



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:27 PM GMT

PDB ID : 1PF9  
Title : GroEL-GroES-ADP  
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 : 2003-05-24  
Resolution : 2.99 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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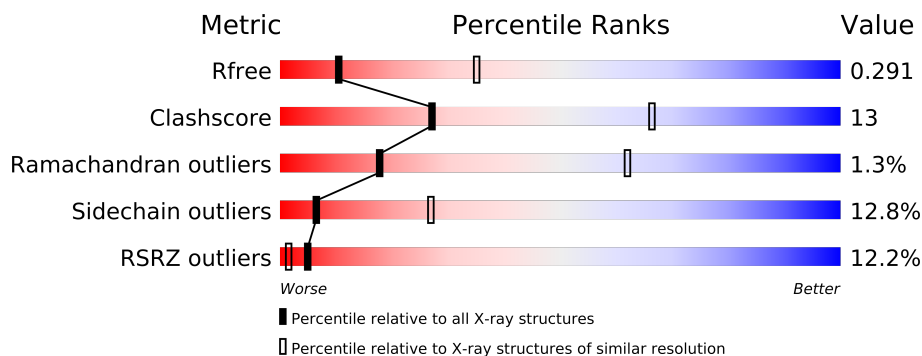
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	524	
1	B	524	
1	C	524	
1	D	524	
1	E	524	
1	F	524	
1	G	524	
1	H	524	
1	I	524	
1	J	524	
1	K	524	
1	L	524	
1	M	524	
1	N	524	

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Mol	Chain	Length	Quality of chain
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	601	-	X
3	MG	D	604	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 59283 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			3856	2397	665	774	20			
1	B	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	C	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	D	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	E	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	F	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	G	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	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			

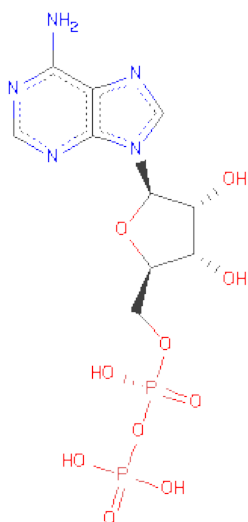
- Molecule 2 is a protein called groES protein.

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 ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		

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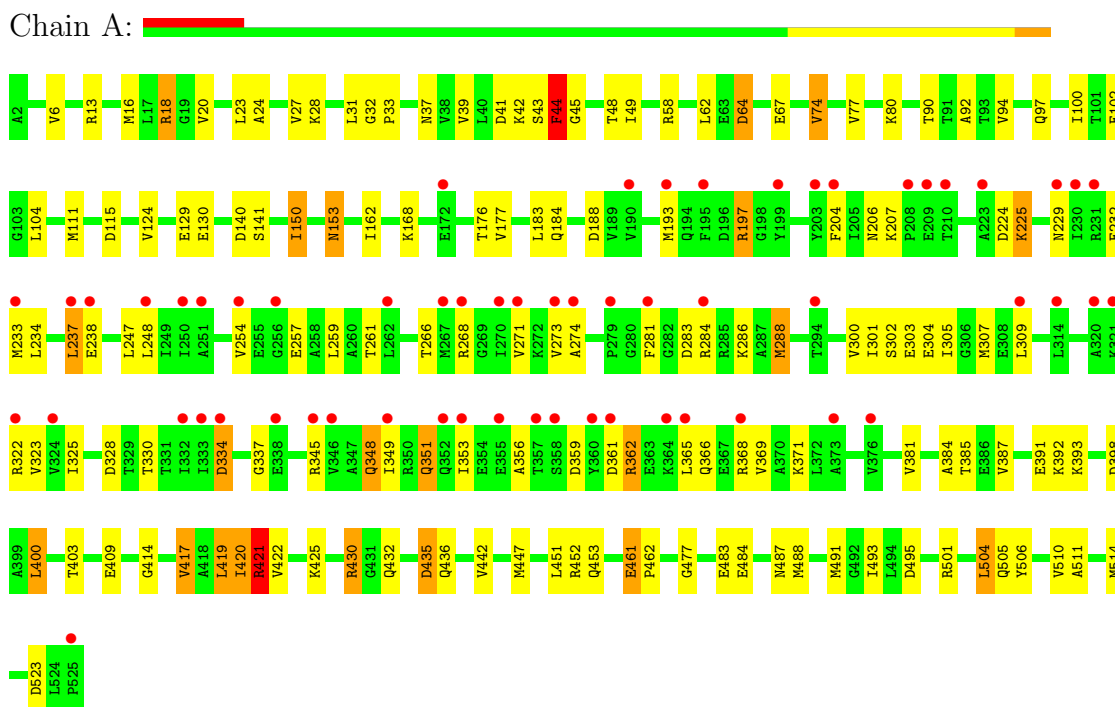
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	O	0	0
			1	1		
5	G	1	Total	O	0	0
			1	1		

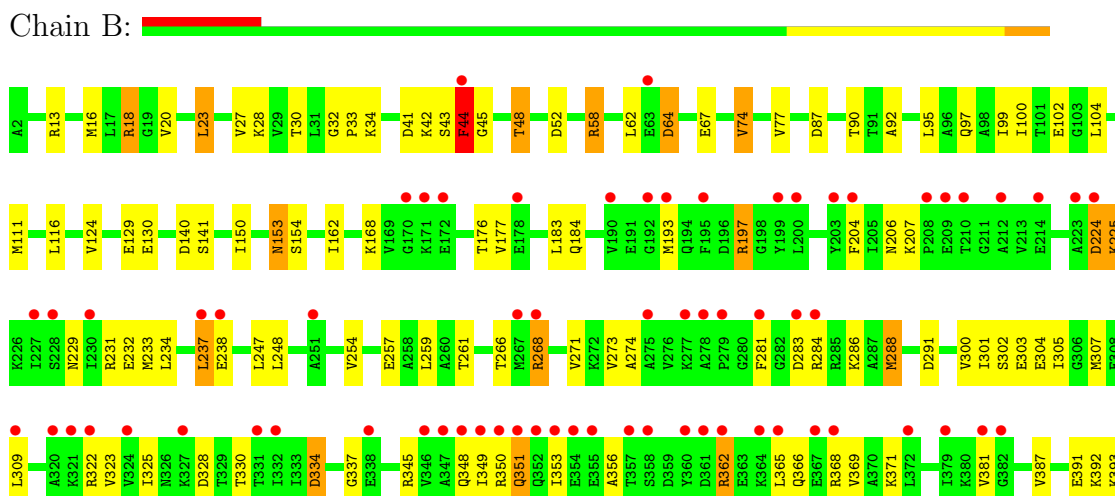
### 3 Residue-property plots

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.

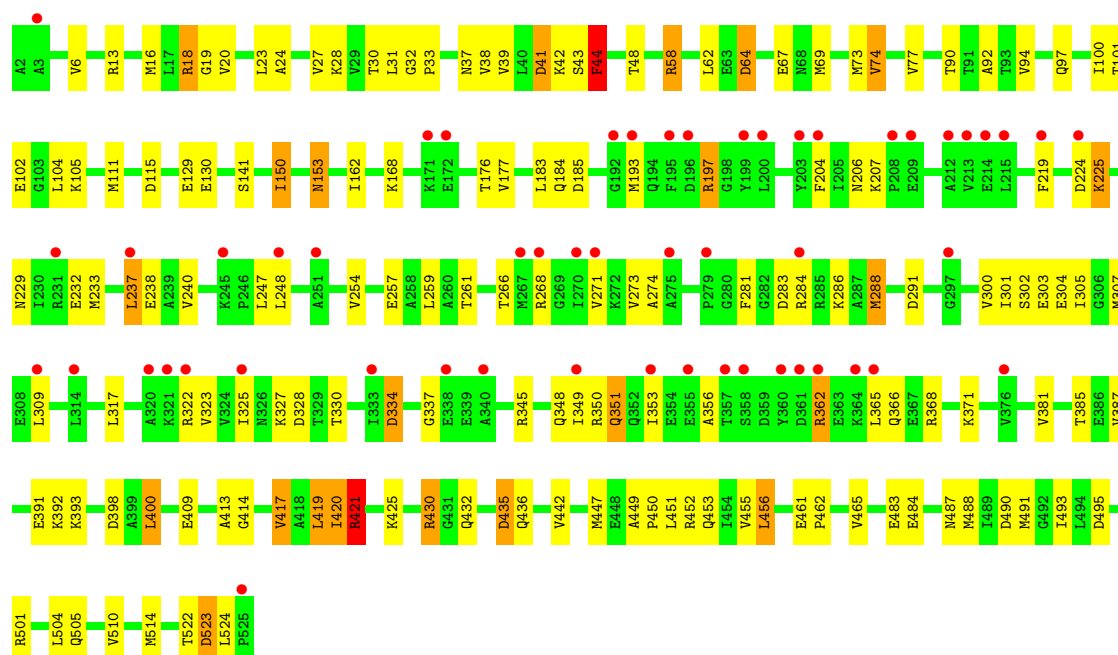
- Molecule 1: groEL protein



- Molecule 1: groEL protein

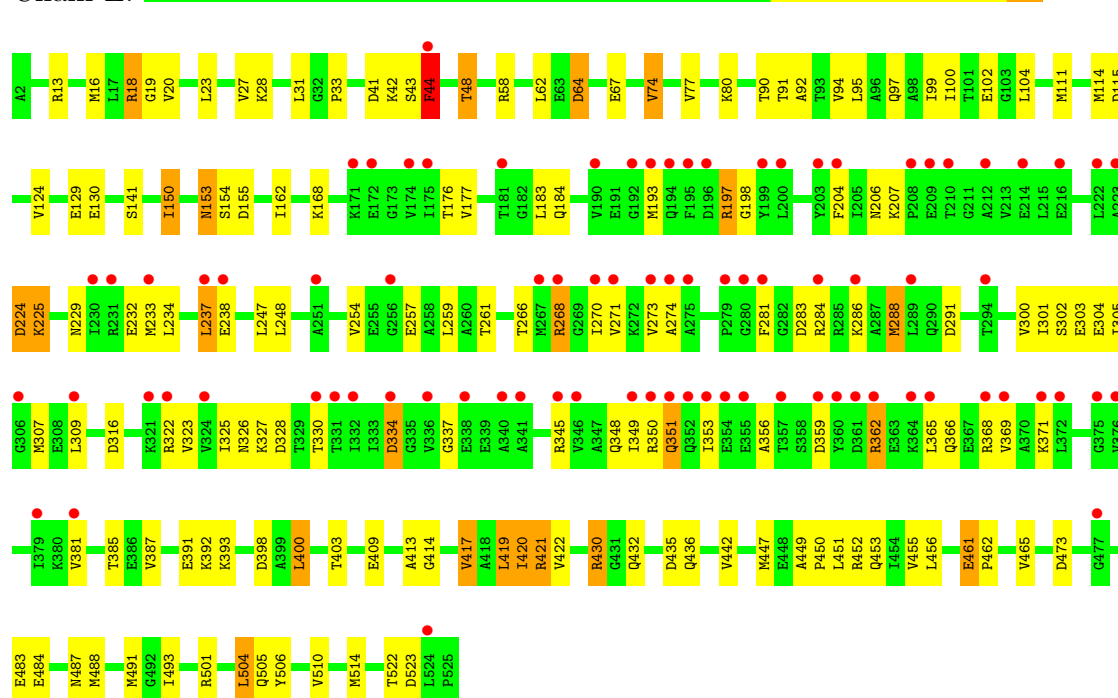






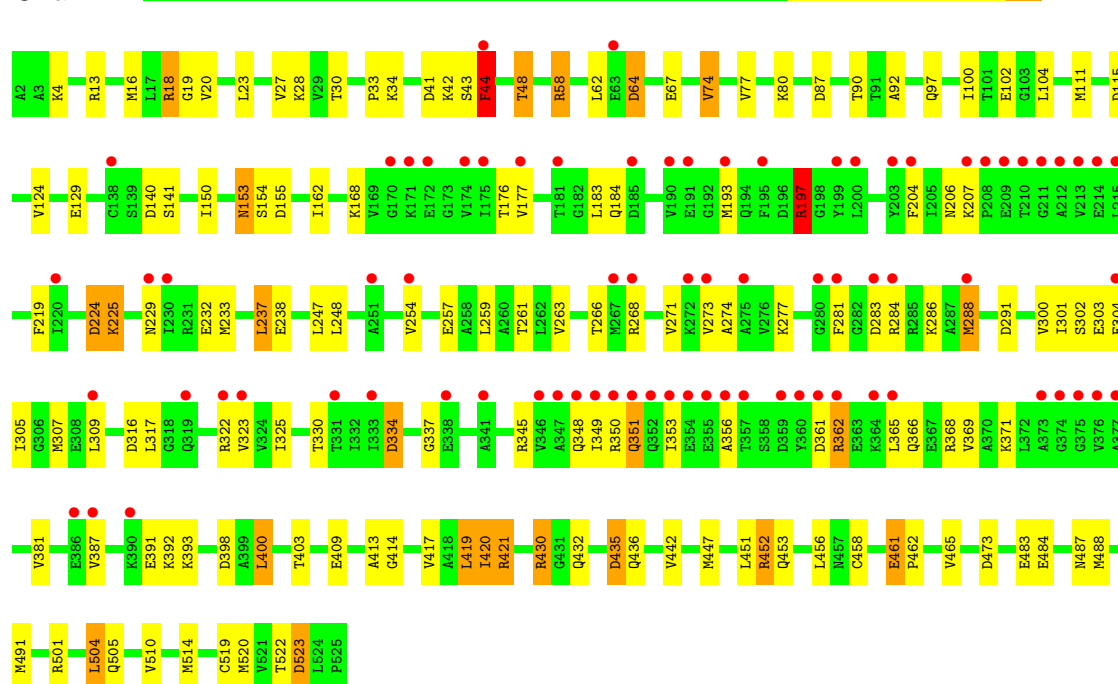
• Molecule 1: groEL protein

Chain E:



• Molecule 1: groEL protein

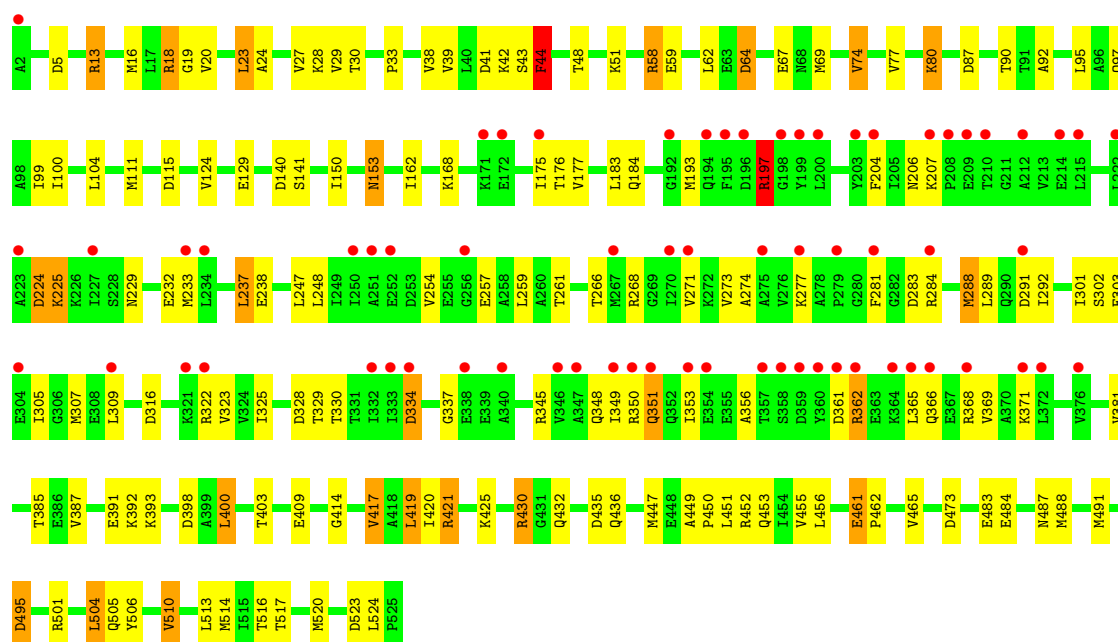
Chain F:

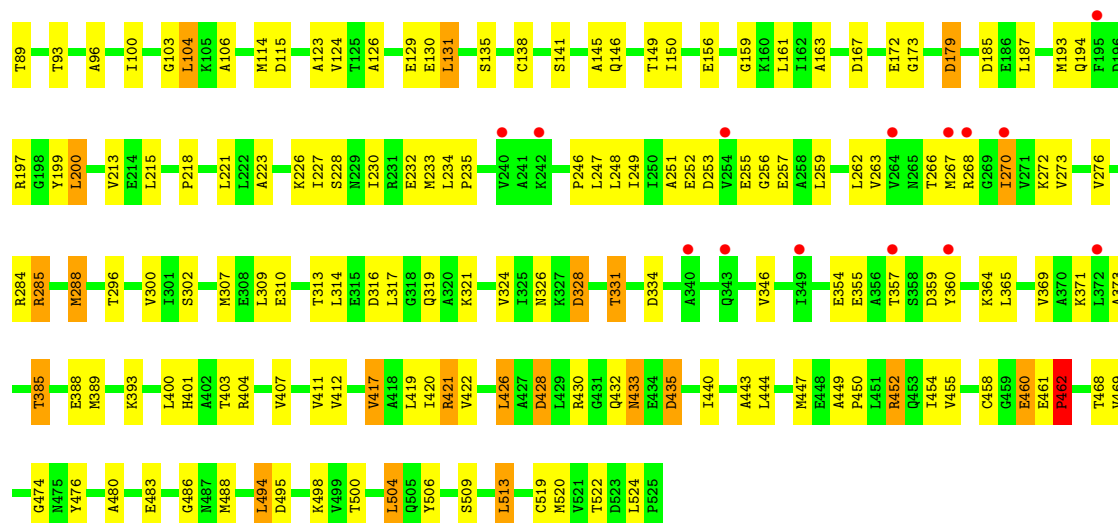


• Molecule 1: groEL protein

Chain G:

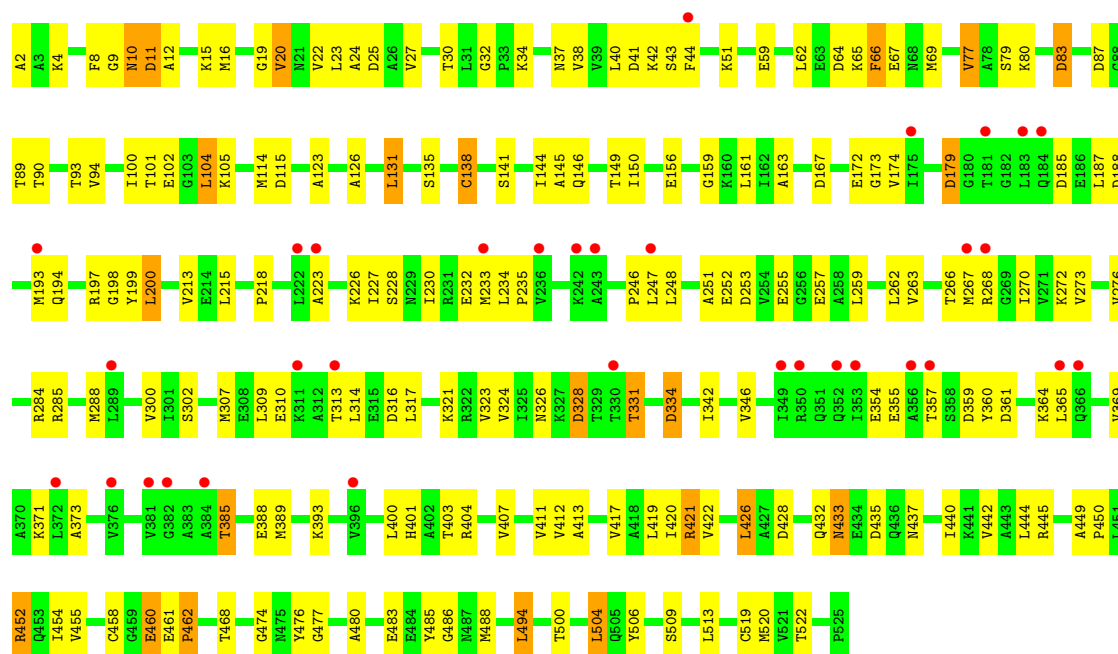






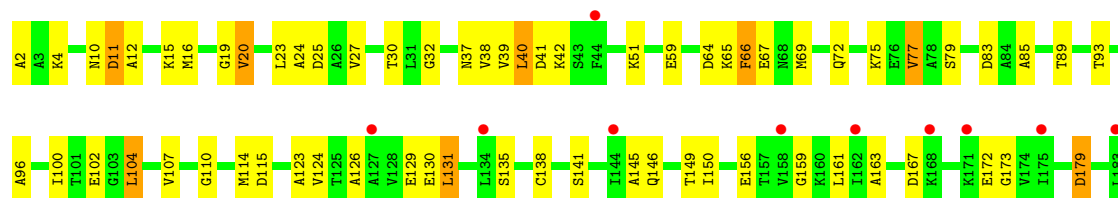
• Molecule 1: groEL protein

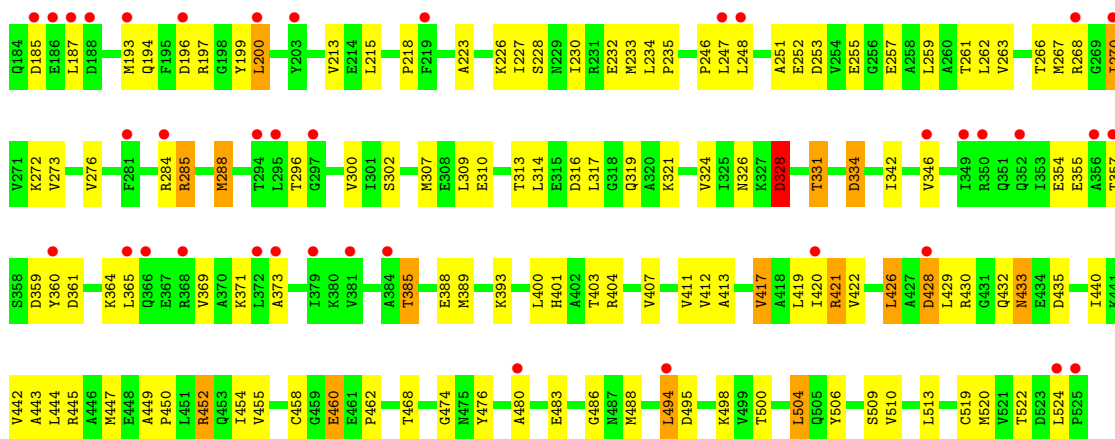
Chain J:



• Molecule 1: groEL protein

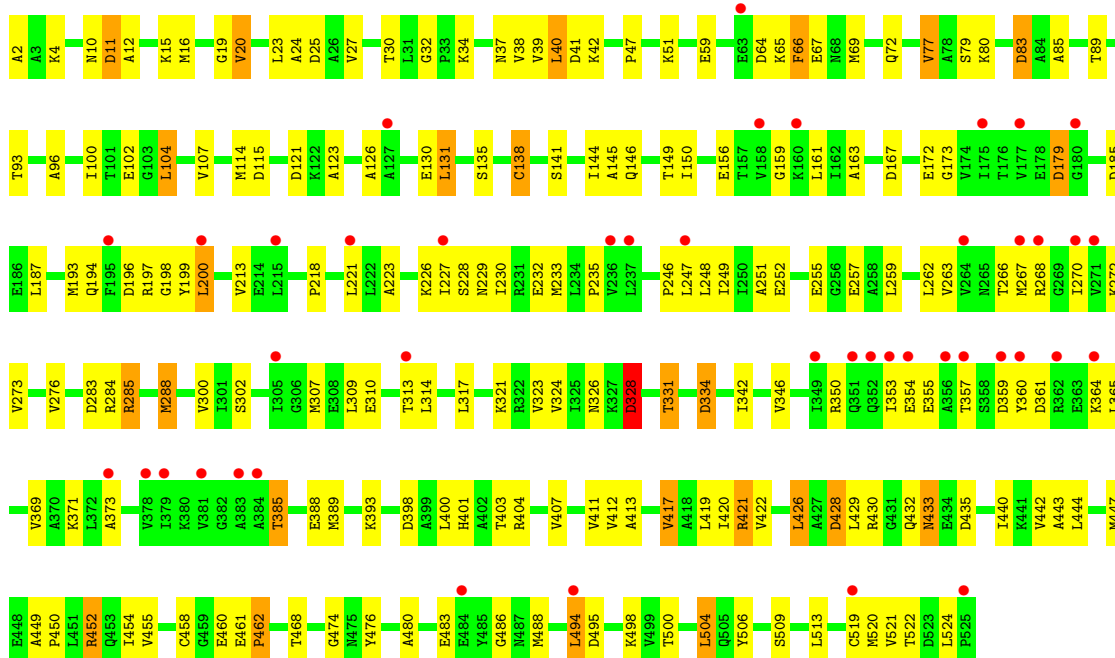
Chain K:





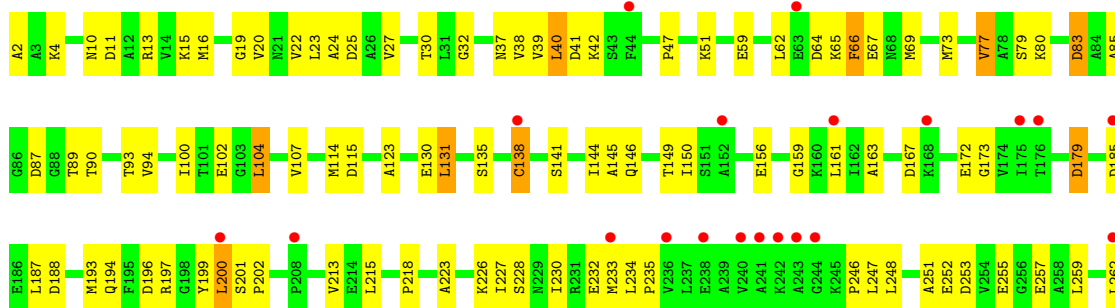
• Molecule 1: groEL protein

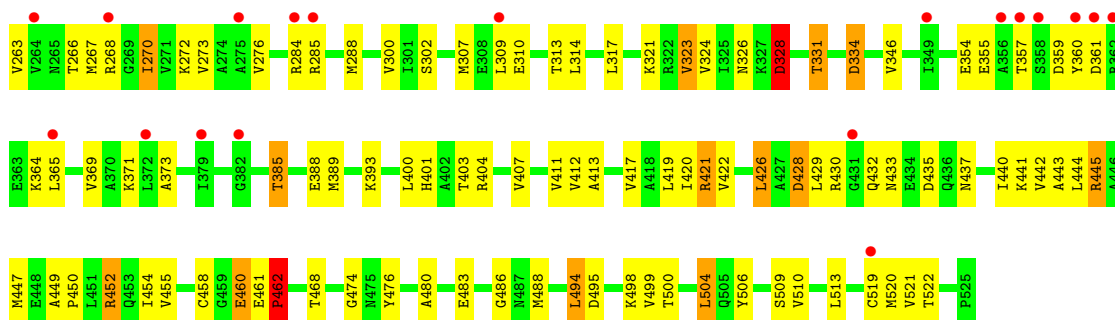
Chain L:



• Molecule 1: groEL protein

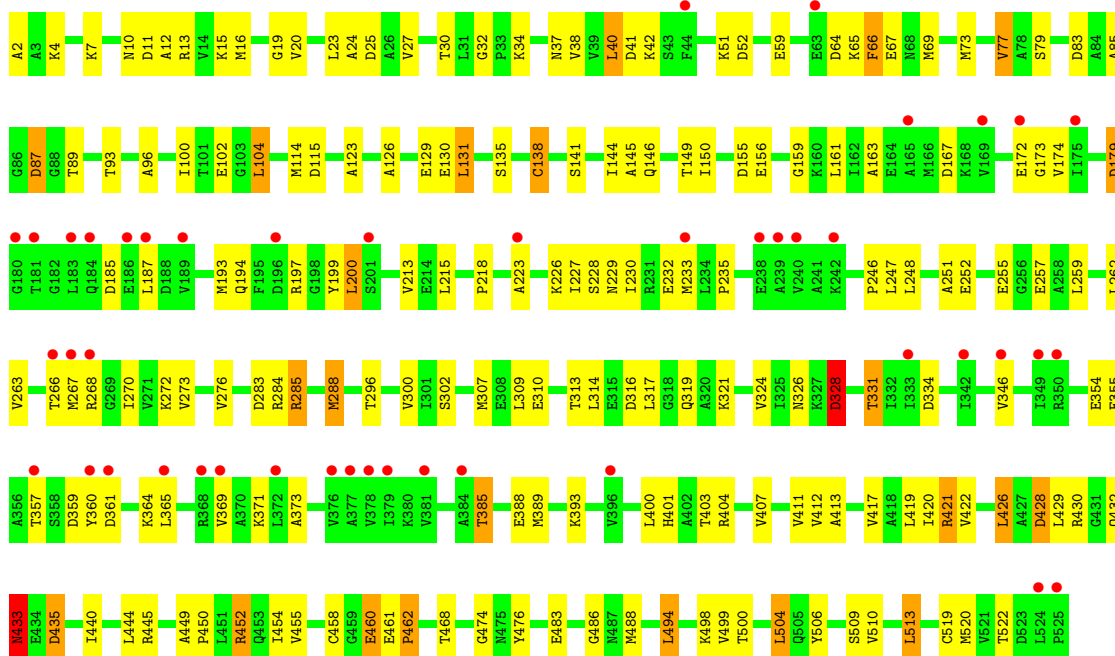
Chain M:





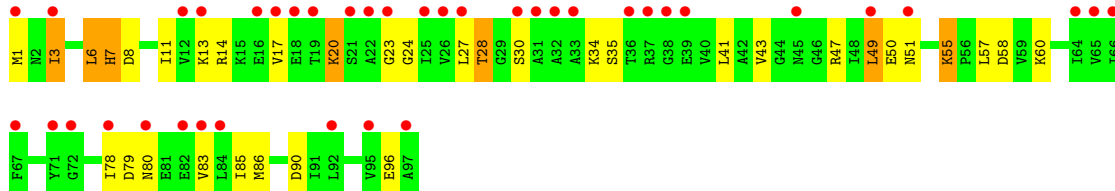
• Molecule 1: groEL protein

Chain N:



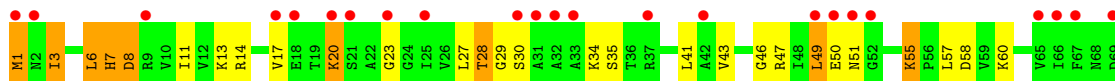
• Molecule 2: groES protein

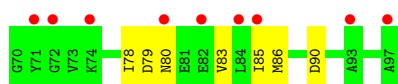
Chain O:



• Molecule 2: groES protein

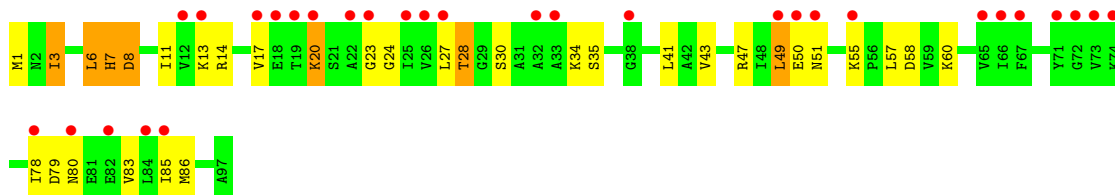
Chain P:





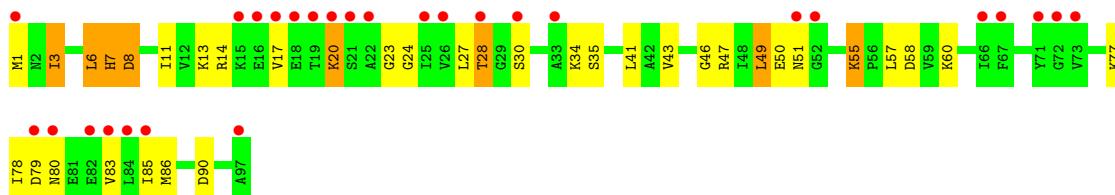
- Molecule 2: groES protein

Chain Q:



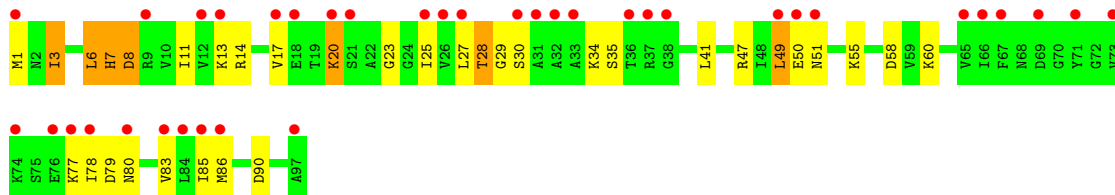
- Molecule 2: groES protein

Chain R:



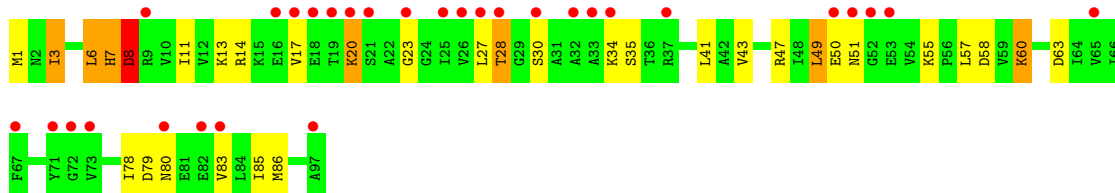
- Molecule 2: groES protein

Chain S:



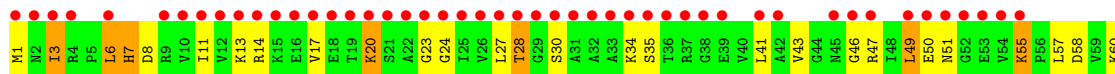
- Molecule 2: groES protein

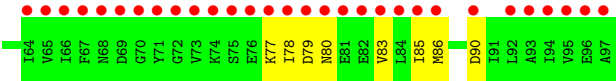
Chain T:



- Molecule 2: groES protein

Chain U:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.26Å 265.25Å 184.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.16 – 2.99 40.07 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.16-2.99) 96.7 (40.07-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.269 , 0.287 0.274 , 0.291	Depositor DCC
$R_{free}$ test set	12081 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 23.5	EDS
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 242645 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	59283	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.67	0/3884	0.90	18/5243 (0.3%)
1	B	0.60	0/3884	0.95	18/5243 (0.3%)
1	C	0.64	0/3884	0.91	20/5243 (0.4%)
1	D	0.66	1/3884 (0.0%)	0.90	17/5243 (0.3%)
1	E	0.57	0/3884	0.86	15/5243 (0.3%)
1	F	0.55	0/3884	0.86	17/5243 (0.3%)
1	G	0.64	0/3884	0.91	20/5243 (0.4%)
1	H	0.59	0/3884	0.85	14/5243 (0.3%)
1	I	0.64	0/3884	0.86	15/5243 (0.3%)
1	J	0.61	0/3884	0.87	18/5243 (0.3%)
1	K	0.54	0/3884	0.83	17/5243 (0.3%)
1	L	0.51	0/3884	0.87	20/5243 (0.4%)
1	M	0.59	0/3884	0.90	20/5243 (0.4%)
1	N	0.59	0/3884	0.85	17/5243 (0.3%)
2	O	0.37	0/732	0.73	3/983 (0.3%)
2	P	0.37	0/732	0.73	4/983 (0.4%)
2	Q	0.38	0/732	0.73	2/983 (0.2%)
2	R	0.41	0/732	0.74	4/983 (0.4%)
2	S	0.39	0/732	0.74	4/983 (0.4%)
2	T	0.39	0/732	0.74	3/983 (0.3%)
2	U	0.38	0/732	0.72	3/983 (0.3%)
All	All	0.59	1/59500 (0.0%)	0.87	269/80283 (0.3%)

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	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	GLU	CD-OE1	5.35	1.31	1.25

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	NE-CZ-NH1	-19.37	110.61	120.30
1	B	231	ARG	NE-CZ-NH2	18.28	129.44	120.30
1	L	268	ARG	NE-CZ-NH2	14.85	127.72	120.30
1	M	268	ARG	NE-CZ-NH2	14.77	127.68	120.30
1	M	268	ARG	NE-CZ-NH1	-14.67	112.97	120.30
1	L	268	ARG	NE-CZ-NH1	-14.62	112.99	120.30
1	G	268	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	D	268	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	A	268	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	A	268	ARG	NE-CZ-NH2	-11.46	114.57	120.30
1	D	268	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	G	268	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	G	197	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	F	197	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	C	197	ARG	NE-CZ-NH1	-10.17	115.22	120.30
1	G	197	ARG	NE-CZ-NH2	9.95	125.28	120.30
1	C	197	ARG	NE-CZ-NH2	9.68	125.14	120.30
1	F	197	ARG	NE-CZ-NH2	9.57	125.08	120.30
1	C	268	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	B	268	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	E	268	ARG	NE-CZ-NH2	9.47	125.04	120.30
1	C	268	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	B	268	ARG	NE-CZ-NH1	-9.26	115.67	120.30
1	B	231	ARG	CD-NE-CZ	9.20	136.48	123.60
1	E	268	ARG	NE-CZ-NH1	-9.19	115.70	120.30
1	F	268	ARG	NE-CZ-NH1	-9.17	115.72	120.30
1	F	268	ARG	NE-CZ-NH2	9.14	124.87	120.30
1	J	25	ASP	CB-CG-OD2	9.01	126.41	118.30
1	E	197	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	B	197	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	K	25	ASP	CB-CG-OD2	7.63	125.16	118.30
1	A	197	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	N	25	ASP	CB-CG-OD2	7.51	125.06	118.30
1	H	25	ASP	CB-CG-OD2	7.47	125.03	118.30
1	L	25	ASP	CB-CG-OD2	7.22	124.80	118.30
1	L	268	ARG	CD-NE-CZ	7.21	133.69	123.60
1	N	83	ASP	CB-CG-OD2	7.18	124.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	268	ARG	CD-NE-CZ	7.12	133.57	123.60
1	E	64	ASP	CB-CG-OD2	7.12	124.70	118.30
1	E	197	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	D	495	ASP	CB-CG-OD2	7.05	124.64	118.30
1	D	197	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	D	64	ASP	CB-CG-OD2	6.88	124.49	118.30
1	M	41	ASP	CB-CG-OD2	6.82	124.44	118.30
1	M	25	ASP	CB-CG-OD2	6.82	124.43	118.30
1	J	428	ASP	CB-CG-OD2	6.79	124.41	118.30
1	B	197	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	K	41	ASP	CB-CG-OD2	6.64	124.28	118.30
1	K	428	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	197	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	M	115	ASP	CB-CG-OD2	6.58	124.23	118.30
1	G	64	ASP	CB-CG-OD2	6.57	124.22	118.30
1	A	421	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	435	ASP	CB-CG-OD2	6.53	124.18	118.30
1	K	83	ASP	CB-CG-OD2	6.50	124.15	118.30
1	D	197	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	K	268	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	25	ASP	CB-CG-OD2	6.39	124.05	118.30
1	L	83	ASP	CB-CG-OD2	6.39	124.05	118.30
1	N	41	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	334	ASP	CB-CG-OD2	6.33	123.99	118.30
1	M	11	ASP	CB-CG-OD2	6.32	123.99	118.30
1	H	268	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	G	140	ASP	CB-CG-OD2	6.30	123.97	118.30
1	E	41	ASP	CB-CG-OD2	6.30	123.97	118.30
1	C	334	ASP	CB-CG-OD2	6.28	123.95	118.30
1	J	83	ASP	CB-CG-OD2	6.27	123.94	118.30
1	I	268	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	F	334	ASP	CB-CG-OD2	6.19	123.87	118.30
1	L	428	ASP	CB-CG-OD2	6.19	123.87	118.30
1	G	334	ASP	CB-CG-OD2	6.18	123.87	118.30
1	K	268	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	87	ASP	CB-CG-OD2	6.16	123.85	118.30
1	D	334	ASP	CB-CG-OD2	6.16	123.84	118.30
1	L	115	ASP	CB-CG-OD2	6.15	123.84	118.30
1	E	334	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	435	ASP	CB-CG-OD2	6.12	123.81	118.30
1	J	268	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	334	ASP	CB-CG-OD2	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	CB-CG-OD2	6.09	123.78	118.30
1	J	41	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	140	ASP	CB-CG-OD2	6.05	123.74	118.30
1	D	421	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	I	41	ASP	CB-CG-OD2	6.03	123.72	118.30
1	M	428	ASP	CB-CG-OD2	6.03	123.72	118.30
1	D	41	ASP	CB-CG-OD2	6.02	123.72	118.30
1	L	11	ASP	CB-CG-OD2	6.01	123.70	118.30
1	I	25	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	283	ASP	CB-CG-OD2	5.96	123.66	118.30
1	D	435	ASP	CB-CG-OD2	5.94	123.64	118.30
1	F	64	ASP	CB-CG-OD2	5.94	123.64	118.30
1	J	115	ASP	CB-CG-OD2	5.94	123.64	118.30
1	H	334	ASP	CB-CG-OD2	5.93	123.64	118.30
1	J	11	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	64	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	523	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	140	ASP	CB-CG-OD2	5.91	123.62	118.30
1	N	268	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	F	283	ASP	CB-CG-OD2	5.89	123.60	118.30
1	I	268	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	I	428	ASP	CB-CG-OD2	5.87	123.58	118.30
1	N	268	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	115	ASP	CB-CG-OD2	5.86	123.57	118.30
2	R	8	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	283	ASP	CB-CG-OD2	5.85	123.57	118.30
2	Q	58	ASP	CB-CG-OD2	5.85	123.57	118.30
1	J	435	ASP	CB-CG-OD2	5.84	123.56	118.30
1	H	268	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	P	58	ASP	CB-CG-OD2	5.83	123.55	118.30
1	F	41	ASP	CB-CG-OD2	5.83	123.55	118.30
1	D	523	ASP	CB-CG-OD2	5.80	123.52	118.30
1	H	428	ASP	CB-CG-OD2	5.79	123.51	118.30
1	H	495	ASP	CB-CG-OD2	5.79	123.51	118.30
1	C	41	ASP	CB-CG-OD2	5.77	123.49	118.30
1	D	268	ARG	CD-NE-CZ	5.77	131.67	123.60
1	I	495	ASP	CB-CG-OD2	5.76	123.48	118.30
1	M	83	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	268	ARG	CD-NE-CZ	5.75	131.66	123.60
2	T	58	ASP	CB-CG-OD2	5.75	123.47	118.30
1	N	428	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	41	ASP	CB-CG-OD2	5.72	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	435	ASP	CB-CG-OD2	5.69	123.42	118.30
1	I	115	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	283	ASP	CB-CG-OD2	5.68	123.41	118.30
1	I	435	ASP	CB-CG-OD2	5.68	123.41	118.30
1	J	334	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	473	ASP	CB-CG-OD2	5.66	123.39	118.30
2	R	58	ASP	CB-CG-OD2	5.66	123.39	118.30
1	F	140	ASP	CB-CG-OD2	5.66	123.39	118.30
1	M	328	ASP	CB-CG-OD2	5.65	123.39	118.30
1	G	495	ASP	CB-CG-OD2	5.65	123.38	118.30
2	O	58	ASP	CB-CG-OD2	5.65	123.38	118.30
1	G	13	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	G	268	ARG	CD-NE-CZ	5.62	131.47	123.60
1	G	283	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	495	ASP	CB-CG-OD2	5.61	123.35	118.30
1	N	87	ASP	CB-CG-OD2	5.60	123.34	118.30
1	E	283	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	283	ASP	CB-CG-OD2	5.58	123.32	118.30
1	J	268	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	224	ASP	CB-CG-OD2	5.55	123.29	118.30
2	P	8	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	473	ASP	CB-CG-OD2	5.53	123.28	118.30
1	M	334	ASP	CB-CG-OD2	5.51	123.26	118.30
1	M	179	ASP	CB-CG-OD2	5.48	123.24	118.30
1	G	87	ASP	CB-CG-OD2	5.48	123.23	118.30
1	K	115	ASP	CB-CG-OD2	5.48	123.23	118.30
1	E	155	ASP	CB-CG-OD2	5.48	123.23	118.30
1	G	523	ASP	CB-CG-OD2	5.48	123.23	118.30
1	F	523	ASP	CB-CG-OD2	5.47	123.22	118.30
1	H	83	ASP	CB-CG-OD2	5.47	123.23	118.30
2	U	90	ASP	CB-CG-OD2	5.47	123.22	118.30
1	L	334	ASP	CB-CG-OD2	5.47	123.22	118.30
1	G	473	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	523	ASP	CB-CG-OD2	5.46	123.21	118.30
1	H	359	ASP	CB-CG-OD2	5.45	123.20	118.30
1	H	196	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	64	ASP	CB-CG-OD2	5.44	123.19	118.30
1	L	359	ASP	CB-CG-OD2	5.44	123.19	118.30
1	G	224	ASP	CB-CG-OD2	5.43	123.19	118.30
1	K	196	ASP	CB-CG-OD2	5.42	123.18	118.30
1	J	316	ASP	CB-CG-OD2	5.42	123.18	118.30
1	J	179	ASP	CB-CG-OD2	5.41	123.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	316	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	115	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	155	ASP	CB-CG-OD2	5.37	123.13	118.30
2	T	79	ASP	CB-CG-OD2	5.37	123.13	118.30
1	K	179	ASP	CB-CG-OD2	5.36	123.12	118.30
1	M	253	ASP	CB-CG-OD2	5.34	123.11	118.30
1	F	155	ASP	CB-CG-OD2	5.34	123.10	118.30
1	N	179	ASP	CB-CG-OD2	5.33	123.10	118.30
1	L	121	ASP	CB-CG-OD2	5.33	123.10	118.30
1	F	473	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	140	ASP	CB-CG-OD2	5.33	123.09	118.30
2	Q	79	ASP	CB-CG-OD2	5.32	123.09	118.30
1	J	253	ASP	CB-CG-OD2	5.31	123.08	118.30
1	L	462	PRO	N-CD-CG	-5.31	95.23	103.20
1	E	473	ASP	CB-CG-OD2	5.31	123.08	118.30
1	G	5	ASP	CB-CG-OD2	5.30	123.07	118.30
1	I	87	ASP	CB-CG-OD2	5.30	123.07	118.30
1	K	359	ASP	CB-CG-OD2	5.30	123.07	118.30
1	K	495	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	188	ASP	CB-CG-OD2	5.29	123.06	118.30
1	I	359	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	64	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	185	ASP	CB-CG-OD2	5.29	123.06	118.30
1	J	359	ASP	CB-CG-OD2	5.29	123.06	118.30
1	M	361	ASP	CB-CG-OD2	5.29	123.06	118.30
1	M	435	ASP	CB-CG-OD2	5.28	123.06	118.30
1	K	316	ASP	CB-CG-OD2	5.28	123.05	118.30
1	H	283	ASP	CB-CG-OD2	5.27	123.05	118.30
2	P	79	ASP	CB-CG-OD2	5.27	123.05	118.30
1	F	87	ASP	CB-CG-OD2	5.27	123.04	118.30
1	M	359	ASP	CB-CG-OD2	5.26	123.04	118.30
1	C	452	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	L	495	ASP	CB-CG-OD2	5.25	123.03	118.30
1	L	41	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	115	ASP	CB-CG-OD2	5.25	123.03	118.30
1	L	179	ASP	CB-CG-OD2	5.25	123.03	118.30
1	E	328	ASP	CB-CG-OD2	5.25	123.02	118.30
1	L	196	ASP	CB-CG-OD2	5.25	123.02	118.30
1	N	328	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	185	ASP	CB-CG-OD2	5.24	123.02	118.30
2	O	90	ASP	CB-CG-OD2	5.24	123.02	118.30
1	F	224	ASP	CB-CG-OD2	5.24	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	495	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	115	ASP	CB-CG-OD2	5.22	123.00	118.30
1	L	361	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	224	ASP	CB-CG-OD2	5.22	123.00	118.30
2	O	79	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	361	ASP	CB-CG-OD2	5.21	122.99	118.30
1	N	435	ASP	CB-CG-OD2	5.21	122.99	118.30
1	L	328	ASP	CB-CG-OD2	5.20	122.98	118.30
1	M	462	PRO	N-CD-CG	-5.20	95.40	103.20
1	I	253	ASP	CB-CG-OD2	5.20	122.98	118.30
1	K	334	ASP	CB-CG-OD2	5.20	122.98	118.30
1	G	41	ASP	CB-CG-OD2	5.20	122.98	118.30
1	I	316	ASP	CB-CG-OD2	5.19	122.97	118.30
2	R	79	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	361	ASP	CB-CG-OD2	5.19	122.97	118.30
1	H	435	ASP	CB-CG-OD2	5.19	122.97	118.30
1	J	188	ASP	CB-CG-OD2	5.19	122.97	118.30
2	U	58	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	490	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	421	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	I	11	ASP	CB-CG-OD2	5.16	122.95	118.30
1	N	155	ASP	CB-CG-OD2	5.16	122.94	118.30
1	N	115	ASP	CB-CG-OD2	5.15	122.94	118.30
1	G	316	ASP	CB-CG-OD2	5.15	122.93	118.30
1	H	316	ASP	CB-CG-OD2	5.15	122.93	118.30
1	I	179	ASP	CB-CG-OD2	5.14	122.93	118.30
1	M	196	ASP	CB-CG-OD2	5.14	122.93	118.30
1	L	398	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	196	ASP	CB-CG-OD2	5.14	122.92	118.30
2	S	79	ASP	CB-CG-OD2	5.13	122.92	118.30
1	N	52	ASP	CB-CG-OD2	5.13	122.91	118.30
1	E	316	ASP	CB-CG-OD2	5.12	122.91	118.30
1	N	359	ASP	CB-CG-OD2	5.12	122.90	118.30
1	H	462	PRO	N-CD-CG	-5.11	95.53	103.20
1	K	253	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	167	ASP	CB-CG-OD2	5.11	122.90	118.30
1	K	328	ASP	CB-CG-OD2	5.11	122.90	118.30
2	S	8	ASP	CB-CG-OD2	5.11	122.90	118.30
2	S	90	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	224	ASP	CB-CG-OD2	5.10	122.89	118.30
1	K	361	ASP	CB-CG-OD2	5.09	122.89	118.30
2	U	79	ASP	CB-CG-OD2	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	90	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	328	ASP	CB-CG-OD2	5.08	122.87	118.30
1	N	361	ASP	CB-CG-OD2	5.08	122.87	118.30
1	G	115	ASP	CB-CG-OD2	5.07	122.86	118.30
2	R	90	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	328	ASP	CB-CG-OD2	5.06	122.86	118.30
2	S	58	ASP	CB-CG-OD2	5.06	122.86	118.30
1	L	283	ASP	CB-CG-OD2	5.06	122.86	118.30
1	I	462	PRO	N-CD-CG	-5.06	95.61	103.20
1	A	328	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	316	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	359	ASP	CB-CG-OD2	5.04	122.84	118.30
1	M	188	ASP	CB-CG-OD2	5.04	122.84	118.30
1	G	328	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	52	ASP	CB-CG-OD2	5.02	122.82	118.30
2	T	8	ASP	CB-CG-OD2	5.02	122.82	118.30
1	C	359	ASP	CB-CG-OD2	5.02	122.82	118.30
1	J	87	ASP	CB-CG-OD2	5.02	122.81	118.30
1	J	328	ASP	CB-CG-OD2	5.01	122.81	118.30
1	N	283	ASP	CB-CG-OD2	5.01	122.81	118.30
1	K	11	ASP	CB-CG-OD2	5.01	122.81	118.30
1	E	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	N	433	ASN	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3976	105	0
1	B	3856	0	3976	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3856	0	3976	109	0
1	D	3856	0	3976	115	0
1	E	3856	0	3976	104	0
1	F	3856	0	3976	99	0
1	G	3856	0	3976	113	0
1	H	3856	0	3976	107	0
1	I	3856	0	3976	104	0
1	J	3856	0	3976	106	0
1	K	3856	0	3976	110	0
1	L	3856	0	3976	112	0
1	M	3856	0	3976	115	0
1	N	3856	0	3976	111	0
2	O	728	0	762	20	0
2	P	728	0	762	21	0
2	Q	728	0	762	18	0
2	R	728	0	762	17	0
2	S	728	0	762	19	0
2	T	728	0	762	15	0
2	U	728	0	762	17	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	27	0	12	2	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	3	0
4	E	27	0	12	1	0
4	F	27	0	12	1	0
4	G	27	0	12	3	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	D	1	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	1	0
All	All	59283	0	61082	1567	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 13.

All (1567) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:114:MET:CE	1:E:114:MET:SD	2.05	1.45
1:C:73:MET:SD	1:C:73:MET:CE	2.05	1.42
1:C:18:ARG:HG2	1:C:18:ARG:HH11	1.07	1.19
1:G:18:ARG:HH11	1:G:18:ARG:HG2	1.07	1.17
1:D:432:GLN:NE2	1:D:436:GLN:HE22	1.47	1.13
1:F:18:ARG:HH11	1:F:18:ARG:HG2	1.03	1.11
1:E:18:ARG:HH11	1:E:18:ARG:HG2	1.11	1.11
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.14	1.11
1:B:18:ARG:HH11	1:B:18:ARG:HG2	1.00	1.10
1:B:414:GLY:O	1:B:417:VAL:HG12	1.52	1.09
1:A:432:GLN:NE2	1:A:436:GLN:HE22	1.51	1.09
1:G:432:GLN:NE2	1:G:436:GLN:HE22	1.52	1.07
1:A:414:GLY:O	1:A:417:VAL:HG12	1.51	1.07
1:G:414:GLY:O	1:G:417:VAL:HG12	1.54	1.06
1:C:432:GLN:NE2	1:C:436:GLN:HE22	1.53	1.05
1:B:18:ARG:CG	1:B:18:ARG:HH11	1.71	1.03
1:B:432:GLN:NE2	1:B:436:GLN:HE22	1.56	1.02
1:F:414:GLY:O	1:F:417:VAL:HG12	1.59	1.02
1:D:414:GLY:O	1:D:417:VAL:HG12	1.58	1.02
1:C:414:GLY:O	1:C:417:VAL:HG12	1.57	1.02
1:E:432:GLN:NE2	1:E:436:GLN:HE22	1.57	1.02
1:F:432:GLN:NE2	1:F:436:GLN:HE22	1.58	1.01
1:D:18:ARG:HH11	1:D:18:ARG:HG2	1.24	1.01
1:D:432:GLN:HE21	1:D:436:GLN:NE2	1.58	1.00
1:F:18:ARG:CG	1:F:18:ARG:HH11	1.73	1.00
1:E:414:GLY:O	1:E:417:VAL:HG12	1.62	0.99
1:M:65:LYS:O	1:M:66:PHE:HB2	1.61	0.99
1:D:44:PHE:HD1	1:D:44:PHE:H	1.03	0.98
1:G:18:ARG:CG	1:G:18:ARG:HH11	1.77	0.97
1:C:18:ARG:CG	1:C:18:ARG:HH11	1.76	0.97
1:L:426:LEU:HD12	1:L:444:LEU:HD21	1.48	0.95
1:E:44:PHE:H	1:E:44:PHE:HD1	1.06	0.95
1:F:18:ARG:NH1	1:F:18:ARG:HG2	1.76	0.95
1:B:204:PHE:HE2	1:B:266:THR:HG21	1.32	0.95
1:B:18:ARG:NH1	1:B:18:ARG:HG2	1.72	0.95
1:A:204:PHE:HE2	1:A:266:THR:HG21	1.31	0.94
1:C:432:GLN:HE21	1:C:436:GLN:HE22	0.96	0.94
1:G:204:PHE:HE2	1:G:266:THR:HG21	1.32	0.94
1:A:432:GLN:HE21	1:A:436:GLN:NE2	1.64	0.94
1:D:18:ARG:CG	1:D:18:ARG:HH11	1.81	0.94

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:204:PHE:HE2	1:D:266:THR:HG21	1.33	0.93
1:E:204:PHE:HE2	1:E:266:THR:HG21	1.31	0.93
1:E:18:ARG:HH11	1:E:18:ARG:CG	1.80	0.93
1:K:65:LYS:O	1:K:66:PHE:HB2	1.66	0.93
1:F:204:PHE:HE2	1:F:266:THR:HG21	1.30	0.93
1:N:65:LYS:O	1:N:66:PHE:HB2	1.64	0.93
1:B:432:GLN:HE21	1:B:436:GLN:HE22	0.96	0.93
1:C:44:PHE:HD1	1:C:44:PHE:H	0.99	0.93
1:I:404:ARG:HH11	1:I:404:ARG:HG2	1.34	0.93
1:J:65:LYS:O	1:J:66:PHE:HB2	1.68	0.93
1:C:204:PHE:HE2	1:C:266:THR:HG21	1.32	0.92
1:F:44:PHE:HD1	1:F:44:PHE:H	1.11	0.92
1:A:18:ARG:CG	1:A:18:ARG:HH11	1.81	0.92
1:C:432:GLN:HE21	1:C:436:GLN:NE2	1.66	0.92
1:G:432:GLN:HE21	1:G:436:GLN:HE22	0.94	0.92
1:G:18:ARG:NH1	1:G:18:ARG:HG2	1.81	0.91
1:E:432:GLN:HE21	1:E:436:GLN:HE22	0.96	0.91
1:D:430:ARG:HH11	1:D:430:ARG:HG2	1.32	0.91
1:I:65:LYS:O	1:I:66:PHE:HB2	1.70	0.91
1:L:65:LYS:O	1:L:66:PHE:HB2	1.71	0.91
1:H:65:LYS:O	1:H:66:PHE:HB2	1.66	0.91
1:A:44:PHE:H	1:A:44:PHE:HD1	1.07	0.91
1:L:69:MET:HE1	1:L:522:THR:HB	1.52	0.90
1:J:426:LEU:HD12	1:J:444:LEU:HD21	1.53	0.90
1:G:432:GLN:HE21	1:G:436:GLN:NE2	1.70	0.90
1:C:18:ARG:NH1	1:C:18:ARG:HG2	1.77	0.89
1:I:426:LEU:HD12	1:I:444:LEU:HD21	1.53	0.89
1:E:432:GLN:HE21	1:E:436:GLN:NE2	1.69	0.89
1:M:426:LEU:HD12	1:M:444:LEU:HD21	1.54	0.89
1:B:44:PHE:HD1	1:B:44:PHE:H	1.00	0.89
1:G:44:PHE:H	1:G:44:PHE:HD1	1.08	0.88
1:B:432:GLN:HE21	1:B:436:GLN:NE2	1.70	0.88
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.36	0.88
1:F:432:GLN:HE21	1:F:436:GLN:NE2	1.70	0.88
1:N:426:LEU:HD12	1:N:444:LEU:HD21	1.53	0.88
1:E:18:ARG:HG2	1:E:18:ARG:NH1	1.82	0.88
1:F:432:GLN:HE21	1:F:436:GLN:HE22	0.95	0.87
1:I:69:MET:HE1	1:I:522:THR:HB	1.56	0.87
1:K:426:LEU:HD12	1:K:444:LEU:HD21	1.55	0.86
1:G:430:ARG:HG2	1:G:430:ARG:HH11	1.40	0.85
1:A:432:GLN:HE21	1:A:436:GLN:HE22	0.86	0.85
1:H:426:LEU:HD12	1:H:444:LEU:HD21	1.57	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:69:MET:HE1	1:K:522:THR:HB	1.57	0.84
1:A:74:VAL:O	1:A:77:VAL:HG13	1.78	0.84
1:H:69:MET:HE1	1:H:522:THR:HB	1.58	0.84
1:C:430:ARG:HG2	1:C:430:ARG:HH11	1.43	0.84
1:A:18:ARG:HG2	1:A:18:ARG:NH1	1.83	0.83
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.43	0.83
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.43	0.83
1:E:44:PHE:N	1:E:44:PHE:CD1	2.47	0.83
1:D:74:VAL:O	1:D:77:VAL:HG13	1.79	0.82
1:E:430:ARG:HH11	1:E:430:ARG:HG2	1.43	0.82
1:C:100:ILE:HD11	1:C:514:MET:HE1	1.60	0.82
1:F:44:PHE:N	1:F:44:PHE:CD1	2.48	0.81
1:D:44:PHE:N	1:D:44:PHE:CD1	2.48	0.81
1:F:204:PHE:CE2	1:F:266:THR:HG21	2.16	0.81
1:N:69:MET:HE1	1:N:522:THR:HB	1.62	0.81
1:A:204:PHE:CE2	1:A:266:THR:HG21	2.16	0.81
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.46	0.81
1:C:204:PHE:CE2	1:C:266:THR:HG21	2.17	0.80
1:F:430:ARG:HH11	1:F:430:ARG:HG2	1.45	0.79
1:E:204:PHE:CE2	1:E:266:THR:HG21	2.17	0.79
1:J:69:MET:HE1	1:J:522:THR:HB	1.62	0.79
1:B:204:PHE:CE2	1:B:266:THR:HG21	2.17	0.79
1:J:131:LEU:HD13	1:J:422:VAL:HG11	1.63	0.78
1:K:419:LEU:CD2	1:K:500:THR:HG23	2.13	0.78
1:D:18:ARG:HG2	1:D:18:ARG:NH1	1.91	0.78
1:B:44:PHE:CD1	1:B:44:PHE:N	2.46	0.78
1:G:204:PHE:CE2	1:G:266:THR:HG21	2.18	0.78
1:G:44:PHE:N	1:G:44:PHE:CD1	2.48	0.78
1:H:419:LEU:CD2	1:H:500:THR:HG23	2.14	0.77
1:I:131:LEU:HD13	1:I:422:VAL:HG11	1.65	0.77
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.66	0.77
1:N:69:MET:CE	1:N:522:THR:HB	2.15	0.77
1:C:44:PHE:CD1	1:C:44:PHE:N	2.46	0.77
1:D:432:GLN:HE21	1:D:436:GLN:HE22	0.79	0.77
1:C:74:VAL:O	1:C:77:VAL:HG13	1.85	0.77
1:A:409:GLU:OE2	1:A:501:ARG:NH2	2.17	0.77
1:M:421:ARG:HD2	1:M:474:GLY:O	1.85	0.76
1:M:131:LEU:HD13	1:M:422:VAL:HG11	1.66	0.76
1:F:197:ARG:HD2	1:F:277:LYS:HB2	1.68	0.76
1:G:197:ARG:HD2	1:G:277:LYS:HB2	1.66	0.76
1:L:38:VAL:HG22	1:M:519:CYS:HB3	1.67	0.76
1:E:33:PRO:HA	1:E:153:ASN:HD21	1.50	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:VAL:O	1:B:77:VAL:HG13	1.85	0.76
1:C:197:ARG:HD2	1:C:277:LYS:HB2	1.66	0.76
1:J:69:MET:CE	1:J:522:THR:HB	2.15	0.76
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.51	0.75
1:K:100:ILE:O	1:K:104:LEU:HB2	1.86	0.75
1:H:69:MET:CE	1:H:522:THR:HB	2.16	0.75
1:A:44:PHE:CD1	1:A:44:PHE:N	2.46	0.75
1:D:204:PHE:CE2	1:D:266:THR:HG21	2.18	0.75
1:C:44:PHE:HD1	1:C:44:PHE:N	1.81	0.75
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.51	0.75
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.67	0.75
1:G:74:VAL:O	1:G:77:VAL:HG13	1.85	0.75
1:N:452:ARG:HH11	1:N:452:ARG:HG2	1.52	0.75
1:J:149:THR:HG23	1:J:159:GLY:HA3	1.68	0.75
1:J:404:ARG:HH11	1:J:404:ARG:HG2	1.52	0.74
1:K:232:GLU:HB3	1:K:309:LEU:HB2	1.68	0.74
1:N:232:GLU:HB3	1:N:309:LEU:HB2	1.69	0.74
1:M:69:MET:CE	1:M:522:THR:HB	2.17	0.74
1:L:69:MET:CE	1:L:522:THR:HB	2.17	0.74
1:L:232:GLU:HB3	1:L:309:LEU:HB2	1.69	0.74
1:K:419:LEU:CD2	1:K:500:THR:CG2	2.65	0.74
1:I:421:ARG:HD2	1:I:474:GLY:O	1.86	0.74
1:A:100:ILE:HD11	1:A:514:MET:HE1	1.70	0.74
1:N:65:LYS:O	1:N:66:PHE:CB	2.36	0.74
1:B:44:PHE:HD1	1:B:44:PHE:N	1.82	0.74
1:A:385:THR:HG21	1:G:510:VAL:HG12	1.71	0.73
1:N:419:LEU:CD2	1:N:500:THR:HG23	2.18	0.73
1:M:100:ILE:O	1:M:104:LEU:HB2	1.88	0.73
1:J:421:ARG:HD2	1:J:474:GLY:O	1.87	0.73
1:I:149:THR:HG23	1:I:159:GLY:HA3	1.70	0.73
1:H:131:LEU:HD13	1:H:422:VAL:HG11	1.70	0.73
1:J:419:LEU:CD2	1:J:500:THR:CG2	2.66	0.73
1:E:44:PHE:N	1:E:44:PHE:HD1	1.85	0.73
1:H:32:GLY:HA2	1:H:454:ILE:HD13	1.70	0.73
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.70	0.73
1:E:74:VAL:O	1:E:77:VAL:HG13	1.88	0.73
1:M:232:GLU:HB3	1:M:309:LEU:HB2	1.71	0.73
1:H:149:THR:HG23	1:H:159:GLY:HA3	1.71	0.73
1:H:232:GLU:HB3	1:H:309:LEU:HB2	1.69	0.72
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.71	0.72
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.70	0.72
1:J:32:GLY:HA2	1:J:454:ILE:HD13	1.70	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:33:PRO:HA	1:G:153:ASN:HD21	1.53	0.72
1:G:417:VAL:HG11	1:G:488:MET:HG3	1.72	0.72
1:M:419:LEU:CD2	1:M:500:THR:HG23	2.20	0.72
1:J:232:GLU:HB3	1:J:309:LEU:HB2	1.70	0.72
1:N:421:ARG:HD2	1:N:474:GLY:O	1.89	0.72
1:H:421:ARG:HD2	1:H:474:GLY:O	1.89	0.72
1:H:100:ILE:O	1:H:104:LEU:HB2	1.90	0.72
1:N:100:ILE:O	1:N:104:LEU:HB2	1.90	0.72
1:K:149:THR:HG23	1:K:159:GLY:HA3	1.70	0.72
1:D:100:ILE:HD11	1:D:514:MET:HE1	1.72	0.72
1:L:32:GLY:HA2	1:L:454:ILE:HD13	1.71	0.72
1:I:131:LEU:CD1	1:I:422:VAL:HG11	2.20	0.72
1:J:100:ILE:O	1:J:104:LEU:HB2	1.90	0.71
1:F:74:VAL:O	1:F:77:VAL:HG13	1.90	0.71
1:I:232:GLU:HB3	1:I:309:LEU:HB2	1.71	0.71
1:D:409:GLU:OE2	1:D:501:ARG:NH2	2.22	0.71
1:G:44:PHE:N	1:G:44:PHE:HD1	1.86	0.71
1:H:227:ILE:HD12	1:H:309:LEU:HD11	1.72	0.71
1:L:421:ARG:HD2	1:L:474:GLY:O	1.90	0.71
1:L:227:ILE:HD12	1:L:309:LEU:HD11	1.73	0.71
1:K:32:GLY:HA2	1:K:454:ILE:HD13	1.71	0.71
1:N:227:ILE:HD12	1:N:309:LEU:HD11	1.72	0.71
1:I:227:ILE:HD12	1:I:309:LEU:HD11	1.72	0.71
1:M:149:THR:HG23	1:M:159:GLY:HA3	1.71	0.71
1:N:149:THR:HG23	1:N:159:GLY:HA3	1.73	0.71
1:K:131:LEU:HD13	1:K:422:VAL:HG11	1.70	0.71
1:L:131:LEU:HD13	1:L:422:VAL:HG11	1.71	0.71
1:M:69:MET:HE1	1:M:522:THR:HB	1.72	0.71
1:I:404:ARG:HG2	1:I:404:ARG:NH1	2.05	0.71
1:K:227:ILE:HD12	1:K:309:LEU:HD11	1.72	0.70
1:M:227:ILE:HD12	1:M:309:LEU:HD11	1.72	0.70
1:A:417:VAL:HG11	1:A:488:MET:HG3	1.73	0.70
1:K:421:ARG:HD2	1:K:474:GLY:O	1.90	0.70
1:K:69:MET:CE	1:K:522:THR:HB	2.21	0.70
1:H:419:LEU:CD2	1:H:500:THR:CG2	2.69	0.70
1:B:33:PRO:HA	1:B:153:ASN:HD21	1.55	0.70
1:I:69:MET:CE	1:I:522:THR:HB	2.22	0.70
1:J:227:ILE:HD12	1:J:309:LEU:HD11	1.72	0.70
1:L:100:ILE:O	1:L:104:LEU:HB2	1.92	0.70
1:A:430:ARG:NH1	1:A:430:ARG:HG2	2.07	0.70
1:I:419:LEU:CD2	1:I:500:THR:CG2	2.69	0.70
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:20:VAL:HG13	1:A:74:VAL:HG11	1.73	0.69
1:M:419:LEU:CD2	1:M:500:THR:CG2	2.69	0.69
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.73	0.69
1:C:64:ASP:HB3	1:C:67:GLU:HB2	1.74	0.69
1:M:27:VAL:HG11	1:M:93:THR:HG21	1.73	0.69
1:L:419:LEU:CD2	1:L:500:THR:HG23	2.23	0.69
1:I:173:GLY:O	1:I:404:ARG:NH2	2.24	0.69
1:J:419:LEU:CD2	1:J:500:THR:HG23	2.22	0.69
1:K:27:VAL:HG11	1:K:93:THR:HG21	1.75	0.69
1:I:419:LEU:CD2	1:I:500:THR:HG23	2.23	0.69
1:F:33:PRO:HA	1:F:153:ASN:HD21	1.57	0.69
1:M:404:ARG:NH1	1:M:404:ARG:HG2	2.08	0.69
1:J:200:LEU:HD12	1:J:276:VAL:HA	1.75	0.69
1:D:44:PHE:N	1:D:44:PHE:HD1	1.84	0.68
1:A:44:PHE:HD1	1:A:44:PHE:N	1.85	0.68
1:M:173:GLY:O	1:M:404:ARG:NH2	2.25	0.68
1:K:200:LEU:HD12	1:K:276:VAL:HA	1.74	0.68
1:M:32:GLY:HA2	1:M:454:ILE:HD13	1.75	0.68
1:H:200:LEU:HD12	1:H:276:VAL:HA	1.75	0.68
1:H:452:ARG:HH11	1:H:452:ARG:HG2	1.58	0.68
1:G:430:ARG:HG2	1:G:430:ARG:NH1	2.08	0.68
1:C:417:VAL:HG11	1:C:488:MET:HG3	1.75	0.68
1:M:194:GLN:HB2	1:M:331:THR:HB	1.74	0.68
2:T:7:HIS:O	2:T:8:ASP:HB3	1.94	0.68
1:N:404:ARG:HH11	1:N:404:ARG:HG2	1.58	0.67
2:Q:7:HIS:O	2:Q:8:ASP:HB3	1.94	0.67
1:N:200:LEU:HD12	1:N:276:VAL:HA	1.75	0.67
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.57	0.67
1:K:65:LYS:O	1:K:66:PHE:CB	2.38	0.67
1:J:131:LEU:CD1	1:J:422:VAL:HG11	2.25	0.67
1:M:131:LEU:CD1	1:M:422:VAL:HG11	2.23	0.67
1:D:430:ARG:NH1	1:D:430:ARG:HG2	2.05	0.67
1:I:65:LYS:O	1:I:66:PHE:CB	2.40	0.67
1:B:430:ARG:HG2	1:B:430:ARG:NH1	2.10	0.67
1:C:487:ASN:O	1:C:491:MET:HG3	1.94	0.67
1:L:200:LEU:HD12	1:L:276:VAL:HA	1.76	0.67
1:I:200:LEU:HD12	1:I:276:VAL:HA	1.76	0.67
1:C:16:MET:O	1:C:20:VAL:HG23	1.95	0.66
2:P:7:HIS:O	2:P:8:ASP:HB3	1.95	0.66
1:F:100:ILE:HD11	1:F:514:MET:HE3	1.77	0.66
1:L:194:GLN:HB2	1:L:331:THR:HB	1.77	0.66
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:C:702:ADP:O3B	5:C:802:HOH:O	2.12	0.66
1:G:487:ASN:O	1:G:491:MET:HG3	1.95	0.66
1:I:100:ILE:O	1:I:104:LEU:HB2	1.95	0.66
1:C:510:VAL:HG12	1:D:385:THR:HG21	1.77	0.66
1:M:200:LEU:HD12	1:M:276:VAL:HA	1.76	0.66
1:D:417:VAL:HG11	1:D:488:MET:HG3	1.77	0.66
1:G:100:ILE:HD11	1:G:514:MET:HE1	1.78	0.66
1:L:419:LEU:CD2	1:L:500:THR:CG2	2.74	0.66
1:A:13:ARG:HD2	1:A:104:LEU:HD22	1.78	0.66
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.59	0.66
1:I:452:ARG:HH11	1:I:452:ARG:HG2	1.60	0.66
1:B:74:VAL:HG13	1:B:514:MET:HE3	1.78	0.66
1:M:38:VAL:HG22	1:N:519:CYS:HB3	1.77	0.66
2:O:7:HIS:O	2:O:8:ASP:HB3	1.96	0.66
1:E:74:VAL:HG13	1:E:514:MET:HE1	1.78	0.65
1:I:194:GLN:HB2	1:I:331:THR:HB	1.78	0.65
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.78	0.65
1:N:32:GLY:HA2	1:N:454:ILE:HD13	1.77	0.65
1:M:452:ARG:HG2	1:M:452:ARG:HH11	1.59	0.65
2:U:7:HIS:O	2:U:8:ASP:HB3	1.97	0.65
1:C:33:PRO:HA	1:C:153:ASN:ND2	2.11	0.65
1:E:100:ILE:HD11	1:E:514:MET:HE1	1.77	0.65
4:B:701:ADP:O3B	5:B:801:HOH:O	2.13	0.65
2:S:7:HIS:O	2:S:8:ASP:HB3	1.95	0.65
1:I:32:GLY:HA2	1:I:454:ILE:HD13	1.77	0.65
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.78	0.65
1:H:65:LYS:O	1:H:66:PHE:CB	2.37	0.65
1:A:39:VAL:HG23	1:G:517:THR:HG23	1.78	0.65
1:M:385:THR:HG23	1:M:388:GLU:HB2	1.79	0.64
1:F:44:PHE:N	1:F:44:PHE:HD1	1.87	0.64
1:M:65:LYS:O	1:M:66:PHE:CB	2.34	0.64
1:C:430:ARG:NH1	1:C:430:ARG:HG2	2.10	0.64
1:C:516:THR:OG1	1:D:37:ASN:ND2	2.29	0.64
1:K:452:ARG:HH11	1:K:452:ARG:HG2	1.62	0.64
1:E:417:VAL:HG11	1:E:488:MET:HG3	1.79	0.64
1:L:131:LEU:CD1	1:L:422:VAL:HG11	2.28	0.64
1:G:288:MET:HG2	1:G:368:ARG:HD2	1.79	0.64
1:J:173:GLY:O	1:J:404:ARG:NH2	2.30	0.64
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.79	0.64
1:K:194:GLN:HB2	1:K:331:THR:HB	1.80	0.64
1:F:111:MET:HG2	1:F:435:ASP:OD1	1.98	0.63
1:N:194:GLN:HB2	1:N:331:THR:HB	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:288:MET:HG2	1:A:368:ARG:HD2	1.80	0.63
2:O:20:LYS:HB3	2:O:27:LEU:HG	1.81	0.63
1:B:288:MET:HG2	1:B:368:ARG:HD2	1.80	0.63
1:N:419:LEU:CD2	1:N:500:THR:CG2	2.75	0.63
1:F:417:VAL:HG11	1:F:488:MET:HG3	1.79	0.63
1:H:173:GLY:O	1:H:404:ARG:NH2	2.31	0.63
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.81	0.63
1:H:194:GLN:HB2	1:H:331:THR:HB	1.81	0.63
1:J:65:LYS:O	1:J:66:PHE:CB	2.40	0.63
1:I:30:THR:HB	1:I:51:LYS:O	1.99	0.63
1:H:96:ALA:O	1:H:100:ILE:HG13	1.98	0.62
1:D:18:ARG:CB	1:D:18:ARG:HH11	2.11	0.62
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.79	0.62
1:L:47:PRO:HG2	1:M:73:MET:HG3	1.80	0.62
1:E:288:MET:HG2	1:E:368:ARG:HD2	1.80	0.62
1:B:100:ILE:HD11	1:B:514:MET:HE3	1.80	0.62
1:G:409:GLU:OE2	1:G:501:ARG:NH2	2.29	0.62
2:T:20:LYS:HB3	2:T:27:LEU:HG	1.82	0.62
1:F:430:ARG:NH1	1:F:430:ARG:HG2	2.12	0.62
1:B:64:ASP:HB3	1:B:67:GLU:HB2	1.81	0.62
1:L:173:GLY:O	1:L:404:ARG:NH2	2.32	0.62
1:J:194:GLN:HB2	1:J:331:THR:HB	1.82	0.62
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.82	0.62
1:K:131:LEU:CD1	1:K:422:VAL:HG11	2.30	0.62
2:R:20:LYS:HB3	2:R:27:LEU:HG	1.81	0.62
1:B:111:MET:HG2	1:B:435:ASP:OD1	1.99	0.62
2:R:7:HIS:O	2:R:8:ASP:HB3	1.98	0.62
2:U:20:LYS:HB3	2:U:27:LEU:HG	1.82	0.62
1:H:419:LEU:HD21	1:H:500:THR:HG23	1.82	0.61
1:J:149:THR:CG2	1:J:159:GLY:HA3	2.29	0.61
2:Q:20:LYS:HB3	2:Q:27:LEU:HG	1.81	0.61
1:G:510:VAL:HG23	1:G:514:MET:CE	2.30	0.61
1:H:131:LEU:CD1	1:H:422:VAL:HG11	2.30	0.61
4:A:700:ADP:O3B	5:A:800:HOH:O	2.16	0.61
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.82	0.61
1:D:64:ASP:HB3	1:D:67:GLU:HB2	1.83	0.61
1:N:173:GLY:O	1:N:404:ARG:NH2	2.33	0.61
1:F:288:MET:HG2	1:F:368:ARG:HD2	1.81	0.61
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.81	0.61
1:J:426:LEU:CD1	1:J:444:LEU:HD21	2.30	0.61
1:I:2:ALA:O	1:I:4:LYS:HE3	1.99	0.61
1:A:414:GLY:O	1:A:417:VAL:CG1	2.40	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:20:LYS:HB3	2:S:27:LEU:HG	1.83	0.61
2:P:20:LYS:HB3	2:P:27:LEU:HG	1.83	0.61
1:N:131:LEU:HD13	1:N:422:VAL:HG11	1.82	0.61
1:L:426:LEU:CD1	1:L:444:LEU:HD21	2.27	0.61
1:K:199:TYR:HA	1:K:276:VAL:HG12	1.83	0.61
1:F:409:GLU:OE2	1:F:501:ARG:NH2	2.31	0.61
1:A:234:LEU:HD22	2:O:23:GLY:HA3	1.81	0.61
1:C:288:MET:HG2	1:C:368:ARG:HD2	1.81	0.61
1:H:385:THR:HG23	1:H:388:GLU:HB2	1.81	0.61
1:K:419:LEU:HD21	1:K:500:THR:HG23	1.82	0.60
1:F:419:LEU:HG	1:F:447:MET:HG2	1.82	0.60
1:B:419:LEU:HG	1:B:447:MET:HG2	1.83	0.60
1:B:417:VAL:HG11	1:B:488:MET:HG3	1.82	0.60
1:I:149:THR:CG2	1:I:159:GLY:HA3	2.30	0.60
1:K:149:THR:CG2	1:K:159:GLY:HA3	2.31	0.60
1:N:174:VAL:HG21	1:N:194:GLN:HB3	1.84	0.60
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.83	0.60
1:N:385:THR:HG23	1:N:388:GLU:HB2	1.83	0.60
1:G:33:PRO:HA	1:G:153:ASN:ND2	2.17	0.60
1:F:193:MET:HG3	1:F:371:LYS:HB3	1.84	0.60
1:L:452:ARG:HG2	1:L:452:ARG:HH11	1.66	0.60
1:E:33:PRO:HA	1:E:153:ASN:ND2	2.16	0.60
1:E:193:MET:HG3	1:E:371:LYS:HB3	1.84	0.60
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.11	0.60
1:G:302:SER:H	1:G:307:MET:HE3	1.66	0.60
1:L:24:ALA:HA	1:L:27:VAL:HG12	1.84	0.59
1:B:510:VAL:HG12	1:C:385:THR:HG21	1.84	0.59
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.83	0.59
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.84	0.59
1:I:385:THR:HG23	1:I:388:GLU:HB2	1.82	0.59
1:H:2:ALA:O	1:H:4:LYS:HE3	2.02	0.59
1:L:385:THR:HG23	1:L:388:GLU:HB2	1.83	0.59
1:B:16:MET:O	1:B:20:VAL:HG23	2.03	0.59
1:D:193:MET:HG3	1:D:371:LYS:HB3	1.85	0.59
1:K:173:GLY:O	1:K:404:ARG:NH2	2.35	0.59
1:M:411:VAL:HG21	1:M:494:LEU:HD12	1.83	0.59
2:R:23:GLY:H	2:S:80:ASN:ND2	2.00	0.59
1:F:325:ILE:HG12	1:F:330:THR:HG23	1.83	0.59
1:L:149:THR:CG2	1:L:159:GLY:HA3	2.32	0.59
1:A:420:ILE:HD13	1:A:451:LEU:HD13	1.83	0.59
1:B:487:ASN:O	1:B:491:MET:HG3	2.03	0.59
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.83	0.59
1:M:426:LEU:CD1	1:M:444:LEU:HD21	2.30	0.59
1:M:149:THR:CG2	1:M:159:GLY:HA3	2.31	0.59
1:M:146:GLN:HE21	1:M:150:ILE:HD11	1.68	0.59
1:N:27:VAL:HG11	1:N:93:THR:HG21	1.85	0.59
1:C:520:MET:HG2	1:D:39:VAL:HB	1.84	0.58
1:A:193:MET:HG3	1:A:371:LYS:HB3	1.85	0.58
1:C:111:MET:HG2	1:C:435:ASP:OD1	2.03	0.58
1:A:432:GLN:NE2	1:A:436:GLN:NE2	2.35	0.58
1:K:146:GLN:HE21	1:K:150:ILE:HD11	1.67	0.58
1:I:411:VAL:HG21	1:I:494:LEU:HD12	1.86	0.58
1:A:325:ILE:HG12	1:A:330:THR:HG23	1.85	0.58
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.85	0.58
1:A:419:LEU:HG	1:A:447:MET:HG2	1.85	0.58
1:G:64:ASP:HB3	1:G:67:GLU:HB2	1.86	0.58
1:J:146:GLN:HE21	1:J:150:ILE:HD11	1.68	0.58
1:B:33:PRO:HA	1:B:153:ASN:ND2	2.18	0.58
1:J:174:VAL:HG21	1:J:194:GLN:HB3	1.86	0.58
1:B:325:ILE:HG12	1:B:330:THR:HG23	1.86	0.58
1:L:64:ASP:HB3	1:L:67:GLU:HB2	1.85	0.58
1:E:268:ARG:HH21	2:S:27:LEU:CD2	2.16	0.58
1:L:223:ALA:HB3	1:L:251:ALA:HB2	1.86	0.58
1:F:510:VAL:HG12	1:G:385:THR:HG21	1.85	0.58
1:M:30:THR:HB	1:M:51:LYS:O	2.04	0.58
1:I:199:TYR:HA	1:I:276:VAL:HG12	1.86	0.58
1:N:313:THR:HG22	1:N:314:LEU:H	1.69	0.58
1:C:432:GLN:NE2	1:C:436:GLN:NE2	2.34	0.57
1:H:149:THR:CG2	1:H:159:GLY:HA3	2.33	0.57
1:A:162:ILE:HG12	1:A:400:LEU:HD23	1.86	0.57
1:C:102:GLU:HB3	1:C:442:VAL:HG22	1.86	0.57
1:D:33:PRO:HA	1:D:153:ASN:HD21	1.68	0.57
1:K:223:ALA:HB3	1:K:251:ALA:HB2	1.87	0.57
1:L:39:VAL:HB	1:M:520:MET:HG2	1.86	0.57
1:N:426:LEU:CD1	1:N:444:LEU:HD21	2.31	0.57
1:D:325:ILE:HG12	1:D:330:THR:HG23	1.85	0.57
1:L:313:THR:HG22	1:L:314:LEU:H	1.69	0.57
1:J:199:TYR:HA	1:J:276:VAL:HG12	1.87	0.57
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.87	0.57
1:L:146:GLN:HE21	1:L:150:ILE:HD11	1.69	0.57
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.86	0.57
1:N:404:ARG:NH1	1:N:404:ARG:HG2	2.20	0.57
1:A:39:VAL:HB	1:G:520:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:P:3:ILE:HD13	2:P:11:ILE:HG21	1.87	0.57
1:A:37:ASN:ND2	1:G:516:THR:OG1	2.31	0.57
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.70	0.57
1:M:270:ILE:HA	1:N:257:GLU:OE2	2.04	0.57
1:B:193:MET:HG3	1:B:371:LYS:HB3	1.87	0.57
1:J:24:ALA:HA	1:J:27:VAL:HG12	1.86	0.57
1:E:419:LEU:HG	1:E:447:MET:HG2	1.86	0.57
1:B:18:ARG:CG	1:B:18:ARG:NH1	2.43	0.57
1:C:193:MET:HG3	1:C:371:LYS:HB3	1.87	0.57
1:G:432:GLN:NE2	1:G:436:GLN:NE2	2.36	0.57
1:K:426:LEU:CD1	1:K:444:LEU:HD21	2.33	0.57
1:K:385:THR:HG23	1:K:388:GLU:HB2	1.86	0.57
1:N:223:ALA:HB3	1:N:251:ALA:HB2	1.87	0.57
1:H:223:ALA:HB3	1:H:251:ALA:HB2	1.87	0.57
1:L:19:GLY:HA3	1:L:67:GLU:O	2.04	0.56
1:G:111:MET:HG2	1:G:435:ASP:OD1	2.05	0.56
1:H:16:MET:HG3	1:H:520:MET:SD	2.44	0.56
1:F:18:ARG:NH1	1:F:18:ARG:CG	2.45	0.56
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.15	0.56
1:J:145:ALA:O	1:J:149:THR:HG23	2.05	0.56
1:I:419:LEU:HD21	1:I:500:THR:HG23	1.87	0.56
1:G:419:LEU:HG	1:G:447:MET:HG2	1.88	0.56
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.87	0.56
1:J:313:THR:HG22	1:J:314:LEU:H	1.69	0.56
1:I:64:ASP:HB3	1:I:67:GLU:HB2	1.87	0.56
1:N:24:ALA:HA	1:N:27:VAL:HG12	1.87	0.56
1:D:288:MET:HG2	1:D:368:ARG:HD2	1.86	0.56
1:N:403:THR:O	1:N:407:VAL:HG23	2.06	0.56
1:A:64:ASP:HB3	1:A:67:GLU:HB2	1.88	0.56
1:N:19:GLY:HA3	1:N:67:GLU:O	2.05	0.56
1:E:430:ARG:NH1	1:E:430:ARG:HG2	2.13	0.56
1:K:96:ALA:O	1:K:100:ILE:HG13	2.05	0.56
1:M:24:ALA:HA	1:M:27:VAL:HG12	1.88	0.56
1:F:33:PRO:HA	1:F:153:ASN:ND2	2.21	0.56
1:F:64:ASP:HB3	1:F:67:GLU:HB2	1.88	0.56
1:L:199:TYR:HA	1:L:276:VAL:HG12	1.87	0.56
1:J:385:THR:HG23	1:J:388:GLU:HB2	1.86	0.56
1:H:313:THR:HG22	1:H:314:LEU:H	1.70	0.56
1:H:426:LEU:CD1	1:H:444:LEU:HD21	2.34	0.56
1:C:268:ARG:HD2	2:Q:27:LEU:CD2	2.34	0.56
1:N:146:GLN:HE21	1:N:150:ILE:HD11	1.69	0.56
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.86	0.56
1:J:123:ALA:HB2	1:J:440:ILE:HG23	1.88	0.56
1:M:69:MET:HE2	1:M:522:THR:HB	1.88	0.56
1:J:64:ASP:HB3	1:J:67:GLU:HB2	1.88	0.56
1:L:65:LYS:O	1:L:66:PHE:CB	2.43	0.56
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.20	0.56
1:M:199:TYR:HA	1:M:276:VAL:HG12	1.86	0.56
1:C:519:CYS:HB3	1:D:38:VAL:HG22	1.88	0.56
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.88	0.56
1:A:111:MET:HG2	1:A:435:ASP:OD1	2.05	0.56
2:T:3:ILE:HD13	2:T:11:ILE:HG21	1.87	0.56
1:C:419:LEU:HG	1:C:447:MET:HG2	1.86	0.56
1:M:47:PRO:HG2	1:N:73:MET:HG3	1.88	0.56
1:H:199:TYR:HA	1:H:276:VAL:HG12	1.87	0.56
1:M:90:THR:O	1:M:94:VAL:HG23	2.05	0.56
1:I:326:ASN:ND2	1:I:328:ASP:H	2.03	0.56
1:J:403:THR:O	1:J:407:VAL:HG23	2.06	0.56
1:D:432:GLN:NE2	1:D:436:GLN:NE2	2.30	0.55
1:J:419:LEU:HD21	1:J:500:THR:CG2	2.36	0.55
2:O:3:ILE:HD13	2:O:11:ILE:HG21	1.88	0.55
1:K:2:ALA:O	1:K:4:LYS:HE3	2.05	0.55
1:A:16:MET:O	1:A:20:VAL:HG23	2.05	0.55
1:E:487:ASN:O	1:E:491:MET:HG3	2.05	0.55
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.88	0.55
1:L:417:VAL:HG21	1:L:488:MET:HG3	1.87	0.55
1:K:24:ALA:HA	1:K:27:VAL:HG12	1.88	0.55
2:R:3:ILE:HD13	2:R:11:ILE:HG21	1.87	0.55
1:I:419:LEU:HD21	1:I:500:THR:CG2	2.36	0.55
1:N:326:ASN:ND2	1:N:328:ASP:H	2.03	0.55
1:H:146:GLN:HE21	1:H:150:ILE:HD11	1.70	0.55
1:M:413:ALA:HB1	1:M:417:VAL:HB	1.88	0.55
1:F:124:VAL:HG13	1:F:504:LEU:HD13	1.88	0.55
1:C:100:ILE:CD1	1:C:514:MET:HE1	2.33	0.55
1:G:20:VAL:HG13	1:G:74:VAL:HG11	1.87	0.55
1:I:24:ALA:HA	1:I:27:VAL:HG12	1.87	0.55
1:C:18:ARG:CB	1:C:18:ARG:HH11	2.18	0.55
1:N:77:VAL:HG22	1:N:506:TYR:HD1	1.71	0.55
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.88	0.55
1:F:74:VAL:HG13	1:F:514:MET:HE3	1.88	0.55
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.88	0.55
1:D:111:MET:HG2	1:D:435:ASP:OD1	2.06	0.55
1:I:426:LEU:CD1	1:I:444:LEU:HD21	2.31	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:346:VAL:HG21	1:M:373:ALA:HB2	1.89	0.55
1:K:313:THR:HG22	1:K:314:LEU:H	1.72	0.55
1:G:238:GLU:HA	1:G:238:GLU:OE2	2.07	0.55
1:N:452:ARG:NH1	1:N:452:ARG:HG2	2.22	0.55
1:N:419:LEU:HD21	1:N:500:THR:HG23	1.89	0.55
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.07	0.55
1:N:149:THR:CG2	1:N:159:GLY:HA3	2.36	0.55
1:J:326:ASN:ND2	1:J:328:ASP:H	2.04	0.55
1:L:193:MET:HG3	1:L:371:LYS:HB3	1.89	0.55
1:A:238:GLU:OE2	1:A:238:GLU:HA	2.07	0.55
1:H:24:ALA:HA	1:H:27:VAL:HG12	1.88	0.54
2:R:13:LYS:HB3	2:R:41:LEU:HD11	1.89	0.54
1:I:223:ALA:HB3	1:I:251:ALA:HB2	1.88	0.54
1:M:313:THR:HG22	1:M:314:LEU:H	1.71	0.54
1:E:64:ASP:HB3	1:E:67:GLU:HB2	1.90	0.54
1:M:419:LEU:HD21	1:M:500:THR:HG23	1.89	0.54
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.88	0.54
1:D:487:ASN:O	1:D:491:MET:HG3	2.08	0.54
2:Q:3:ILE:HD13	2:Q:11:ILE:HG21	1.88	0.54
1:C:238:GLU:HA	1:C:238:GLU:OE2	2.07	0.54
1:K:417:VAL:HG21	1:K:488:MET:HG3	1.88	0.54
1:M:403:THR:O	1:M:407:VAL:HG23	2.07	0.54
1:G:18:ARG:NH1	1:G:18:ARG:CG	2.49	0.54
1:J:404:ARG:NH1	1:J:404:ARG:HG2	2.16	0.54
1:N:199:TYR:HA	1:N:276:VAL:HG12	1.88	0.54
1:J:476:TYR:HA	1:J:486:GLY:O	2.08	0.54
1:N:433:ASN:OD1	1:N:435:ASP:HB2	2.07	0.54
1:N:419:LEU:HD11	1:N:504:LEU:HG	1.89	0.54
2:S:3:ILE:HD13	2:S:11:ILE:HG21	1.89	0.54
2:T:13:LYS:HB3	2:T:41:LEU:HD11	1.89	0.54
1:H:346:VAL:HG21	1:H:373:ALA:HB2	1.90	0.54
1:K:326:ASN:ND2	1:K:328:ASP:H	2.06	0.54
1:D:510:VAL:HG23	1:D:514:MET:CE	2.38	0.54
1:N:96:ALA:O	1:N:100:ILE:HG13	2.07	0.54
1:N:149:THR:CG2	1:N:156:GLU:HA	2.37	0.54
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.89	0.54
1:A:510:VAL:HG23	1:A:514:MET:CE	2.38	0.54
1:E:16:MET:O	1:E:20:VAL:HG23	2.08	0.54
2:U:3:ILE:HD13	2:U:11:ILE:HG21	1.89	0.54
1:E:302:SER:H	1:E:307:MET:HE3	1.73	0.54
1:H:149:THR:CG2	1:H:156:GLU:HA	2.38	0.54
2:O:6:LEU:O	2:O:7:HIS:O	2.26	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:23:GLY:H	2:S:80:ASN:HD21	1.56	0.54
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.89	0.54
1:C:153:ASN:O	1:C:154:SER:HB2	2.07	0.54
1:J:346:VAL:HG21	1:J:373:ALA:HB2	1.88	0.54
1:J:77:VAL:HG22	1:J:506:TYR:HD1	1.73	0.54
1:A:18:ARG:CB	1:A:18:ARG:HH11	2.21	0.53
1:J:419:LEU:HD11	1:J:504:LEU:HG	1.89	0.53
1:J:16:MET:O	1:J:20:VAL:HG12	2.08	0.53
2:Q:13:LYS:HB3	2:Q:41:LEU:HD11	1.90	0.53
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.90	0.53
1:D:452:ARG:HH11	1:D:452:ARG:HG2	1.73	0.53
1:H:130:GLU:HG3	1:H:426:LEU:HD23	1.91	0.53
1:G:510:VAL:CG2	1:G:514:MET:HE2	2.38	0.53
1:I:313:THR:HG22	1:I:314:LEU:H	1.74	0.53
1:D:150:ILE:HD13	1:D:493:ILE:HA	1.90	0.53
1:L:218:PRO:HB3	1:L:246:PRO:HB2	1.91	0.53
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.89	0.53
1:B:238:GLU:HA	1:B:238:GLU:OE2	2.09	0.53
1:G:124:VAL:HG13	1:G:504:LEU:HD13	1.91	0.53
1:H:64:ASP:HB3	1:H:67:GLU:HB2	1.89	0.53
1:J:30:THR:HB	1:J:51:LYS:O	2.07	0.53
1:D:74:VAL:HG13	1:D:514:MET:HE1	1.90	0.53
4:D:703:ADP:O3B	5:D:803:HOH:O	2.19	0.53
1:N:346:VAL:HG21	1:N:373:ALA:HB2	1.90	0.53
1:B:42:LYS:HE2	1:B:48:THR:OG1	2.08	0.53
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.90	0.53
1:M:218:PRO:HB3	1:M:246:PRO:HB2	1.91	0.53
1:G:510:VAL:HG23	1:G:514:MET:HE2	1.89	0.53
1:J:149:THR:CG2	1:J:156:GLU:HA	2.38	0.53
1:A:238:GLU:OE1	2:O:24:GLY:HA3	2.09	0.53
1:K:403:THR:O	1:K:407:VAL:HG23	2.09	0.53
1:G:162:ILE:HG21	1:G:403:THR:HG21	1.90	0.53
1:J:419:LEU:HD21	1:J:500:THR:HG23	1.90	0.53
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.90	0.53
1:D:16:MET:O	1:D:20:VAL:HG23	2.08	0.53
1:D:419:LEU:HG	1:D:447:MET:HG2	1.89	0.53
1:G:452:ARG:HH11	1:G:452:ARG:HG2	1.73	0.53
1:C:18:ARG:NH1	1:C:18:ARG:CG	2.46	0.53
1:E:20:VAL:HG13	1:E:74:VAL:HG11	1.90	0.53
1:L:419:LEU:HD21	1:L:500:THR:HG23	1.91	0.53
2:U:6:LEU:O	2:U:7:HIS:O	2.27	0.53
1:B:302:SER:H	1:B:307:MET:HE3	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:161:LEU:HD21	1:L:185:ASP:HB3	1.90	0.53
1:D:302:SER:H	1:D:307:MET:HE3	1.73	0.53
1:J:161:LEU:HD21	1:J:185:ASP:HB3	1.91	0.53
1:E:42:LYS:HE2	1:E:48:THR:OG1	2.09	0.52
1:J:16:MET:HG3	1:J:520:MET:SD	2.49	0.52
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.91	0.52
1:K:161:LEU:HD21	1:K:185:ASP:HB3	1.90	0.52
1:D:162:ILE:HG12	1:D:400:LEU:HD23	1.90	0.52
1:B:18:ARG:CB	1:B:18:ARG:HH11	2.20	0.52
1:K:419:LEU:HD11	1:K:504:LEU:HG	1.92	0.52
1:I:145:ALA:O	1:I:149:THR:HG23	2.09	0.52
1:I:149:THR:CG2	1:I:156:GLU:HA	2.38	0.52
2:Q:47:ARG:HD2	2:Q:49:LEU:HB2	1.91	0.52
1:C:409:GLU:OE2	1:C:501:ARG:NH2	2.33	0.52
1:H:123:ALA:HB2	1:H:440:ILE:HG23	1.92	0.52
1:E:238:GLU:HA	1:E:238:GLU:OE2	2.09	0.52
1:N:66:PHE:H	1:N:69:MET:HG3	1.75	0.52
1:A:162:ILE:HG21	1:A:403:THR:HG21	1.90	0.52
1:L:403:THR:O	1:L:407:VAL:HG23	2.08	0.52
1:A:18:ARG:CG	1:A:18:ARG:NH1	2.52	0.52
1:I:16:MET:HG3	1:I:520:MET:SD	2.49	0.52
1:B:20:VAL:HG13	1:B:74:VAL:HG11	1.92	0.52
1:L:145:ALA:O	1:L:149:THR:HG23	2.09	0.52
1:K:145:ALA:O	1:K:149:THR:HG23	2.10	0.52
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.92	0.52
1:F:77:VAL:HG23	1:F:92:ALA:HB1	1.91	0.52
2:O:23:GLY:H	2:P:80:ASN:HD21	1.58	0.52
1:M:326:ASN:ND2	1:M:328:ASP:H	2.07	0.52
1:B:162:ILE:HG12	1:B:400:LEU:HD23	1.91	0.52
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.90	0.52
2:Q:23:GLY:H	2:R:80:ASN:HD21	1.58	0.52
1:H:218:PRO:HB3	1:H:246:PRO:HB2	1.92	0.52
2:O:80:ASN:HD21	2:U:23:GLY:H	1.58	0.52
1:A:74:VAL:HG13	1:A:514:MET:HE1	1.91	0.52
1:A:224:ASP:HB3	1:A:302:SER:HA	1.91	0.52
1:L:326:ASN:ND2	1:L:328:ASP:H	2.08	0.52
1:F:487:ASN:O	1:F:491:MET:HG3	2.09	0.52
1:L:123:ALA:HB2	1:L:440:ILE:HG23	1.92	0.52
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.92	0.52
1:F:452:ARG:HG2	1:F:452:ARG:HH11	1.74	0.52
1:E:77:VAL:HG23	1:E:92:ALA:HB1	1.92	0.52
1:E:268:ARG:HH21	2:S:27:LEU:HD23	1.75	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:443:ALA:O	1:H:447:MET:HG3	2.10	0.52
1:H:161:LEU:HD21	1:H:185:ASP:HB3	1.92	0.52
2:T:47:ARG:HD2	2:T:49:LEU:HB2	1.92	0.52
1:F:238:GLU:HA	1:F:238:GLU:OE2	2.08	0.52
1:N:411:VAL:HG21	1:N:494:LEU:HD12	1.92	0.52
1:K:19:GLY:HA3	1:K:67:GLU:O	2.09	0.52
1:H:130:GLU:HG3	1:H:426:LEU:CD2	2.40	0.52
1:H:102:GLU:OE2	1:H:445:ARG:NH1	2.43	0.52
2:S:47:ARG:HD2	2:S:49:LEU:HB2	1.92	0.52
1:G:33:PRO:HG3	4:G:706:ADP:C6	2.45	0.51
2:P:6:LEU:O	2:P:7:HIS:O	2.28	0.51
1:M:145:ALA:O	1:M:149:THR:HG23	2.10	0.51
1:N:131:LEU:CD1	1:N:422:VAL:HG11	2.40	0.51
1:C:501:ARG:HD3	1:C:505:GLN:OE1	2.11	0.51
1:C:381:VAL:CG1	1:C:392:LYS:HG2	2.40	0.51
1:K:346:VAL:HG21	1:K:373:ALA:HB2	1.91	0.51
1:M:161:LEU:HD21	1:M:185:ASP:HB3	1.91	0.51
2:P:23:GLY:H	2:Q:80:ASN:HD21	1.58	0.51
1:M:2:ALA:O	1:M:4:LYS:HE3	2.11	0.51
1:E:162:ILE:HG12	1:E:400:LEU:HD23	1.91	0.51
1:D:6:VAL:HG23	1:D:6:VAL:O	2.11	0.51
1:D:32:GLY:HA2	4:D:703:ADP:H5'1	1.91	0.51
1:C:302:SER:H	1:C:307:MET:HE3	1.75	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.10	0.51
1:D:510:VAL:HG23	1:D:514:MET:HE2	1.92	0.51
2:P:13:LYS:HB3	2:P:41:LEU:HD11	1.92	0.51
1:M:64:ASP:HB3	1:M:67:GLU:HB2	1.91	0.51
1:G:510:VAL:HG23	1:G:514:MET:HE3	1.93	0.51
1:H:145:ALA:O	1:H:149:THR:HG23	2.09	0.51
1:K:149:THR:CG2	1:K:156:GLU:HA	2.41	0.51
1:J:16:MET:O	1:J:20:VAL:CG1	2.59	0.51
2:T:47:ARG:HD3	2:T:49:LEU:HD12	1.93	0.51
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.92	0.51
1:C:452:ARG:HG2	1:C:452:ARG:HH11	1.74	0.51
1:E:432:GLN:NE2	1:E:436:GLN:NE2	2.39	0.51
1:H:66:PHE:H	1:H:69:MET:HG3	1.76	0.51
1:J:452:ARG:HG2	1:J:452:ARG:NH1	2.26	0.51
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.91	0.51
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.92	0.51
1:L:149:THR:CG2	1:L:156:GLU:HA	2.41	0.51
1:N:419:LEU:HD22	1:N:500:THR:CG2	2.41	0.51
1:C:268:ARG:HH21	2:Q:27:LEU:HD23	1.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:162:ILE:HG12	1:F:400:LEU:HD23	1.92	0.51
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.93	0.51
1:L:346:VAL:HG21	1:L:373:ALA:HB2	1.92	0.51
1:J:19:GLY:HA3	1:J:67:GLU:O	2.09	0.51
1:K:419:LEU:HD21	1:K:500:THR:CG2	2.37	0.51
1:E:224:ASP:HB3	1:E:302:SER:HA	1.92	0.51
1:L:77:VAL:HG22	1:L:506:TYR:HD1	1.75	0.51
1:F:18:ARG:HH11	1:F:18:ARG:CB	2.21	0.51
1:E:153:ASN:O	1:E:154:SER:HB2	2.11	0.51
2:U:11:ILE:HG12	2:U:85:ILE:HG12	1.93	0.51
1:N:476:TYR:HA	1:N:486:GLY:O	2.10	0.51
1:J:218:PRO:HB3	1:J:246:PRO:HB2	1.93	0.51
1:I:161:LEU:HD21	1:I:185:ASP:HB3	1.92	0.51
1:D:510:VAL:HG12	1:E:385:THR:HG21	1.93	0.51
1:I:38:VAL:HG12	1:I:40:LEU:HD13	1.92	0.51
1:I:218:PRO:HB3	1:I:246:PRO:HB2	1.93	0.51
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.51	0.51
1:I:146:GLN:HE21	1:I:150:ILE:HD11	1.74	0.51
2:U:13:LYS:HB3	2:U:41:LEU:HD11	1.91	0.51
2:U:47:ARG:HD2	2:U:49:LEU:HB2	1.93	0.51
1:L:64:ASP:C	1:L:65:LYS:O	2.46	0.50
1:G:238:GLU:OE1	2:U:24:GLY:HA3	2.11	0.50
1:B:420:ILE:HD13	1:B:451:LEU:HD13	1.93	0.50
1:A:28:LYS:HD2	1:A:453:GLN:CD	2.31	0.50
1:D:238:GLU:HA	1:D:238:GLU:OE2	2.11	0.50
1:N:135:SER:HA	1:N:412:VAL:HG12	1.94	0.50
1:N:259:LEU:O	1:N:263:VAL:HG23	2.11	0.50
2:O:13:LYS:HB3	2:O:41:LEU:HD11	1.93	0.50
1:L:228:SER:O	1:L:257:GLU:HB3	2.11	0.50
1:J:66:PHE:H	1:J:69:MET:HG3	1.77	0.50
1:A:409:GLU:CD	1:A:501:ARG:HH21	2.10	0.50
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.92	0.50
1:H:163:ALA:O	1:H:167:ASP:HB2	2.11	0.50
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.93	0.50
1:D:204:PHE:HE1	1:D:274:ALA:HB2	1.77	0.50
1:K:102:GLU:OE2	1:K:445:ARG:NH1	2.44	0.50
2:P:47:ARG:HD2	2:P:49:LEU:HB2	1.94	0.50
2:O:50:GLU:HA	2:U:50:GLU:OE1	2.11	0.50
1:A:300:VAL:O	1:A:307:MET:HE3	2.11	0.50
1:H:11:ASP:O	1:H:12:ALA:C	2.50	0.50
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.94	0.50
1:C:42:LYS:HE2	1:C:48:THR:OG1	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:145:ALA:O	1:N:149:THR:HG23	2.11	0.50
1:L:96:ALA:O	1:L:100:ILE:HG13	2.11	0.50
2:R:6:LEU:O	2:R:7:HIS:O	2.29	0.50
2:R:11:ILE:HG12	2:R:85:ILE:HG12	1.92	0.50
2:U:78:ILE:HD13	2:U:83:VAL:HG21	1.94	0.50
1:H:417:VAL:HG21	1:H:488:MET:HG3	1.92	0.50
1:B:237:LEU:HD21	1:B:271:VAL:HG21	1.93	0.50
1:N:2:ALA:O	1:N:4:LYS:HE3	2.11	0.50
2:T:6:LEU:O	2:T:7:HIS:O	2.29	0.50
1:B:268:ARG:HH21	2:P:27:LEU:HD23	1.77	0.50
1:H:19:GLY:HA3	1:H:67:GLU:O	2.11	0.50
2:O:47:ARG:HD2	2:O:49:LEU:HB2	1.94	0.50
1:J:413:ALA:HB1	1:J:417:VAL:HB	1.92	0.50
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.93	0.50
1:K:218:PRO:HB3	1:K:246:PRO:HB2	1.93	0.50
1:F:356:ALA:HB3	1:F:362:ARG:HG3	1.94	0.50
1:J:135:SER:HA	1:J:412:VAL:HG12	1.94	0.50
1:I:346:VAL:HG21	1:I:373:ALA:HB2	1.93	0.50
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.94	0.50
1:C:28:LYS:HD2	1:C:453:GLN:CD	2.32	0.50
1:B:452:ARG:HG2	1:B:452:ARG:HH11	1.75	0.50
1:B:224:ASP:HB3	1:B:302:SER:HA	1.93	0.50
2:U:47:ARG:HD3	2:U:49:LEU:HD12	1.94	0.50
1:D:28:LYS:HD2	1:D:453:GLN:CD	2.32	0.50
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.92	0.50
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.93	0.50
1:N:161:LEU:HD21	1:N:185:ASP:HB3	1.93	0.50
1:A:356:ALA:HB3	1:A:362:ARG:HG3	1.94	0.50
1:M:102:GLU:OE2	1:M:445:ARG:NH1	2.45	0.50
1:F:224:ASP:HB3	1:F:302:SER:HA	1.93	0.50
1:N:30:THR:HB	1:N:51:LYS:O	2.12	0.50
1:I:19:GLY:HA3	1:I:67:GLU:O	2.11	0.50
1:C:77:VAL:HG23	1:C:92:ALA:HB1	1.93	0.50
1:M:149:THR:CG2	1:M:156:GLU:HA	2.42	0.50
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.93	0.50
1:B:381:VAL:CG1	1:B:392:LYS:HG2	2.42	0.50
1:E:111:MET:HG2	1:E:435:ASP:OD1	2.12	0.50
1:A:124:VAL:HG13	1:A:504:LEU:HD13	1.94	0.50
1:C:162:ILE:HG12	1:C:400:LEU:HD23	1.93	0.50
1:B:34:LYS:HD2	1:B:458:CYS:SG	2.52	0.50
1:M:19:GLY:HA3	1:M:67:GLU:O	2.12	0.49
1:H:419:LEU:HD11	1:H:504:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:501:ARG:HD3	1:D:505:GLN:OE1	2.12	0.49
1:C:237:LEU:HD21	1:C:271:VAL:HG21	1.93	0.49
1:A:42:LYS:HG2	1:A:44:PHE:CE2	2.47	0.49
1:F:16:MET:O	1:F:20:VAL:HG23	2.12	0.49
1:F:20:VAL:HG13	1:F:74:VAL:HG11	1.93	0.49
1:G:224:ASP:HB3	1:G:302:SER:HA	1.93	0.49
1:D:224:ASP:HB3	1:D:302:SER:HA	1.93	0.49
1:G:237:LEU:HD21	1:G:271:VAL:HG21	1.93	0.49
1:E:356:ALA:HB3	1:E:362:ARG:HG3	1.94	0.49
1:C:124:VAL:HG13	1:C:504:LEU:HD13	1.93	0.49
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.94	0.49
2:R:47:ARG:HD2	2:R:49:LEU:HB2	1.94	0.49
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.94	0.49
1:K:419:LEU:HD22	1:K:500:THR:CG2	2.42	0.49
1:M:419:LEU:HD11	1:M:504:LEU:HG	1.93	0.49
1:N:417:VAL:HG21	1:N:488:MET:HG3	1.93	0.49
1:K:228:SER:O	1:K:257:GLU:HB3	2.12	0.49
1:N:218:PRO:HB3	1:N:246:PRO:HB2	1.95	0.49
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.94	0.49
1:H:259:LEU:O	1:H:263:VAL:HG23	2.13	0.49
1:F:237:LEU:HD21	1:F:271:VAL:HG21	1.93	0.49
1:D:522:THR:OG1	1:D:523:ASP:N	2.46	0.49
1:G:74:VAL:HG13	1:G:514:MET:HE1	1.95	0.49
2:Q:47:ARG:HD3	2:Q:49:LEU:HD12	1.94	0.49
1:H:77:VAL:HG22	1:H:506:TYR:HD1	1.76	0.49
1:L:163:ALA:O	1:L:167:ASP:HB2	2.12	0.49
1:L:2:ALA:O	1:L:4:LYS:HE3	2.13	0.49
1:C:224:ASP:HB3	1:C:302:SER:HA	1.94	0.49
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.94	0.49
1:K:193:MET:HG3	1:K:371:LYS:HB3	1.94	0.49
1:M:360:TYR:O	1:M:364:LYS:HB2	2.12	0.49
2:S:13:LYS:HB3	2:S:41:LEU:HD11	1.93	0.49
1:J:193:MET:HG3	1:J:371:LYS:HB3	1.93	0.49
1:H:179:ASP:OD1	1:H:393:LYS:HD2	2.12	0.49
1:H:321:LYS:HB2	1:H:334:ASP:HB3	1.95	0.49
1:M:135:SER:HA	1:M:412:VAL:HG12	1.95	0.49
2:O:80:ASN:ND2	2:U:23:GLY:H	2.09	0.49
1:L:321:LYS:HB2	1:L:334:ASP:HB3	1.95	0.49
1:N:179:ASP:OD1	1:N:393:LYS:HD2	2.13	0.49
1:G:28:LYS:C	1:G:30:THR:N	2.66	0.49
2:T:11:ILE:HG12	2:T:85:ILE:HG12	1.95	0.49
1:H:360:TYR:O	1:H:364:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:360:TYR:O	1:J:364:LYS:HB2	2.13	0.49
1:G:414:GLY:O	1:G:417:VAL:CG1	2.45	0.48
1:E:204:PHE:HE1	1:E:274:ALA:HB2	1.77	0.48
1:N:64:ASP:HB3	1:N:67:GLU:HB2	1.94	0.48
2:Q:6:LEU:O	2:Q:7:HIS:O	2.31	0.48
1:A:237:LEU:HD21	1:A:271:VAL:HG21	1.95	0.48
1:G:356:ALA:HB3	1:G:362:ARG:HG3	1.95	0.48
1:E:18:ARG:HH11	1:E:18:ARG:CB	2.25	0.48
1:A:18:ARG:HB2	1:A:67:GLU:HG2	1.95	0.48
1:I:66:PHE:H	1:I:69:MET:HG3	1.78	0.48
1:H:419:LEU:HD21	1:H:500:THR:CG2	2.40	0.48
1:H:452:ARG:NH1	1:H:452:ARG:HG2	2.27	0.48
1:L:411:VAL:HG21	1:L:494:LEU:HD12	1.94	0.48
1:C:95:LEU:O	1:C:99:ILE:HG13	2.12	0.48
1:B:356:ALA:HB3	1:B:362:ARG:HG3	1.95	0.48
1:J:38:VAL:HG22	1:K:519:CYS:HB3	1.94	0.48
1:N:15:LYS:HB3	1:N:66:PHE:HB3	1.95	0.48
1:C:517:THR:HG23	1:D:39:VAL:HG23	1.95	0.48
1:C:247:LEU:HB3	1:C:273:VAL:HG12	1.94	0.48
1:M:130:GLU:HG3	1:M:426:LEU:HD23	1.94	0.48
2:O:47:ARG:HD3	2:O:49:LEU:HD12	1.95	0.48
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.95	0.48
1:H:403:THR:O	1:H:407:VAL:HG23	2.13	0.48
1:M:443:ALA:O	1:M:447:MET:HG3	2.13	0.48
1:N:266:THR:CG2	1:N:273:VAL:H	2.26	0.48
1:I:179:ASP:OD1	1:I:393:LYS:HD2	2.13	0.48
1:K:413:ALA:HB1	1:K:417:VAL:HB	1.95	0.48
1:F:247:LEU:HB3	1:F:273:VAL:HG12	1.95	0.48
1:G:23:LEU:CD1	1:G:23:LEU:C	2.81	0.48
1:N:130:GLU:HG3	1:N:426:LEU:CD2	2.44	0.48
2:P:11:ILE:HG12	2:P:85:ILE:HG12	1.94	0.48
2:O:11:ILE:HG12	2:O:85:ILE:HG12	1.95	0.48
1:L:428:ASP:O	1:L:430:ARG:HG2	2.13	0.48
1:I:80:LYS:HA	1:I:83:ASP:HB2	1.94	0.48
1:C:204:PHE:HE1	1:C:274:ALA:HB2	1.77	0.48
1:M:130:GLU:HG3	1:M:426:LEU:CD2	2.43	0.48
1:D:356:ALA:HB3	1:D:362:ARG:HG3	1.95	0.48
1:A:257:GLU:O	1:A:261:THR:HG23	2.13	0.48
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.95	0.48
1:H:193:MET:HG3	1:H:371:LYS:HB3	1.94	0.48
1:D:420:ILE:HD13	1:D:451:LEU:HD13	1.95	0.48
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.51	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:124:VAL:HG13	1:I:504:LEU:HD13	1.96	0.48
1:I:419:LEU:HD11	1:I:504:LEU:HG	1.94	0.48
1:G:162:ILE:HG12	1:G:400:LEU:HD23	1.95	0.48
1:B:381:VAL:CG1	1:B:392:LYS:CG	2.91	0.48
1:K:30:THR:HB	1:K:51:LYS:O	2.13	0.48
1:J:102:GLU:HB3	1:J:442:VAL:HG22	1.96	0.48
1:D:102:GLU:HB3	1:D:442:VAL:HG22	1.96	0.48
1:M:163:ALA:O	1:M:167:ASP:HB2	2.14	0.48
1:N:428:ASP:O	1:N:430:ARG:HG2	2.14	0.48
1:J:321:LYS:HB2	1:J:334:ASP:HB3	1.96	0.48
1:E:95:LEU:O	1:E:99:ILE:HG13	2.13	0.48
1:I:15:LYS:HB3	1:I:66:PHE:HB3	1.96	0.48
1:K:102:GLU:HB3	1:K:442:VAL:HG22	1.96	0.48
1:A:232:GLU:HB3	1:A:309:LEU:HB3	1.96	0.48
1:E:237:LEU:HD21	1:E:271:VAL:HG21	1.95	0.48
1:I:77:VAL:HG22	1:I:506:TYR:HD1	1.78	0.48
2:R:34:LYS:HG3	2:R:35:SER:H	1.79	0.48
1:H:519:CYS:HB3	1:N:38:VAL:HG22	1.96	0.48
1:L:179:ASP:OD1	1:L:393:LYS:HD2	2.14	0.48
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.54	0.48
1:D:237:LEU:HD21	1:D:271:VAL:HG21	1.96	0.48
1:K:135:SER:HA	1:K:412:VAL:HG12	1.96	0.48
1:L:85:ALA:HA	1:L:498:LYS:HD3	1.96	0.48
1:C:356:ALA:HB3	1:C:362:ARG:HG3	1.95	0.48
1:K:123:ALA:HB2	1:K:440:ILE:HG23	1.96	0.48
1:E:247:LEU:HB3	1:E:273:VAL:HG12	1.96	0.48
1:E:413:ALA:CB	1:E:417:VAL:HG13	2.44	0.47
1:G:204:PHE:HE1	1:G:274:ALA:HB2	1.78	0.47
1:A:510:VAL:HG23	1:A:514:MET:HE2	1.96	0.47
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.95	0.47
1:A:32:GLY:HA2	4:A:700:ADP:H5'1	1.96	0.47
1:B:206:ASN:O	1:B:207:LYS:HG2	2.14	0.47
1:N:11:ASP:O	1:N:12:ALA:C	2.50	0.47
1:H:266:THR:CG2	1:H:273:VAL:H	2.27	0.47
1:K:163:ALA:O	1:K:167:ASP:HB2	2.13	0.47
1:B:257:GLU:O	1:B:261:THR:HG23	2.14	0.47
1:L:130:GLU:HG3	1:L:426:LEU:HD23	1.94	0.47
1:M:428:ASP:O	1:M:430:ARG:HG2	2.14	0.47
1:K:259:LEU:O	1:K:263:VAL:HG23	2.14	0.47
1:K:16:MET:HG3	1:K:520:MET:SD	2.54	0.47
1:H:226:LYS:HG3	1:H:252:GLU:HB3	1.96	0.47
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:204:PHE:HE1	1:F:274:ALA:HB2	1.79	0.47
1:F:197:ARG:HD3	1:F:197:ARG:HA	1.62	0.47
2:S:47:ARG:HD3	2:S:49:LEU:HD12	1.95	0.47
1:I:259:LEU:O	1:I:263:VAL:HG23	2.14	0.47
1:I:163:ALA:O	1:I:167:ASP:HB2	2.14	0.47
1:H:455:VAL:HG11	1:H:461:GLU:O	2.13	0.47
1:J:266:THR:CG2	1:J:273:VAL:H	2.27	0.47
1:A:204:PHE:HE1	1:A:274:ALA:HB2	1.78	0.47
1:N:69:MET:HE2	1:N:522:THR:HB	1.93	0.47
1:C:74:VAL:HG13	1:C:514:MET:HE1	1.95	0.47
2:P:47:ARG:HD3	2:P:49:LEU:HD12	1.95	0.47
1:J:417:VAL:HG21	1:J:488:MET:HG3	1.96	0.47
1:I:103:GLY:O	1:I:106:ALA:HB3	2.14	0.47
1:B:232:GLU:HB3	1:B:309:LEU:HB3	1.96	0.47
1:F:461:GLU:HA	1:F:462:PRO:HD3	1.79	0.47
1:J:138:CYS:SG	1:J:144:ILE:HD13	2.54	0.47
1:I:266:THR:CG2	1:I:273:VAL:H	2.27	0.47
1:A:80:LYS:HD2	1:A:506:TYR:CE1	2.50	0.47
1:K:124:VAL:HG13	1:K:504:LEU:HD13	1.96	0.47
1:K:360:TYR:O	1:K:364:LYS:HB2	2.14	0.47
1:H:135:SER:HA	1:H:412:VAL:HG12	1.97	0.47
1:N:163:ALA:O	1:N:167:ASP:HB2	2.14	0.47
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.96	0.47
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.97	0.47
1:J:179:ASP:OD1	1:J:393:LYS:HD2	2.15	0.47
1:G:42:LYS:HG2	1:G:44:PHE:CE2	2.50	0.47
1:D:510:VAL:CG2	1:D:514:MET:HE2	2.44	0.47
1:E:206:ASN:O	1:E:207:LYS:HG2	2.15	0.47
1:E:522:THR:OG1	1:E:523:ASP:N	2.48	0.47
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.96	0.47
1:F:432:GLN:NE2	1:F:436:GLN:NE2	2.41	0.47
1:N:15:LYS:HD3	1:N:15:LYS:HA	1.70	0.47
1:G:510:VAL:CG2	1:G:514:MET:CE	2.92	0.47
2:S:11:ILE:HG12	2:S:85:ILE:HG12	1.95	0.47
1:B:233:MET:HB3	1:B:237:LEU:HD12	1.97	0.47
1:E:381:VAL:CG1	1:E:392:LYS:HG2	2.45	0.47
1:F:300:VAL:O	1:F:307:MET:HE3	2.14	0.47
2:R:47:ARG:HD3	2:R:49:LEU:HD12	1.95	0.47
1:F:381:VAL:CG1	1:F:392:LYS:HG2	2.45	0.47
1:G:455:VAL:HG21	1:G:465:VAL:HG11	1.96	0.47
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.97	0.47
2:O:78:ILE:HD13	2:O:83:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:18:ARG:CB	1:G:18:ARG:HH11	2.26	0.47
1:L:130:GLU:HG3	1:L:426:LEU:CD2	2.44	0.47
1:J:15:LYS:HB3	1:J:66:PHE:HB3	1.97	0.47
1:E:510:VAL:HG23	1:E:514:MET:CE	2.45	0.47
1:B:268:ARG:HH21	2:P:27:LEU:CD2	2.27	0.47
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.97	0.47
1:B:234:LEU:HD22	2:P:23:GLY:HA3	1.96	0.47
1:K:443:ALA:O	1:K:447:MET:HG3	2.14	0.47
1:G:232:GLU:HB3	1:G:309:LEU:HB3	1.97	0.47
1:L:360:TYR:O	1:L:364:LYS:HB2	2.15	0.47
1:K:179:ASP:OD1	1:K:393:LYS:HD2	2.14	0.47
1:G:247:LEU:HB3	1:G:273:VAL:HG12	1.97	0.47
1:E:232:GLU:HB3	1:E:309:LEU:HB3	1.96	0.47
1:F:232:GLU:HB3	1:F:309:LEU:HB3	1.96	0.47
1:J:228:SER:O	1:J:257:GLU:HB3	2.15	0.47
1:I:365:LEU:O	1:I:369:VAL:HG23	2.15	0.47
1:F:18:ARG:HB2	1:F:67:GLU:HG2	1.96	0.47
1:I:130:GLU:HG3	1:I:426:LEU:HD23	1.97	0.47
1:M:444:LEU:HD23	1:M:444:LEU:HA	1.72	0.47
1:L:38:VAL:HG12	1:L:40:LEU:HD13	1.97	0.47
1:L:40:LEU:HD12	1:M:521:VAL:HB	1.96	0.47
1:C:90:THR:O	1:C:94:VAL:HG23	2.15	0.47
1:E:162:ILE:HG21	1:E:403:THR:HG21	1.97	0.47
2:Q:50:GLU:OE1	2:R:50:GLU:HA	2.15	0.47
1:L:266:THR:CG2	1:L:273:VAL:H	2.27	0.47
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.96	0.47
1:L:30:THR:HB	1:L:51:LYS:O	2.14	0.47
1:A:247:LEU:HB3	1:A:273:VAL:HG12	1.96	0.47
1:I:360:TYR:O	1:I:364:LYS:HB2	2.15	0.47
1:M:66:PHE:H	1:M:69:MET:HG3	1.80	0.47
2:S:6:LEU:O	2:S:7:HIS:O	2.32	0.47
1:D:233:MET:HB3	1:D:237:LEU:HD12	1.96	0.47
1:I:135:SER:HA	1:I:412:VAL:HG12	1.96	0.47
1:K:411:VAL:HG21	1:K:494:LEU:HD12	1.97	0.47
1:I:321:LYS:HB2	1:I:334:ASP:HB3	1.97	0.47
1:G:206:ASN:O	1:G:207:LYS:HG2	2.15	0.47
1:C:73:MET:CG	1:C:73:MET:CE	2.92	0.46
1:M:77:VAL:HG11	1:M:510:VAL:HB	1.97	0.46
1:L:11:ASP:O	1:L:12:ALA:C	2.51	0.46
1:H:326:ASN:ND2	1:H:328:ASP:H	2.12	0.46
1:G:257:GLU:O	1:G:261:THR:HG23	2.15	0.46
1:B:247:LEU:HB3	1:B:273:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:228:SER:O	1:H:257:GLU:HB3	2.15	0.46
1:I:428:ASP:O	1:I:430:ARG:HG2	2.14	0.46
1:N:360:TYR:O	1:N:364:LYS:HB2	2.15	0.46
1:D:247:LEU:HB3	1:D:273:VAL:HG12	1.97	0.46
1:B:414:GLY:O	1:B:417:VAL:CG1	2.43	0.46
1:L:16:MET:HG3	1:L:520:MET:SD	2.56	0.46
1:M:266:THR:CG2	1:M:273:VAL:H	2.28	0.46
1:L:476:TYR:HA	1:L:486:GLY:O	2.15	0.46
1:J:259:LEU:O	1:J:263:VAL:HG23	2.15	0.46
1:E:18:ARG:HB2	1:E:67:GLU:HG2	1.97	0.46
1:M:13:ARG:HD2	1:M:104:LEU:HD11	1.96	0.46
1:K:40:LEU:HD12	1:L:521:VAL:HB	1.96	0.46
1:F:302:SER:H	1:F:307:MET:HE3	1.79	0.46
1:C:233:MET:HB3	1:C:237:LEU:HD12	1.96	0.46
1:K:262:LEU:O	1:K:266:THR:HG23	2.15	0.46
1:E:420:ILE:HD13	1:E:451:LEU:HD13	1.97	0.46
1:K:433:ASN:OD1	1:K:435:ASP:HB2	2.16	0.46
1:A:206:ASN:O	1:A:207:LYS:HG2	2.15	0.46
1:G:351:GLN:HG2	1:G:351:GLN:O	2.15	0.46
1:B:162:ILE:HG21	1:B:403:THR:HG21	1.96	0.46
1:C:31:LEU:HD23	1:C:453:GLN:HB3	1.98	0.46
1:G:233:MET:HB3	1:G:237:LEU:HD12	1.98	0.46
1:C:232:GLU:HB3	1:C:309:LEU:HB3	1.98	0.46
1:D:232:GLU:HB3	1:D:309:LEU:HB3	1.98	0.46
1:C:351:GLN:O	1:C:351:GLN:HG2	2.16	0.46
1:J:100:ILE:HG23	1:J:104:LEU:HD22	1.97	0.46
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.97	0.46
1:L:135:SER:HA	1:L:412:VAL:HG12	1.98	0.46
1:B:204:PHE:HE1	1:B:274:ALA:HB2	1.80	0.46
1:A:430:ARG:CG	1:A:430:ARG:NH1	2.78	0.46
1:A:510:VAL:CG2	1:A:514:MET:HE2	2.45	0.46
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.98	0.46
1:N:413:ALA:HB1	1:N:417:VAL:HB	1.98	0.46
1:M:77:VAL:HG22	1:M:506:TYR:HD1	1.81	0.46
1:H:85:ALA:HA	1:H:498:LYS:HD3	1.98	0.46
1:E:461:GLU:HA	1:E:462:PRO:HD3	1.82	0.46
1:M:259:LEU:O	1:M:263:VAL:HG23	2.15	0.46
1:I:403:THR:O	1:I:407:VAL:HG23	2.15	0.46
1:N:321:LYS:HB2	1:N:334:ASP:HB3	1.98	0.46
1:C:381:VAL:CG1	1:C:392:LYS:CG	2.93	0.46
1:D:24:ALA:O	1:D:28:LYS:HG3	2.15	0.46
1:E:381:VAL:CG1	1:E:392:LYS:CG	2.94	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:455:VAL:HG21	1:D:465:VAL:HG11	1.98	0.46
1:F:381:VAL:CG1	1:F:392:LYS:CG	2.94	0.46
1:H:411:VAL:HG21	1:H:494:LEU:HD12	1.98	0.46
1:H:428:ASP:O	1:H:430:ARG:HG2	2.16	0.46
1:C:248:LEU:HD22	1:C:323:VAL:HG11	1.97	0.46
1:G:28:LYS:O	1:G:30:THR:N	2.48	0.46
1:H:262:LEU:O	1:H:266:THR:HG23	2.16	0.46
1:K:85:ALA:HA	1:K:498:LYS:HD3	1.98	0.46
1:E:501:ARG:HD3	1:E:505:GLN:OE1	2.16	0.46
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.98	0.46
1:A:351:GLN:HG2	1:A:351:GLN:O	2.15	0.46
1:N:130:GLU:HG3	1:N:426:LEU:HD23	1.98	0.46
1:E:91:THR:O	1:E:92:ALA:C	2.53	0.46
1:A:225:LYS:HG2	1:A:303:GLU:HB2	1.98	0.46
1:D:206:ASN:O	1:D:207:LYS:HG2	2.16	0.46
1:J:411:VAL:HG21	1:J:494:LEU:HD12	1.97	0.46
1:F:206:ASN:O	1:F:207:LYS:HG2	2.16	0.46
1:H:476:TYR:HA	1:H:486:GLY:O	2.16	0.46
1:M:38:VAL:HG12	1:M:40:LEU:HD13	1.96	0.46
1:B:32:GLY:HA2	4:B:701:ADP:H5'1	1.98	0.46
2:T:78:ILE:HD13	2:T:83:VAL:HG21	1.98	0.46
1:C:206:ASN:O	1:C:207:LYS:HG2	2.16	0.46
1:F:28:LYS:HD2	1:F:453:GLN:CD	2.36	0.46
1:E:124:VAL:HG13	1:E:504:LEU:HD13	1.96	0.46
1:D:254:VAL:HG12	1:D:259:LEU:HB2	1.97	0.46
1:K:426:LEU:O	1:K:444:LEU:HD11	2.16	0.45
1:G:501:ARG:HD3	1:G:505:GLN:OE1	2.15	0.45
1:A:381:VAL:CG1	1:A:392:LYS:CG	2.94	0.45
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.56	0.45
1:B:351:GLN:O	1:B:351:GLN:HG2	2.16	0.45
1:A:501:ARG:HD3	1:A:505:GLN:OE1	2.16	0.45
1:G:225:LYS:HG2	1:G:303:GLU:HB2	1.99	0.45
1:L:433:ASN:OD1	1:L:435:ASP:HB2	2.17	0.45
1:I:23:LEU:HD11	1:I:75:LYS:HG3	1.97	0.45
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.99	0.45
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.98	0.45
1:F:351:GLN:O	1:F:351:GLN:HG2	2.16	0.45
1:K:428:ASP:O	1:K:430:ARG:HG2	2.16	0.45
1:L:262:LEU:O	1:L:266:THR:HG23	2.16	0.45
2:Q:78:ILE:HD13	2:Q:83:VAL:HG21	1.98	0.45
1:I:226:LYS:HG3	1:I:252:GLU:HB3	1.98	0.45
1:K:321:LYS:HB2	1:K:334:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:270:ILE:HA	1:J:257:GLU:OE2	2.16	0.45
1:A:49:ILE:HD13	1:G:513:LEU:HB3	1.97	0.45
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.97	0.45
1:D:381:VAL:CG1	1:D:392:LYS:HG2	2.47	0.45
1:E:261:THR:HG22	2:S:29:GLY:HA3	1.97	0.45
2:S:78:ILE:HD13	2:S:83:VAL:HG21	1.99	0.45
1:B:77:VAL:HG23	1:B:92:ALA:HB1	1.98	0.45
1:C:197:ARG:HG2	1:C:277:LYS:O	2.16	0.45
1:I:104:LEU:HA	1:I:104:LEU:HD12	1.75	0.45
1:E:300:VAL:O	1:E:307:MET:HE3	2.17	0.45
1:F:522:THR:OG1	1:F:523:ASP:N	2.50	0.45
1:I:85:ALA:HA	1:I:498:LYS:HD3	1.98	0.45
1:D:225:LYS:HG2	1:D:303:GLU:HB2	1.98	0.45
2:R:78:ILE:HD13	2:R:83:VAL:HG21	1.98	0.45
1:A:384:ALA:O	1:G:506:TYR:HE1	1.99	0.45
1:M:179:ASP:OD1	1:M:393:LYS:HD2	2.17	0.45
1:K:270:ILE:HG23	1:L:229:ASN:HD21	1.82	0.45
1:H:413:ALA:HB1	1:H:417:VAL:HB	1.99	0.45
1:K:266:THR:CG2	1:K:273:VAL:H	2.29	0.45
1:M:321:LYS:HB2	1:M:334:ASP:HB3	1.99	0.45
1:C:23:LEU:CD1	1:C:23:LEU:C	2.84	0.45
1:M:138:CYS:SG	1:M:144:ILE:HD13	2.56	0.45
1:A:77:VAL:HG23	1:A:92:ALA:HB1	1.99	0.45
1:N:228:SER:O	1:N:257:GLU:HB3	2.17	0.45
1:B:300:VAL:O	1:B:307:MET:HE3	2.17	0.45
1:K:365:LEU:O	1:K:369:VAL:HG23	2.17	0.45
1:K:476:TYR:HA	1:K:486:GLY:O	2.17	0.45
2:S:23:GLY:H	2:T:80:ASN:HD21	1.64	0.45
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.57	0.45
1:L:444:LEU:HD23	1:L:444:LEU:HA	1.74	0.45
1:G:197:ARG:HG2	1:G:277:LYS:O	2.17	0.45
1:M:270:ILE:HG23	1:N:229:ASN:ND2	2.32	0.45
1:C:409:GLU:CD	1:C:501:ARG:HH21	2.19	0.45
1:F:28:LYS:HD2	1:F:453:GLN:NE2	2.32	0.45
1:L:433:ASN:HD22	1:L:433:ASN:HA	1.59	0.45
1:L:365:LEU:O	1:L:369:VAL:HG23	2.16	0.45
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.57	0.45
1:F:413:ALA:CB	1:F:417:VAL:HG13	2.47	0.45
1:M:16:MET:HG3	1:M:520:MET:SD	2.57	0.45
1:A:28:LYS:HD2	1:A:453:GLN:NE2	2.31	0.45
1:F:233:MET:HB3	1:F:237:LEU:HD12	1.98	0.45
1:I:417:VAL:HG21	1:I:488:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:105:LYS:HB2	1:D:105:LYS:HE3	1.74	0.45
1:C:257:GLU:O	1:C:261:THR:HG23	2.17	0.45
1:E:351:GLN:HG2	1:E:351:GLN:O	2.16	0.45
1:L:419:LEU:HD11	1:L:504:LEU:HG	1.99	0.45
1:L:47:PRO:CG	1:M:73:MET:HG3	2.44	0.45
1:L:16:MET:O	1:L:20:VAL:HG12	2.17	0.45
1:D:381:VAL:CG1	1:D:392:LYS:CG	2.95	0.45
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.99	0.45
1:F:420:ILE:HD13	1:F:451:LEU:HD13	1.98	0.45
1:D:351:GLN:O	1:D:351:GLN:HG2	2.16	0.45
1:J:64:ASP:OD1	1:J:65:LYS:O	2.34	0.44
2:Q:11:ILE:HG12	2:Q:85:ILE:HG12	1.98	0.44
1:L:259:LEU:O	1:L:263:VAL:HG23	2.18	0.44
1:J:365:LEU:O	1:J:369:VAL:HG23	2.17	0.44
1:H:15:LYS:HB3	1:H:66:PHE:HB3	1.99	0.44
1:K:444:LEU:HA	1:K:444:LEU:HD23	1.69	0.44
1:C:32:GLY:HA2	4:C:702:ADP:H5'1	1.98	0.44
1:N:429:LEU:HB3	1:N:440:ILE:HG21	2.00	0.44
1:D:28:LYS:C	1:D:30:THR:H	2.21	0.44
1:N:262:LEU:O	1:N:266:THR:HG23	2.17	0.44
1:I:213:VAL:O	1:I:324:VAL:HA	2.17	0.44
2:P:34:LYS:HG3	2:P:35:SER:H	1.82	0.44
1:F:510:VAL:HG23	1:F:514:MET:CE	2.47	0.44
1:B:153:ASN:O	1:B:154:SER:HB2	2.17	0.44
1:M:417:VAL:HG21	1:M:488:MET:HG3	1.99	0.44
1:K:16:MET:O	1:K:20:VAL:HG12	2.17	0.44
1:E:257:GLU:O	1:E:261:THR:HG23	2.17	0.44
1:E:28:LYS:HD2	1:E:453:GLN:CD	2.38	0.44
1:N:226:LYS:HG3	1:N:252:GLU:HB3	1.98	0.44
2:P:78:ILE:HD13	2:P:83:VAL:HG21	1.99	0.44
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.57	0.44
1:B:18:ARG:HB2	1:B:67:GLU:HG2	1.99	0.44
1:N:77:VAL:HG11	1:N:510:VAL:HB	1.99	0.44
1:F:254:VAL:HG12	1:F:259:LEU:HB2	2.00	0.44
2:Q:43:VAL:HG13	2:Q:57:LEU:HD12	2.00	0.44
1:N:16:MET:HG3	1:N:520:MET:SD	2.57	0.44
1:C:420:ILE:HD13	1:C:451:LEU:HD13	1.99	0.44
1:J:163:ALA:O	1:J:167:ASP:HB2	2.17	0.44
1:G:18:ARG:HB2	1:G:67:GLU:HG2	1.99	0.44
1:J:69:MET:HE2	1:J:522:THR:HB	1.95	0.44
1:H:15:LYS:HD3	1:H:15:LYS:HA	1.72	0.44
1:J:444:LEU:HA	1:J:444:LEU:HD23	1.71	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:126:ALA:HB1	1:K:426:LEU:HD22	2.00	0.44
1:C:100:ILE:HD11	1:C:514:MET:CE	2.38	0.44
1:C:510:VAL:CG2	1:C:514:MET:HE2	2.48	0.44
1:G:197:ARG:HA	1:G:197:ARG:HD3	1.64	0.44
1:G:16:MET:O	1:G:20:VAL:HG23	2.18	0.44
1:K:38:VAL:HG12	1:K:40:LEU:HD13	1.98	0.44
1:M:419:LEU:HD21	1:M:500:THR:CG2	2.42	0.44
1:L:342:ILE:O	1:L:346:VAL:HG23	2.17	0.44
1:G:24:ALA:O	1:G:28:LYS:HG3	2.17	0.44
1:E:233:MET:HB3	1:E:237:LEU:HD12	1.98	0.44
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.58	0.44
1:L:226:LYS:HG3	1:L:252:GLU:HB3	1.99	0.44
1:A:461:GLU:HA	1:A:462:PRO:HD3	1.89	0.44
1:C:413:ALA:CB	1:C:417:VAL:HG13	2.47	0.44
4:G:706:ADP:O3B	5:G:806:HOH:O	2.21	0.44
1:F:33:PRO:HG3	4:F:705:ADP:C6	2.53	0.44
2:O:43:VAL:HG13	2:O:57:LEU:HD12	2.00	0.44
2:P:43:VAL:HG13	2:P:57:LEU:HD12	2.00	0.44
1:J:90:THR:O	1:J:94:VAL:HG23	2.17	0.44
1:E:150:ILE:HD13	1:E:493:ILE:HA	1.99	0.44
1:N:513:LEU:HD12	1:N:513:LEU:HA	1.90	0.44
1:C:365:LEU:O	1:C:369:VAL:HG13	2.18	0.44
1:C:28:LYS:HD2	1:C:453:GLN:NE2	2.33	0.44
1:A:233:MET:HB3	1:A:237:LEU:HD12	2.00	0.44
1:H:34:LYS:HB2	1:H:458:CYS:SG	2.58	0.44
1:E:31:LEU:HD23	1:E:453:GLN:HB3	2.00	0.44
1:C:225:LYS:HG2	1:C:303:GLU:HB2	2.00	0.44
1:E:225:LYS:HG2	1:E:303:GLU:HB2	1.99	0.44
1:E:421:ARG:HD3	1:E:421:ARG:HA	1.72	0.44
1:D:42:LYS:HG2	1:D:44:PHE:CE2	2.52	0.44
1:J:126:ALA:HB1	1:J:426:LEU:HD22	2.00	0.44
1:D:100:ILE:HD11	1:D:514:MET:CE	2.46	0.44
1:G:495:ASP:CG	4:G:706:ADP:HO2'	2.21	0.44
1:D:300:VAL:O	1:D:307:MET:HE3	2.18	0.44
1:F:162:ILE:HG21	1:F:403:THR:HG21	2.00	0.44
1:K:270:ILE:HG23	1:L:229:ASN:ND2	2.33	0.44
1:G:451:LEU:HD21	1:G:465:VAL:HG12	1.99	0.44
1:D:301:ILE:O	1:D:301:ILE:HG22	2.18	0.44
1:G:80:LYS:HD2	1:G:506:TYR:CE1	2.53	0.44
1:A:130:GLU:HB3	1:A:422:VAL:HB	1.99	0.44
1:M:85:ALA:HA	1:M:498:LYS:HD3	2.00	0.44
1:M:15:LYS:HB3	1:M:66:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:64:ASP:HB3	1:K:67:GLU:HB2	1.98	0.44
1:L:419:LEU:HD21	1:L:500:THR:CG2	2.45	0.44
1:I:228:SER:O	1:I:257:GLU:HB3	2.18	0.44
1:M:15:LYS:HD3	1:M:15:LYS:HA	1.73	0.43
1:J:64:ASP:C	1:J:65:LYS:O	2.55	0.43
1:I:326:ASN:HD22	1:I:328:ASP:H	1.65	0.43
1:D:28:LYS:C	1:D:30:THR:N	2.68	0.43
1:G:28:LYS:HD2	1:G:453:GLN:NE2	2.32	0.43
1:M:262:LEU:O	1:M:266:THR:HG23	2.17	0.43
1:F:451:LEU:HD21	1:F:465:VAL:HG12	1.98	0.43
1:I:296:THR:HB	1:I:319:GLN:H	1.82	0.43
1:I:285:ARG:HA	1:I:288:MET:HB2	1.99	0.43
1:A:254:VAL:HG12	1:A:259:LEU:HB2	2.00	0.43
1:L:455:VAL:HG11	1:L:461:GLU:O	2.17	0.43
1:F:4:LYS:HG3	1:G:59:GLU:O	2.18	0.43
1:F:225:LYS:HG2	1:F:303:GLU:HB2	2.00	0.43
2:T:43:VAL:HG13	2:T:57:LEU:HD12	2.00	0.43
1:D:327:LYS:HG2	1:D:327:LYS:O	2.18	0.43
1:K:130:GLU:HG3	1:K:426:LEU:CD2	2.48	0.43
1:M:227:ILE:CD1	1:M:309:LEU:HD11	2.47	0.43
1:J:104:LEU:HA	1:J:104:LEU:HD12	1.66	0.43
1:A:361:ASP:O	1:A:365:LEU:HD23	2.18	0.43
1:A:349:ILE:HG23	1:A:365:LEU:HD12	2.00	0.43
1:N:38:VAL:HG12	1:N:40:LEU:HD13	1.99	0.43
1:E:234:LEU:HD22	2:S:23:GLY:HA3	1.99	0.43
2:O:96:GLU:O	2:P:1:MET:HB2	2.18	0.43
1:M:87:ASP:HB3	1:M:499:VAL:HG21	2.00	0.43
1:B:413:ALA:CB	1:B:417:VAL:HG13	2.48	0.43
1:D:414:GLY:O	1:D:417:VAL:CG1	2.48	0.43
1:A:381:VAL:HG11	1:A:392:LYS:HG3	2.01	0.43
2:T:34:LYS:HG3	2:T:35:SER:H	1.82	0.43
1:C:254:VAL:HG12	1:C:259:LEU:HB2	2.00	0.43
1:A:102:GLU:HB3	1:A:442:VAL:HG22	2.01	0.43
1:B:519:CYS:HB3	1:C:38:VAL:HG22	2.01	0.43
1:I:476:TYR:HA	1:I:486:GLY:O	2.18	0.43
1:D:18:ARG:HH11	1:D:18:ARG:HB3	1.83	0.43
1:N:104:LEU:HD12	1:N:104:LEU:HA	1.71	0.43
1:K:452:ARG:HG2	1:K:452:ARG:NH1	2.32	0.43
1:D:6:VAL:CG2	1:D:6:VAL:O	2.66	0.43
2:O:50:GLU:OE1	2:P:50:GLU:HA	2.18	0.43
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.90	0.43
1:N:102:GLU:OE2	1:N:445:ARG:NH1	2.50	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:365:LEU:O	1:H:369:VAL:HG23	2.19	0.43
1:H:30:THR:HB	1:H:51:LYS:O	2.18	0.43
1:A:421:ARG:HA	1:A:421:ARG:HD3	1.68	0.43
1:K:130:GLU:HG3	1:K:426:LEU:HD23	1.99	0.43
1:G:175:ILE:HG21	1:G:400:LEU:HD21	2.01	0.43
1:N:213:VAL:O	1:N:324:VAL:HA	2.18	0.43
1:J:80:LYS:HA	1:J:83:ASP:HB2	2.00	0.43
1:K:77:VAL:HG11	1:K:510:VAL:HB	1.98	0.43
1:K:77:VAL:HG22	1:K:506:TYR:HD1	1.82	0.43
1:K:226:LYS:HG3	1:K:252:GLU:HB3	2.00	0.43
2:O:34:LYS:HG3	2:O:35:SER:H	1.83	0.43
1:A:44:PHE:HB2	1:A:45:GLY:H	1.72	0.43
1:F:197:ARG:HG2	1:F:277:LYS:O	2.18	0.43
1:N:77:VAL:HG22	1:N:506:TYR:CD1	2.53	0.43
1:C:300:VAL:O	1:C:307:MET:HE3	2.19	0.43
1:L:102:GLU:HB3	1:L:442:VAL:HG22	2.01	0.43
1:B:225:LYS:HG2	1:B:303:GLU:HB2	2.01	0.43
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.52	0.43
1:C:510:VAL:HG23	1:C:514:MET:CE	2.49	0.43
2:P:50:GLU:OE1	2:Q:50:GLU:HA	2.19	0.43
1:D:257:GLU:O	1:D:261:THR:HG23	2.18	0.43
2:Q:34:LYS:HG3	2:Q:35:SER:H	1.83	0.43
1:H:409:GLU:OE2	1:H:501:ARG:NH2	2.47	0.43
2:T:23:GLY:H	2:U:80:ASN:HD21	1.66	0.43
1:N:34:LYS:HB2	1:N:458:CYS:SG	2.58	0.43
1:I:443:ALA:O	1:I:447:MET:HG3	2.19	0.43
1:N:126:ALA:HB1	1:N:426:LEU:HD22	2.00	0.43
1:D:452:ARG:NH1	1:D:452:ARG:HG2	2.33	0.43
1:G:254:VAL:HG12	1:G:259:LEU:HB2	2.00	0.43
2:R:46:GLY:HA3	2:R:55:LYS:O	2.19	0.43
1:E:248:LEU:HD22	1:E:323:VAL:HG11	2.00	0.43
1:K:524:LEU:HD23	1:K:524:LEU:HA	1.87	0.43
1:G:421:ARG:HD3	1:G:421:ARG:HA	1.69	0.43
1:K:66:PHE:H	1:K:69:MET:HG3	1.83	0.43
1:N:69:MET:CE	1:N:522:THR:CB	2.93	0.43
1:L:34:LYS:HB2	1:L:458:CYS:SG	2.58	0.43
1:G:381:VAL:CG1	1:G:392:LYS:CG	2.97	0.43
1:M:80:LYS:HA	1:M:83:ASP:HB2	2.00	0.43
1:B:28:LYS:C	1:B:30:THR:N	2.72	0.43
1:B:449:ALA:HB3	1:B:450:PRO:HD3	2.00	0.43
1:G:524:LEU:HA	1:G:524:LEU:HD23	1.84	0.43
1:L:72:GLN:HA	1:L:72:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:19:GLY:HA3	1:G:67:GLU:O	2.19	0.43
1:E:42:LYS:HG2	1:E:44:PHE:CE2	2.53	0.43
1:N:7:LYS:HD2	1:N:66:PHE:CE2	2.54	0.43
1:H:7:LYS:HD2	1:H:66:PHE:CE2	2.54	0.43
1:G:77:VAL:HG23	1:G:92:ALA:HB1	2.01	0.43
1:M:419:LEU:HD22	1:M:500:THR:CG2	2.47	0.43
1:G:28:LYS:HD2	1:G:453:GLN:CD	2.39	0.43
1:J:262:LEU:O	1:J:266:THR:HG23	2.18	0.43
1:E:409:GLU:OE2	1:E:501:ARG:NH2	2.42	0.43
1:B:130:GLU:HB3	1:B:422:VAL:HB	2.01	0.43
1:F:248:LEU:HD22	1:F:323:VAL:HG11	1.99	0.43
1:H:433:ASN:OD1	1:H:435:ASP:HB2	2.18	0.43
1:M:64:ASP:C	1:M:65:LYS:O	2.56	0.42
1:K:64:ASP:OD1	1:K:65:LYS:O	2.37	0.42
1:H:444:LEU:HA	1:H:444:LEU:HD23	1.72	0.42
1:I:96:ALA:O	1:I:100:ILE:HG13	2.18	0.42
1:K:270:ILE:HA	1:L:257:GLU:OE2	2.19	0.42
1:B:301:ILE:HG22	1:B:301:ILE:O	2.19	0.42
1:F:257:GLU:O	1:F:261:THR:HG23	2.19	0.42
1:M:365:LEU:O	1:M:369:VAL:HG23	2.19	0.42
1:N:365:LEU:O	1:N:369:VAL:HG23	2.19	0.42
2:S:50:GLU:OE1	2:T:50:GLU:HA	2.19	0.42
1:B:432:GLN:NE2	1:B:436:GLN:NE2	2.39	0.42
1:K:285:ARG:HA	1:K:288:MET:HB2	2.01	0.42
1:B:102:GLU:HB3	1:B:442:VAL:HG22	2.01	0.42
1:J:226:LYS:HG3	1:J:252:GLU:HB3	2.01	0.42
1:F:520:MET:HG2	1:G:39:VAL:HB	2.00	0.42
1:A:477:GLY:HA3	1:A:488:MET:SD	2.59	0.42
1:A:365:LEU:O	1:A:369:VAL:HG13	2.19	0.42
1:G:349:ILE:HG23	1:G:365:LEU:HD12	2.01	0.42
1:D:349:ILE:HG23	1:D:365:LEU:HD12	2.01	0.42
1:K:429:LEU:HB3	1:K:440:ILE:HG21	2.01	0.42
1:G:455:VAL:HG11	1:G:462:PRO:HA	2.02	0.42
2:U:43:VAL:HG13	2:U:57:LEU:HD12	2.01	0.42
2:U:34:LYS:HG3	2:U:35:SER:H	1.84	0.42
1:D:421:ARG:HA	1:D:421:ARG:HD3	1.73	0.42
1:M:426:LEU:H	1:M:426:LEU:HG	1.67	0.42
1:A:510:VAL:HG23	1:A:514:MET:HE3	2.02	0.42
1:D:100:ILE:O	1:D:101:THR:C	2.56	0.42
1:J:32:GLY:HA2	1:J:454:ILE:CD1	2.46	0.42
1:G:288:MET:O	1:G:291:ASP:HB2	2.19	0.42
1:J:77:VAL:HG22	1:J:506:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:215:LEU:HB3	1:N:218:PRO:HG3	2.01	0.42
1:D:451:LEU:HD21	1:D:465:VAL:HG12	2.01	0.42
1:D:105:LYS:HD3	1:K:110:GLY:O	2.19	0.42
1:J:477:GLY:O	1:J:485:TYR:HA	2.19	0.42
1:M:441:LYS:O	1:M:442:VAL:C	2.58	0.42
1:A:286:LYS:HE2	1:A:304:GLU:OE1	2.19	0.42
1:D:248:LEU:HD22	1:D:323:VAL:HG11	2.01	0.42
1:N:285:ARG:HA	1:N:288:MET:HB2	2.01	0.42
1:L:524:LEU:HD23	1:L:524:LEU:HA	1.82	0.42
1:I:15:LYS:HD3	1:I:15:LYS:HA	1.73	0.42
1:D:77:VAL:HG23	1:D:92:ALA:HB1	2.01	0.42
1:M:22:VAL:HG11	1:M:62:LEU:HD21	2.02	0.42
1:E:80:LYS:HD2	1:E:506:TYR:CE1	2.54	0.42
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.54	0.42
1:B:510:VAL:HG23	1:B:514:MET:CE	2.49	0.42
1:A:90:THR:O	1:A:94:VAL:HG23	2.19	0.42
1:D:28:LYS:O	1:D:30:THR:N	2.52	0.42
1:A:381:VAL:CG1	1:A:392:LYS:HG2	2.49	0.42
1:I:461:GLU:HA	1:I:462:PRO:HD3	1.90	0.42
1:M:228:SER:O	1:M:257:GLU:HB3	2.20	0.42
1:D:18:ARG:HB2	1:D:67:GLU:HG2	2.00	0.42
1:K:15:LYS:HD3	1:K:15:LYS:HA	1.74	0.42
1:H:419:LEU:HD22	1:H:500:THR:CG2	2.47	0.42
1:L:213:VAL:O	1:L:324:VAL:HA	2.20	0.42
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.60	0.42
1:L:126:ALA:HB1	1:L:426:LEU:HD22	2.02	0.42
1:D:430:ARG:CG	1:D:430:ARG:NH1	2.75	0.42
1:M:104:LEU:HD12	1:M:104:LEU:HA	1.72	0.42
1:J:419:LEU:HD22	1:J:500:THR:CG2	2.47	0.42
1:G:361:ASP:O	1:G:365:LEU:HD23	2.19	0.42
1:G:365:LEU:O	1:G:369:VAL:HG13	2.19	0.42
1:M:413:ALA:CB	1:M:417:VAL:HB	2.50	0.42
1:A:301:ILE:HG21	1:A:309:LEU:HD12	2.02	0.42
1:I:262:LEU:O	1:I:266:THR:HG23	2.19	0.42
1:N:87:ASP:HB3	1:N:499:VAL:HG21	2.02	0.42
1:J:8:PHE:O	1:J:9:GLY:C	2.57	0.42
1:F:34:LYS:HD2	1:F:458:CYS:SG	2.60	0.42
1:D:41:ASP:O	1:D:42:LYS:HG3	2.20	0.42
1:F:204:PHE:CG	1:F:204:PHE:O	2.73	0.42
1:I:130:GLU:HG3	1:I:426:LEU:CD2	2.49	0.42
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.55	0.42
1:N:444:LEU:HD23	1:N:444:LEU:HA	1.68	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:33:PRO:HG3	4:D:703:ADP:C6	2.55	0.42
1:M:215:LEU:HB3	1:M:218:PRO:HG3	2.01	0.42
1:J:215:LEU:HB3	1:J:218:PRO:HG3	2.02	0.42
1:B:381:VAL:HG11	1:B:392:LYS:HG3	2.02	0.42
1:M:234:LEU:N	1:M:235:PRO:HD2	2.34	0.42
1:A:150:ILE:HD13	1:A:493:ILE:HA	2.02	0.42
1:K:213:VAL:O	1:K:324:VAL:HA	2.20	0.42
1:E:286:LYS:HE2	1:E:304:GLU:OE1	2.20	0.42
1:H:285:ARG:HA	1:H:288:MET:HB2	2.01	0.42
1:C:455:VAL:HG21	1:C:465:VAL:HG11	2.01	0.42
1:L:15:LYS:HB3	1:L:66:PHE:HB3	2.02	0.42
1:A:288:MET:CG	1:A:368:ARG:HD2	2.50	0.42
1:F:501:ARG:HD3	1:F:505:GLN:OE1	2.19	0.42
1:K:342:ILE:O	1:K:346:VAL:HG23	2.20	0.42
1:F:301:ILE:HG22	1:F:301:ILE:O	2.20	0.42
1:E:455:VAL:HG21	1:E:465:VAL:HG11	2.02	0.42
1:M:455:VAL:HG13	1:M:460:GLU:HB2	2.01	0.42
1:K:11:ASP:O	1:K:12:ALA:C	2.59	0.42
1:L:80:LYS:HA	1:L:83:ASP:HB2	2.02	0.42
1:F:219:PHE:HB3	1:F:317:LEU:HD13	2.01	0.42
1:F:413:ALA:HB3	1:F:417:VAL:HG13	2.02	0.41
1:L:15:LYS:HA	1:L:15:LYS:HD3	1.76	0.41
1:N:149:THR:HG22	1:N:156:GLU:HA	2.02	0.41
1:H:234:LEU:N	1:H:235:PRO:HD2	2.35	0.41
1:B:381:VAL:HG12	1:B:392:LYS:HG2	2.02	0.41
1:G:28:LYS:C	1:G:30:THR:H	2.22	0.41
1:M:39:VAL:HB	1:N:520:MET:HG2	2.02	0.41
1:L:443:ALA:O	1:L:447:MET:HG3	2.20	0.41
1:L:285:ARG:HA	1:L:288:MET:HB2	2.02	0.41
1:J:213:VAL:O	1:J:324:VAL:HA	2.19	0.41
1:B:23:LEU:C	1:B:23:LEU:CD1	2.88	0.41
1:N:64:ASP:OD1	1:N:65:LYS:O	2.37	0.41
1:L:104:LEU:HA	1:L:104:LEU:HD12	1.74	0.41
1:L:428:ASP:O	1:L:429:LEU:C	2.59	0.41
1:M:429:LEU:HB3	1:M:440:ILE:HG21	2.03	0.41
1:G:301:ILE:HG21	1:G:309:LEU:HD12	2.02	0.41
1:A:381:VAL:CG1	1:A:392:LYS:HG3	2.50	0.41
1:N:85:ALA:HA	1:N:498:LYS:HD3	2.02	0.41
1:C:130:GLU:HB3	1:C:422:VAL:HB	2.03	0.41
2:S:34:LYS:HG3	2:S:35:SER:H	1.84	0.41
1:K:296:THR:HB	1:K:319:GLN:H	1.84	0.41
1:B:44:PHE:HB2	1:B:45:GLY:H	1.76	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:197:ARG:HD3	1:C:197:ARG:HA	1.66	0.41
1:H:342:ILE:O	1:H:346:VAL:HG23	2.20	0.41
1:A:24:ALA:O	1:A:28:LYS:HG3	2.20	0.41
1:K:428:ASP:O	1:K:429:LEU:C	2.58	0.41
1:K:39:VAL:HB	1:L:520:MET:HG2	2.02	0.41
1:F:28:LYS:O	1:F:30:THR:N	2.53	0.41
1:B:286:LYS:HE2	1:B:304:GLU:OE1	2.20	0.41
1:J:2:ALA:O	1:J:4:LYS:HE3	2.20	0.41
1:M:476:TYR:HA	1:M:486:GLY:O	2.20	0.41
1:E:130:GLU:HB3	1:E:422:VAL:HB	2.01	0.41
1:H:524:LEU:HA	1:H:524:LEU:HD23	1.84	0.41
1:I:524:LEU:HD23	1:I:524:LEU:HA	1.85	0.41
1:M:226:LYS:HG3	1:M:252:GLU:HB3	2.01	0.41
1:I:64:ASP:C	1:I:65:LYS:O	2.58	0.41
1:K:104:LEU:HA	1:K:104:LEU:HD12	1.80	0.41
1:H:104:LEU:HD12	1:H:104:LEU:HA	1.74	0.41
1:N:100:ILE:HG23	1:N:104:LEU:HD22	2.01	0.41
1:D:28:LYS:HD2	1:D:453:GLN:NE2	2.36	0.41
1:K:16:MET:O	1:K:20:VAL:CG1	2.69	0.41
1:E:102:GLU:HB3	1:E:442:VAL:HG22	2.03	0.41
2:T:60:LYS:HG2	2:T:63:ASP:OD2	2.20	0.41
1:C:286:LYS:HE2	1:C:304:GLU:OE1	2.21	0.41
1:B:501:ARG:HD3	1:B:505:GLN:OE1	2.20	0.41
1:E:270:ILE:HG23	2:S:25:ILE:HG22	2.03	0.41
1:C:114:MET:HE3	1:C:114:MET:O	2.20	0.41
1:C:204:PHE:CG	1:C:204:PHE:O	2.73	0.41
1:C:197:ARG:H	1:C:329:THR:HA	1.84	0.41
1:N:13:ARG:HD2	1:N:104:LEU:HD11	2.03	0.41
1:F:349:ILE:HG23	1:F:365:LEU:HD12	2.01	0.41
1:D:238:GLU:OE1	2:R:24:GLY:HA3	2.20	0.41
1:L:16:MET:O	1:L:20:VAL:CG1	2.69	0.41
1:H:428:ASP:O	1:H:429:LEU:C	2.58	0.41
1:E:150:ILE:CD1	1:E:493:ILE:HA	2.50	0.41
1:D:69:MET:O	1:D:73:MET:HG3	2.21	0.41
1:G:289:LEU:HA	1:G:292:ILE:HD12	2.02	0.41
1:F:421:ARG:HA	1:F:421:ARG:HD3	1.74	0.41
1:M:66:PHE:HD1	1:M:520:MET:HE2	1.85	0.41
1:E:365:LEU:O	1:E:369:VAL:HG13	2.20	0.41
1:H:102:GLU:HB3	1:H:442:VAL:HG22	2.02	0.41
1:I:215:LEU:HB3	1:I:218:PRO:HG3	2.03	0.41
1:K:215:LEU:HB3	1:K:218:PRO:HG3	2.02	0.41
1:B:261:THR:HG22	2:P:29:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:301:ILE:HG21	1:F:309:LEU:HD12	2.03	0.41
1:I:455:VAL:HG13	1:I:460:GLU:HB2	2.02	0.41
1:J:10:ASN:O	1:J:11:ASP:C	2.59	0.41
1:H:69:MET:HE2	1:H:522:THR:HB	2.00	0.41
1:G:16:MET:HE1	1:G:514:MET:HB3	2.03	0.41
1:E:288:MET:CG	1:E:368:ARG:HD2	2.49	0.41
1:J:437:ASN:HA	1:J:440:ILE:HD12	2.01	0.41
1:H:10:ASN:O	1:H:11:ASP:C	2.59	0.41
1:F:28:LYS:C	1:F:30:THR:N	2.73	0.41
1:A:248:LEU:HD22	1:A:323:VAL:HG11	2.02	0.41
1:N:296:THR:HB	1:N:319:GLN:H	1.85	0.41
1:G:248:LEU:HD22	1:G:323:VAL:HG11	2.02	0.41
1:J:101:THR:HG22	1:J:105:LYS:HE3	2.02	0.41
1:B:95:LEU:O	1:B:99:ILE:HG13	2.21	0.41
1:M:461:GLU:HA	1:M:462:PRO:HD3	1.89	0.41
1:I:11:ASP:O	1:I:12:ALA:C	2.58	0.41
1:C:421:ARG:HD3	1:C:421:ARG:HA	1.74	0.41
1:A:204:PHE:O	1:A:204:PHE:CG	2.74	0.41
1:F:153:ASN:O	1:F:154:SER:HB2	2.21	0.41
1:F:365:LEU:O	1:F:369:VAL:HG13	2.20	0.41
1:M:270:ILE:HG23	1:N:229:ASN:HD21	1.86	0.41
1:L:198:GLY:HA3	1:L:328:ASP:HA	2.03	0.41
1:C:452:ARG:HH12	1:C:463:SER:HB3	1.85	0.41
1:C:162:ILE:HG21	1:C:403:THR:HG21	2.03	0.41
1:D:240:VAL:HG11	1:D:247:LEU:HB2	2.03	0.41
1:E:451:LEU:HD21	1:E:465:VAL:HG12	2.02	0.41
1:H:433:ASN:HA	1:H:433:ASN:HD22	1.54	0.41
1:B:248:LEU:HD22	1:B:323:VAL:HG11	2.01	0.41
1:I:221:LEU:HD12	1:I:249:ILE:HG23	2.02	0.41
1:E:198:GLY:HA2	1:E:326:ASN:O	2.21	0.41
1:C:30:THR:HB	1:C:51:LYS:HG2	2.03	0.41
1:D:524:LEU:HA	1:D:524:LEU:HD23	1.99	0.41
1:D:456:LEU:HD13	1:D:462:PRO:CG	2.51	0.41
1:D:413:ALA:CB	1:D:417:VAL:HG13	2.51	0.41
1:D:19:GLY:HA3	1:D:67:GLU:O	2.20	0.41
1:K:15:LYS:HB3	1:K:66:PHE:HB3	2.03	0.41
1:A:510:VAL:O	1:A:511:ALA:C	2.57	0.41
1:B:16:MET:HE1	1:B:514:MET:HB3	2.03	0.41
1:I:421:ARG:NH2	1:I:469:VAL:O	2.51	0.41
1:E:16:MET:HE1	1:E:514:MET:HB3	2.03	0.41
1:H:200:LEU:CD1	1:H:276:VAL:HA	2.49	0.41
1:M:452:ARG:HG2	1:M:452:ARG:NH1	2.29	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:VAL:HG12	1:G:69:MET:CE	2.51	0.41
1:E:288:MET:O	1:E:291:ASP:HB2	2.21	0.41
1:F:288:MET:CG	1:F:368:ARG:HD2	2.49	0.41
1:B:444:LEU:O	1:B:447:MET:HB2	2.20	0.41
1:F:361:ASP:O	1:F:365:LEU:HD23	2.21	0.41
1:D:288:MET:O	1:D:291:ASP:HB2	2.21	0.41
1:B:365:LEU:O	1:B:369:VAL:HG13	2.21	0.41
1:C:238:GLU:OE1	2:Q:24:GLY:HA3	2.21	0.41
1:J:342:ILE:O	1:J:346:VAL:HG23	2.21	0.41
1:D:150:ILE:CD1	1:D:493:ILE:HA	2.51	0.41
1:J:234:LEU:N	1:J:235:PRO:HD2	2.36	0.41
1:K:234:LEU:N	1:K:235:PRO:HD2	2.36	0.41
1:L:266:THR:HG22	1:L:273:VAL:H	1.85	0.41
1:B:247:LEU:O	1:B:273:VAL:HA	2.21	0.41
1:F:259:LEU:O	1:F:263:VAL:HG23	2.21	0.41
1:J:43:SER:HB2	1:J:44:PHE:CD1	2.55	0.41
1:N:138:CYS:SG	1:N:144:ILE:HD13	2.61	0.41
1:K:455:VAL:HG13	1:K:460:GLU:HB2	2.02	0.41
1:D:286:LYS:HE2	1:D:304:GLU:OE1	2.20	0.41
1:F:519:CYS:HB3	1:G:38:VAL:HG22	2.03	0.41
1:A:6:VAL:HG23	1:A:6:VAL:O	2.20	0.41
1:M:213:VAL:O	1:M:324:VAL:HA	2.21	0.41
1:H:213:VAL:O	1:H:324:VAL:HA	2.20	0.41
1:H:221:LEU:HD12	1:H:249:ILE:HG23	2.02	0.41
1:F:102:GLU:HB3	1:F:442:VAL:HG22	2.03	0.41
1:A:348:GLN:HE21	1:A:348:GLN:HB3	1.68	0.41
1:E:19:GLY:HA3	1:E:67:GLU:O	2.21	0.41
1:I:100:ILE:HG23	1:I:104:LEU:HD22	2.02	0.41
1:C:288:MET:CG	1:C:368:ARG:HD2	2.49	0.41
1:J:34:LYS:HB2	1:J:458:CYS:SG	2.61	0.41
1:G:95:LEU:O	1:G:99:ILE:HG13	2.21	0.41
1:J:22:VAL:HG11	1:J:62:LEU:HD21	2.02	0.41
1:N:461:GLU:HA	1:N:462:PRO:HD3	1.93	0.41
1:L:221:LEU:HD12	1:L:249:ILE:HG23	2.02	0.41
1:I:513:LEU:HA	1:I:513:LEU:HD12	1.94	0.41
1:F:19:GLY:HA3	1:F:67:GLU:O	2.21	0.40
1:B:204:PHE:CG	1:B:204:PHE:O	2.74	0.40
1:I:444:LEU:HD23	1:I:444:LEU:HA	1.67	0.40
1:I:452:ARG:NH1	1:I:452:ARG:HG2	2.31	0.40
1:F:288:MET:O	1:F:291:ASP:HB2	2.21	0.40
1:E:349:ILE:HG23	1:E:365:LEU:HD12	2.01	0.40
1:M:428:ASP:O	1:M:429:LEU:C	2.59	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:437:ASN:HA	1:M:440:ILE:HD12	2.03	0.40
1:H:381:VAL:HG21	1:H:393:LYS:HA	2.03	0.40
2:U:46:GLY:HA3	2:U:55:LYS:O	2.21	0.40
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.92	0.40
1:F:42:LYS:HE2	1:F:48:THR:OG1	2.22	0.40
1:L:419:LEU:HD22	1:L:500:THR:CG2	2.50	0.40
1:C:361:ASP:O	1:C:365:LEU:HD23	2.21	0.40
1:H:521:VAL:HB	1:N:40:LEU:HD12	2.04	0.40
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.84	0.40
1:J:11:ASP:O	1:J:12:ALA:C	2.59	0.40
1:C:404:ARG:O	1:C:408:GLU:HG2	2.21	0.40
2:R:43:VAL:HG13	2:R:57:LEU:HD12	2.04	0.40
1:C:301:ILE:HG22	1:C:301:ILE:O	2.22	0.40
1:J:433:ASN:HA	1:J:433:ASN:HD22	1.57	0.40
1:E:327:LYS:O	1:E:327:LYS:HG2	2.20	0.40
1:C:413:ALA:HB3	1:C:417:VAL:HG13	2.02	0.40
1:B:16:MET:CE	1:B:514:MET:HB3	2.51	0.40
1:G:288:MET:CG	1:G:368:ARG:HD2	2.48	0.40
1:B:288:MET:O	1:B:291:ASP:HB2	2.22	0.40
1:B:349:ILE:HG23	1:B:365:LEU:HD12	2.02	0.40
1:L:429:LEU:HB3	1:L:440:ILE:HG21	2.04	0.40
1:H:38:VAL:HG12	1:H:40:LEU:HD13	2.03	0.40
1:I:234:LEU:N	1:I:235:PRO:HD2	2.36	0.40
1:I:266:THR:HG22	1:I:273:VAL:H	1.85	0.40
1:E:301:ILE:HG21	1:E:309:LEU:HD12	2.04	0.40
1:D:301:ILE:HG21	1:D:309:LEU:HD12	2.04	0.40
1:H:496:PRO:HB2	1:H:499:VAL:HG13	2.04	0.40
1:L:350:ARG:HA	1:L:353:ILE:HD12	2.04	0.40
1:I:433:ASN:OD1	1:I:435:ASP:HB2	2.22	0.40
1:B:461:GLU:HA	1:B:462:PRO:HD3	1.83	0.40
1:M:201:SER:HA	1:M:202:PRO:HD3	1.95	0.40
1:A:452:ARG:HH11	1:A:452:ARG:HG2	1.86	0.40
1:D:204:PHE:O	1:D:204:PHE:CG	2.74	0.40
1:E:33:PRO:HG3	4:E:704:ADP:C6	2.56	0.40
1:N:32:GLY:CA	1:N:454:ILE:HG23	2.52	0.40
1:A:301:ILE:O	1:A:301:ILE:HG22	2.21	0.40
1:E:247:LEU:O	1:E:273:VAL:HA	2.21	0.40
1:M:266:THR:HG22	1:M:273:VAL:H	1.86	0.40
1:G:381:VAL:CG1	1:G:392:LYS:HG3	2.52	0.40
1:D:219:PHE:HB3	1:D:317:LEU:HD13	2.02	0.40
1:F:286:LYS:HE2	1:F:304:GLU:OE1	2.22	0.40
1:H:201:SER:HA	1:H:202:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:55:LYS:H	2:O:55:LYS:HE2	1.87	0.40
1:E:452:ARG:HG2	1:E:452:ARG:HH11	1.86	0.40
1:E:413:ALA:HB3	1:E:417:VAL:HG13	2.04	0.40
1:G:197:ARG:H	1:G:329:THR:HA	1.87	0.40
1:D:90:THR:O	1:D:94:VAL:HG23	2.21	0.40
1:H:149:THR:HG22	1:H:156:GLU:HA	2.04	0.40
1:E:90:THR:O	1:E:94:VAL:HG23	2.21	0.40
1:J:198:GLY:HA3	1:J:328:ASP:HA	2.03	0.40
1:G:28:LYS:O	1:G:29:VAL:C	2.59	0.40
1:H:461:GLU:HA	1:H:462:PRO:HD3	1.90	0.40
1:B:301:ILE:HG21	1:B:309:LEU:HD12	2.04	0.40
2:P:46:GLY:HA3	2:P:55:LYS:O	2.22	0.40
1:D:449:ALA:HB3	1:D:450:PRO:HD3	2.04	0.40
1:B:404:ARG:O	1:B:408:GLU:HG2	2.21	0.40
1:K:72:GLN:HE22	1:K:75:LYS:NZ	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/524 (100%)	485 (93%)	33 (6%)	4 (1%)	27	76
1	B	522/524 (100%)	484 (93%)	33 (6%)	5 (1%)	22	70
1	C	522/524 (100%)	484 (93%)	34 (6%)	4 (1%)	27	76
1	D	522/524 (100%)	485 (93%)	32 (6%)	5 (1%)	22	70
1	E	522/524 (100%)	489 (94%)	29 (6%)	4 (1%)	27	76
1	F	522/524 (100%)	490 (94%)	27 (5%)	5 (1%)	22	70
1	G	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	22	70
1	H	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	22	70
1	I	522/524 (100%)	483 (92%)	32 (6%)	7 (1%)	18	62
1	J	522/524 (100%)	480 (92%)	38 (7%)	4 (1%)	27	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	522/524 (100%)	479 (92%)	38 (7%)	5 (1%)	22	70
1	L	522/524 (100%)	483 (92%)	34 (6%)	5 (1%)	22	70
1	M	522/524 (100%)	480 (92%)	37 (7%)	5 (1%)	22	70
1	N	522/524 (100%)	483 (92%)	35 (7%)	4 (1%)	27	76
2	O	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	3	18
2	P	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	3	18
2	Q	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	2	12
2	R	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	3	18
2	S	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	3	18
2	T	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	2	12
2	U	95/97 (98%)	76 (80%)	14 (15%)	5 (5%)	3	18
All	All	7973/8015 (100%)	7303 (92%)	566 (7%)	104 (1%)	18	62

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	B	44	PHE
1	C	44	PHE
1	D	44	PHE
1	E	44	PHE
1	F	44	PHE
1	G	44	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	A	337	GLY
1	B	337	GLY
1	C	337	GLY
1	D	337	GLY
1	E	337	GLY
1	F	337	GLY
1	G	337	GLY
1	H	66	PHE

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Mol	Chain	Res	Type
1	H	270	ILE
1	I	66	PHE
1	I	270	ILE
1	J	270	ILE
1	K	270	ILE
1	L	270	ILE
1	M	66	PHE
1	M	270	ILE
1	N	66	PHE
1	N	270	ILE
2	O	28	THR
2	P	28	THR
2	Q	28	THR
2	R	28	THR
2	S	28	THR
2	T	28	THR
2	U	28	THR
1	A	334	ASP
1	C	334	ASP
1	D	58	ARG
1	F	58	ARG
1	G	58	ARG
1	H	267	MET
1	H	462	PRO
1	I	267	MET
1	I	462	PRO
1	J	66	PHE
1	J	267	MET
1	K	66	PHE
1	K	267	MET
1	K	462	PRO
1	L	462	PRO
1	M	267	MET
1	M	462	PRO
1	N	267	MET
1	N	462	PRO
2	O	51	ASN
2	P	51	ASN
2	Q	49	LEU
2	Q	51	ASN
2	R	51	ASN
2	S	51	ASN

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Mol	Chain	Res	Type
2	T	51	ASN
2	U	49	LEU
2	U	51	ASN
1	B	58	ARG
1	B	334	ASP
1	D	334	ASP
1	E	334	ASP
1	F	334	ASP
1	G	334	ASP
1	J	462	PRO
1	L	66	PHE
1	L	267	MET
2	O	49	LEU
2	P	49	LEU
2	R	49	LEU
2	S	49	LEU
2	T	49	LEU
1	I	417	VAL
1	L	417	VAL
2	Q	8	ASP
2	T	8	ASP
2	R	17	VAL
1	C	305	ILE
1	G	305	ILE
2	O	17	VAL
2	S	17	VAL
1	A	305	ILE
1	B	305	ILE
1	D	305	ILE
1	E	305	ILE
1	F	305	ILE
1	H	323	VAL
1	I	9	GLY
1	M	323	VAL
2	P	17	VAL
2	Q	17	VAL
2	T	17	VAL
2	U	17	VAL
1	I	256	GLY
1	K	417	VAL

### 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%)	359 (89%)	45 (11%)	9	34
1	B	404/404 (100%)	358 (89%)	46 (11%)	8	33
1	C	404/404 (100%)	356 (88%)	48 (12%)	8	30
1	D	404/404 (100%)	357 (88%)	47 (12%)	8	31
1	E	404/404 (100%)	358 (89%)	46 (11%)	8	33
1	F	404/404 (100%)	357 (88%)	47 (12%)	8	31
1	G	404/404 (100%)	354 (88%)	50 (12%)	7	28
1	H	404/404 (100%)	347 (86%)	57 (14%)	5	23
1	I	404/404 (100%)	349 (86%)	55 (14%)	5	24
1	J	404/404 (100%)	349 (86%)	55 (14%)	5	24
1	K	404/404 (100%)	347 (86%)	57 (14%)	5	23
1	L	404/404 (100%)	348 (86%)	56 (14%)	5	23
1	M	404/404 (100%)	347 (86%)	57 (14%)	5	23
1	N	404/404 (100%)	349 (86%)	55 (14%)	5	24
2	O	80/80 (100%)	70 (88%)	10 (12%)	7	28
2	P	80/80 (100%)	70 (88%)	10 (12%)	7	28
2	Q	80/80 (100%)	70 (88%)	10 (12%)	7	28
2	R	80/80 (100%)	69 (86%)	11 (14%)	5	24
2	S	80/80 (100%)	69 (86%)	11 (14%)	5	24
2	T	80/80 (100%)	70 (88%)	10 (12%)	7	28
2	U	80/80 (100%)	69 (86%)	11 (14%)	5	24
All	All	6216/6216 (100%)	5422 (87%)	794 (13%)	6	27

All (794) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	23	LEU
1	A	43	SER

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Mol	Chain	Res	Type
1	A	44	PHE
1	A	48	THR
1	A	58	ARG
1	A	62	LEU
1	A	74	VAL
1	A	97	GLN
1	A	129	GLU
1	A	141	SER
1	A	150	ILE
1	A	153	ASN
1	A	168	LYS
1	A	176	THR
1	A	177	VAL
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	281	PHE
1	A	284	ARG
1	A	288	MET
1	A	322	ARG
1	A	345	ARG
1	A	348	GLN
1	A	351	GLN
1	A	362	ARG
1	A	366	GLN
1	A	387	VAL
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	425	LYS
1	A	430	ARG
1	A	461	GLU
1	A	483	GLU
1	A	484	GLU
1	A	504	LEU

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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	58	ARG
1	B	62	LEU
1	B	74	VAL
1	B	97	GLN
1	B	129	GLU
1	B	141	SER
1	B	150	ILE
1	B	153	ASN
1	B	168	LYS
1	B	176	THR
1	B	177	VAL
1	B	183	LEU
1	B	184	GLN
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	348	GLN
1	B	350	ARG
1	B	351	GLN
1	B	362	ARG
1	B	366	GLN
1	B	387	VAL
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	430	ARG
1	B	456	LEU

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Mol	Chain	Res	Type
1	B	461	GLU
1	B	483	GLU
1	B	484	GLU
1	B	504	LEU
1	C	18	ARG
1	C	23	LEU
1	C	43	SER
1	C	44	PHE
1	C	48	THR
1	C	58	ARG
1	C	62	LEU
1	C	74	VAL
1	C	80	LYS
1	C	97	GLN
1	C	129	GLU
1	C	141	SER
1	C	150	ILE
1	C	153	ASN
1	C	168	LYS
1	C	176	THR
1	C	177	VAL
1	C	183	LEU
1	C	184	GLN
1	C	197	ARG
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	348	GLN
1	C	350	ARG
1	C	351	GLN
1	C	362	ARG
1	C	366	GLN
1	C	387	VAL
1	C	390	LYS
1	C	391	GLU
1	C	398	ASP
1	C	400	LEU

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Mol	Chain	Res	Type
1	C	419	LEU
1	C	420	ILE
1	C	421	ARG
1	C	425	LYS
1	C	430	ARG
1	C	452	ARG
1	C	461	GLU
1	C	483	GLU
1	C	504	LEU
1	C	510	VAL
1	D	18	ARG
1	D	23	LEU
1	D	43	SER
1	D	44	PHE
1	D	48	THR
1	D	58	ARG
1	D	62	LEU
1	D	74	VAL
1	D	97	GLN
1	D	129	GLU
1	D	141	SER
1	D	150	ILE
1	D	153	ASN
1	D	168	LYS
1	D	176	THR
1	D	177	VAL
1	D	183	LEU
1	D	184	GLN
1	D	197	ARG
1	D	225	LYS
1	D	229	ASN
1	D	237	LEU
1	D	281	PHE
1	D	284	ARG
1	D	288	MET
1	D	322	ARG
1	D	345	ARG
1	D	348	GLN
1	D	350	ARG
1	D	351	GLN
1	D	362	ARG
1	D	366	GLN

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Mol	Chain	Res	Type
1	D	387	VAL
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	425	LYS
1	D	430	ARG
1	D	456	LEU
1	D	461	GLU
1	D	483	GLU
1	D	484	GLU
1	D	504	LEU
1	E	18	ARG
1	E	23	LEU
1	E	43	SER
1	E	44	PHE
1	E	48	THR
1	E	58	ARG
1	E	62	LEU
1	E	74	VAL
1	E	97	GLN
1	E	129	GLU
1	E	141	SER
1	E	150	ILE
1	E	153	ASN
1	E	168	LYS
1	E	176	THR
1	E	177	VAL
1	E	183	LEU
1	E	184	GLN
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

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Mol	Chain	Res	Type
1	E	348	GLN
1	E	350	ARG
1	E	351	GLN
1	E	362	ARG
1	E	366	GLN
1	E	387	VAL
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	430	ARG
1	E	456	LEU
1	E	461	GLU
1	E	483	GLU
1	E	484	GLU
1	E	504	LEU
1	F	18	ARG
1	F	23	LEU
1	F	43	SER
1	F	44	PHE
1	F	48	THR
1	F	58	ARG
1	F	62	LEU
1	F	74	VAL
1	F	80	LYS
1	F	97	GLN
1	F	129	GLU
1	F	141	SER
1	F	150	ILE
1	F	153	ASN
1	F	168	LYS
1	F	176	THR
1	F	177	VAL
1	F	183	LEU
1	F	184	GLN
1	F	197	ARG
1	F	225	LYS
1	F	229	ASN
1	F	237	LEU

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Mol	Chain	Res	Type
1	F	281	PHE
1	F	284	ARG
1	F	288	MET
1	F	322	ARG
1	F	345	ARG
1	F	348	GLN
1	F	350	ARG
1	F	351	GLN
1	F	362	ARG
1	F	366	GLN
1	F	387	VAL
1	F	391	GLU
1	F	398	ASP
1	F	400	LEU
1	F	419	LEU
1	F	420	ILE
1	F	421	ARG
1	F	430	ARG
1	F	452	ARG
1	F	456	LEU
1	F	461	GLU
1	F	483	GLU
1	F	484	GLU
1	F	504	LEU
1	G	18	ARG
1	G	23	LEU
1	G	43	SER
1	G	44	PHE
1	G	48	THR
1	G	51	LYS
1	G	58	ARG
1	G	62	LEU
1	G	74	VAL
1	G	80	LYS
1	G	97	GLN
1	G	129	GLU
1	G	141	SER
1	G	150	ILE
1	G	153	ASN
1	G	168	LYS
1	G	176	THR
1	G	177	VAL

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Mol	Chain	Res	Type
1	G	183	LEU
1	G	184	GLN
1	G	197	ARG
1	G	225	LYS
1	G	229	ASN
1	G	237	LEU
1	G	281	PHE
1	G	284	ARG
1	G	288	MET
1	G	322	ARG
1	G	345	ARG
1	G	348	GLN
1	G	350	ARG
1	G	351	GLN
1	G	362	ARG
1	G	366	GLN
1	G	387	VAL
1	G	391	GLU
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	425	LYS
1	G	430	ARG
1	G	456	LEU
1	G	461	GLU
1	G	483	GLU
1	G	484	GLU
1	G	504	LEU
1	G	510	VAL
1	H	10	ASN
1	H	20	VAL
1	H	23	LEU
1	H	37	ASN
1	H	40	LEU
1	H	42	LYS
1	H	59	GLU
1	H	77	VAL
1	H	79	SER
1	H	89	THR

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Mol	Chain	Res	Type
1	H	104	LEU
1	H	114	MET
1	H	129	GLU
1	H	131	LEU
1	H	138	CYS
1	H	141	SER
1	H	172	GLU
1	H	187	LEU
1	H	197	ARG
1	H	200	LEU
1	H	230	ILE
1	H	233	MET
1	H	247	LEU
1	H	248	LEU
1	H	255	GLU
1	H	261	THR
1	H	272	LYS
1	H	284	ARG
1	H	285	ARG
1	H	288	MET
1	H	300	VAL
1	H	302	SER
1	H	307	MET
1	H	317	LEU
1	H	323	VAL
1	H	328	ASP
1	H	331	THR
1	H	354	GLU
1	H	355	GLU
1	H	357	THR
1	H	385	THR
1	H	389	MET
1	H	400	LEU
1	H	401	HIS
1	H	420	ILE
1	H	421	ARG
1	H	426	LEU
1	H	432	GLN
1	H	433	ASN
1	H	445	ARG
1	H	452	ARG
1	H	460	GLU

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Mol	Chain	Res	Type
1	H	468	THR
1	H	483	GLU
1	H	494	LEU
1	H	504	LEU
1	H	513	LEU
1	I	10	ASN
1	I	20	VAL
1	I	23	LEU
1	I	37	ASN
1	I	40	LEU
1	I	42	LYS
1	I	59	GLU
1	I	77	VAL
1	I	79	SER
1	I	89	THR
1	I	104	LEU
1	I	114	MET
1	I	129	GLU
1	I	131	LEU
1	I	138	CYS
1	I	141	SER
1	I	172	GLU
1	I	187	LEU
1	I	197	ARG
1	I	200	LEU
1	I	230	ILE
1	I	233	MET
1	I	247	LEU
1	I	248	LEU
1	I	255	GLU
1	I	272	LYS
1	I	284	ARG
1	I	285	ARG
1	I	288	MET
1	I	300	VAL
1	I	302	SER
1	I	307	MET
1	I	317	LEU
1	I	328	ASP
1	I	331	THR
1	I	354	GLU
1	I	355	GLU

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Mol	Chain	Res	Type
1	I	357	THR
1	I	385	THR
1	I	389	MET
1	I	400	LEU
1	I	401	HIS
1	I	420	ILE
1	I	421	ARG
1	I	426	LEU
1	I	432	GLN
1	I	433	ASN
1	I	452	ARG
1	I	460	GLU
1	I	468	THR
1	I	483	GLU
1	I	494	LEU
1	I	504	LEU
1	I	509	SER
1	I	513	LEU
1	J	10	ASN
1	J	20	VAL
1	J	23	LEU
1	J	37	ASN
1	J	40	LEU
1	J	42	LYS
1	J	59	GLU
1	J	77	VAL
1	J	79	SER
1	J	89	THR
1	J	104	LEU
1	J	114	MET
1	J	131	LEU
1	J	138	CYS
1	J	141	SER
1	J	172	GLU
1	J	187	LEU
1	J	197	ARG
1	J	200	LEU
1	J	230	ILE
1	J	233	MET
1	J	247	LEU
1	J	248	LEU
1	J	255	GLU

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Mol	Chain	Res	Type
1	J	272	LYS
1	J	284	ARG
1	J	285	ARG
1	J	288	MET
1	J	300	VAL
1	J	302	SER
1	J	307	MET
1	J	317	LEU
1	J	323	VAL
1	J	331	THR
1	J	354	GLU
1	J	355	GLU
1	J	357	THR
1	J	385	THR
1	J	389	MET
1	J	400	LEU
1	J	401	HIS
1	J	420	ILE
1	J	421	ARG
1	J	426	LEU
1	J	432	GLN
1	J	433	ASN
1	J	445	ARG
1	J	452	ARG
1	J	460	GLU
1	J	468	THR
1	J	483	GLU
1	J	494	LEU
1	J	504	LEU
1	J	509	SER
1	J	513	LEU
1	K	10	ASN
1	K	20	VAL
1	K	23	LEU
1	K	37	ASN
1	K	40	LEU
1	K	42	LYS
1	K	59	GLU
1	K	77	VAL
1	K	79	SER
1	K	89	THR
1	K	104	LEU

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Mol	Chain	Res	Type
1	K	107	VAL
1	K	114	MET
1	K	129	GLU
1	K	131	LEU
1	K	138	CYS
1	K	141	SER
1	K	172	GLU
1	K	187	LEU
1	K	197	ARG
1	K	200	LEU
1	K	230	ILE
1	K	233	MET
1	K	247	LEU
1	K	248	LEU
1	K	255	GLU
1	K	261	THR
1	K	272	LYS
1	K	284	ARG
1	K	285	ARG
1	K	288	MET
1	K	300	VAL
1	K	302	SER
1	K	307	MET
1	K	317	LEU
1	K	328	ASP
1	K	331	THR
1	K	354	GLU
1	K	355	GLU
1	K	357	THR
1	K	385	THR
1	K	389	MET
1	K	400	LEU
1	K	401	HIS
1	K	420	ILE
1	K	421	ARG
1	K	426	LEU
1	K	432	GLN
1	K	433	ASN
1	K	452	ARG
1	K	460	GLU
1	K	468	THR
1	K	483	GLU

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Mol	Chain	Res	Type
1	K	494	LEU
1	K	504	LEU
1	K	509	SER
1	K	513	LEU
1	L	10	ASN
1	L	20	VAL
1	L	23	LEU
1	L	37	ASN
1	L	40	LEU
1	L	42	LYS
1	L	59	GLU
1	L	77	VAL
1	L	79	SER
1	L	89	THR
1	L	104	LEU
1	L	107	VAL
1	L	114	MET
1	L	131	LEU
1	L	138	CYS
1	L	141	SER
1	L	172	GLU
1	L	187	LEU
1	L	197	ARG
1	L	200	LEU
1	L	230	ILE
1	L	233	MET
1	L	247	LEU
1	L	248	LEU
1	L	255	GLU
1	L	272	LYS
1	L	284	ARG
1	L	285	ARG
1	L	288	MET
1	L	300	VAL
1	L	302	SER
1	L	307	MET
1	L	317	LEU
1	L	323	VAL
1	L	328	ASP
1	L	331	THR
1	L	354	GLU
1	L	355	GLU

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Mol	Chain	Res	Type
1	L	357	THR
1	L	385	THR
1	L	389	MET
1	L	400	LEU
1	L	401	HIS
1	L	420	ILE
1	L	421	ARG
1	L	426	LEU
1	L	432	GLN
1	L	433	ASN
1	L	452	ARG
1	L	460	GLU
1	L	468	THR
1	L	483	GLU
1	L	494	LEU
1	L	504	LEU
1	L	509	SER
1	L	513	LEU
1	M	10	ASN
1	M	20	VAL
1	M	23	LEU
1	M	37	ASN
1	M	40	LEU
1	M	42	LYS
1	M	59	GLU
1	M	77	VAL
1	M	79	SER
1	M	89	THR
1	M	104	LEU
1	M	107	VAL
1	M	114	MET
1	M	131	LEU
1	M	138	CYS
1	M	141	SER
1	M	172	GLU
1	M	187	LEU
1	M	197	ARG
1	M	200	LEU
1	M	230	ILE
1	M	233	MET
1	M	247	LEU
1	M	248	LEU

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Mol	Chain	Res	Type
1	M	255	GLU
1	M	272	LYS
1	M	284	ARG
1	M	285	ARG
1	M	288	MET
1	M	300	VAL
1	M	302	SER
1	M	307	MET
1	M	317	LEU
1	M	323	VAL
1	M	328	ASP
1	M	331	THR
1	M	354	GLU
1	M	355	GLU
1	M	357	THR
1	M	385	THR
1	M	389	MET
1	M	400	LEU
1	M	401	HIS
1	M	420	ILE
1	M	421	ARG
1	M	426	LEU
1	M	432	GLN
1	M	433	ASN
1	M	445	ARG
1	M	452	ARG
1	M	460	GLU
1	M	468	THR
1	M	483	GLU
1	M	494	LEU
1	M	504	LEU
1	M	509	SER
1	M	513	LEU
1	N	10	ASN
1	N	20	VAL
1	N	23	LEU
1	N	37	ASN
1	N	40	LEU
1	N	42	LYS
1	N	59	GLU
1	N	77	VAL
1	N	79	SER

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Mol	Chain	Res	Type
1	N	89	THR
1	N	104	LEU
1	N	114	MET
1	N	129	GLU
1	N	131	LEU
1	N	138	CYS
1	N	141	SER
1	N	172	GLU
1	N	187	LEU
1	N	197	ARG
1	N	200	LEU
1	N	230	ILE
1	N	233	MET
1	N	247	LEU
1	N	248	LEU
1	N	255	GLU
1	N	272	LYS
1	N	284	ARG
1	N	285	ARG
1	N	288	MET
1	N	300	VAL
1	N	302	SER
1	N	307	MET
1	N	317	LEU
1	N	328	ASP
1	N	331	THR
1	N	354	GLU
1	N	355	GLU
1	N	357	THR
1	N	385	THR
1	N	389	MET
1	N	400	LEU
1	N	401	HIS
1	N	420	ILE
1	N	421	ARG
1	N	426	LEU
1	N	432	GLN
1	N	433	ASN
1	N	452	ARG
1	N	460	GLU
1	N	468	THR
1	N	483	GLU

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Mol	Chain	Res	Type
1	N	494	LEU
1	N	504	LEU
1	N	509	SER
1	N	513	LEU
2	O	1	MET
2	O	3	ILE
2	O	6	LEU
2	O	14	ARG
2	O	20	LYS
2	O	28	THR
2	O	30	SER
2	O	55	LYS
2	O	60	LYS
2	O	86	MET
2	P	1	MET
2	P	3	ILE
2	P	6	LEU
2	P	14	ARG
2	P	20	LYS
2	P	28	THR
2	P	30	SER
2	P	55	LYS
2	P	60	LYS
2	P	86	MET
2	Q	1	MET
2	Q	3	ILE
2	Q	6	LEU
2	Q	14	ARG
2	Q	20	LYS
2	Q	28	THR
2	Q	30	SER
2	Q	55	LYS
2	Q	60	LYS
2	Q	86	MET
2	R	1	MET
2	R	3	ILE
2	R	6	LEU
2	R	14	ARG
2	R	20	LYS
2	R	28	THR
2	R	30	SER
2	R	55	LYS

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Mol	Chain	Res	Type
2	R	60	LYS
2	R	77	LYS
2	R	86	MET
2	S	1	MET
2	S	3	ILE
2	S	6	LEU
2	S	14	ARG
2	S	20	LYS
2	S	28	THR
2	S	30	SER
2	S	55	LYS
2	S	60	LYS
2	S	77	LYS
2	S	86	MET
2	T	1	MET
2	T	3	ILE
2	T	6	LEU
2	T	14	ARG
2	T	20	LYS
2	T	28	THR
2	T	30	SER
2	T	55	LYS
2	T	60	LYS
2	T	86	MET
2	U	1	MET
2	U	3	ILE
2	U	6	LEU
2	U	14	ARG
2	U	20	LYS
2	U	28	THR
2	U	30	SER
2	U	55	LYS
2	U	60	LYS
2	U	77	LYS
2	U	86	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	37	ASN
1	A	97	GLN

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Mol	Chain	Res	Type
1	A	146	GLN
1	A	153	ASN
1	A	348	GLN
1	A	432	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
1	B	348	GLN
1	B	432	GLN
1	B	453	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	432	GLN
1	C	453	GLN
1	C	457	ASN
1	C	475	ASN
1	D	21	ASN
1	D	37	ASN
1	D	146	GLN
1	D	153	ASN
1	D	265	ASN
1	D	348	GLN
1	D	432	GLN
1	D	453	GLN
1	D	457	ASN
1	D	475	ASN
1	E	21	ASN
1	E	146	GLN
1	E	153	ASN
1	E	348	GLN
1	E	432	GLN
1	E	453	GLN

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Mol	Chain	Res	Type
1	E	457	ASN
1	E	475	ASN
1	F	21	ASN
1	F	82	ASN
1	F	97	GLN
1	F	146	GLN
1	F	153	ASN
1	F	265	ASN
1	F	348	GLN
1	F	432	GLN
1	F	453	GLN
1	F	457	ASN
1	F	475	ASN
1	G	21	ASN
1	G	97	GLN
1	G	146	GLN
1	G	153	ASN
1	G	265	ASN
1	G	348	GLN
1	G	432	GLN
1	G	453	GLN
1	G	457	ASN
1	G	475	ASN
1	H	21	ASN
1	H	72	GLN
1	H	97	GLN
1	H	146	GLN
1	H	326	ASN
1	H	348	GLN
1	H	433	ASN
1	H	436	GLN
1	I	21	ASN
1	I	72	GLN
1	I	97	GLN
1	I	146	GLN
1	I	153	ASN
1	I	326	ASN
1	I	348	GLN
1	I	433	ASN
1	J	21	ASN
1	J	72	GLN
1	J	97	GLN

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Mol	Chain	Res	Type
1	J	146	GLN
1	J	326	ASN
1	J	348	GLN
1	J	433	ASN
1	J	436	GLN
1	K	21	ASN
1	K	72	GLN
1	K	97	GLN
1	K	146	GLN
1	K	326	ASN
1	K	348	GLN
1	K	433	ASN
1	L	21	ASN
1	L	37	ASN
1	L	72	GLN
1	L	97	GLN
1	L	146	GLN
1	L	326	ASN
1	L	348	GLN
1	L	433	ASN
1	M	21	ASN
1	M	37	ASN
1	M	72	GLN
1	M	97	GLN
1	M	146	GLN
1	M	326	ASN
1	M	348	GLN
1	M	433	ASN
1	N	21	ASN
1	N	72	GLN
1	N	97	GLN
1	N	146	GLN
1	N	326	ASN
1	N	348	GLN
1	N	433	ASN
1	N	436	GLN
2	O	80	ASN
2	P	68	ASN
2	P	80	ASN
2	Q	68	ASN
2	Q	80	ASN
2	R	68	ASN

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Mol	Chain	Res	Type
2	R	80	ASN
2	S	68	ASN
2	S	80	ASN
2	T	80	ASN
2	U	68	ASN
2	U	80	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\# Z  > 2$
4	ADP	A	700	3	29,29,29	1.15	3 (10%)	45,45,45	2.64	18 (40%)
4	ADP	B	701	3	29,29,29	1.24	3 (10%)	45,45,45	2.53	14 (31%)
4	ADP	C	702	3	29,29,29	1.12	3 (10%)	45,45,45	2.63	17 (37%)
4	ADP	D	703	3	29,29,29	1.34	5 (17%)	45,45,45	2.67	15 (33%)
4	ADP	E	704	3	29,29,29	1.12	3 (10%)	45,45,45	2.52	14 (31%)
4	ADP	F	705	3	29,29,29	0.99	2 (6%)	45,45,45	2.38	12 (26%)
4	ADP	G	706	3	29,29,29	1.09	1 (3%)	45,45,45	2.51	17 (37%)

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
4	ADP	A	700	3	-	0/16/32/32	0/1/3/3
4	ADP	B	701	3	-	0/16/32/32	0/1/3/3
4	ADP	C	702	3	-	0/16/32/32	0/1/3/3
4	ADP	D	703	3	-	0/16/32/32	0/1/3/3
4	ADP	E	704	3	-	0/16/32/32	0/1/3/3
4	ADP	F	705	3	-	0/16/32/32	0/1/3/3
4	ADP	G	706	3	-	0/16/32/32	0/1/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	706	ADP	C2-N3	3.57	1.39	1.32
4	B	701	ADP	C2-N3	3.36	1.38	1.32
4	D	703	ADP	C2-N3	3.12	1.38	1.32
4	A	700	ADP	C2-N3	3.03	1.38	1.32
4	E	704	ADP	C2-N3	3.01	1.38	1.32
4	B	701	ADP	C2-N1	2.96	1.39	1.33
4	D	703	ADP	C2'-C1'	-2.88	1.49	1.53
4	D	703	ADP	C2-N1	2.86	1.39	1.33
4	C	702	ADP	C2-N3	2.85	1.37	1.32
4	F	705	ADP	C2-N3	2.81	1.37	1.32
4	D	703	ADP	O4'-C1'	-2.58	1.37	1.41
4	C	702	ADP	C2-N1	2.53	1.38	1.33
4	F	705	ADP	C2-N1	2.43	1.38	1.33
4	E	704	ADP	C2-N1	2.41	1.38	1.33
4	B	701	ADP	C2'-C1'	-2.36	1.50	1.53
4	A	700	ADP	O4'-C4'	-2.23	1.39	1.45
4	A	700	ADP	C2-N1	2.16	1.38	1.33
4	D	703	ADP	O4'-C4'	-2.11	1.40	1.45
4	C	702	ADP	C2'-C1'	-2.08	1.50	1.53
4	E	704	ADP	C2'-C1'	-2.05	1.50	1.53

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	ADP	N3-C2-N1	-12.03	118.65	128.71
4	A	700	ADP	N3-C2-N1	-11.33	119.24	128.71
4	F	705	ADP	N3-C2-N1	-10.79	119.69	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	ADP	N3-C2-N1	-10.43	119.99	128.71
4	E	704	ADP	N3-C2-N1	-10.40	120.02	128.71
4	B	701	ADP	N3-C2-N1	-10.24	120.14	128.71
4	G	706	ADP	N3-C2-N1	-9.92	120.42	128.71
4	C	702	ADP	PA-O3A-PB	-5.30	116.14	131.68
4	E	704	ADP	PA-O3A-PB	-5.17	116.52	131.68
4	G	706	ADP	PA-O3A-PB	-5.11	116.71	131.68
4	F	705	ADP	PA-O3A-PB	-5.02	116.96	131.68
4	A	700	ADP	PA-O3A-PB	-5.01	117.00	131.68
4	D	703	ADP	PA-O3A-PB	-5.00	117.01	131.68
4	B	701	ADP	PA-O3A-PB	-4.85	117.47	131.68
4	G	706	ADP	C4-C5-N7	-4.60	105.58	109.52
4	C	702	ADP	O3'-C3'-C4'	-4.50	97.82	111.08
4	B	701	ADP	C8-N9-C4	4.47	110.31	106.90
4	B	701	ADP	C4-C5-N7	-4.47	105.70	109.52
4	C	702	ADP	C4-C5-N7	-4.20	105.93	109.52
4	G	706	ADP	O3'-C3'-C4'	-4.07	99.09	111.08
4	E	704	ADP	C8-N9-C4	4.02	109.97	106.90
4	B	701	ADP	O3'-C3'-C4'	-3.99	99.31	111.08
4	E	704	ADP	C4-C5-N7	-3.98	106.11	109.52
4	A	700	ADP	C1'-N9-C4	-3.75	120.16	126.64
4	D	703	ADP	C8-N9-C4	3.75	109.76	106.90
4	C	702	ADP	C8-N9-C4	3.74	109.75	106.90
4	E	704	ADP	C1'-N9-C4	-3.72	120.20	126.64
4	A	700	ADP	C4-C5-N7	-3.68	106.37	109.52
4	B	701	ADP	C1'-N9-C4	-3.63	120.37	126.64
4	A	700	ADP	O4'-C1'-N9	3.53	111.73	108.44
4	A	700	ADP	C8-N9-C4	3.53	109.59	106.90
4	B	701	ADP	N3-C4-N9	3.53	131.81	125.43
4	D	703	ADP	C1'-N9-C4	-3.47	120.64	126.64
4	F	705	ADP	C4-C5-N7	-3.47	106.55	109.52
4	G	706	ADP	C4'-O4'-C1'	3.39	113.43	109.75
4	D	703	ADP	O3'-C3'-C4'	-3.34	101.23	111.08
4	D	703	ADP	N3-C4-N9	3.31	131.40	125.43
4	A	700	ADP	N3-C4-N9	3.19	131.19	125.43
4	E	704	ADP	N3-C4-N9	3.18	131.18	125.43
4	G	706	ADP	N3-C4-N9	3.17	131.15	125.43
4	C	702	ADP	C4'-O4'-C1'	3.12	113.14	109.75
4	G	706	ADP	C8-N9-C4	3.12	109.28	106.90
4	D	703	ADP	O2'-C2'-C1'	-3.12	101.80	111.23
4	C	702	ADP	N3-C4-N9	3.11	131.05	125.43
4	E	704	ADP	O5'-C5'-C4'	3.11	120.35	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	704	ADP	N7-C8-N9	-3.11	105.56	114.36
4	F	705	ADP	N3-C4-N9	3.07	130.98	125.43
4	C	702	ADP	C1'-N9-C4	-3.06	121.35	126.64
4	D	703	ADP	C4-C5-N7	-3.05	106.91	109.52
4	B	701	ADP	N7-C8-N9	-3.02	105.82	114.36
4	A	700	ADP	O3'-C3'-C4'	-2.99	102.27	111.08
4	C	702	ADP	O2'-C2'-C1'	-2.97	102.25	111.23
4	D	703	ADP	O5'-C5'-C4'	2.95	119.78	108.94
4	E	704	ADP	O4'-C1'-N9	2.95	111.18	108.44
4	F	705	ADP	C1'-N9-C4	-2.88	121.65	126.64
4	C	702	ADP	N7-C8-N9	-2.88	106.20	114.36
4	F	705	ADP	O5'-C5'-C4'	2.88	119.50	108.94
4	G	706	ADP	N7-C8-N9	-2.87	106.25	114.36
4	B	701	ADP	O5'-C5'-C4'	2.84	119.36	108.94
4	G	706	ADP	C2'-C3'-C4'	2.83	108.29	102.65
4	G	706	ADP	C1'-N9-C4	-2.82	121.76	126.64
4	D	703	ADP	N7-C8-N9	-2.82	106.39	114.36
4	A	700	ADP	N7-C8-N9	-2.81	106.42	114.36
4	A	700	ADP	O5'-C5'-C4'	2.77	119.11	108.94
4	D	703	ADP	C4'-O4'-C1'	2.76	112.75	109.75
4	F	705	ADP	C8-N9-C4	2.76	109.01	106.90
4	C	702	ADP	O5'-C5'-C4'	2.74	119.00	108.94
4	E	704	ADP	O2'-C2'-C1'	-2.73	102.98	111.23
4	F	705	ADP	O3'-C3'-C4'	-2.72	103.07	111.08
4	G	706	ADP	O5'-C5'-C4'	2.67	118.75	108.94
4	F	705	ADP	N7-C8-N9	-2.67	106.80	114.36
4	A	700	ADP	C4'-O4'-C1'	2.67	112.65	109.75
4	E	704	ADP	O3'-C3'-C4'	-2.57	103.51	111.08
4	A	700	ADP	N6-C6-N1	-2.53	114.40	119.36
4	A	700	ADP	C2-N3-C4	2.53	121.21	114.01
4	A	700	ADP	C2'-C3'-C4'	2.48	107.59	102.65
4	G	706	ADP	O2'-C2'-C1'	-2.47	103.74	111.23
4	C	702	ADP	O4'-C1'-N9	2.45	110.72	108.44
4	D	703	ADP	C2-N3-C4	2.44	120.95	114.01
4	E	704	ADP	C8-N7-C5	2.42	111.08	103.58
4	B	701	ADP	C8-N7-C5	2.41	111.06	103.58
4	B	701	ADP	O2'-C2'-C1'	-2.39	104.00	111.23
4	D	703	ADP	O2B-PB-O1B	2.38	118.21	110.44
4	G	706	ADP	C5-C4-N3	-2.37	120.55	125.70
4	F	705	ADP	C2-N3-C4	2.36	120.73	114.01
4	C	702	ADP	C2'-C3'-C4'	2.35	107.33	102.65
4	B	701	ADP	C2-N3-C4	2.31	120.58	114.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	ADP	O2B-PB-O1B	2.29	117.93	110.44
4	G	706	ADP	O3'-C3'-C2'	-2.28	104.43	111.83
4	G	706	ADP	C8-N7-C5	2.25	110.57	103.58
4	C	702	ADP	C8-N7-C5	2.23	110.49	103.58
4	E	704	ADP	C2-N3-C4	2.20	120.27	114.01
4	G	706	ADP	N6-C6-N1	-2.17	115.10	119.36
4	C	702	ADP	C2-N3-C4	2.17	120.18	114.01
4	A	700	ADP	O2'-C2'-C1'	-2.16	104.70	111.23
4	G	706	ADP	C2-N3-C4	2.16	120.15	114.01
4	C	702	ADP	O3B-PB-O3A	2.14	115.28	105.14
4	E	704	ADP	C2'-C3'-C4'	2.13	106.90	102.65
4	D	703	ADP	C3'-C2'-C1'	2.12	104.23	100.91
4	B	701	ADP	C5-C4-N3	-2.12	121.09	125.70
4	B	701	ADP	C2'-C3'-C4'	2.10	106.83	102.65
4	A	700	ADP	C8-N7-C5	2.08	110.03	103.58
4	A	700	ADP	O3'-C3'-C2'	-2.07	105.11	111.83
4	A	700	ADP	C5-C4-N3	-2.05	121.23	125.70
4	D	703	ADP	C8-N7-C5	2.05	109.93	103.58
4	F	705	ADP	C5-C4-N3	-2.04	121.25	125.70
4	F	705	ADP	C8-N7-C5	2.03	109.87	103.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	0.62	59 (11%) 6 2	5, 7, 9, 10	0
1	B	524/524 (100%)	0.70	69 (13%) 4 1	5, 7, 9, 10	0
1	C	524/524 (100%)	0.48	50 (9%) 8 2	5, 7, 9, 10	0
1	D	524/524 (100%)	0.55	53 (10%) 7 2	5, 7, 9, 10	0
1	E	524/524 (100%)	0.83	84 (16%) 3 1	5, 7, 9, 10	0
1	F	524/524 (100%)	0.89	78 (14%) 3 1	5, 7, 9, 10	0
1	G	524/524 (100%)	0.70	67 (12%) 4 1	5, 7, 9, 10	0
1	H	524/524 (100%)	0.40	22 (4%) 35 7	6, 7, 9, 10	0
1	I	524/524 (100%)	0.32	15 (2%) 49 9	5, 7, 9, 10	0
1	J	524/524 (100%)	0.45	33 (6%) 19 5	5, 7, 9, 10	0
1	K	524/524 (100%)	0.63	49 (9%) 9 2	5, 7, 9, 10	0
1	L	524/524 (100%)	0.63	43 (8%) 12 3	5, 7, 9, 10	0
1	M	524/524 (100%)	0.50	39 (7%) 14 3	5, 7, 9, 10	0
1	N	524/524 (100%)	0.55	45 (8%) 11 3	5, 7, 9, 10	0
2	O	97/97 (100%)	1.83	39 (40%) 1 0	7, 7, 8, 8	0
2	P	97/97 (100%)	1.74	32 (32%) 1 0	7, 7, 8, 8	0
2	Q	97/97 (100%)	1.47	30 (30%) 1 0	7, 7, 8, 8	0
2	R	97/97 (100%)	1.52	28 (28%) 1 0	7, 7, 8, 8	0
2	S	97/97 (100%)	1.87	37 (38%) 1 0	7, 7, 8, 8	0
2	T	97/97 (100%)	1.74	30 (30%) 1 0	7, 7, 8, 8	0
2	U	97/97 (100%)	3.40	78 (80%) 0 0	7, 7, 8, 8	0
All	All	8015/8015 (100%)	0.70	980 (12%) 5 1	5, 7, 9, 10	0

All (980) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	C	361	ASP	15.0
1	F	361	ASP	10.3
1	A	361	ASP	9.8
1	F	210	THR	9.2
1	G	208	PRO	8.8
1	E	361	ASP	8.7
2	U	32	ALA	8.5
1	G	199	TYR	8.1
2	U	33	ALA	7.8
1	D	212	ALA	7.8
1	L	357	THR	7.7
1	A	357	THR	7.4
2	S	33	ALA	7.3
1	F	172	GLU	7.2
1	I	268	ARG	7.2
2	P	23	GLY	7.1
1	E	353	ILE	7.0
1	E	338	GLU	7.0
2	T	18	GLU	7.0
1	G	361	ASP	7.0
1	D	361	ASP	7.0
2	R	17	VAL	6.9
2	U	22	ALA	6.8
1	B	357	THR	6.6
1	A	353	ILE	6.6
2	S	17	VAL	6.5
2	O	25	ILE	6.5
1	G	357	THR	6.4
1	K	186	GLU	6.4
2	P	32	ALA	6.4
2	U	17	VAL	6.4
1	F	349	ILE	6.4
1	C	210	THR	6.4
2	S	51	ASN	6.3
1	C	212	ALA	6.2
2	U	31	ALA	6.2
1	N	183	LEU	6.2
2	O	97	ALA	6.2
1	F	357	THR	6.2
1	F	355	GLU	6.1
1	G	195	PHE	6.1
2	S	97	ALA	6.1
1	D	357	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	LYS	6.1
1	E	281	PHE	6.1
2	T	97	ALA	6.1
1	B	361	ASP	6.1
1	D	365	LEU	6.0
2	U	71	TYR	6.0
1	E	357	THR	6.0
2	U	51	ASN	6.0
1	E	209	GLU	5.9
2	U	18	GLU	5.9
2	Q	25	ILE	5.9
2	U	97	ALA	5.8
1	C	360	TYR	5.8
1	B	353	ILE	5.8
1	F	353	ILE	5.8
2	U	25	ILE	5.8
1	B	355	GLU	5.8
2	O	17	VAL	5.8
2	U	19	THR	5.8
2	U	30	SER	5.7
2	S	32	ALA	5.7
2	U	28	THR	5.7
2	U	26	VAL	5.6
2	P	67	PHE	5.6
1	C	199	TYR	5.6
1	K	356	ALA	5.5
1	G	362	ARG	5.5
1	E	340	ALA	5.5
1	G	210	THR	5.5
1	M	357	THR	5.5
1	C	353	ILE	5.4
2	T	25	ILE	5.4
2	P	51	ASN	5.4
1	E	341	ALA	5.4
1	A	360	TYR	5.4
2	Q	32	ALA	5.4
1	D	209	GLU	5.4
1	K	360	TYR	5.3
1	G	256	GLY	5.3
1	M	284	ARG	5.3
1	F	171	LYS	5.2
2	S	30	SER	5.2

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Mol	Chain	Res	Type	RSRZ
2	Q	71	TYR	5.2
1	F	212	ALA	5.2
1	A	365	LEU	5.2
1	A	208	PRO	5.2
1	M	268	ARG	5.2
1	C	357	THR	5.1
1	L	264	VAL	5.1
1	E	210	THR	5.1
2	P	18	GLU	5.1
2	R	51	ASN	5.1
2	O	1	MET	5.1
2	U	23	GLY	5.1
2	O	72	GLY	5.1
1	F	267	MET	5.0
1	A	338	GLU	5.0
2	R	18	GLU	5.0
2	P	17	VAL	5.0
1	D	353	ILE	5.0
2	S	18	GLU	5.0
1	F	350	ARG	5.0
1	M	360	TYR	5.0
2	P	49	LEU	5.0
2	T	33	ALA	4.9
1	E	355	GLU	4.9
1	G	353	ILE	4.9
1	F	374	GLY	4.9
1	A	203	TYR	4.9
1	B	200	LEU	4.9
1	G	271	VAL	4.8
1	G	350	ARG	4.8
1	B	346	VAL	4.8
1	C	267	MET	4.8
2	T	17	VAL	4.8
1	E	346	VAL	4.8
2	U	27	LEU	4.8
2	U	1	MET	4.8
1	E	354	GLU	4.8
2	P	1	MET	4.8
2	S	80	ASN	4.7
1	D	268	ARG	4.7
2	U	21	SER	4.7
1	L	177	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	P	85	ILE	4.7
2	U	65	VAL	4.7
1	G	251	ALA	4.7
2	U	72	GLY	4.7
1	B	284	ARG	4.6
2	R	25	ILE	4.6
2	T	28	THR	4.6
1	G	209	GLU	4.6
2	Q	33	ALA	4.6
2	S	31	ALA	4.6
1	B	349	ILE	4.6
2	T	27	LEU	4.5
1	I	264	VAL	4.5
2	U	83	VAL	4.5
1	H	360	TYR	4.5
1	B	348	GLN	4.5
2	U	69	ASP	4.5
1	F	213	VAL	4.5
1	F	375	GLY	4.5
2	U	80	ASN	4.5
1	F	214	GLU	4.5
1	D	338	GLU	4.4
2	T	52	GLY	4.4
2	T	32	ALA	4.4
1	N	360	TYR	4.4
1	B	199	TYR	4.4
2	T	67	PHE	4.4
2	U	78	ILE	4.4
2	S	83	VAL	4.4
1	F	281	PHE	4.4
1	G	214	GLU	4.3
2	O	66	ILE	4.3
1	I	357	THR	4.3
1	G	222	LEU	4.3
1	G	372	LEU	4.3
2	O	33	ALA	4.3
2	U	16	GLU	4.3
1	I	360	TYR	4.3
1	A	251	ALA	4.2
1	K	187	LEU	4.2
2	P	71	TYR	4.2
1	G	346	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	O	83	VAL	4.2
2	U	38	GLY	4.2
2	P	31	ALA	4.2
1	L	221	LEU	4.2
1	B	212	ALA	4.2
2	U	84	LEU	4.2
2	Q	26	VAL	4.2
2	R	80	ASN	4.2
1	A	284	ARG	4.1
1	L	362	ARG	4.1
2	U	20	LYS	4.1
1	G	212	ALA	4.1
1	J	365	LEU	4.1
2	R	33	ALA	4.1
2	U	79	ASP	4.1
1	F	251	ALA	4.1
1	E	284	ARG	4.1
2	O	27	LEU	4.1
1	K	295	LEU	4.1
2	Q	18	GLU	4.1
1	N	184	GLN	4.1
2	R	30	SER	4.1
1	C	270	ILE	4.0
1	J	223	ALA	4.0
2	S	67	PHE	4.0
1	B	365	LEU	4.0
2	U	49	LEU	4.0
1	F	203	TYR	4.0
2	U	75	SER	4.0
1	A	376	VAL	4.0
2	R	83	VAL	4.0
1	G	284	ARG	4.0
1	C	209	GLU	4.0
2	U	53	GLU	4.0
1	D	321	LYS	4.0
1	F	387	VAL	4.0
1	D	172	GLU	4.0
1	D	192	GLY	3.9
1	K	188	ASP	3.9
1	D	199	TYR	3.9
1	G	354	GLU	3.9
1	N	525	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
2	T	51	ASN	3.9
1	M	358	SER	3.9
1	J	268	ARG	3.9
2	U	52	GLY	3.9
1	F	352	GLN	3.9
1	E	365	LEU	3.8
1	E	332	ILE	3.8
1	J	356	ALA	3.8
2	P	97	ALA	3.8
1	B	192	GLY	3.8
1	E	44	PHE	3.8
1	A	349	ILE	3.8
1	J	353	ILE	3.8
2	T	30	SER	3.8
1	H	525	PRO	3.8
2	O	65	VAL	3.8
1	A	355	GLU	3.8
1	M	264	VAL	3.8
1	G	203	TYR	3.8
1	E	279	PRO	3.8
1	E	195	PHE	3.8
1	A	281	PHE	3.8
1	B	208	PRO	3.8
2	P	30	SER	3.7
2	U	35	SER	3.7
1	F	273	VAL	3.7
1	M	233	MET	3.7
1	F	341	ALA	3.7
1	L	268	ARG	3.7
2	U	82	GLU	3.7
2	Q	78	ILE	3.7
1	G	360	TYR	3.7
1	A	364	LYS	3.7
2	O	26	VAL	3.7
2	R	16	GLU	3.7
1	K	384	ALA	3.7
2	O	32	ALA	3.7
2	Q	67	PHE	3.7
1	F	209	GLU	3.7
1	G	279	PRO	3.7
1	F	364	LYS	3.7
1	I	270	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	O	80	ASN	3.7
1	E	360	TYR	3.7
1	B	203	TYR	3.7
1	F	377	ALA	3.6
1	M	243	ALA	3.6
2	U	67	PHE	3.7
1	G	349	ILE	3.6
1	F	177	VAL	3.6
1	M	275	ALA	3.6
1	D	284	ARG	3.6
1	F	284	ARG	3.6
1	F	360	TYR	3.6
2	T	71	TYR	3.6
2	U	10	VAL	3.6
2	U	85	ILE	3.6
1	J	233	MET	3.6
1	A	320	ALA	3.6
2	O	51	ASN	3.6
2	O	67	PHE	3.6
2	O	23	GLY	3.6
1	B	267	MET	3.6
1	B	360	TYR	3.6
1	E	251	ALA	3.6
1	D	309	LEU	3.6
2	Q	27	LEU	3.6
2	S	85	ILE	3.6
1	F	331	THR	3.6
2	U	12	VAL	3.6
2	U	96	GLU	3.6
1	J	357	THR	3.5
1	J	193	MET	3.5
1	A	172	GLU	3.5
2	S	21	SER	3.5
1	N	357	THR	3.5
2	S	1	MET	3.5
1	N	186	GLU	3.5
1	J	396	VAL	3.5
1	A	250	ILE	3.5
1	L	353	ILE	3.5
1	N	342	ILE	3.5
1	G	172	GLU	3.5
1	H	342	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	S	36	THR	3.5
2	Q	66	ILE	3.5
2	S	66	ILE	3.5
1	E	280	GLY	3.5
1	F	174	VAL	3.5
2	R	28	THR	3.5
2	P	25	ILE	3.5
1	A	230	ILE	3.4
1	B	338	GLU	3.4
1	G	309	LEU	3.4
2	O	78	ILE	3.4
2	P	52	GLY	3.4
1	F	288	MET	3.4
1	B	350	ARG	3.4
1	C	362	ARG	3.4
1	J	372	LEU	3.4
1	B	193	MET	3.4
1	C	203	TYR	3.4
2	U	66	ILE	3.4
1	E	371	LYS	3.4
2	Q	65	VAL	3.4
1	J	183	LEU	3.4
2	T	72	GLY	3.4
2	U	93	ALA	3.4
2	T	20	LYS	3.4
1	G	277	LYS	3.4
1	D	213	VAL	3.4
1	E	368	ARG	3.4
1	M	175	ILE	3.4
2	R	71	TYR	3.3
2	S	84	LEU	3.3
1	B	171	LYS	3.3
1	C	284	ARG	3.3
1	C	350	ARG	3.3
1	H	368	ARG	3.3
1	D	349	ILE	3.3
1	K	352	GLN	3.3
1	K	372	LEU	3.3
1	A	193	MET	3.3
2	U	2	ASN	3.3
1	E	309	LEU	3.3
2	P	33	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	349	ILE	3.3
1	E	270	ILE	3.3
1	E	349	ILE	3.3
1	M	44	PHE	3.3
2	Q	12	VAL	3.3
1	E	199	TYR	3.3
1	G	332	ILE	3.3
1	M	349	ILE	3.3
2	P	20	LYS	3.3
1	G	204	PHE	3.3
1	N	266	THR	3.3
1	G	267	MET	3.2
2	Q	50	GLU	3.2
1	E	375	GLY	3.2
1	A	270	ILE	3.2
1	F	230	ILE	3.2
1	I	44	PHE	3.2
2	T	82	GLU	3.2
1	F	356	ALA	3.2
2	R	97	ALA	3.2
1	K	44	PHE	3.2
1	A	271	VAL	3.2
1	M	176	THR	3.2
2	T	19	THR	3.2
2	U	34	LYS	3.2
1	B	279	PRO	3.2
1	C	279	PRO	3.2
1	B	309	LEU	3.2
2	U	24	GLY	3.2
2	T	73	VAL	3.2
1	F	338	GLU	3.2
2	R	20	LYS	3.2
2	S	20	LYS	3.2
1	B	275	ALA	3.2
1	D	251	ALA	3.2
2	Q	23	GLY	3.2
2	U	29	GLY	3.2
2	O	30	SER	3.2
1	D	360	TYR	3.2
1	G	365	LEU	3.2
1	D	376	VAL	3.1
1	F	323	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	321	LYS	3.1
2	R	79	ASP	3.1
1	N	384	ALA	3.1
1	G	371	LYS	3.1
1	D	195	PHE	3.1
2	U	54	VAL	3.1
1	C	358	SER	3.1
1	H	186	GLU	3.1
2	O	38	GLY	3.1
1	B	223	ALA	3.1
1	K	349	ILE	3.1
2	U	39	GLU	3.1
2	U	81	GLU	3.1
2	S	78	ILE	3.1
1	D	362	ARG	3.1
1	K	284	ARG	3.1
2	S	69	ASP	3.1
1	D	204	PHE	3.1
1	L	180	GLY	3.1
1	F	193	MET	3.1
1	C	138	CYS	3.1
2	U	92	LEU	3.1
1	L	270	ILE	3.1
2	Q	85	ILE	3.1
1	K	127	ALA	3.1
2	S	74	LYS	3.1
1	B	209	GLU	3.1
1	C	271	VAL	3.1
1	D	237	LEU	3.1
1	K	268	ARG	3.1
1	A	209	GLU	3.1
1	F	283	ASP	3.1
1	K	185	ASP	3.1
1	N	350	ARG	3.0
2	U	70	GLY	3.0
1	E	372	LEU	3.0
1	H	193	MET	3.0
1	H	268	ARG	3.0
2	O	19	THR	3.0
1	F	386	GLU	3.0
2	T	53	GLU	3.0
1	F	333	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	242	LYS	3.0
1	E	334	ASP	3.0
1	F	215	LEU	3.0
1	N	172	GLU	3.0
1	J	366	GLN	3.0
2	R	72	GLY	3.0
2	U	36	THR	3.0
1	E	364	LYS	3.0
1	D	203	TYR	3.0
1	E	256	GLY	3.0
1	H	372	LEU	3.0
2	U	13	LYS	3.0
2	O	3	ILE	3.0
2	O	64	ILE	3.0
1	F	170	GLY	3.0
1	L	378	VAL	3.0
2	Q	73	VAL	3.0
1	H	44	PHE	3.0
2	U	41	LEU	3.0
2	U	3	ILE	3.0
2	O	18	GLU	3.0
2	U	77	LYS	3.0
1	B	44	PHE	3.0
1	K	193	MET	3.0
1	C	349	ILE	3.0
2	U	50	GLU	3.0
2	U	76	GLU	3.0
1	G	364	LYS	3.0
1	G	322	ARG	3.0
1	K	346	VAL	3.0
1	K	368	ARG	3.0
1	G	171	LYS	3.0
1	B	351	GLN	2.9
1	C	278	ALA	2.9
2	P	84	LEU	2.9
1	J	330	THR	2.9
1	F	195	PHE	2.9
1	B	354	GLU	2.9
2	S	25	ILE	2.9
1	D	322	ARG	2.9
1	J	181	THR	2.9
2	O	22	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	267	MET	2.9
1	D	297	GLY	2.9
1	K	494	LEU	2.9
2	O	37	ARG	2.9
1	G	207	LYS	2.9
1	B	224	ASP	2.9
2	Q	49	LEU	2.9
1	A	223	ALA	2.9
1	B	381	VAL	2.9
1	F	322	ARG	2.9
1	B	382	GLY	2.9
1	N	267	MET	2.9
2	R	82	GLU	2.9
2	U	68	ASN	2.9
2	R	21	SER	2.9
1	E	362	ARG	2.9
1	B	238	GLU	2.9
1	G	338	GLU	2.9
1	A	195	PHE	2.9
1	K	247	LEU	2.9
2	S	13	LYS	2.9
2	T	23	GLY	2.9
1	F	390	LYS	2.9
2	O	21	SER	2.9
1	G	376	VAL	2.8
2	O	31	ALA	2.8
2	Q	38	GLY	2.8
2	U	64	ILE	2.8
2	S	37	ARG	2.8
1	J	381	VAL	2.8
1	M	431	GLY	2.8
1	N	180	GLY	2.8
2	S	73	VAL	2.8
1	B	278	ALA	2.8
1	E	203	TYR	2.8
1	A	229	ASN	2.8
1	C	268	ARG	2.8
1	C	191	GLU	2.8
1	A	358	SER	2.8
1	B	327	LYS	2.8
1	E	330	THR	2.8
1	F	199	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	351	GLN	2.8
1	N	372	LEU	2.8
1	A	279	PRO	2.8
1	B	352	GLN	2.8
1	G	347	ALA	2.8
1	A	238	GLU	2.8
1	C	195	PHE	2.8
1	C	322	ARG	2.8
1	E	174	VAL	2.8
1	A	373	ALA	2.8
1	L	360	TYR	2.8
1	G	270	ILE	2.8
1	L	484	GLU	2.8
2	Q	82	GLU	2.8
2	R	1	MET	2.8
2	Q	13	LYS	2.8
1	G	281	PHE	2.8
2	T	80	ASN	2.8
1	M	244	GLY	2.8
1	A	368	ARG	2.8
2	T	37	ARG	2.8
1	N	365	LEU	2.8
2	P	80	ASN	2.8
1	B	268	ARG	2.8
1	E	350	ARG	2.8
2	U	14	ARG	2.8
1	C	251	ALA	2.8
1	M	240	VAL	2.8
2	U	73	VAL	2.8
1	F	275	ALA	2.8
1	K	144	ILE	2.8
1	C	214	GLU	2.7
1	D	214	GLU	2.7
1	N	369	VAL	2.7
1	D	340	ALA	2.7
1	L	267	MET	2.7
1	M	168	LYS	2.7
1	A	248	LEU	2.7
1	E	237	LEU	2.7
1	F	309	LEU	2.7
2	R	66	ILE	2.7
1	N	165	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	281	PHE	2.7
1	C	355	GLU	2.7
1	K	366	GLN	2.7
2	O	36	THR	2.7
1	B	364	LYS	2.7
1	N	396	VAL	2.7
1	D	320	ALA	2.7
1	H	283	ASP	2.7
1	K	171	LYS	2.7
1	L	381	VAL	2.7
1	L	215	LEU	2.7
1	F	204	PHE	2.7
1	F	280	GLY	2.7
1	L	127	ALA	2.7
2	R	22	ALA	2.7
2	P	82	GLU	2.7
1	N	349	ILE	2.7
1	J	384	ALA	2.7
2	S	71	TYR	2.7
1	J	267	MET	2.7
1	H	284	ARG	2.7
1	M	365	LEU	2.7
1	B	230	ILE	2.7
1	D	208	PRO	2.7
1	D	364	LYS	2.7
1	K	525	PRO	2.7
1	A	322	ARG	2.7
2	P	2	ASN	2.7
1	G	321	LYS	2.7
1	D	358	SER	2.7
2	P	37	ARG	2.7
1	A	274	ALA	2.7
1	D	275	ALA	2.7
1	C	276	VAL	2.6
1	L	227	ILE	2.6
2	O	95	VAL	2.6
2	R	52	GLY	2.6
1	E	268	ARG	2.6
2	U	4	ARG	2.6
1	E	196	ASP	2.6
2	Q	22	ALA	2.6
1	A	273	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	322	ARG	2.6
2	O	82	GLU	2.6
1	E	172	GLU	2.6
1	M	236	VAL	2.6
1	J	44	PHE	2.6
1	N	238	GLU	2.6
2	R	73	VAL	2.6
2	S	65	VAL	2.6
1	E	294	THR	2.6
1	E	267	MET	2.6
1	F	373	ALA	2.6
1	K	350	ARG	2.6
1	C	192	GLY	2.6
2	O	13	LYS	2.6
1	F	346	VAL	2.6
1	N	361	ASP	2.6
1	L	356	ALA	2.6
1	B	172	GLU	2.6
2	U	45	ASN	2.6
2	R	26	VAL	2.6
2	R	85	ILE	2.6
1	B	368	ARG	2.6
1	I	340	ALA	2.6
1	C	200	LEU	2.6
1	E	238	GLU	2.6
1	F	200	LEU	2.6
1	F	348	GLN	2.6
1	D	325	ILE	2.6
1	J	311	LYS	2.6
1	H	343	GLN	2.6
2	Q	51	ASN	2.6
1	D	171	LYS	2.6
1	E	208	PRO	2.6
1	L	63	GLU	2.6
1	D	3	ALA	2.6
2	O	49	LEU	2.6
1	J	242	LYS	2.6
1	G	198	GLY	2.5
1	A	199	TYR	2.5
1	L	247	LEU	2.5
1	N	181	THR	2.5
2	U	86	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	175	ILE	2.5
1	J	382	GLY	2.5
1	L	352	GLN	2.5
1	C	223	ALA	2.5
1	F	191	GLU	2.5
1	N	63	GLU	2.5
1	C	359	ASP	2.5
1	D	196	ASP	2.5
1	G	196	ASP	2.5
2	U	55	LYS	2.5
1	B	237	LEU	2.5
1	M	208	PRO	2.5
1	E	231	ARG	2.5
1	D	193	MET	2.5
1	C	213	VAL	2.5
1	I	254	VAL	2.5
2	Q	74	LYS	2.5
2	S	77	LYS	2.5
1	B	372	LEU	2.5
1	E	222	LEU	2.5
2	U	47	ARG	2.5
1	D	355	GLU	2.5
1	H	356	ALA	2.5
1	E	204	PHE	2.5
2	R	67	PHE	2.5
2	U	95	VAL	2.5
1	E	194	GLN	2.5
1	F	44	PHE	2.5
1	G	250	ILE	2.5
1	F	359	ASP	2.5
1	N	189	VAL	2.5
1	H	524	LEU	2.5
1	M	238	GLU	2.5
1	C	208	PRO	2.5
1	K	373	ALA	2.5
1	N	379	ILE	2.5
2	U	11	ILE	2.5
1	M	309	LEU	2.5
1	B	195	PHE	2.5
2	O	71	TYR	2.5
2	U	42	ALA	2.5
1	A	332	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	362	ARG	2.5
1	K	270	ILE	2.5
1	E	214	GLU	2.5
1	C	365	LEU	2.5
1	D	525	PRO	2.4
1	F	208	PRO	2.4
1	D	270	ILE	2.4
1	F	185	ASP	2.4
1	B	320	ALA	2.4
1	L	354	GLU	2.4
1	M	242	LYS	2.4
2	U	46	GLY	2.4
1	B	210	THR	2.4
1	M	362	ARG	2.4
1	A	267	MET	2.4
1	A	352	GLN	2.4
1	B	379	ILE	2.4
1	F	220	ILE	2.4
2	P	42	ALA	2.4
2	P	93	ALA	2.4
1	G	192	GLY	2.4
1	C	372	LEU	2.4
1	E	524	LEU	2.4
1	K	381	VAL	2.4
2	P	65	VAL	2.4
1	B	347	ALA	2.4
1	E	233	MET	2.4
1	K	480	ALA	2.4
1	L	384	ALA	2.4
1	N	175	ILE	2.4
1	A	268	ARG	2.4
1	E	324	VAL	2.4
1	J	236	VAL	2.4
1	L	160	LYS	2.4
2	U	37	ARG	2.4
1	F	319	GLN	2.4
2	P	72	GLY	2.4
1	D	333	ILE	2.4
1	G	340	ALA	2.4
2	U	9	ARG	2.4
1	E	200	LEU	2.4
1	K	281	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	477	GLY	2.4
1	F	211	GLY	2.4
1	K	379	ILE	2.4
1	L	305	ILE	2.4
2	Q	55	LYS	2.4
2	U	74	LYS	2.4
1	K	183	LEU	2.4
2	S	50	GLU	2.4
1	A	254	VAL	2.4
1	K	294	THR	2.4
1	D	200	LEU	2.4
1	D	271	VAL	2.4
1	B	321	LYS	2.4
1	L	519	CYS	2.4
1	C	224	ASP	2.4
1	G	252	GLU	2.4
1	I	349	ILE	2.4
1	J	175	ILE	2.4
1	N	196	ASP	2.4
1	A	237	LEU	2.3
1	A	262	LEU	2.3
1	K	168	LYS	2.3
1	L	379	ILE	2.3
1	G	215	LEU	2.3
1	L	200	LEU	2.3
1	N	239	ALA	2.3
2	Q	84	LEU	2.3
1	A	345	ARG	2.3
1	B	332	ILE	2.3
1	G	227	ILE	2.3
1	L	313	THR	2.3
1	M	379	ILE	2.3
2	P	66	ILE	2.3
1	C	314	LEU	2.3
2	Q	19	THR	2.3
1	I	267	MET	2.3
1	L	383	ALA	2.3
1	M	356	ALA	2.3
1	A	346	VAL	2.3
1	C	324	VAL	2.3
2	T	34	LYS	2.3
1	M	361	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	190	VAL	2.3
1	E	381	VAL	2.3
1	L	236	VAL	2.3
1	L	271	VAL	2.3
1	B	277	LYS	2.3
1	L	195	PHE	2.3
1	J	247	LEU	2.3
1	L	175	ILE	2.3
2	T	21	SER	2.3
1	A	309	LEU	2.3
1	F	365	LEU	2.3
1	N	187	LEU	2.3
1	H	384	ALA	2.3
1	F	190	VAL	2.3
1	F	376	VAL	2.3
1	G	368	ARG	2.3
1	K	365	LEU	2.3
1	M	372	LEU	2.3
1	C	340	ALA	2.3
1	F	181	THR	2.3
1	N	223	ALA	2.3
1	E	336	VAL	2.3
1	F	229	ASN	2.3
1	B	358	SER	2.3
1	H	270	ILE	2.3
1	K	248	LEU	2.3
2	P	69	ASP	2.3
2	R	84	LEU	2.3
1	E	352	GLN	2.3
1	E	275	ALA	2.3
1	M	382	GLY	2.3
2	R	15	LYS	2.3
1	G	351	GLN	2.3
1	G	358	SER	2.3
1	K	420	ILE	2.3
1	G	233	MET	2.3
1	B	251	ALA	2.3
1	C	347	ALA	2.3
1	G	275	ALA	2.3
1	N	377	ALA	2.3
1	J	376	VAL	2.3
2	U	15	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	172	GLU	2.2
1	C	354	GLU	2.2
1	G	194	GLN	2.2
1	G	200	LEU	2.2
2	S	27	LEU	2.2
1	A	233	MET	2.2
1	E	286	LYS	2.2
1	H	381	VAL	2.2
1	C	308	GLU	2.2
1	G	366	GLN	2.2
2	O	84	LEU	2.2
1	G	333	ILE	2.2
1	N	201	SER	2.2
1	E	376	VAL	2.2
2	T	65	VAL	2.2
1	B	426	LEU	2.2
1	N	524	LEU	2.2
1	A	231	ARG	2.2
1	D	279	PRO	2.2
1	A	324	VAL	2.2
1	G	2	ALA	2.2
1	I	240	VAL	2.2
1	J	352	GLN	2.2
1	K	134	LEU	2.2
1	K	357	THR	2.2
1	L	237	LEU	2.2
1	F	175	ILE	2.2
1	B	190	VAL	2.2
2	T	50	GLU	2.2
1	B	204	PHE	2.2
1	E	274	ALA	2.2
1	E	351	GLN	2.2
1	M	241	ALA	2.2
2	O	12	VAL	2.2
1	H	187	LEU	2.2
1	A	210	THR	2.2
1	E	379	ILE	2.2
1	J	313	THR	2.2
1	E	171	LYS	2.2
1	L	525	PRO	2.2
1	H	273	VAL	2.2
1	I	343	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	368	ARG	2.2
2	T	26	VAL	2.2
1	E	289	LEU	2.2
1	F	138	CYS	2.2
1	J	289	LEU	2.2
1	B	214	GLU	2.2
1	G	359	ASP	2.2
1	K	196	ASP	2.2
2	U	90	ASP	2.2
1	K	175	ILE	2.2
1	K	297	GLY	2.2
1	A	525	PRO	2.2
2	P	9	ARG	2.2
1	E	212	ALA	2.2
2	O	92	LEU	2.2
1	G	175	ILE	2.2
1	E	345	ARG	2.1
2	S	9	ARG	2.1
1	H	288	MET	2.1
1	N	233	MET	2.1
2	S	76	GLU	2.1
1	B	324	VAL	2.1
1	C	275	ALA	2.1
1	M	200	LEU	2.1
2	S	49	LEU	2.1
2	P	74	LYS	2.1
1	M	138	CYS	2.1
1	C	238	GLU	2.1
1	F	354	GLU	2.1
1	K	219	PHE	2.1
1	D	245	LYS	2.1
1	A	314	LEU	2.1
1	H	369	VAL	2.1
2	Q	17	VAL	2.1
1	B	283	ASP	2.1
1	K	428	ASP	2.1
1	E	230	ILE	2.1
1	B	331	THR	2.1
1	C	338	GLU	2.1
1	E	181	THR	2.1
1	F	272	LYS	2.1
2	S	86	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	158	VAL	2.1
1	N	346	VAL	2.1
2	T	83	VAL	2.1
1	B	362	ARG	2.1
1	E	322	ARG	2.1
1	N	268	ARG	2.1
1	F	304	GLU	2.1
1	I	242	LYS	2.1
2	P	50	GLU	2.1
1	A	204	PHE	2.1
1	D	219	PHE	2.1
1	G	234	LEU	2.1
1	E	271	VAL	2.1
1	N	378	VAL	2.1
1	G	291	ASP	2.1
1	G	334	ASP	2.1
2	Q	20	LYS	2.1
2	O	45	ASN	2.1
1	A	294	THR	2.1
1	J	222	LEU	2.1
1	K	524	LEU	2.1
1	K	158	VAL	2.1
1	N	240	VAL	2.1
1	M	185	ASP	2.1
1	B	178	GLU	2.1
1	B	367	GLU	2.1
1	M	63	GLU	2.1
1	A	333	ILE	2.1
1	L	351	GLN	2.1
2	T	9	ARG	2.1
1	E	369	VAL	2.1
2	O	39	GLU	2.1
2	S	26	VAL	2.1
1	G	223	ALA	2.1
1	C	250	ILE	2.1
1	J	349	ILE	2.1
1	M	519	CYS	2.1
2	P	21	SER	2.1
1	D	224	ASP	2.1
1	E	193	MET	2.1
1	E	273	VAL	2.1
1	N	169	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	376	VAL	2.1
2	S	12	VAL	2.1
1	K	162	ILE	2.1
2	U	94	ILE	2.1
1	K	203	TYR	2.1
1	I	195	PHE	2.1
1	A	256	GLY	2.1
1	C	215	LEU	2.1
1	D	215	LEU	2.1
1	E	192	GLY	2.1
1	H	484	GLU	2.1
1	K	200	LEU	2.1
1	M	262	LEU	2.1
2	O	16	GLU	2.1
1	F	254	VAL	2.0
1	N	381	VAL	2.0
1	J	184	GLN	2.0
1	N	333	ILE	2.0
1	D	231	ARG	2.0
1	M	285	ARG	2.0
1	N	44	PHE	2.0
2	Q	80	ASN	2.0
1	B	63	GLU	2.0
1	B	170	GLY	2.0
1	D	248	LEU	2.0
1	I	372	LEU	2.0
1	L	494	LEU	2.0
2	Q	72	GLY	2.0
1	B	228	SER	2.0
1	E	359	ASP	2.0
1	L	359	ASP	2.0
1	L	364	LYS	2.0
1	F	347	ALA	2.0
1	M	152	ALA	2.0
1	F	268	ARG	2.0
1	J	350	ARG	2.0
1	G	304	GLU	2.0
2	T	16	GLU	2.0
1	E	306	GLY	2.0
1	A	190	VAL	2.0
1	B	227	ILE	2.0
1	E	223	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	331	THR	2.0
1	C	211	GLY	2.0
1	D	314	LEU	2.0
2	U	6	LEU	2.0
1	F	207	LYS	2.0
1	A	334	ASP	2.0
1	E	216	GLU	2.0
1	F	63	GLU	2.0
1	J	243	ALA	2.0
1	L	373	ALA	2.0
2	R	19	THR	2.0
1	M	161	LEU	2.0
2	S	38	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	D	604	1/1	0.32	14.84	2,2,2,2	0
3	MG	A	601	1/1	0.29	12.83	2,2,2,2	0
3	MG	G	607	1/1	0.21	1.28	2,2,2,2	0
3	MG	B	602	1/1	0.23	0.95	2,2,2,2	0
3	MG	C	603	1/1	0.20	0.74	2,2,2,2	0
4	ADP	B	701	27/27	0.21	0.13	6,8,9,10	0
4	ADP	A	700	27/27	0.18	0.06	6,8,9,11	0
3	MG	F	606	1/1	0.25	-0.12	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ADP	F	705	27/27	0.21	-0.17	6,8,9,10	0
4	ADP	E	704	27/27	0.20	-0.26	6,8,9,10	0
4	ADP	D	703	27/27	0.16	-0.71	6,8,9,10	0
4	ADP	G	706	27/27	0.16	-0.78	6,8,9,10	0
3	MG	E	605	1/1	0.20	-1.24	2,2,2,2	0
4	ADP	C	702	27/27	0.14	-1.63	6,8,9,10	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.