.43
2:S:7:HIS:HB3	2:S:45:ASN:HD22	1.83	0.43
1:M:247:LEU:HB3	1:M:273:VAL:HG12	2.00	0.43
1:I:198:GLY:O	1:I:276:VAL:HG12	2.19	0.43
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.84	0.43
2:S:20:LYS:HB3	2:S:27:LEU:HG	1.99	0.43
1:D:247:LEU:HB3	1:D:273:VAL:HG12	2.00	0.43
1:M:16:MET:CG	1:M:16:MET:CE	2.93	0.43
1:D:302:SER:HB3	1:D:305:ILE:HG12	2.00	0.43
1:G:233:MET:HB3	1:G:237:LEU:HD12	1.99	0.43
1:L:44:PHE:N	1:L:44:PHE:CD1	2.87	0.43
1:F:464:VAL:O	1:F:468:THR:HG23	2.18	0.43
1:J:286:LYS:NZ	1:J:304:GLU:OE1	2.51	0.43
1:G:130:GLU:OE1	1:G:425:LYS:HD2	2.18	0.43
1:B:259:LEU:O	1:B:263:VAL:HG23	2.18	0.43
1:F:225:LYS:HG2	1:F:303:GLU:HB2	1.99	0.43
2:O:50:GLU:HG2	2:P:51:ASN:CB	2.38	0.43
1:H:313:THR:HG22	1:H:314:LEU:HD12	1.99	0.43
1:B:225:LYS:HG2	1:B:303:GLU:HB2	1.99	0.43
1:C:259:LEU:O	1:C:263:VAL:HG23	2.18	0.43
1:I:161:LEU:HD21	1:I:185:ASP:HB3	2.01	0.43
1:N:419:LEU:HA	1:N:419:LEU:HD13	1.76	0.43
1:D:146:GLN:HE21	1:D:146:GLN:HB2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:LEU:HD22	1:B:451:LEU:O	2.19	0.43
1:M:451:LEU:O	1:M:452:ARG:C	2.57	0.43
2:T:7:HIS:HB3	2:T:45:ASN:HD22	1.84	0.43
1:M:73:MET:HE1	1:M:514:MET:CE	2.49	0.43
1:M:268:ARG:HD2	1:M:268:ARG:HA	1.36	0.43
1:C:419:LEU:HG	1:C:447:MET:HG2	2.01	0.43
1:H:44:PHE:CD1	1:H:44:PHE:N	2.86	0.43
1:M:124:VAL:O	1:M:128:VAL:HG23	2.19	0.43
1:J:43:SER:HB2	1:J:44:PHE:HD1	1.84	0.43
1:L:247:LEU:HB3	1:L:273:VAL:HG12	2.01	0.43
1:M:82:ASN:HB2	1:M:89:THR:OG1	2.19	0.43
1:H:197:ARG:HG2	1:H:277:LYS:O	2.18	0.43
1:E:512:GLY:O	1:E:515:ILE:HG13	2.18	0.43
1:N:64:ASP:HB3	1:N:67:GLU:HB2	2.00	0.43
1:M:65:LYS:H	1:M:65:LYS:HG3	1.47	0.43
1:H:421:ARG:CD	1:H:474:GLY:O	2.65	0.43
1:F:302:SER:HB3	1:F:305:ILE:HG12	2.01	0.43
1:C:302:SER:HB3	1:C:305:ILE:HG12	2.01	0.43
1:L:35:GLY:O	1:L:51:LYS:HE3	2.18	0.43
1:A:455:VAL:HG11	1:A:462:PRO:HA	2.00	0.43
1:H:404:ARG:CG	1:H:404:ARG:HH11	2.32	0.43
1:J:43:SER:HB2	1:J:44:PHE:CD1	2.53	0.43
1:E:225:LYS:HG2	1:E:303:GLU:HB2	1.99	0.43
1:D:320:ALA:HA	1:D:335:GLY:HA2	2.00	0.43
1:N:197:ARG:HG2	1:N:277:LYS:O	2.19	0.43
1:K:149:THR:HG23	1:K:159:GLY:HA3	2.00	0.43
1:A:233:MET:HB3	1:A:237:LEU:HD12	1.99	0.43
1:H:38:VAL:HG22	1:I:519:CYS:HB3	2.01	0.43
1:D:22:VAL:HG11	1:D:62:LEU:HD11	2.01	0.43
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.99	0.43
2:Q:78:ILE:HD13	2:Q:83:VAL:HG21	2.00	0.43
1:I:247:LEU:HB3	1:I:273:VAL:HG12	2.01	0.43
1:M:504:LEU:O	1:M:504:LEU:HD22	2.19	0.43
1:D:444:LEU:O	1:D:447:MET:HB2	2.18	0.43
1:B:421:ARG:HA	1:B:421:ARG:HD3	1.78	0.43
1:J:16:MET:HG2	1:J:70:GLY:HA2	2.01	0.43
1:E:77:VAL:HG12	1:E:510:VAL:HG21	1.99	0.43
1:G:16:MET:HG3	1:G:520:MET:HE3	2.01	0.43
1:D:233:MET:HB3	1:D:237:LEU:HD12	2.00	0.43
1:J:221:LEU:HD23	1:J:317:LEU:HD11	2.00	0.43
1:N:262:LEU:O	1:N:266:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:HB2	1:A:93:THR:OG1	2.19	0.43
1:A:147:VAL:HG22	1:A:403:THR:HG22	1.99	0.43
1:I:63:GLU:HA	1:J:3:ALA:CB	2.49	0.43
1:A:193:MET:HG3	1:A:371:LYS:HB3	2.01	0.43
1:H:198:GLY:O	1:H:276:VAL:HG12	2.18	0.43
1:E:234:LEU:HB2	1:E:235:PRO:HD3	2.01	0.43
1:M:31:LEU:O	1:M:32:GLY:O	2.37	0.42
1:L:77:VAL:HG12	1:L:78:ALA:N	2.33	0.42
1:D:455:VAL:HG11	1:D:462:PRO:HA	2.00	0.42
1:I:16:MET:HG2	1:I:70:GLY:HA2	2.01	0.42
2:U:78:ILE:HD13	2:U:83:VAL:HG21	2.00	0.42
1:L:131:LEU:HD12	1:L:422:VAL:HG11	2.00	0.42
1:I:38:VAL:HG12	1:I:40:LEU:HD13	2.01	0.42
1:I:172:GLU:HA	1:I:172:GLU:OE1	2.19	0.42
1:C:381:VAL:CG1	1:C:392:LYS:HG2	2.49	0.42
1:N:452:ARG:HH11	1:N:452:ARG:HG2	1.83	0.42
1:D:130:GLU:O	1:D:133:ALA:HB3	2.19	0.42
1:G:461:GLU:HB2	1:G:464:VAL:HB	2.01	0.42
1:K:247:LEU:HB3	1:K:273:VAL:HG12	2.01	0.42
1:D:259:LEU:O	1:D:263:VAL:HG23	2.19	0.42
1:E:381:VAL:CG1	1:E:392:LYS:HG2	2.50	0.42
1:C:225:LYS:HG2	1:C:303:GLU:HB2	2.00	0.42
1:H:247:LEU:HB3	1:H:273:VAL:HG12	2.02	0.42
2:P:78:ILE:HD13	2:P:83:VAL:HG21	2.01	0.42
1:J:147:VAL:HG21	1:J:411:VAL:HG11	2.01	0.42
1:M:37:ASN:H	1:M:37:ASN:ND2	2.17	0.42
1:J:38:VAL:HG12	1:J:40:LEU:HD13	2.02	0.42
1:I:64:ASP:OD1	1:I:65:LYS:O	2.38	0.42
1:C:77:VAL:HG12	1:C:510:VAL:HG21	2.00	0.42
1:L:285:ARG:HA	1:L:288:MET:HB2	2.01	0.42
1:N:404:ARG:HG2	1:N:404:ARG:NH1	2.34	0.42
1:N:313:THR:HG22	1:N:314:LEU:HD12	1.99	0.42
1:J:266:THR:HG22	1:J:273:VAL:H	1.84	0.42
1:M:504:LEU:HA	1:M:504:LEU:HD23	1.73	0.42
1:F:433:ASN:OD1	1:F:436:GLN:HG3	2.19	0.42
1:F:441:LYS:HB3	1:F:445:ARG:HH21	1.83	0.42
1:F:31:LEU:CD1	5:F:1100:ADP:H5'2	2.50	0.42
1:L:96:ALA:O	1:L:100:ILE:HG13	2.19	0.42
1:E:320:ALA:HA	1:E:335:GLY:HA2	2.01	0.42
1:E:519:CYS:HB3	1:F:38:VAL:HG22	2.00	0.42
1:H:513:LEU:HA	1:H:513:LEU:HD12	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:VAL:HG12	1:E:514:MET:HE1	2.01	0.42
1:I:449:ALA:N	1:I:450:PRO:CD	2.83	0.42
1:B:233:MET:HB3	1:B:237:LEU:HD12	1.99	0.42
1:B:31:LEU:HD23	1:B:453:GLN:HB3	2.01	0.42
1:F:320:ALA:HA	1:F:335:GLY:HA2	2.01	0.42
1:I:96:ALA:O	1:I:100:ILE:HG13	2.18	0.42
1:G:234:LEU:HB2	1:G:235:PRO:HD3	2.01	0.42
1:B:130:GLU:OE1	1:B:425:LYS:HD2	2.19	0.42
1:C:193:MET:HG3	1:C:371:LYS:HB3	2.02	0.42
1:M:286:LYS:NZ	1:M:304:GLU:OE1	2.53	0.42
1:E:247:LEU:HB3	1:E:273:VAL:HG12	2.01	0.42
1:N:37:ASN:ND2	1:N:37:ASN:H	2.17	0.42
1:N:66:PHE:O	1:N:67:GLU:C	2.56	0.42
1:H:285:ARG:HA	1:H:288:MET:HB2	2.01	0.42
1:B:224:ASP:CB	1:B:302:SER:HA	2.49	0.42
1:H:38:VAL:HG12	1:H:40:LEU:HD13	2.02	0.42
1:K:43:SER:HB2	1:K:44:PHE:HD1	1.84	0.42
1:K:262:LEU:O	1:K:266:THR:HG23	2.20	0.42
1:L:266:THR:HG22	1:L:273:VAL:H	1.84	0.42
1:H:200:LEU:HD13	1:H:276:VAL:HA	2.01	0.42
1:H:419:LEU:HA	1:H:419:LEU:HD13	1.79	0.42
1:K:513:LEU:HD12	1:K:513:LEU:HA	1.85	0.42
2:S:50:GLU:O	2:S:50:GLU:HG3	2.20	0.42
1:I:285:ARG:HA	1:I:288:MET:HB2	2.01	0.42
1:H:496:PRO:HB2	1:H:499:VAL:HG13	2.02	0.42
1:K:295:LEU:HD23	1:K:332:ILE:HD11	2.02	0.42
1:B:23:LEU:C	1:B:23:LEU:CD1	2.88	0.42
1:A:20:VAL:HG13	1:A:74:VAL:HG11	2.00	0.42
2:R:7:HIS:HB3	2:R:45:ASN:HD22	1.84	0.42
1:B:302:SER:HB3	1:B:305:ILE:HG12	2.02	0.42
1:N:38:VAL:HG12	1:N:40:LEU:HD13	2.02	0.42
1:A:236:VAL:O	1:A:240:VAL:HG23	2.20	0.42
1:L:295:LEU:HD23	1:L:332:ILE:HD11	2.02	0.42
1:A:247:LEU:HB3	1:A:273:VAL:HG12	2.01	0.42
1:C:320:ALA:HA	1:C:335:GLY:HA2	2.01	0.42
2:P:15:LYS:HB3	2:P:16:GLU:H	1.69	0.42
1:D:23:LEU:C	1:D:23:LEU:CD1	2.88	0.42
1:I:441:LYS:HD2	1:I:441:LYS:HA	1.84	0.42
1:I:37:ASN:N	1:I:37:ASN:ND2	2.68	0.42
1:N:413:ALA:CB	1:N:417:VAL:HB	2.50	0.42
1:M:404:ARG:NH1	1:M:404:ARG:CG	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:ASN:N	1:K:37:ASN:ND2	2.68	0.42
1:F:162:ILE:HG12	1:F:400:LEU:HD23	2.02	0.42
1:G:444:LEU:O	1:G:447:MET:HB2	2.19	0.42
2:P:60:LYS:H	2:P:60:LYS:HG2	1.73	0.42
1:D:514:MET:HB2	1:D:514:MET:HE3	1.92	0.42
1:A:302:SER:HB3	1:A:305:ILE:HG12	2.02	0.42
1:M:267:MET:O	1:M:268:ARG:CB	2.68	0.42
1:J:404:ARG:HH11	1:J:404:ARG:HG2	1.84	0.42
1:D:419:LEU:HG	1:D:447:MET:HG2	2.02	0.42
1:B:222:LEU:HD12	1:B:293:ALA:HB2	2.00	0.42
1:J:96:ALA:O	1:J:100:ILE:HG13	2.20	0.42
1:C:464:VAL:O	1:C:468:THR:HG23	2.19	0.42
1:F:247:LEU:HB3	1:F:273:VAL:HG12	2.02	0.42
1:D:76:GLU:O	1:D:80:LYS:HB2	2.20	0.42
1:B:461:GLU:HB2	1:B:464:VAL:HB	2.01	0.42
1:N:336:VAL:HG12	1:N:336:VAL:O	2.20	0.42
1:C:421:ARG:HD3	1:C:421:ARG:HA	1.76	0.42
1:M:31:LEU:HD22	1:M:94:VAL:HG21	2.02	0.42
1:H:444:LEU:HA	1:H:447:MET:CE	2.50	0.42
1:D:477:GLY:HA3	1:D:488:MET:SD	2.60	0.42
1:E:366:GLN:O	1:E:369:VAL:HG22	2.19	0.42
1:N:44:PHE:N	1:N:44:PHE:CD1	2.87	0.42
1:J:262:LEU:HD22	1:J:273:VAL:HG21	2.02	0.42
1:I:44:PHE:N	1:I:44:PHE:CD1	2.87	0.42
1:H:85:ALA:HB1	1:H:499:VAL:HG12	2.01	0.42
1:I:37:ASN:ND2	1:I:37:ASN:H	2.18	0.42
1:I:286:LYS:NZ	1:I:304:GLU:OE1	2.53	0.42
1:K:197:ARG:HG2	1:K:277:LYS:O	2.20	0.42
1:D:487:ASN:O	1:D:491:MET:HG3	2.20	0.42
1:B:247:LEU:HB3	1:B:273:VAL:HG12	2.01	0.42
1:C:234:LEU:HB2	1:C:235:PRO:HD3	2.02	0.42
2:R:78:ILE:HD13	2:R:83:VAL:HG21	2.01	0.42
1:M:336:VAL:O	1:M:336:VAL:HG12	2.20	0.42
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.02	0.41
1:M:285:ARG:HA	1:M:288:MET:HB2	2.02	0.41
1:N:451:LEU:O	1:N:452:ARG:C	2.58	0.41
1:J:413:ALA:HB1	1:J:417:VAL:HB	2.01	0.41
1:J:415:GLY:N	1:J:417:VAL:HG23	2.35	0.41
1:N:404:ARG:HH11	1:N:404:ARG:CG	2.33	0.41
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.32	0.41
1:J:44:PHE:N	1:J:44:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:LEU:HB2	1:B:235:PRO:HD3	2.02	0.41
1:D:33:PRO:HA	1:D:153:ASN:HD21	1.85	0.41
1:E:150:ILE:HD13	1:E:492:GLY:O	2.20	0.41
1:J:336:VAL:HG12	1:J:336:VAL:O	2.19	0.41
1:M:95:LEU:O	1:M:98:ALA:N	2.51	0.41
1:K:77:VAL:HG13	1:K:506:TYR:HB3	2.01	0.41
1:H:77:VAL:HG12	1:H:78:ALA:N	2.35	0.41
1:M:449:ALA:N	1:M:450:PRO:CD	2.83	0.41
1:C:42:LYS:O	1:C:43:SER:C	2.59	0.41
1:M:413:ALA:CB	1:M:417:VAL:HB	2.50	0.41
1:M:385:THR:HG23	1:M:388:GLU:CB	2.49	0.41
1:K:285:ARG:HA	1:K:288:MET:HB2	2.02	0.41
1:G:100:ILE:HG13	1:G:511:ALA:CB	2.50	0.41
1:I:415:GLY:N	1:I:417:VAL:HG23	2.34	0.41
1:N:415:GLY:N	1:N:417:VAL:HG23	2.35	0.41
1:A:32:GLY:HA2	5:A:600:ADP:H5'1	2.01	0.41
1:A:39:VAL:HB	1:G:520:MET:HG2	2.02	0.41
1:E:225:LYS:HG3	1:E:225:LYS:H	1.66	0.41
1:H:262:LEU:O	1:H:266:THR:HG23	2.20	0.41
1:C:124:VAL:HG21	1:C:508:ALA:HB2	2.02	0.41
1:L:286:LYS:NZ	1:L:304:GLU:OE1	2.54	0.41
1:K:433:ASN:HD22	1:K:433:ASN:HA	1.63	0.41
1:L:77:VAL:HG13	1:L:506:TYR:HB3	2.01	0.41
1:M:462:PRO:O	1:M:463:SER:C	2.59	0.41
1:K:417:VAL:HG21	1:K:488:MET:HG3	2.03	0.41
1:L:262:LEU:O	1:L:266:THR:HG23	2.20	0.41
1:N:147:VAL:HG21	1:N:411:VAL:HG11	2.02	0.41
1:G:259:LEU:O	1:G:263:VAL:HG23	2.19	0.41
1:H:336:VAL:O	1:H:336:VAL:HG12	2.20	0.41
2:T:50:GLU:O	2:T:50:GLU:HG3	2.20	0.41
2:R:50:GLU:O	2:R:50:GLU:HG3	2.21	0.41
1:K:38:VAL:HG12	1:K:40:LEU:HD13	2.02	0.41
1:D:100:ILE:HG13	1:D:511:ALA:CB	2.50	0.41
1:K:44:PHE:CD1	1:K:44:PHE:N	2.88	0.41
1:J:40:LEU:HD12	1:K:521:VAL:HB	2.01	0.41
1:C:162:ILE:HG12	1:C:400:LEU:HD23	2.02	0.41
1:A:222:LEU:HD12	1:A:293:ALA:HB2	2.01	0.41
1:A:238:GLU:OE2	1:A:238:GLU:HA	2.20	0.41
1:J:479:ASN:C	1:J:479:ASN:OD1	2.58	0.41
1:C:513:LEU:HA	1:C:513:LEU:HD23	1.81	0.41
1:J:504:LEU:HD23	1:J:504:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:PRO:HB3	1:G:272:LYS:HB3	2.03	0.41
1:J:285:ARG:HA	1:J:288:MET:HB2	2.03	0.41
1:G:302:SER:HB3	1:G:305:ILE:HG12	2.03	0.41
1:L:455:VAL:HG13	1:L:460:GLU:HB2	2.02	0.41
1:I:200:LEU:HD13	1:I:276:VAL:HA	2.02	0.41
1:K:63:GLU:HB2	1:L:524:LEU:HD11	2.02	0.41
1:A:259:LEU:O	1:A:263:VAL:HG23	2.19	0.41
1:K:200:LEU:HD13	1:K:276:VAL:HA	2.03	0.41
1:C:247:LEU:HB3	1:C:273:VAL:HG12	2.01	0.41
1:I:104:LEU:HA	1:I:104:LEU:HD12	1.76	0.41
1:J:15:LYS:HA	1:J:15:LYS:HD2	1.96	0.41
1:G:33:PRO:HA	1:G:153:ASN:ND2	2.33	0.41
1:D:501:ARG:HD3	1:D:505:GLN:OE1	2.20	0.41
1:I:175:ILE:CG2	1:I:400:LEU:HD11	2.51	0.41
1:H:295:LEU:HD23	1:H:332:ILE:HD11	2.03	0.41
1:G:247:LEU:HB3	1:G:273:VAL:HG12	2.02	0.41
1:C:130:GLU:OE1	1:C:425:LYS:HD2	2.20	0.41
1:M:49:ILE:HG21	1:N:513:LEU:HG	2.02	0.41
1:C:433:ASN:OD1	1:C:436:GLN:HG3	2.20	0.41
1:J:198:GLY:O	1:J:276:VAL:HG12	2.20	0.41
1:A:103:GLY:HA3	1:A:515:ILE:HG21	2.02	0.41
1:L:336:VAL:O	1:L:336:VAL:HG12	2.20	0.41
1:B:111:MET:HG3	1:B:435:ASP:OD1	2.21	0.41
2:Q:50:GLU:HG3	2:Q:50:GLU:O	2.20	0.41
1:I:426:LEU:HD12	1:I:444:LEU:HD21	2.02	0.41
1:N:285:ARG:HA	1:N:288:MET:HB2	2.03	0.41
1:A:224:ASP:CB	1:A:302:SER:HA	2.51	0.41
1:K:267:MET:O	1:K:268:ARG:CB	2.68	0.41
1:B:444:LEU:O	1:B:447:MET:HB2	2.21	0.41
1:H:82:ASN:HB2	1:H:89:THR:OG1	2.21	0.41
1:K:286:LYS:NZ	1:K:304:GLU:OE1	2.54	0.41
1:E:193:MET:HG3	1:E:371:LYS:HB3	2.02	0.41
1:K:85:ALA:HB1	1:K:499:VAL:HG12	2.02	0.41
1:D:236:VAL:O	1:D:240:VAL:HG23	2.21	0.41
1:G:479:ASN:ND2	1:G:493:ILE:HD11	2.34	0.41
1:N:198:GLY:O	1:N:276:VAL:HG12	2.19	0.41
1:I:77:VAL:HG12	1:I:78:ALA:N	2.36	0.41
2:P:7:HIS:NE2	2:P:48:ILE:HD11	2.36	0.41
1:E:302:SER:HB3	1:E:305:ILE:HG12	2.03	0.41
1:J:262:LEU:O	1:J:266:THR:HG23	2.21	0.41
1:C:461:GLU:HB2	1:C:464:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:263:VAL:HG12	1:G:267:MET:HE3	2.03	0.41
2:O:78:ILE:HD13	2:O:83:VAL:HG21	2.02	0.41
1:D:234:LEU:HB2	1:D:235:PRO:HD3	2.03	0.41
1:I:448:GLU:O	1:I:452:ARG:HD2	2.21	0.41
1:I:358:SER:HB3	1:I:361:ASP:OD1	2.21	0.41
1:M:447:MET:CG	1:M:447:MET:CE	2.95	0.41
2:U:50:GLU:HG3	2:U:50:GLU:O	2.20	0.41
1:A:477:GLY:CA	1:A:488:MET:SD	3.07	0.41
1:C:20:VAL:HG13	1:C:74:VAL:HG21	2.03	0.41
1:K:444:LEU:HA	1:K:444:LEU:HD23	1.92	0.41
1:H:37:ASN:ND2	1:H:37:ASN:N	2.68	0.41
1:N:266:THR:HG22	1:N:273:VAL:H	1.85	0.41
1:H:262:LEU:HD22	1:H:273:VAL:HG21	2.03	0.41
1:A:512:GLY:O	1:A:515:ILE:HG13	2.20	0.41
1:D:78:ALA:HB2	1:D:93:THR:OG1	2.21	0.41
1:M:197:ARG:HG2	1:M:277:LYS:O	2.21	0.41
1:F:147:VAL:HG22	1:F:403:THR:HG22	2.02	0.41
1:M:198:GLY:O	1:M:276:VAL:HG12	2.21	0.41
1:B:381:VAL:CG1	1:B:392:LYS:HG2	2.51	0.41
2:U:60:LYS:HG2	2:U:60:LYS:H	1.75	0.41
1:H:21:ASN:HA	1:H:21:ASN:HD22	1.61	0.41
1:D:193:MET:HG3	1:D:371:LYS:HB3	2.03	0.41
1:E:130:GLU:O	1:E:133:ALA:HB3	2.21	0.41
2:T:78:ILE:HD13	2:T:83:VAL:HG21	2.03	0.41
1:C:246:PRO:HB3	1:C:272:LYS:HB3	2.03	0.41
1:A:514:MET:HB2	1:A:514:MET:HE3	1.86	0.41
1:C:455:VAL:CG1	1:C:462:PRO:HA	2.51	0.41
1:M:193:MET:HG2	1:M:194:GLN:N	2.37	0.41
1:K:100:ILE:CG2	1:K:104:LEU:HD22	2.51	0.41
1:N:221:LEU:HD23	1:N:317:LEU:HD11	2.03	0.41
1:M:262:LEU:HD22	1:M:273:VAL:HG21	2.03	0.41
1:I:266:THR:HG22	1:I:273:VAL:H	1.85	0.41
1:D:263:VAL:HG12	1:D:267:MET:HE3	2.03	0.41
1:N:513:LEU:HA	1:N:513:LEU:HD12	1.85	0.41
1:G:147:VAL:HG22	1:G:403:THR:HG22	2.02	0.41
1:J:21:ASN:HD22	1:J:21:ASN:HA	1.63	0.41
1:F:451:LEU:O	1:F:451:LEU:HD22	2.21	0.41
1:N:66:PHE:HA	1:N:69:MET:HE3	2.03	0.40
1:H:232:GLU:HA	1:H:310:GLU:HG2	2.03	0.40
1:M:455:VAL:HG21	1:M:465:VAL:HG11	2.03	0.40
1:N:193:MET:HG2	1:N:194:GLN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:247:LEU:HB3	1:N:273:VAL:HG12	2.03	0.40
1:B:247:LEU:O	1:B:273:VAL:HA	2.22	0.40
1:J:197:ARG:HG2	1:J:277:LYS:O	2.21	0.40
5:G:1200:ADP:O3B	6:G:1202:AF3:F3	2.30	0.40
1:M:172:GLU:HA	1:M:172:GLU:OE1	2.21	0.40
1:L:104:LEU:HA	1:L:104:LEU:HD12	1.77	0.40
1:M:415:GLY:O	1:M:451:LEU:HD12	2.22	0.40
1:D:16:MET:HG3	1:D:520:MET:HE3	2.02	0.40
1:I:31:LEU:O	1:I:32:GLY:O	2.39	0.40
1:K:266:THR:HG22	1:K:273:VAL:H	1.86	0.40
1:H:266:THR:HG22	1:H:273:VAL:H	1.86	0.40
1:F:31:LEU:HD12	5:F:1100:ADP:H5'2	2.04	0.40
1:C:124:VAL:HG13	1:C:504:LEU:HD13	2.03	0.40
1:I:106:ALA:O	1:I:109:ALA:HB3	2.21	0.40
1:C:466:ALA:O	1:C:467:ASN:C	2.58	0.40
1:N:504:LEU:HD23	1:N:504:LEU:HA	1.90	0.40
1:D:429:LEU:HA	1:D:429:LEU:HD12	1.91	0.40
1:N:479:ASN:OD1	1:N:479:ASN:C	2.59	0.40
1:E:246:PRO:HB3	1:E:272:LYS:HB3	2.04	0.40
1:K:107:VAL:HG11	1:K:515:ILE:HG23	2.02	0.40
1:K:31:LEU:HD22	1:K:94:VAL:HG21	2.02	0.40
1:G:224:ASP:CB	1:G:302:SER:HA	2.51	0.40
1:F:32:GLY:HA2	5:F:1100:ADP:H5'1	2.04	0.40
1:G:419:LEU:HG	1:G:447:MET:HG2	2.03	0.40
1:A:165:ALA:O	1:A:169:VAL:HG22	2.22	0.40
1:I:270:ILE:HG23	1:J:229:ASN:HD21	1.86	0.40
1:M:450:PRO:O	1:M:454:ILE:HG12	2.21	0.40
1:I:413:ALA:HB1	1:I:417:VAL:HB	2.02	0.40
1:N:267:MET:O	1:N:268:ARG:CB	2.70	0.40
1:M:58:ARG:HB2	1:M:58:ARG:CZ	2.51	0.40
1:I:262:LEU:HD22	1:I:273:VAL:HG21	2.03	0.40
1:I:262:LEU:O	1:I:266:THR:HG23	2.22	0.40
1:G:502:SER:O	1:G:503:ALA:C	2.57	0.40
1:J:131:LEU:HD12	1:J:422:VAL:HG11	2.03	0.40
1:M:100:ILE:CG2	1:M:104:LEU:HD22	2.52	0.40
1:I:336:VAL:O	1:I:336:VAL:HG12	2.21	0.40
1:B:246:PRO:HB3	1:B:272:LYS:HB3	2.04	0.40
1:C:224:ASP:CB	1:C:302:SER:HA	2.51	0.40
2:T:7:HIS:NE2	2:T:48:ILE:HD11	2.37	0.40
1:E:461:GLU:HB2	1:E:464:VAL:HB	2.04	0.40
1:M:43:SER:HB2	1:M:44:PHE:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:LYS:HG3	1:D:225:LYS:H	1.66	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	522/524 (100%)	486 (93%)	32 (6%)	4 (1%)	24	58
1	B	522/524 (100%)	486 (93%)	32 (6%)	4 (1%)	24	58
1	C	522/524 (100%)	484 (93%)	34 (6%)	4 (1%)	24	58
1	D	522/524 (100%)	486 (93%)	31 (6%)	5 (1%)	19	52
1	E	522/524 (100%)	488 (94%)	30 (6%)	4 (1%)	24	58
1	F	522/524 (100%)	487 (93%)	31 (6%)	4 (1%)	24	58
1	G	522/524 (100%)	489 (94%)	29 (6%)	4 (1%)	24	58
1	H	522/524 (100%)	483 (92%)	33 (6%)	6 (1%)	17	50
1	I	522/524 (100%)	480 (92%)	36 (7%)	6 (1%)	17	50
1	J	522/524 (100%)	477 (91%)	39 (8%)	6 (1%)	17	50
1	K	522/524 (100%)	483 (92%)	33 (6%)	6 (1%)	17	50
1	L	522/524 (100%)	485 (93%)	31 (6%)	6 (1%)	17	50
1	M	522/524 (100%)	468 (90%)	42 (8%)	12 (2%)	8	26
1	N	522/524 (100%)	479 (92%)	37 (7%)	6 (1%)	17	50
2	O	95/97 (98%)	74 (78%)	18 (19%)	3 (3%)	5	17
2	P	95/97 (98%)	74 (78%)	17 (18%)	4 (4%)	3	11
2	Q	95/97 (98%)	74 (78%)	16 (17%)	5 (5%)	2	7
2	R	95/97 (98%)	74 (78%)	17 (18%)	4 (4%)	3	11
2	S	95/97 (98%)	74 (78%)	18 (19%)	3 (3%)	5	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	95/97 (98%)	74 (78%)	16 (17%)	5 (5%)	2	7
2	U	95/97 (98%)	73 (77%)	18 (19%)	4 (4%)	3	11
All	All	7973/8015 (100%)	7278 (91%)	590 (7%)	105 (1%)	15	44

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	A	337	GLY
1	B	44	PHE
1	B	337	GLY
1	C	44	PHE
1	C	337	GLY
1	D	44	PHE
1	D	337	GLY
1	E	44	PHE
1	E	337	GLY
1	F	44	PHE
1	F	337	GLY
1	G	44	PHE
1	G	337	GLY
1	K	66	PHE
1	M	66	PHE
1	N	66	PHE
2	O	7	HIS
2	P	7	HIS
2	Q	7	HIS
2	R	7	HIS
2	S	7	HIS
2	T	7	HIS
2	U	7	HIS
1	H	32	GLY
1	H	43	SER
1	H	66	PHE
1	H	270	ILE
1	I	32	GLY
1	I	43	SER
1	I	66	PHE
1	I	270	ILE
1	J	32	GLY
1	J	43	SER

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Mol	Chain	Res	Type
1	J	66	PHE
1	J	270	ILE
1	K	32	GLY
1	K	43	SER
1	K	270	ILE
1	L	32	GLY
1	L	43	SER
1	L	66	PHE
1	L	270	ILE
1	M	32	GLY
1	M	43	SER
1	M	270	ILE
1	N	32	GLY
1	N	43	SER
1	N	270	ILE
2	O	21	SER
2	O	52	GLY
2	P	21	SER
2	P	52	GLY
2	Q	21	SER
2	Q	52	GLY
2	R	21	SER
2	R	52	GLY
2	S	21	SER
2	S	52	GLY
2	T	52	GLY
2	U	21	SER
2	U	52	GLY
1	A	205	ILE
1	M	85	ALA
1	M	463	SER
2	T	21	SER
1	B	205	ILE
1	C	205	ILE
1	D	205	ILE
1	E	205	ILE
1	F	205	ILE
1	G	205	ILE
1	M	462	PRO
1	D	58	ARG
1	I	462	PRO
1	M	413	ALA

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Mol	Chain	Res	Type
1	M	457	ASN
1	M	509	SER
2	P	53	GLU
2	R	20	LYS
2	T	20	LYS
2	T	53	GLU
2	U	49	LEU
1	H	462	PRO
1	K	462	PRO
1	L	462	PRO
1	M	89	THR
2	Q	20	LYS
2	Q	53	GLU
1	I	256	GLY
1	J	256	GLY
1	J	462	PRO
1	K	256	GLY
1	H	256	GLY
1	L	256	GLY
1	M	256	GLY
1	N	256	GLY
1	A	305	ILE
1	E	305	ILE
1	F	305	ILE
1	G	305	ILE
1	N	462	PRO
1	B	305	ILE
1	C	305	ILE
1	D	305	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	352 (87%)	52 (13%)	5	16
1	B	404/404 (100%)	354 (88%)	50 (12%)	6	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	404/404 (100%)	353 (87%)	51 (13%)	5	17
1	D	404/404 (100%)	351 (87%)	53 (13%)	5	15
1	E	404/404 (100%)	352 (87%)	52 (13%)	5	16
1	F	404/404 (100%)	352 (87%)	52 (13%)	5	16
1	G	404/404 (100%)	352 (87%)	52 (13%)	5	16
1	H	404/404 (100%)	344 (85%)	60 (15%)	4	11
1	I	404/404 (100%)	343 (85%)	61 (15%)	3	10
1	J	404/404 (100%)	344 (85%)	60 (15%)	4	11
1	K	404/404 (100%)	342 (85%)	62 (15%)	3	10
1	L	404/404 (100%)	345 (85%)	59 (15%)	4	11
1	M	404/404 (100%)	342 (85%)	62 (15%)	3	10
1	N	404/404 (100%)	345 (85%)	59 (15%)	4	11
2	O	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	P	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	Q	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	R	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	S	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	T	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	U	80/80 (100%)	67 (84%)	13 (16%)	3	8
All	All	6216/6216 (100%)	5340 (86%)	876 (14%)	4	12

All (876) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	18	ARG
1	A	23	LEU
1	A	28	LYS
1	A	43	SER
1	A	44	PHE
1	A	48	THR
1	A	62	LEU
1	A	74	VAL
1	A	97	GLN
1	A	111	MET

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Mol	Chain	Res	Type
1	A	129	GLU
1	A	132	LYS
1	A	138	CYS
1	A	147	VAL
1	A	153	ASN
1	A	168	LYS
1	A	176	THR
1	A	177	VAL
1	A	178	GLU
1	A	183	LEU
1	A	184	GLN
1	A	197	ARG
1	A	225	LYS
1	A	229	ASN
1	A	237	LEU
1	A	268	ARG
1	A	281	PHE
1	A	284	ARG
1	A	288	MET
1	A	322	ARG
1	A	345	ARG
1	A	350	ARG
1	A	351	GLN
1	A	366	GLN
1	A	391	GLU
1	A	398	ASP
1	A	400	LEU
1	A	417	VAL
1	A	419	LEU
1	A	420	ILE
1	A	421	ARG
1	A	422	VAL
1	A	430	ARG
1	A	445	ARG
1	A	451	LEU
1	A	452	ARG
1	A	461	GLU
1	A	494	LEU
1	A	504	LEU
1	A	510	VAL
1	A	514	MET
1	B	6	VAL

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Mol	Chain	Res	Type
1	B	18	ARG
1	B	23	LEU
1	B	43	SER
1	B	44	PHE
1	B	48	THR
1	B	62	LEU
1	B	74	VAL
1	B	97	GLN
1	B	111	MET
1	B	129	GLU
1	B	132	LYS
1	B	147	VAL
1	B	153	ASN
1	B	168	LYS
1	B	176	THR
1	B	177	VAL
1	B	178	GLU
1	B	183	LEU
1	B	184	GLN
1	B	185	ASP
1	B	197	ARG
1	B	225	LYS
1	B	229	ASN
1	B	237	LEU
1	B	281	PHE
1	B	284	ARG
1	B	288	MET
1	B	322	ARG
1	B	345	ARG
1	B	351	GLN
1	B	366	GLN
1	B	391	GLU
1	B	398	ASP
1	B	400	LEU
1	B	417	VAL
1	B	419	LEU
1	B	420	ILE
1	B	421	ARG
1	B	422	VAL
1	B	445	ARG
1	B	451	LEU
1	B	452	ARG

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Mol	Chain	Res	Type
1	B	461	GLU
1	B	462	PRO
1	B	463	SER
1	B	494	LEU
1	B	504	LEU
1	B	510	VAL
1	B	514	MET
1	C	6	VAL
1	C	18	ARG
1	C	23	LEU
1	C	28	LYS
1	C	43	SER
1	C	44	PHE
1	C	48	THR
1	C	62	LEU
1	C	74	VAL
1	C	80	LYS
1	C	97	GLN
1	C	111	MET
1	C	129	GLU
1	C	132	LYS
1	C	138	CYS
1	C	147	VAL
1	C	153	ASN
1	C	168	LYS
1	C	176	THR
1	C	177	VAL
1	C	178	GLU
1	C	183	LEU
1	C	184	GLN
1	C	185	ASP
1	C	225	LYS
1	C	229	ASN
1	C	237	LEU
1	C	281	PHE
1	C	284	ARG
1	C	288	MET
1	C	322	ARG
1	C	345	ARG
1	C	350	ARG
1	C	351	GLN
1	C	366	GLN

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Mol	Chain	Res	Type
1	C	391	GLU
1	C	398	ASP
1	C	400	LEU
1	C	417	VAL
1	C	419	LEU
1	C	420	ILE
1	C	421	ARG
1	C	422	VAL
1	C	430	ARG
1	C	445	ARG
1	C	451	LEU
1	C	452	ARG
1	C	461	GLU
1	C	494	LEU
1	C	504	LEU
1	C	510	VAL
1	D	6	VAL
1	D	18	ARG
1	D	23	LEU
1	D	28	LYS
1	D	43	SER
1	D	44	PHE
1	D	48	THR
1	D	62	LEU
1	D	74	VAL
1	D	80	LYS
1	D	97	GLN
1	D	111	MET
1	D	129	GLU
1	D	132	LYS
1	D	138	CYS
1	D	147	VAL
1	D	153	ASN
1	D	168	LYS
1	D	176	THR
1	D	177	VAL
1	D	178	GLU
1	D	183	LEU
1	D	184	GLN
1	D	197	ARG
1	D	225	LYS
1	D	229	ASN

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Mol	Chain	Res	Type
1	D	237	LEU
1	D	268	ARG
1	D	281	PHE
1	D	284	ARG
1	D	288	MET
1	D	322	ARG
1	D	345	ARG
1	D	350	ARG
1	D	351	GLN
1	D	366	GLN
1	D	391	GLU
1	D	398	ASP
1	D	400	LEU
1	D	417	VAL
1	D	419	LEU
1	D	420	ILE
1	D	421	ARG
1	D	422	VAL
1	D	445	ARG
1	D	451	LEU
1	D	452	ARG
1	D	461	GLU
1	D	463	SER
1	D	494	LEU
1	D	504	LEU
1	D	510	VAL
1	D	514	MET
1	E	6	VAL
1	E	18	ARG
1	E	23	LEU
1	E	43	SER
1	E	44	PHE
1	E	62	LEU
1	E	74	VAL
1	E	80	LYS
1	E	97	GLN
1	E	111	MET
1	E	129	GLU
1	E	132	LYS
1	E	138	CYS
1	E	147	VAL
1	E	153	ASN

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Mol	Chain	Res	Type
1	E	168	LYS
1	E	176	THR
1	E	177	VAL
1	E	178	GLU
1	E	183	LEU
1	E	184	GLN
1	E	185	ASP
1	E	197	ARG
1	E	225	LYS
1	E	229	ASN
1	E	237	LEU
1	E	281	PHE
1	E	284	ARG
1	E	288	MET
1	E	322	ARG
1	E	345	ARG
1	E	350	ARG
1	E	351	GLN
1	E	366	GLN
1	E	391	GLU
1	E	398	ASP
1	E	400	LEU
1	E	417	VAL
1	E	419	LEU
1	E	420	ILE
1	E	421	ARG
1	E	422	VAL
1	E	430	ARG
1	E	445	ARG
1	E	451	LEU
1	E	452	ARG
1	E	461	GLU
1	E	462	PRO
1	E	494	LEU
1	E	504	LEU
1	E	510	VAL
1	E	514	MET
1	F	6	VAL
1	F	18	ARG
1	F	23	LEU
1	F	28	LYS
1	F	43	SER

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Mol	Chain	Res	Type
1	F	44	PHE
1	F	48	THR
1	F	62	LEU
1	F	74	VAL
1	F	80	LYS
1	F	97	GLN
1	F	111	MET
1	F	129	GLU
1	F	132	LYS
1	F	138	CYS
1	F	147	VAL
1	F	153	ASN
1	F	168	LYS
1	F	176	THR
1	F	177	VAL
1	F	178	GLU
1	F	183	LEU
1	F	184	GLN
1	F	185	ASP
1	F	225	LYS
1	F	229	ASN
1	F	237	LEU
1	F	281	PHE
1	F	284	ARG
1	F	288	MET
1	F	322	ARG
1	F	345	ARG
1	F	350	ARG
1	F	351	GLN
1	F	366	GLN
1	F	391	GLU
1	F	398	ASP
1	F	400	LEU
1	F	417	VAL
1	F	419	LEU
1	F	420	ILE
1	F	421	ARG
1	F	422	VAL
1	F	445	ARG
1	F	451	LEU
1	F	452	ARG
1	F	461	GLU

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Mol	Chain	Res	Type
1	F	463	SER
1	F	494	LEU
1	F	504	LEU
1	F	510	VAL
1	F	514	MET
1	G	6	VAL
1	G	18	ARG
1	G	23	LEU
1	G	28	LYS
1	G	43	SER
1	G	44	PHE
1	G	48	THR
1	G	62	LEU
1	G	74	VAL
1	G	80	LYS
1	G	97	GLN
1	G	111	MET
1	G	129	GLU
1	G	132	LYS
1	G	138	CYS
1	G	147	VAL
1	G	153	ASN
1	G	168	LYS
1	G	176	THR
1	G	177	VAL
1	G	178	GLU
1	G	183	LEU
1	G	184	GLN
1	G	185	ASP
1	G	225	LYS
1	G	229	ASN
1	G	237	LEU
1	G	268	ARG
1	G	281	PHE
1	G	284	ARG
1	G	288	MET
1	G	322	ARG
1	G	345	ARG
1	G	350	ARG
1	G	351	GLN
1	G	366	GLN
1	G	391	GLU

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Mol	Chain	Res	Type
1	G	398	ASP
1	G	400	LEU
1	G	417	VAL
1	G	419	LEU
1	G	420	ILE
1	G	421	ARG
1	G	422	VAL
1	G	445	ARG
1	G	451	LEU
1	G	461	GLU
1	G	463	SER
1	G	494	LEU
1	G	504	LEU
1	G	510	VAL
1	G	514	MET
1	H	7	LYS
1	H	16	MET
1	H	23	LEU
1	H	37	ASN
1	H	40	LEU
1	H	42	LYS
1	H	43	SER
1	H	55	SER
1	H	65	LYS
1	H	67	GLU
1	H	77	VAL
1	H	87	ASP
1	H	104	LEU
1	H	114	MET
1	H	129	GLU
1	H	141	SER
1	H	147	VAL
1	H	172	GLU
1	H	189	VAL
1	H	197	ARG
1	H	210	THR
1	H	221	LEU
1	H	230	ILE
1	H	232	GLU
1	H	233	MET
1	H	247	LEU
1	H	248	LEU

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Mol	Chain	Res	Type
1	H	255	GLU
1	H	267	MET
1	H	268	ARG
1	H	272	LYS
1	H	284	ARG
1	H	288	MET
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	343	GLN
1	H	354	GLU
1	H	355	GLU
1	H	359	ASP
1	H	364	LYS
1	H	378	VAL
1	H	385	THR
1	H	389	MET
1	H	401	HIS
1	H	404	ARG
1	H	419	LEU
1	H	420	ILE
1	H	421	ARG
1	H	426	LEU
1	H	432	GLN
1	H	433	ASN
1	H	436	GLN
1	H	441	LYS
1	H	454	ILE
1	H	468	THR
1	H	483	GLU
1	H	504	LEU
1	H	509	SER
1	H	513	LEU
1	I	7	LYS
1	I	16	MET
1	I	23	LEU
1	I	37	ASN
1	I	40	LEU
1	I	42	LYS
1	I	43	SER
1	I	55	SER
1	I	65	LYS

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Mol	Chain	Res	Type
1	I	77	VAL
1	I	87	ASP
1	I	104	LEU
1	I	107	VAL
1	I	114	MET
1	I	129	GLU
1	I	141	SER
1	I	147	VAL
1	I	172	GLU
1	I	189	VAL
1	I	197	ARG
1	I	210	THR
1	I	221	LEU
1	I	230	ILE
1	I	232	GLU
1	I	233	MET
1	I	247	LEU
1	I	248	LEU
1	I	255	GLU
1	I	267	MET
1	I	268	ARG
1	I	272	LYS
1	I	284	ARG
1	I	288	MET
1	I	328	ASP
1	I	329	THR
1	I	331	THR
1	I	343	GLN
1	I	354	GLU
1	I	355	GLU
1	I	359	ASP
1	I	364	LYS
1	I	378	VAL
1	I	385	THR
1	I	389	MET
1	I	401	HIS
1	I	404	ARG
1	I	419	LEU
1	I	420	ILE
1	I	421	ARG
1	I	426	LEU
1	I	432	GLN

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Mol	Chain	Res	Type
1	I	433	ASN
1	I	436	GLN
1	I	441	LYS
1	I	451	LEU
1	I	454	ILE
1	I	468	THR
1	I	483	GLU
1	I	504	LEU
1	I	509	SER
1	I	513	LEU
1	J	7	LYS
1	J	16	MET
1	J	23	LEU
1	J	37	ASN
1	J	40	LEU
1	J	42	LYS
1	J	43	SER
1	J	55	SER
1	J	65	LYS
1	J	77	VAL
1	J	87	ASP
1	J	104	LEU
1	J	107	VAL
1	J	114	MET
1	J	129	GLU
1	J	141	SER
1	J	147	VAL
1	J	172	GLU
1	J	189	VAL
1	J	197	ARG
1	J	210	THR
1	J	221	LEU
1	J	230	ILE
1	J	232	GLU
1	J	233	MET
1	J	247	LEU
1	J	248	LEU
1	J	255	GLU
1	J	267	MET
1	J	268	ARG
1	J	272	LYS
1	J	284	ARG

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Mol	Chain	Res	Type
1	J	288	MET
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	343	GLN
1	J	354	GLU
1	J	355	GLU
1	J	359	ASP
1	J	364	LYS
1	J	378	VAL
1	J	385	THR
1	J	389	MET
1	J	401	HIS
1	J	404	ARG
1	J	419	LEU
1	J	420	ILE
1	J	421	ARG
1	J	426	LEU
1	J	432	GLN
1	J	433	ASN
1	J	441	LYS
1	J	452	ARG
1	J	454	ILE
1	J	468	THR
1	J	483	GLU
1	J	504	LEU
1	J	509	SER
1	J	513	LEU
1	K	7	LYS
1	K	16	MET
1	K	23	LEU
1	K	27	VAL
1	K	37	ASN
1	K	40	LEU
1	K	42	LYS
1	K	43	SER
1	K	55	SER
1	K	59	GLU
1	K	65	LYS
1	K	77	VAL
1	K	87	ASP
1	K	101	THR

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Mol	Chain	Res	Type
1	K	104	LEU
1	K	107	VAL
1	K	114	MET
1	K	129	GLU
1	K	141	SER
1	K	147	VAL
1	K	172	GLU
1	K	189	VAL
1	K	197	ARG
1	K	210	THR
1	K	221	LEU
1	K	230	ILE
1	K	232	GLU
1	K	233	MET
1	K	247	LEU
1	K	248	LEU
1	K	255	GLU
1	K	267	MET
1	K	268	ARG
1	K	272	LYS
1	K	284	ARG
1	K	288	MET
1	K	328	ASP
1	K	329	THR
1	K	331	THR
1	K	343	GLN
1	K	354	GLU
1	K	355	GLU
1	K	359	ASP
1	K	364	LYS
1	K	385	THR
1	K	389	MET
1	K	401	HIS
1	K	404	ARG
1	K	419	LEU
1	K	420	ILE
1	K	421	ARG
1	K	426	LEU
1	K	432	GLN
1	K	433	ASN
1	K	441	LYS
1	K	452	ARG

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Mol	Chain	Res	Type
1	K	454	ILE
1	K	468	THR
1	K	483	GLU
1	K	504	LEU
1	K	509	SER
1	K	513	LEU
1	L	7	LYS
1	L	16	MET
1	L	23	LEU
1	L	37	ASN
1	L	40	LEU
1	L	42	LYS
1	L	43	SER
1	L	55	SER
1	L	65	LYS
1	L	77	VAL
1	L	87	ASP
1	L	104	LEU
1	L	107	VAL
1	L	114	MET
1	L	129	GLU
1	L	141	SER
1	L	147	VAL
1	L	172	GLU
1	L	189	VAL
1	L	197	ARG
1	L	210	THR
1	L	221	LEU
1	L	230	ILE
1	L	232	GLU
1	L	233	MET
1	L	247	LEU
1	L	248	LEU
1	L	255	GLU
1	L	267	MET
1	L	268	ARG
1	L	272	LYS
1	L	284	ARG
1	L	288	MET
1	L	328	ASP
1	L	329	THR
1	L	331	THR

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Mol	Chain	Res	Type
1	L	343	GLN
1	L	354	GLU
1	L	355	GLU
1	L	359	ASP
1	L	364	LYS
1	L	378	VAL
1	L	385	THR
1	L	389	MET
1	L	401	HIS
1	L	404	ARG
1	L	419	LEU
1	L	420	ILE
1	L	421	ARG
1	L	426	LEU
1	L	432	GLN
1	L	433	ASN
1	L	441	LYS
1	L	454	ILE
1	L	468	THR
1	L	483	GLU
1	L	504	LEU
1	L	509	SER
1	L	513	LEU
1	M	7	LYS
1	M	16	MET
1	M	21	ASN
1	M	23	LEU
1	M	37	ASN
1	M	40	LEU
1	M	42	LYS
1	M	43	SER
1	M	55	SER
1	M	65	LYS
1	M	77	VAL
1	M	87	ASP
1	M	104	LEU
1	M	107	VAL
1	M	114	MET
1	M	129	GLU
1	M	141	SER
1	M	147	VAL
1	M	172	GLU

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Mol	Chain	Res	Type
1	M	189	VAL
1	M	197	ARG
1	M	210	THR
1	M	230	ILE
1	M	232	GLU
1	M	233	MET
1	M	247	LEU
1	M	248	LEU
1	M	255	GLU
1	M	267	MET
1	M	268	ARG
1	M	272	LYS
1	M	284	ARG
1	M	288	MET
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	343	GLN
1	M	354	GLU
1	M	355	GLU
1	M	359	ASP
1	M	364	LYS
1	M	378	VAL
1	M	385	THR
1	M	389	MET
1	M	401	HIS
1	M	404	ARG
1	M	419	LEU
1	M	420	ILE
1	M	421	ARG
1	M	426	LEU
1	M	432	GLN
1	M	433	ASN
1	M	436	GLN
1	M	441	LYS
1	M	452	ARG
1	M	454	ILE
1	M	468	THR
1	M	483	GLU
1	M	498	LYS
1	M	504	LEU
1	M	509	SER

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Mol	Chain	Res	Type
1	M	513	LEU
1	N	7	LYS
1	N	16	MET
1	N	23	LEU
1	N	37	ASN
1	N	40	LEU
1	N	42	LYS
1	N	43	SER
1	N	55	SER
1	N	59	GLU
1	N	65	LYS
1	N	87	ASP
1	N	104	LEU
1	N	114	MET
1	N	129	GLU
1	N	141	SER
1	N	147	VAL
1	N	172	GLU
1	N	189	VAL
1	N	197	ARG
1	N	210	THR
1	N	221	LEU
1	N	230	ILE
1	N	232	GLU
1	N	233	MET
1	N	247	LEU
1	N	248	LEU
1	N	255	GLU
1	N	267	MET
1	N	268	ARG
1	N	272	LYS
1	N	284	ARG
1	N	288	MET
1	N	328	ASP
1	N	329	THR
1	N	331	THR
1	N	343	GLN
1	N	354	GLU
1	N	355	GLU
1	N	359	ASP
1	N	364	LYS
1	N	378	VAL

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Mol	Chain	Res	Type
1	N	385	THR
1	N	389	MET
1	N	401	HIS
1	N	404	ARG
1	N	419	LEU
1	N	420	ILE
1	N	421	ARG
1	N	426	LEU
1	N	432	GLN
1	N	433	ASN
1	N	441	LYS
1	N	452	ARG
1	N	454	ILE
1	N	468	THR
1	N	483	GLU
1	N	504	LEU
1	N	509	SER
1	N	513	LEU
2	O	1	MET
2	O	3	ILE
2	O	4	ARG
2	O	6	LEU
2	O	20	LYS
2	O	27	LEU
2	O	28	THR
2	O	30	SER
2	O	55	LYS
2	O	60	LYS
2	O	80	ASN
2	O	86	MET
2	O	89	SER
2	P	1	MET
2	P	3	ILE
2	P	4	ARG
2	P	6	LEU
2	P	20	LYS
2	P	27	LEU
2	P	28	THR
2	P	30	SER
2	P	55	LYS
2	P	60	LYS
2	P	80	ASN

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Mol	Chain	Res	Type
2	P	86	MET
2	P	89	SER
2	Q	1	MET
2	Q	3	ILE
2	Q	4	ARG
2	Q	6	LEU
2	Q	20	LYS
2	Q	27	LEU
2	Q	28	THR
2	Q	30	SER
2	Q	55	LYS
2	Q	60	LYS
2	Q	80	ASN
2	Q	86	MET
2	Q	89	SER
2	R	1	MET
2	R	3	ILE
2	R	4	ARG
2	R	6	LEU
2	R	20	LYS
2	R	27	LEU
2	R	28	THR
2	R	30	SER
2	R	55	LYS
2	R	60	LYS
2	R	80	ASN
2	R	86	MET
2	R	89	SER
2	S	1	MET
2	S	3	ILE
2	S	4	ARG
2	S	6	LEU
2	S	20	LYS
2	S	27	LEU
2	S	28	THR
2	S	30	SER
2	S	55	LYS
2	S	60	LYS
2	S	80	ASN
2	S	86	MET
2	S	89	SER
2	T	1	MET

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Mol	Chain	Res	Type
2	T	3	ILE
2	T	4	ARG
2	T	6	LEU
2	T	20	LYS
2	T	27	LEU
2	T	28	THR
2	T	30	SER
2	T	55	LYS
2	T	60	LYS
2	T	80	ASN
2	T	86	MET
2	T	89	SER
2	U	1	MET
2	U	3	ILE
2	U	4	ARG
2	U	6	LEU
2	U	20	LYS
2	U	27	LEU
2	U	28	THR
2	U	30	SER
2	U	55	LYS
2	U	60	LYS
2	U	80	ASN
2	U	86	MET
2	U	89	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	37	ASN
1	A	97	GLN
1	A	146	GLN
1	A	153	ASN
1	A	348	GLN
1	A	453	GLN
1	A	457	ASN
1	A	475	ASN
1	B	21	ASN
1	B	97	GLN
1	B	146	GLN
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	348	GLN
1	B	366	GLN
1	B	457	ASN
1	B	475	ASN
1	C	21	ASN
1	C	97	GLN
1	C	146	GLN
1	C	153	ASN
1	C	265	ASN
1	C	348	GLN
1	C	453	GLN
1	C	457	ASN
1	C	475	ASN
1	D	21	ASN
1	D	37	ASN
1	D	97	GLN
1	D	146	GLN
1	D	153	ASN
1	D	265	ASN
1	D	348	GLN
1	D	457	ASN
1	D	475	ASN
1	E	21	ASN
1	E	97	GLN
1	E	146	GLN
1	E	153	ASN
1	E	348	GLN
1	E	453	GLN
1	E	457	ASN
1	E	475	ASN
1	F	21	ASN
1	F	97	GLN
1	F	146	GLN
1	F	153	ASN
1	F	265	ASN
1	F	348	GLN
1	F	366	GLN
1	F	453	GLN
1	F	457	ASN
1	F	475	ASN
1	G	21	ASN
1	G	97	GLN

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Mol	Chain	Res	Type
1	G	146	GLN
1	G	153	ASN
1	G	265	ASN
1	G	348	GLN
1	G	453	GLN
1	G	457	ASN
1	G	475	ASN
1	H	21	ASN
1	H	37	ASN
1	H	82	ASN
1	H	97	GLN
1	H	319	GLN
1	H	433	ASN
1	H	467	ASN
1	I	21	ASN
1	I	37	ASN
1	I	82	ASN
1	I	97	GLN
1	I	319	GLN
1	I	433	ASN
1	I	436	GLN
1	I	467	ASN
1	J	21	ASN
1	J	37	ASN
1	J	97	GLN
1	J	319	GLN
1	J	433	ASN
1	J	436	GLN
1	J	467	ASN
1	K	21	ASN
1	K	37	ASN
1	K	97	GLN
1	K	319	GLN
1	K	433	ASN
1	K	467	ASN
1	L	21	ASN
1	L	37	ASN
1	L	82	ASN
1	L	97	GLN
1	L	319	GLN
1	L	433	ASN
1	L	467	ASN

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Mol	Chain	Res	Type
1	M	21	ASN
1	M	37	ASN
1	M	97	GLN
1	M	319	GLN
1	M	433	ASN
1	M	467	ASN
1	N	21	ASN
1	N	37	ASN
1	N	97	GLN
1	N	319	GLN
1	N	433	ASN
1	N	436	GLN
1	N	467	ASN
2	O	45	ASN
2	O	80	ASN
2	P	45	ASN
2	P	80	ASN
2	Q	45	ASN
2	Q	68	ASN
2	R	45	ASN
2	R	68	ASN
2	R	80	ASN
2	S	45	ASN
2	S	68	ASN
2	S	80	ASN
2	T	45	ASN
2	T	80	ASN
2	U	45	ASN
2	U	68	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 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$
5	ADP	A	600	3,4,6	22,29,29	1.11	2 (9%)	27,45,45	3.01	9 (33%)
6	AF3	A	602	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	B	700	3,4,6	22,29,29	1.02	2 (9%)	27,45,45	2.79	7 (25%)
6	AF3	B	702	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	C	800	3,4,6	22,29,29	1.05	2 (9%)	27,45,45	2.86	5 (18%)
6	AF3	C	802	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	D	900	3,4,6	22,29,29	1.10	3 (13%)	27,45,45	3.11	7 (25%)
6	AF3	D	902	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	E	1000	3,4,6	22,29,29	1.09	2 (9%)	27,45,45	3.10	8 (29%)
6	AF3	E	1002	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	F	1100	3,4,6	22,29,29	1.14	2 (9%)	27,45,45	2.83	5 (18%)
6	AF3	F	1102	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	G	1200	3,4,6	22,29,29	1.19	2 (9%)	27,45,45	2.99	8 (29%)
6	AF3	G	1202	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	600	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	A	602	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	B	700	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	B	702	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	C	800	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	C	802	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	D	900	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	D	902	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	E	1000	3,4,6	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AF3	E	1002	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	F	1100	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	F	1102	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	G	1200	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	G	1202	1,3,5,4	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	900	ADP	O4'-C4'	-2.03	1.40	1.45
5	E	1000	ADP	C2-N1	2.15	1.38	1.33
5	D	900	ADP	C2-N1	2.33	1.38	1.33
5	A	600	ADP	C2-N1	2.40	1.38	1.33
5	F	1100	ADP	C2-N1	2.58	1.38	1.33
5	B	700	ADP	C2-N1	2.64	1.38	1.33
5	C	800	ADP	C2-N3	2.65	1.36	1.32
5	C	800	ADP	C2-N1	2.74	1.39	1.33
5	B	700	ADP	C2-N3	2.76	1.37	1.32
5	G	1200	ADP	C2-N3	3.00	1.37	1.32
5	D	900	ADP	C2-N3	3.02	1.37	1.32
5	E	1000	ADP	C2-N3	3.14	1.37	1.32
5	G	1200	ADP	C2-N1	3.19	1.40	1.33
5	F	1100	ADP	C2-N3	3.28	1.38	1.32
5	A	600	ADP	C2-N3	3.41	1.38	1.32

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1000	ADP	N3-C2-N1	-12.68	119.18	128.89
5	D	900	ADP	N3-C2-N1	-12.37	119.42	128.89
5	F	1100	ADP	N3-C2-N1	-11.63	119.99	128.89
5	B	700	ADP	N3-C2-N1	-11.55	120.05	128.89
5	A	600	ADP	N3-C2-N1	-11.45	120.13	128.89
5	C	800	ADP	N3-C2-N1	-11.20	120.32	128.89
5	G	1200	ADP	N3-C2-N1	-10.86	120.58	128.89
5	G	1200	ADP	C2'-C1'-N9	-5.88	105.31	114.29
5	C	800	ADP	C2'-C1'-N9	-5.65	105.66	114.29
5	A	600	ADP	C2'-C1'-N9	-5.47	105.93	114.29
5	D	900	ADP	C2'-C1'-N9	-5.29	106.20	114.29
5	E	1000	ADP	C2'-C1'-N9	-5.06	106.55	114.29
5	A	600	ADP	C1'-N9-C4	-4.55	120.08	126.94
5	G	1200	ADP	C1'-N9-C4	-4.53	120.11	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1100	ADP	C2'-C1'-N9	-4.41	107.55	114.29
5	D	900	ADP	C1'-N9-C4	-4.20	120.61	126.94
5	E	1000	ADP	C1'-N9-C4	-3.84	121.15	126.94
5	F	1100	ADP	C1'-N9-C4	-3.83	121.16	126.94
5	B	700	ADP	C2'-C1'-N9	-3.82	108.46	114.29
5	B	700	ADP	C1'-N9-C4	-3.81	121.19	126.94
5	D	900	ADP	PA-O3A-PB	-3.57	120.71	132.67
5	C	800	ADP	C1'-N9-C4	-3.54	121.59	126.94
5	A	600	ADP	PA-O3A-PB	-3.46	121.08	132.67
5	F	1100	ADP	PA-O3A-PB	-3.37	121.36	132.67
5	E	1000	ADP	C4-C5-N7	-3.31	106.43	109.48
5	E	1000	ADP	PA-O3A-PB	-3.22	121.88	132.67
5	D	900	ADP	C4-C5-N7	-3.14	106.59	109.48
5	B	700	ADP	PA-O3A-PB	-3.10	122.28	132.67
5	G	1200	ADP	PA-O3A-PB	-2.97	122.70	132.67
5	C	800	ADP	PA-O3A-PB	-2.53	124.17	132.67
5	G	1200	ADP	O3'-C3'-C4'	-2.28	104.22	111.05
5	A	600	ADP	C4-C5-N7	-2.14	107.51	109.48
5	B	700	ADP	O3'-C3'-C4'	-2.06	104.86	111.05
5	A	600	ADP	O3'-C3'-C4'	-2.05	104.90	111.05
5	D	900	ADP	O3'-C3'-C4'	-2.02	105.00	111.05
5	E	1000	ADP	O2B-PB-O1B	2.05	117.17	110.58
5	G	1200	ADP	C4'-O4'-C1'	2.05	111.97	109.72
5	B	700	ADP	O5'-C5'-C4'	2.10	116.85	109.12
5	A	600	ADP	C2'-C3'-C4'	2.16	107.04	102.61
5	E	1000	ADP	O5'-C5'-C4'	2.22	117.31	109.12
5	A	600	ADP	O2B-PB-O1B	2.29	117.94	110.58
5	G	1200	ADP	C2'-C3'-C4'	2.65	108.05	102.61
5	F	1100	ADP	O4'-C1'-N9	3.33	115.08	108.10
5	E	1000	ADP	O4'-C1'-N9	3.60	115.63	108.10
5	B	700	ADP	O4'-C1'-N9	3.80	116.06	108.10
5	C	800	ADP	O4'-C1'-N9	3.93	116.31	108.10
5	D	900	ADP	O4'-C1'-N9	4.16	116.80	108.10
5	A	600	ADP	O4'-C1'-N9	4.26	117.01	108.10
5	G	1200	ADP	O4'-C1'-N9	4.79	118.12	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ADP	4	0
6	A	602	AF3	1	0
5	B	700	ADP	1	0
5	C	800	ADP	5	0
6	C	802	AF3	1	0
5	D	900	ADP	2	0
5	E	1000	ADP	1	0
5	F	1100	ADP	3	0
5	G	1200	ADP	1	0
6	G	1202	AF3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	524/524 (100%)	0.32	42 (8%) 15 7	2, 2, 4, 6	0
1	B	524/524 (100%)	0.37	50 (9%) 10 5	2, 2, 4, 6	0
1	C	524/524 (100%)	0.37	39 (7%) 17 9	2, 2, 4, 6	0
1	D	524/524 (100%)	0.34	47 (8%) 12 6	2, 2, 4, 6	0
1	E	524/524 (100%)	0.40	58 (11%) 7 3	2, 2, 4, 6	0
1	F	524/524 (100%)	0.66	75 (14%) 4 2	2, 2, 4, 6	0
1	G	524/524 (100%)	0.44	53 (10%) 9 4	2, 2, 4, 6	0
1	H	524/524 (100%)	-0.05	8 (1%) 76 68	2, 2, 4, 6	0
1	I	524/524 (100%)	-0.07	4 (0%) 87 81	2, 2, 4, 6	0
1	J	524/524 (100%)	-0.02	12 (2%) 64 52	2, 2, 4, 6	0
1	K	524/524 (100%)	0.02	4 (0%) 87 81	2, 2, 4, 6	0
1	L	524/524 (100%)	0.21	22 (4%) 40 28	2, 2, 4, 6	0
1	M	524/524 (100%)	0.03	15 (2%) 55 43	2, 2, 4, 6	0
1	N	524/524 (100%)	0.00	12 (2%) 64 52	2, 2, 4, 6	0
2	O	97/97 (100%)	1.27	21 (21%) 1 1	2, 2, 2, 3	0
2	P	97/97 (100%)	0.77	12 (12%) 5 2	2, 2, 2, 3	0
2	Q	97/97 (100%)	0.89	18 (18%) 2 1	2, 2, 2, 2	0
2	R	97/97 (100%)	1.34	30 (30%) 1 0	2, 2, 2, 3	0
2	S	97/97 (100%)	1.08	20 (20%) 1 1	2, 2, 2, 3	0
2	T	97/97 (100%)	1.11	23 (23%) 1 1	2, 2, 2, 3	0
2	U	97/97 (100%)	1.02	23 (23%) 1 1	2, 2, 2, 2	0
All	All	8015/8015 (100%)	0.29	588 (7%) 18 10	2, 2, 4, 6	0

All (588) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	ALA	12.1
2	S	1	MET	10.3
1	F	212	ALA	9.8
2	O	1	MET	9.7
2	O	17	VAL	9.1
1	G	361	ASP	8.9
1	B	353	ILE	8.7
1	G	212	ALA	8.3
1	E	361	ASP	8.0
1	G	270	ILE	7.9
2	R	17	VAL	7.9
1	G	350	ARG	7.9
1	A	204	PHE	7.8
1	F	215	LEU	7.8
1	F	355	GLU	7.8
2	O	30	SER	7.6
1	C	361	ASP	7.5
2	S	27	LEU	7.1
1	D	353	ILE	7.1
1	E	270	ILE	7.1
1	E	309	LEU	7.0
2	Q	25	ILE	6.8
2	R	1	MET	6.8
2	O	3	ILE	6.8
1	G	268	ARG	6.6
1	F	204	PHE	6.4
2	T	25	ILE	6.3
1	G	279	PRO	6.3
2	Q	27	LEU	6.3
1	C	267	MET	6.2
1	F	361	ASP	6.0
1	D	320	ALA	6.0
1	G	320	ALA	6.0
2	S	97	ALA	5.9
1	B	357	THR	5.8
1	F	210	THR	5.8
1	C	270	ILE	5.8
2	O	27	LEU	5.7
1	A	212	ALA	5.7
1	F	273	VAL	5.7
1	B	355	GLU	5.7
1	C	203	TYR	5.7
2	T	29	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	G	267	MET	5.6
1	F	199	TYR	5.6
1	B	270	ILE	5.5
1	F	362	ARG	5.5
1	C	346	VAL	5.4
2	S	17	VAL	5.4
1	A	353	ILE	5.4
2	T	17	VAL	5.3
1	D	361	ASP	5.3
2	R	26	VAL	5.3
1	F	349	ILE	5.2
1	G	353	ILE	5.2
1	A	361	ASP	5.1
1	C	271	VAL	5.1
1	E	365	LEU	5.1
1	F	333	ILE	5.1
2	S	25	ILE	5.0
1	A	360	TYR	5.0
1	E	355	GLU	5.0
2	U	25	ILE	5.0
1	F	338	GLU	5.0
2	R	18	GLU	4.9
1	C	254	VAL	4.9
1	A	337	GLY	4.9
1	G	208	PRO	4.9
2	R	21	SER	4.9
2	T	97	ALA	4.9
2	P	25	ILE	4.9
1	F	357	THR	4.8
1	L	381	VAL	4.8
1	A	338	GLU	4.8
1	C	357	THR	4.7
1	F	309	LEU	4.7
1	D	212	ALA	4.7
1	B	351	GLN	4.7
1	M	353	ILE	4.7
1	D	338	GLU	4.7
2	P	97	ALA	4.6
1	D	321	LYS	4.6
1	B	333	ILE	4.6
1	B	350	ARG	4.6
1	G	199	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	355	GLU	4.6
2	P	17	VAL	4.6
1	A	270	ILE	4.5
2	P	49	LEU	4.5
2	T	27	LEU	4.5
1	F	172	GLU	4.5
1	E	224	ASP	4.5
1	F	203	TYR	4.5
1	A	271	VAL	4.5
1	B	224	ASP	4.5
1	F	323	VAL	4.5
1	C	350	ARG	4.4
1	L	347	ALA	4.4
1	C	214	GLU	4.4
1	H	356	ALA	4.4
1	F	171	LYS	4.4
1	G	209	GLU	4.4
1	D	349	ILE	4.3
1	F	213	VAL	4.3
1	B	309	LEU	4.3
2	U	1	MET	4.3
1	J	353	ILE	4.3
2	O	78	ILE	4.2
1	E	338	GLU	4.2
2	Q	1	MET	4.2
1	F	254	VAL	4.2
1	A	209	GLU	4.2
1	D	209	GLU	4.2
1	F	250	ILE	4.1
1	F	337	GLY	4.1
2	R	25	ILE	4.1
1	A	364	LYS	4.1
1	G	271	VAL	4.1
2	U	27	LEU	4.1
1	D	215	LEU	4.1
1	F	195	PHE	4.1
1	E	337	GLY	4.1
1	D	270	ILE	4.1
1	F	353	ILE	4.1
2	T	20	LYS	4.1
1	B	361	ASP	4.1
1	D	319	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
2	U	84	LEU	4.0
2	T	26	VAL	4.0
1	F	214	GLU	4.0
1	D	204	PHE	4.0
1	E	237	LEU	4.0
1	B	365	LEU	4.0
1	G	365	LEU	4.0
2	R	3	ILE	4.0
2	S	21	SER	3.9
1	F	321	LYS	3.9
1	A	349	ILE	3.9
1	D	337	GLY	3.9
1	E	353	ILE	3.9
1	B	360	TYR	3.9
1	F	270	ILE	3.9
1	F	272	LYS	3.9
2	U	97	ALA	3.8
1	A	332	ILE	3.8
2	O	48	ILE	3.8
1	D	172	GLU	3.8
2	Q	13	LYS	3.8
2	T	31	ALA	3.7
2	R	27	LEU	3.7
1	E	349	ILE	3.7
1	F	332	ILE	3.7
1	N	356	ALA	3.7
1	D	333	ILE	3.7
1	B	295	LEU	3.7
1	L	44	PHE	3.7
1	C	209	GLU	3.6
2	Q	71	TYR	3.6
2	T	80	ASN	3.6
1	E	266	THR	3.6
1	B	209	GLU	3.6
2	S	26	VAL	3.6
1	A	320	ALA	3.6
1	E	336	VAL	3.5
1	C	353	ILE	3.5
2	T	22	ALA	3.5
1	E	350	ARG	3.5
1	E	320	ALA	3.5
1	E	354	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	340	ALA	3.5
1	M	309	LEU	3.5
1	C	224	ASP	3.5
1	E	360	TYR	3.5
1	B	362	ARG	3.5
1	G	224	ASP	3.5
1	F	295	LEU	3.5
1	M	352	GLN	3.5
1	A	273	VAL	3.5
1	A	199	TYR	3.5
1	A	210	THR	3.5
1	B	204	PHE	3.5
1	F	322	ARG	3.5
1	E	265	ASN	3.5
2	S	95	VAL	3.5
1	F	230	ILE	3.5
2	S	80	ASN	3.5
1	E	281	PHE	3.4
1	B	301	ILE	3.4
1	C	210	THR	3.4
1	L	352	GLN	3.4
1	E	273	VAL	3.4
1	F	334	ASP	3.4
2	R	52	GLY	3.4
1	G	342	ILE	3.4
1	M	357	THR	3.4
1	E	172	GLU	3.4
2	Q	26	VAL	3.4
1	G	349	ILE	3.4
1	J	354	GLU	3.3
1	C	199	TYR	3.3
1	F	219	PHE	3.3
1	F	372	LEU	3.3
1	A	333	ILE	3.3
1	F	227	ILE	3.3
1	D	272	LYS	3.3
1	E	340	ALA	3.3
1	E	302	SER	3.3
1	F	240	VAL	3.3
2	R	97	ALA	3.3
1	G	360	TYR	3.3
2	Q	18	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	368	ARG	3.3
2	U	69	ASP	3.3
1	B	240	VAL	3.3
1	H	44	PHE	3.3
1	M	342	ILE	3.3
1	G	256	GLY	3.3
1	L	354	GLU	3.2
2	O	25	ILE	3.2
1	E	294	THR	3.2
1	G	319	GLN	3.2
1	F	192	GLY	3.2
1	G	215	LEU	3.2
2	R	53	GLU	3.2
2	P	31	ALA	3.2
1	B	203	TYR	3.2
1	D	306	GLY	3.2
1	B	373	ALA	3.2
1	D	360	TYR	3.2
1	F	373	ALA	3.2
1	N	355	GLU	3.2
2	R	82	GLU	3.2
1	M	349	ILE	3.2
2	R	29	GLY	3.2
1	B	245	LYS	3.2
1	C	171	LYS	3.2
1	B	217	SER	3.1
1	G	321	LYS	3.1
2	Q	52	GLY	3.1
1	G	254	VAL	3.1
2	O	20	LYS	3.1
1	E	303	GLU	3.1
1	B	284	ARG	3.1
1	D	284	ARG	3.1
1	A	203	TYR	3.1
1	D	369	VAL	3.1
1	F	324	VAL	3.1
1	F	350	ARG	3.1
1	M	284	ARG	3.1
1	C	320	ALA	3.1
2	R	22	ALA	3.1
1	F	354	GLU	3.1
1	E	369	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	302	SER	3.1
1	G	210	THR	3.1
1	C	360	TYR	3.1
2	T	28	THR	3.1
1	E	351	GLN	3.1
2	U	10	VAL	3.0
1	A	297	GLY	3.0
1	D	271	VAL	3.0
1	F	339	GLU	3.0
1	D	305	ILE	3.0
1	E	195	PHE	3.0
1	G	336	VAL	3.0
1	N	365	LEU	3.0
1	D	352	GLN	3.0
1	K	356	ALA	3.0
1	E	212	ALA	3.0
1	E	203	TYR	3.0
1	F	320	ALA	3.0
2	T	69	ASP	2.9
1	B	314	LEU	2.9
2	U	6	LEU	2.9
1	G	203	TYR	2.9
1	L	344	GLY	2.9
1	F	281	PHE	2.9
1	B	369	VAL	2.9
1	D	365	LEU	2.9
1	G	295	LEU	2.9
1	N	233	MET	2.9
1	B	199	TYR	2.9
2	U	35	SER	2.9
1	B	246	PRO	2.9
1	J	268	ARG	2.9
1	A	365	LEU	2.9
1	A	214	GLU	2.9
1	A	215	LEU	2.9
1	F	173	GLY	2.9
2	U	32	ALA	2.9
1	G	364	LYS	2.9
2	S	30	SER	2.9
1	G	303	GLU	2.9
2	P	27	LEU	2.9
2	U	82	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	257	GLU	2.9
2	P	18	GLU	2.9
1	C	309	LEU	2.9
2	T	30	SER	2.9
1	F	340	ALA	2.9
1	G	334	ASP	2.8
2	U	85	ILE	2.8
1	F	279	PRO	2.8
1	I	357	THR	2.8
1	F	315	GLU	2.8
1	D	237	LEU	2.8
1	F	220	ILE	2.8
1	N	351	GLN	2.8
1	F	284	ARG	2.8
1	L	353	ILE	2.8
1	J	284	ARG	2.8
2	O	96	GLU	2.8
1	G	264	VAL	2.8
1	K	44	PHE	2.8
1	F	245	LYS	2.8
1	A	284	ARG	2.8
1	N	267	MET	2.8
1	A	268	ARG	2.8
1	L	268	ARG	2.8
1	E	321	LYS	2.8
2	U	12	VAL	2.8
1	B	200	LEU	2.8
1	F	331	THR	2.8
2	O	19	THR	2.8
2	U	36	THR	2.8
1	G	243	ALA	2.8
1	F	368	ARG	2.8
1	B	291	ASP	2.8
2	P	51	ASN	2.8
2	O	22	ALA	2.8
1	A	254	VAL	2.8
2	T	3	ILE	2.7
2	R	23	GLY	2.7
1	F	224	ASP	2.7
1	D	364	LYS	2.7
1	F	194	GLN	2.7
2	P	52	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	215	LEU	2.7
2	T	82	GLU	2.7
2	U	83	VAL	2.7
1	J	234	LEU	2.7
1	L	221	LEU	2.7
2	Q	49	LEU	2.7
1	C	359	ASP	2.7
2	R	48	ILE	2.7
1	E	271	VAL	2.7
2	U	26	VAL	2.7
1	B	354	GLU	2.7
1	L	374	GLY	2.7
1	E	342	ILE	2.7
1	C	272	LYS	2.7
2	R	30	SER	2.7
1	M	238	GLU	2.7
2	Q	97	ALA	2.7
1	F	369	VAL	2.7
1	D	199	TYR	2.6
1	D	210	THR	2.6
1	J	233	MET	2.6
1	B	208	PRO	2.6
2	O	54	VAL	2.6
2	T	21	SER	2.6
1	B	346	VAL	2.6
1	I	44	PHE	2.6
2	Q	84	LEU	2.6
1	E	375	GLY	2.6
2	U	52	GLY	2.6
1	C	172	GLU	2.6
1	J	365	LEU	2.6
2	R	57	LEU	2.6
1	A	298	GLY	2.6
1	E	341	ALA	2.6
2	T	71	TYR	2.6
1	B	272	LYS	2.6
1	F	288	MET	2.6
1	G	229	ASN	2.6
2	T	1	MET	2.6
1	B	340	ALA	2.6
1	E	335	GLY	2.6
1	G	233	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	341	ALA	2.6
1	L	271	VAL	2.6
1	A	373	ALA	2.6
1	G	366	GLN	2.6
2	O	97	ALA	2.6
1	A	281	PHE	2.5
2	S	28	THR	2.5
1	F	314	LEU	2.5
1	C	349	ILE	2.5
1	G	351	GLN	2.5
2	U	22	ALA	2.5
1	E	267	MET	2.5
1	K	193	MET	2.5
1	C	279	PRO	2.5
1	F	271	VAL	2.5
1	K	354	GLU	2.5
2	P	66	ILE	2.5
2	P	37	ARG	2.5
1	B	321	LYS	2.5
1	A	172	GLU	2.5
1	C	338	GLU	2.5
1	B	266	THR	2.5
1	C	289	LEU	2.5
1	N	306	GLY	2.5
1	C	250	ILE	2.5
1	F	217	SER	2.5
1	G	323	VAL	2.5
2	Q	90	ASP	2.5
1	E	297	GLY	2.5
2	R	51	ASN	2.5
1	B	332	ILE	2.5
1	G	250	ILE	2.5
1	E	345	ARG	2.5
2	S	96	GLU	2.5
1	E	346	VAL	2.5
1	A	259	LEU	2.5
1	C	213	VAL	2.5
1	B	268	ARG	2.4
1	F	268	ARG	2.4
1	B	267	MET	2.4
1	G	346	VAL	2.4
1	A	266	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	357	THR	2.4
1	B	216	GLU	2.4
1	D	243	ALA	2.4
2	O	49	LEU	2.4
2	R	6	LEU	2.4
2	S	20	LYS	2.4
2	T	49	LEU	2.4
1	I	360	TYR	2.4
1	L	372	LEU	2.4
1	B	349	ILE	2.4
1	E	279	PRO	2.4
1	L	281	PHE	2.4
1	G	222	LEU	2.4
1	N	353	ILE	2.4
2	P	10	VAL	2.4
1	L	215	LEU	2.4
1	J	305	ILE	2.4
2	O	18	GLU	2.4
1	D	268	ARG	2.3
1	B	212	ALA	2.3
1	C	204	PHE	2.3
1	D	350	ARG	2.3
1	D	214	GLU	2.3
2	U	20	LYS	2.3
2	O	80	ASN	2.3
2	R	84	LEU	2.3
2	R	96	GLU	2.3
1	F	319	GLN	2.3
1	B	305	ILE	2.3
1	E	343	GLN	2.3
1	D	297	GLY	2.3
1	C	284	ARG	2.3
2	U	66	ILE	2.3
1	E	204	PHE	2.3
1	E	324	VAL	2.3
1	E	314	LEU	2.3
1	E	192	GLY	2.3
1	G	322	ARG	2.3
1	H	268	ARG	2.3
1	M	44	PHE	2.3
2	T	32	ALA	2.3
2	U	33	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	245	LYS	2.3
1	F	346	VAL	2.3
2	R	83	VAL	2.3
1	G	309	LEU	2.3
1	G	340	ALA	2.3
1	D	233	MET	2.3
2	R	85	ILE	2.3
1	D	335	GLY	2.3
1	N	248	LEU	2.3
1	A	205	ILE	2.2
1	C	325	ILE	2.2
1	E	233	MET	2.2
1	F	233	MET	2.2
2	O	37	ARG	2.2
1	L	236	VAL	2.2
1	F	366	GLN	2.2
1	J	351	GLN	2.2
2	R	32	ALA	2.2
2	U	47	ARG	2.2
1	A	314	LEU	2.2
1	G	196	ASP	2.2
1	H	347	ALA	2.2
1	H	355	GLU	2.2
2	R	31	ALA	2.2
1	F	364	LYS	2.2
2	R	55	LYS	2.2
2	Q	12	VAL	2.2
1	G	284	ARG	2.2
1	F	305	ILE	2.2
1	L	233	MET	2.2
2	U	30	SER	2.2
1	A	346	VAL	2.2
1	F	276	VAL	2.2
1	H	354	GLU	2.2
1	D	224	ASP	2.2
1	E	272	LYS	2.2
2	S	32	ALA	2.2
1	A	272	LYS	2.2
1	B	214	GLU	2.2
1	C	355	GLU	2.2
1	E	217	SER	2.2
2	S	51	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	Q	65	VAL	2.2
1	G	289	LEU	2.2
2	O	32	ALA	2.2
2	Q	33	ALA	2.2
1	B	279	PRO	2.2
1	C	230	ILE	2.2
2	O	47	ARG	2.2
1	F	304	GLU	2.2
1	G	368	ARG	2.2
1	D	208	PRO	2.2
1	E	295	LEU	2.2
1	G	251	ALA	2.2
2	Q	32	ALA	2.2
1	B	233	MET	2.2
1	G	362	ARG	2.2
1	M	356	ALA	2.2
1	E	218	PRO	2.1
1	H	238	GLU	2.1
1	G	244	GLY	2.1
1	L	349	ILE	2.1
2	S	78	ILE	2.1
2	T	18	GLU	2.1
1	A	322	ARG	2.1
1	F	294	THR	2.1
2	R	73	VAL	2.1
1	B	303	GLU	2.1
1	B	289	LEU	2.1
1	D	273	VAL	2.1
1	F	209	GLU	2.1
1	E	199	TYR	2.1
1	M	231	ARG	2.1
1	F	311	LYS	2.1
1	E	234	LEU	2.1
1	E	268	ARG	2.1
2	T	84	LEU	2.1
1	M	193	MET	2.1
2	S	31	ALA	2.1
2	R	67	PHE	2.1
1	B	271	VAL	2.1
1	E	240	VAL	2.1
1	D	373	ALA	2.1
1	M	286	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	192	GLY	2.1
1	L	115	ASP	2.1
1	J	238	GLU	2.1
1	M	355	GLU	2.1
1	D	171	LYS	2.1
2	S	10	VAL	2.1
2	S	22	ALA	2.1
1	A	335	GLY	2.1
1	F	330	THR	2.1
2	O	51	ASN	2.1
1	C	242	LYS	2.1
1	D	191	GLU	2.1
1	G	242	LYS	2.1
2	S	53	GLU	2.1
1	N	263	VAL	2.1
1	I	356	ALA	2.1
1	D	211	GLY	2.1
1	D	245	LYS	2.1
1	C	319	GLN	2.1
1	M	340	ALA	2.1
1	C	195	PHE	2.0
1	E	364	LYS	2.0
1	L	167	ASP	2.0
1	J	266	THR	2.0
1	A	289	LEU	2.0
1	D	372	LEU	2.0
1	N	372	LEU	2.0
1	G	246	PRO	2.0
2	Q	3	ILE	2.0
2	R	66	ILE	2.0
1	A	213	VAL	2.0
1	A	295	LEU	2.0
1	F	247	LEU	2.0
2	Q	17	VAL	2.0
1	L	474	GLY	2.0
1	C	314	LEU	2.0
1	H	242	LYS	2.0
1	L	264	VAL	2.0
1	C	251	ALA	2.0
2	T	72	GLY	2.0
1	G	348	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	K	E	1003	1/1	0.98	0.27	1.38	24,24,24,24	0
4	K	D	903	1/1	0.98	0.22	0.02	24,24,24,24	0
5	ADP	E	1000	27/27	0.95	0.18	-0.33	2,2,5,8	0
5	ADP	F	1100	27/27	0.95	0.18	-0.62	2,2,5,8	0
4	K	G	1203	1/1	0.97	0.17	-0.84	24,24,24,24	0
5	ADP	B	700	27/27	0.95	0.15	-0.98	2,2,5,8	0
4	K	B	703	1/1	0.98	0.16	-1.03	24,24,24,24	0
5	ADP	A	600	27/27	0.96	0.12	-1.26	2,2,6,8	0
5	ADP	G	1200	27/27	0.96	0.16	-1.41	2,2,6,8	0
5	ADP	C	800	27/27	0.95	0.15	-1.45	2,2,5,8	0
4	K	A	603	1/1	0.98	0.16	-1.49	24,24,24,24	0
6	AF3	F	1102	4/4	0.86	0.18	-1.59	5,7,8,12	0
4	K	F	1103	1/1	0.98	0.15	-1.60	24,24,24,24	0
6	AF3	D	902	4/4	0.94	0.15	-1.70	5,7,8,12	0
6	AF3	A	602	4/4	0.91	0.14	-1.71	5,7,8,12	0
5	ADP	D	900	27/27	0.97	0.13	-2.02	2,2,5,8	0
6	AF3	C	802	4/4	0.89	0.13	-2.29	5,7,8,12	0
4	K	C	803	1/1	0.98	0.12	-2.32	24,24,24,24	0
6	AF3	G	1202	4/4	0.94	0.10	-2.74	5,7,8,12	0
6	AF3	B	702	4/4	0.90	0.11	-2.90	5,7,8,12	0
6	AF3	E	1002	4/4	0.89	0.12	-3.21	5,7,8,12	0
3	MG	B	701	1/1	0.97	0.06	-	2,2,2,2	0
3	MG	F	1101	1/1	0.97	0.08	-	2,2,2,2	0
3	MG	A	601	1/1	0.98	0.06	-	2,2,2,2	0
3	MG	C	801	1/1	0.97	0.06	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	E	1001	1/1	0.98	0.05	-	2,2,2,2	0
3	MG	D	901	1/1	0.98	0.05	-	2,2,2,2	0
3	MG	G	1201	1/1	0.96	0.06	-	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.