



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 06:07 AM EST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

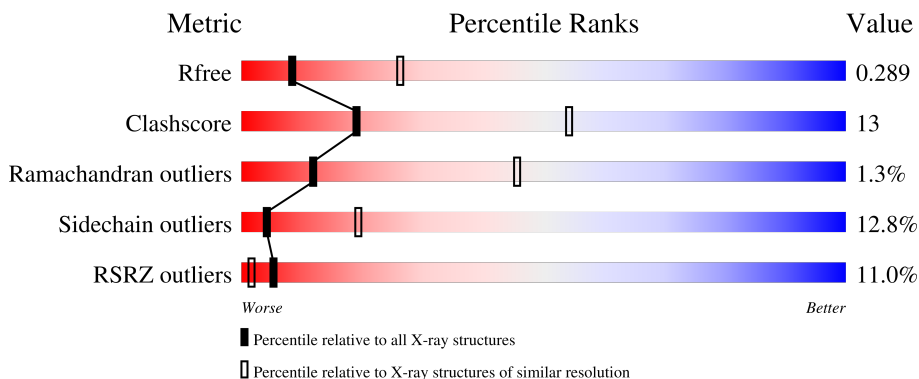
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	524	 11% 71% 25% .
1	B	524	 12% 71% 24% 5%
1	C	524	 9% 69% 27% . .
1	D	524	 10% 69% 26% .
1	E	524	 12% 69% 26% .

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

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called groEL protein.

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

- 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	A	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	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

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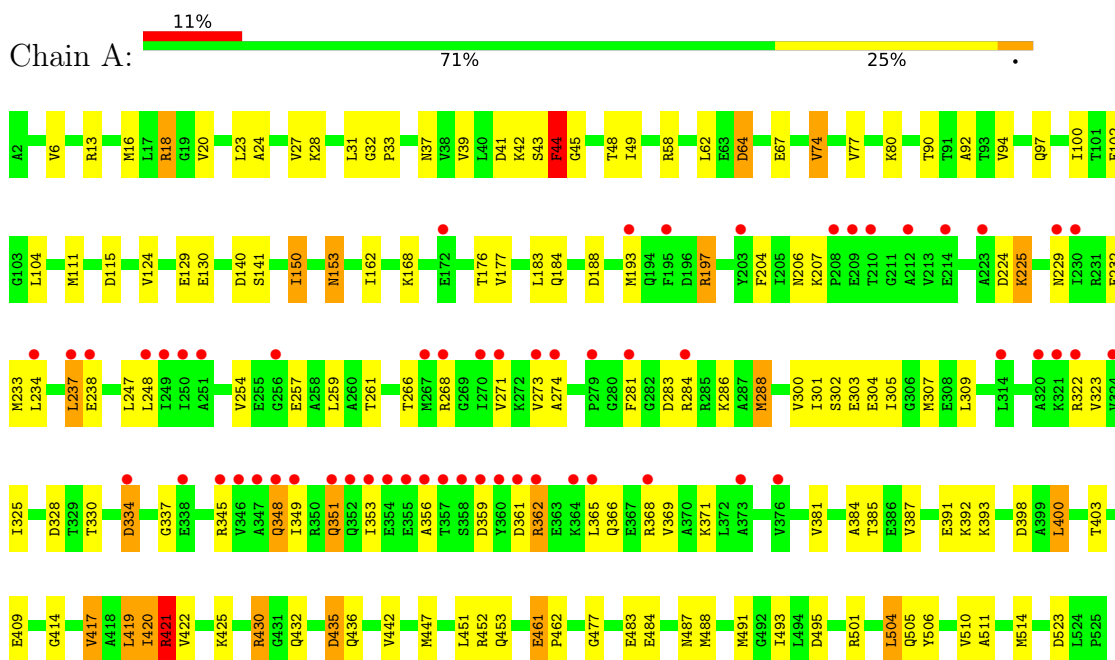
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total O 1 1	0	0
5	G	1	Total O 1 1	0	0

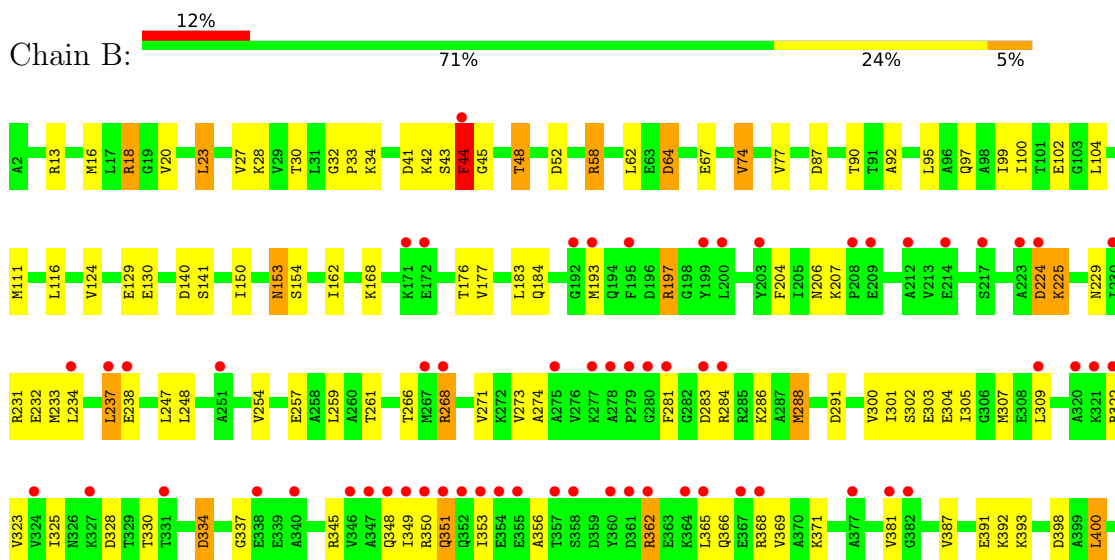
3 Residue-property plots

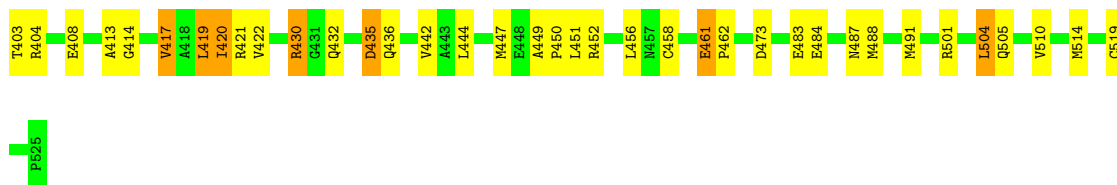
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: groEL protein

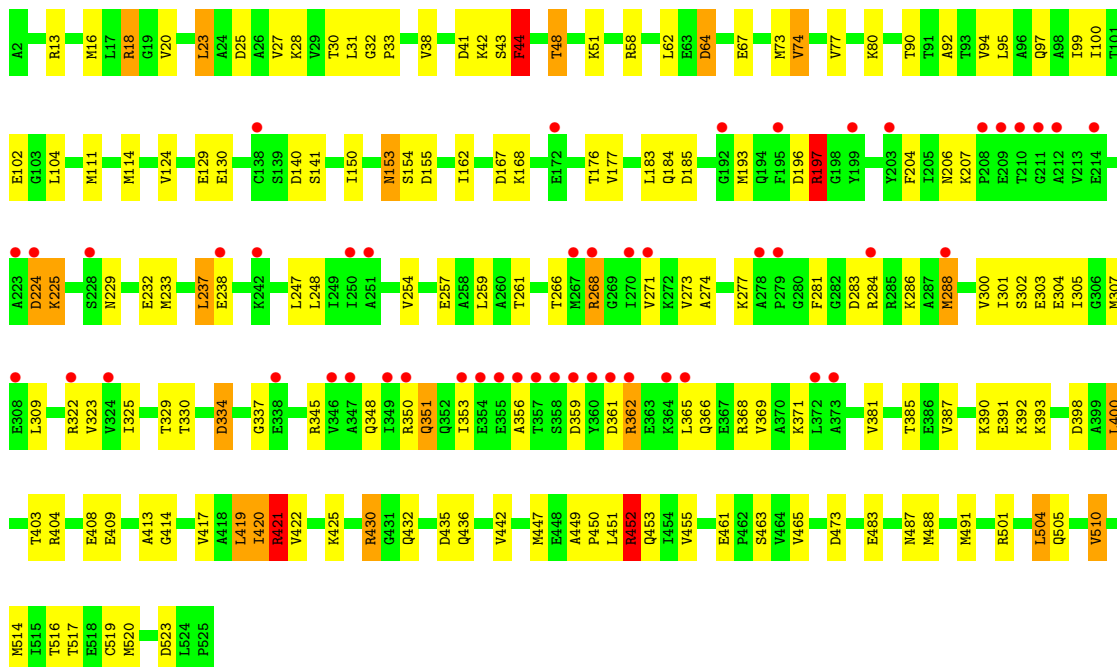


- Molecule 1: groEL protein

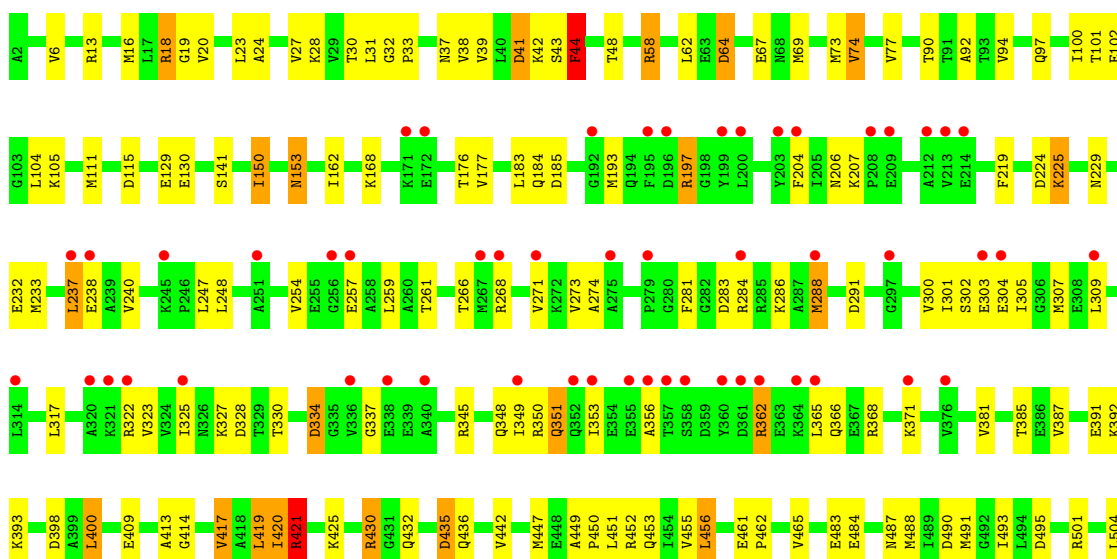




• Molecule 1: groEL protein

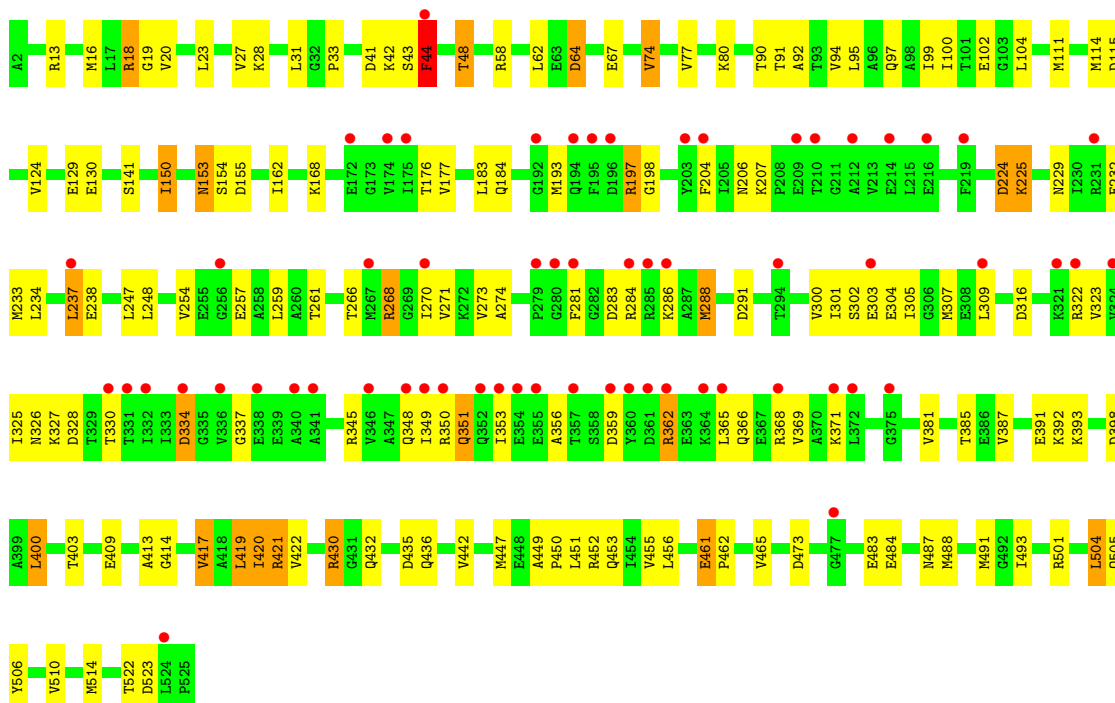


• Molecule 1: groEL protein

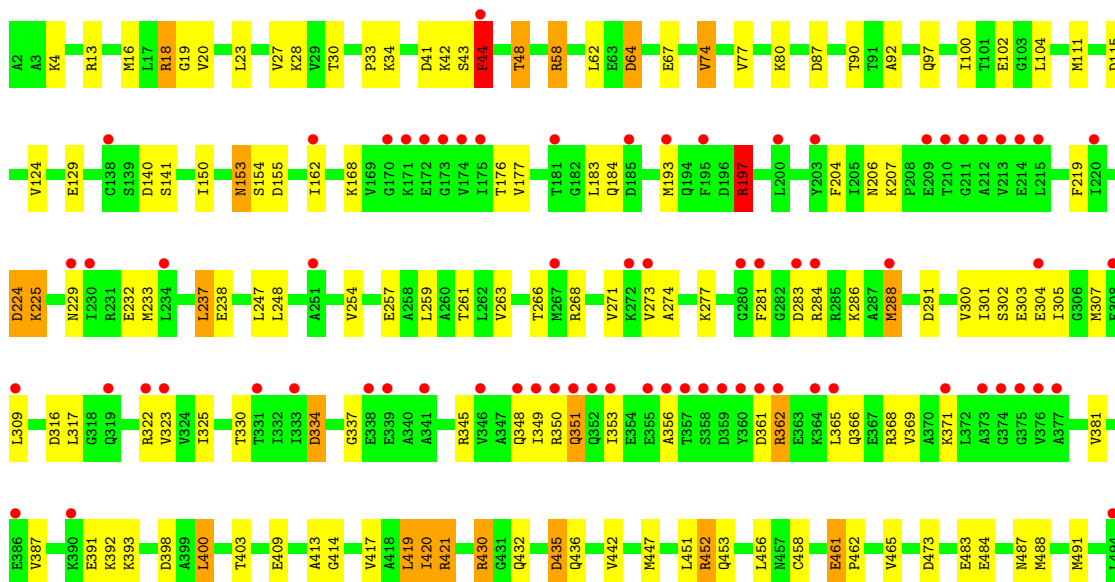
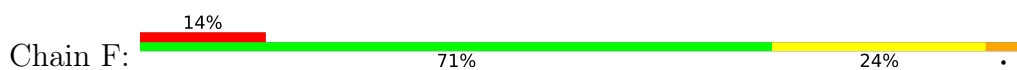




- Molecule 1: groEL protein

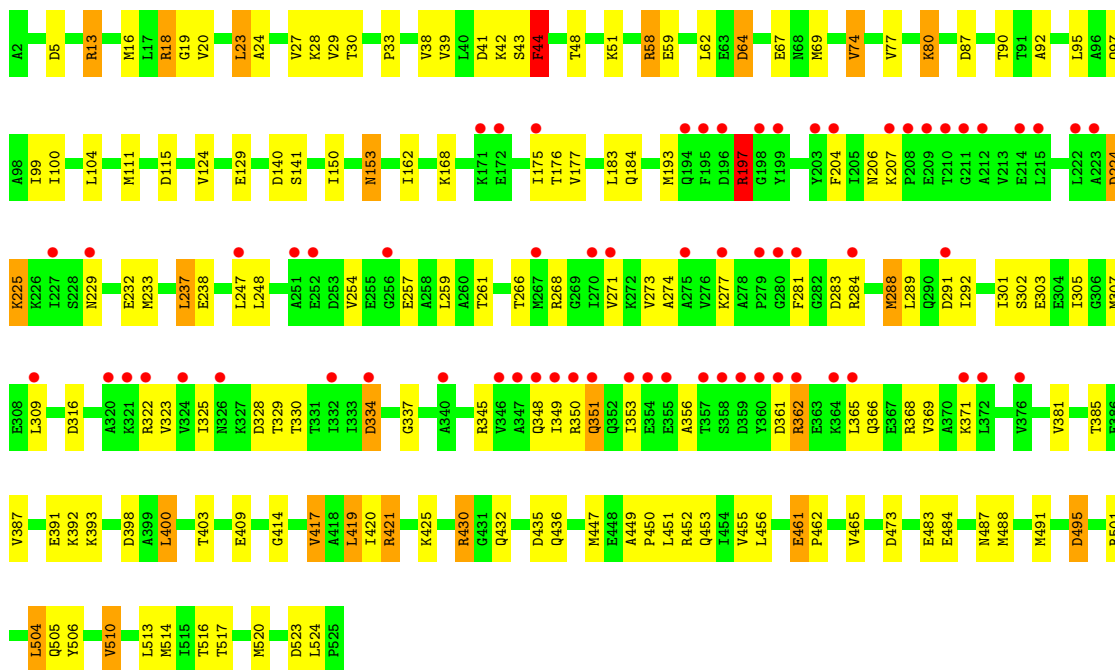


- Molecule 1: groEL protein

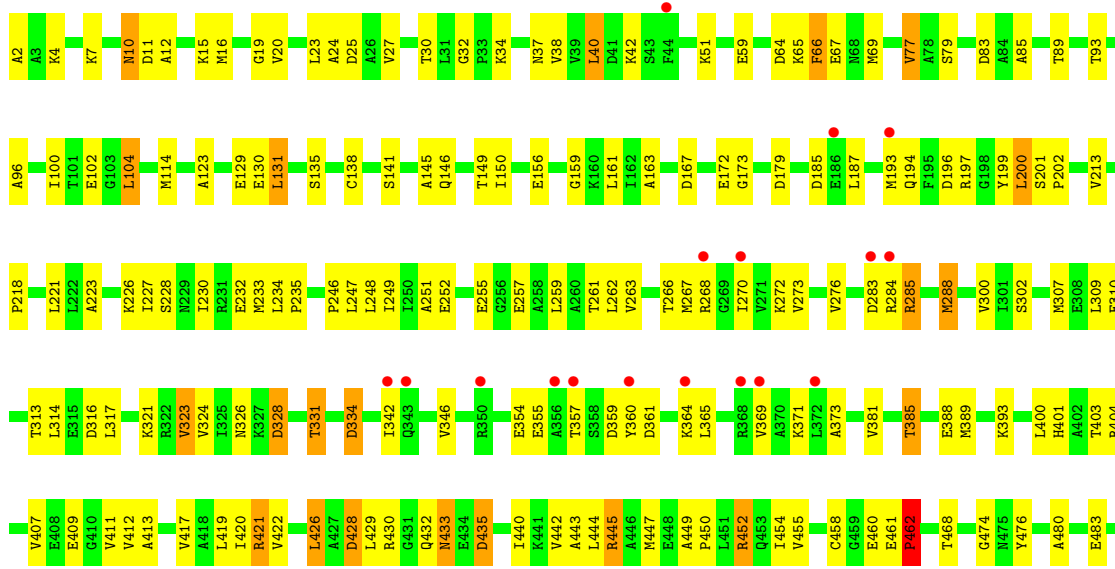


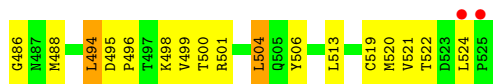


- Molecule 1: groEL protein

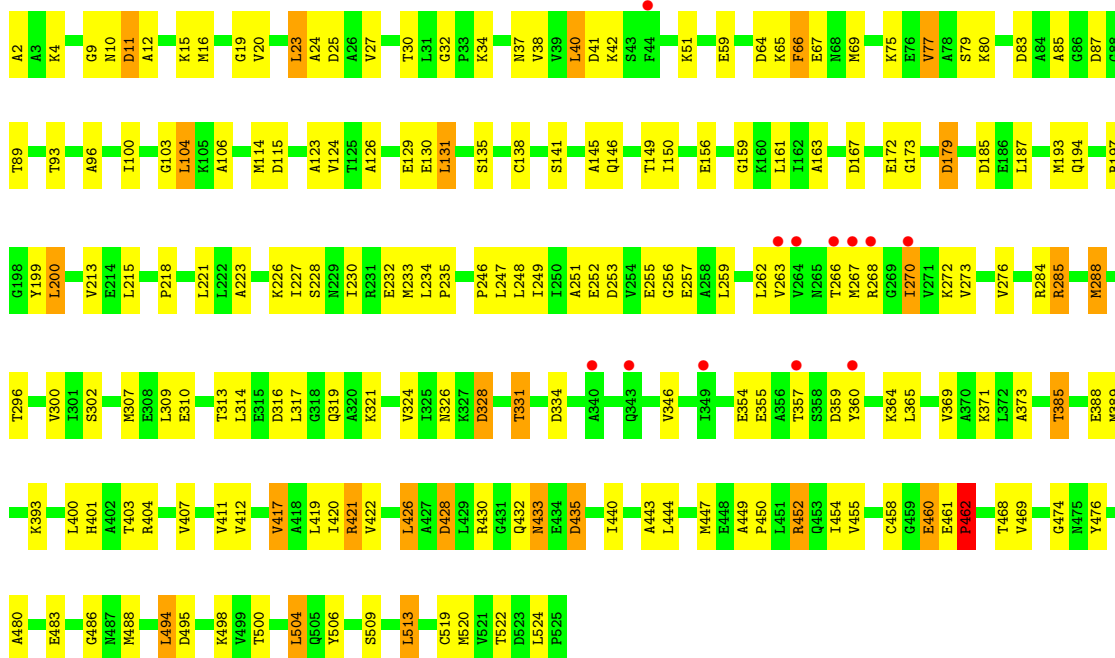


- Molecule 1: groEL protein

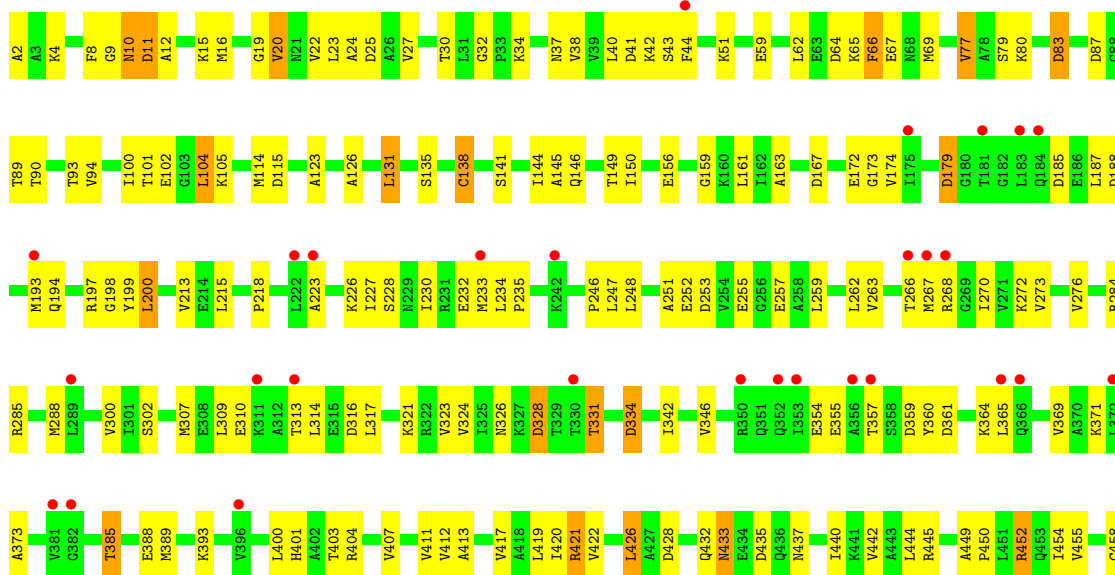


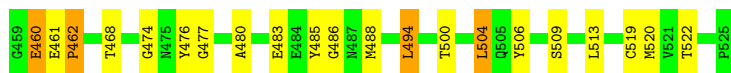


• Molecule 1: groEL protein

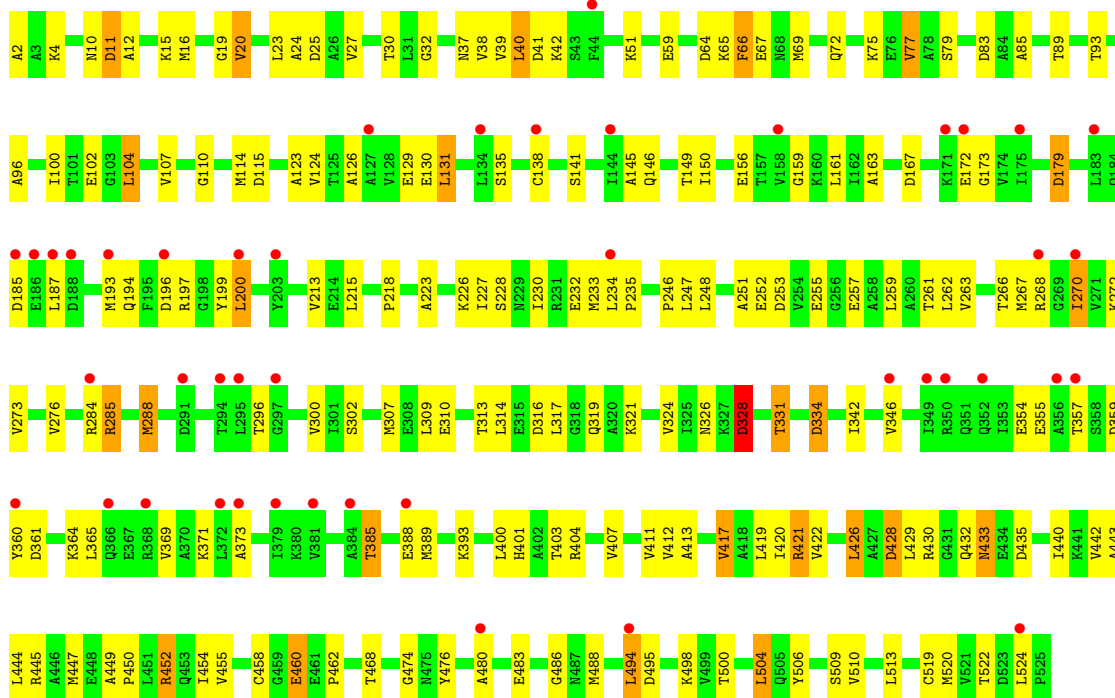


• Molecule 1: groEL protein

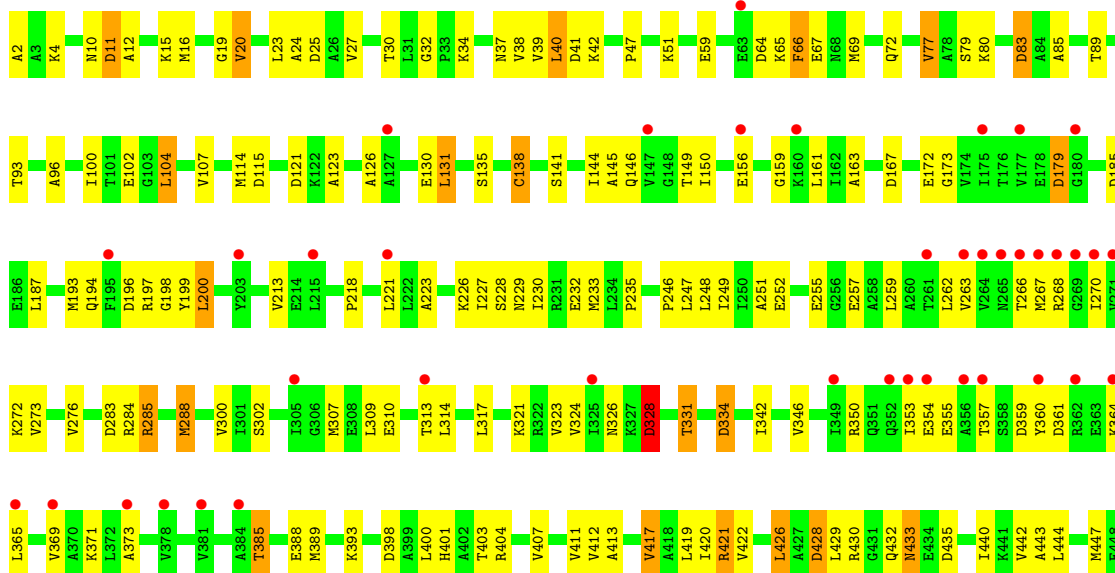


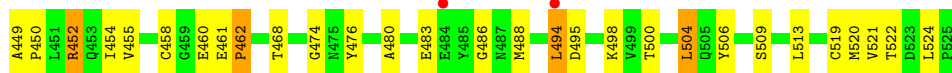


• Molecule 1: groEL protein

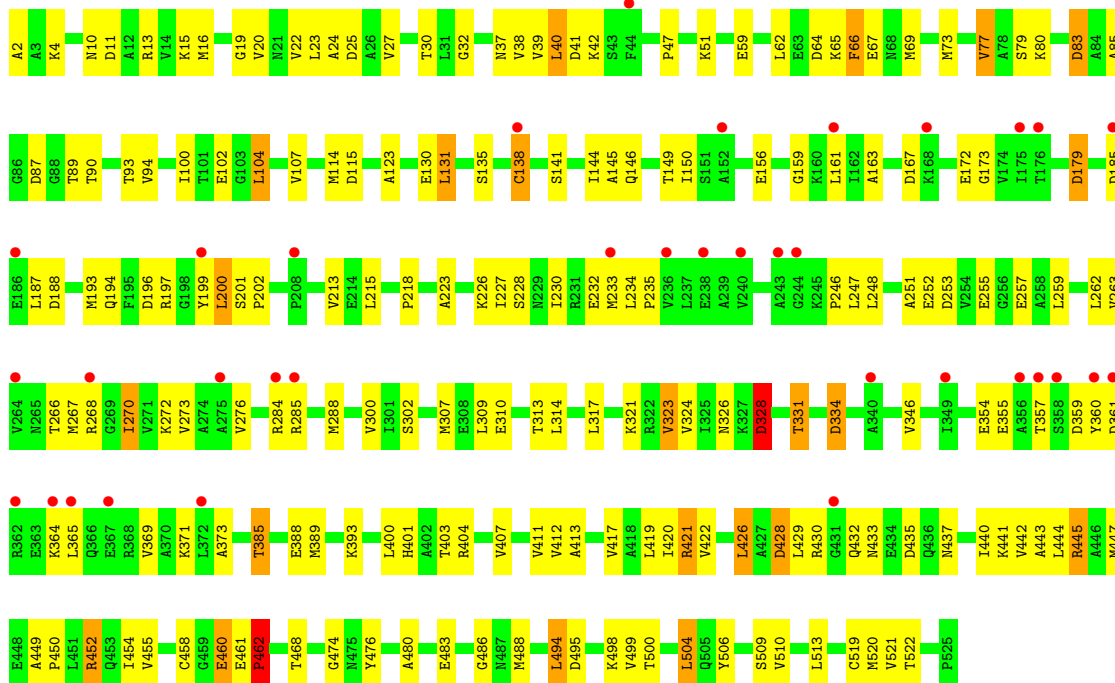


• Molecule 1: groEL protein

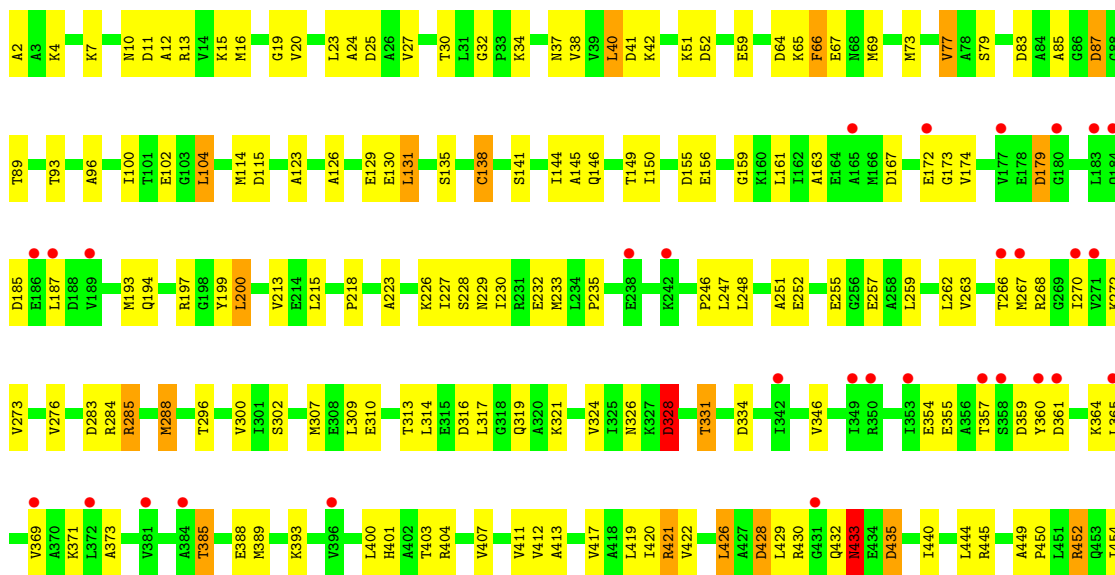


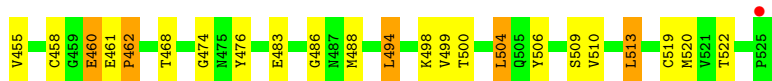


• Molecule 1: groEL protein

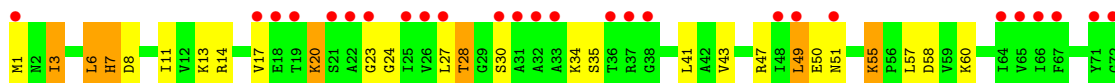


• Molecule 1: groEL protein

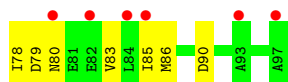
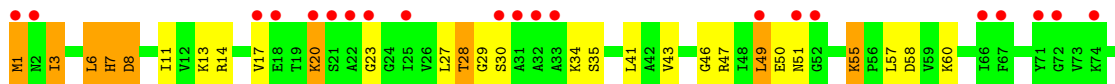




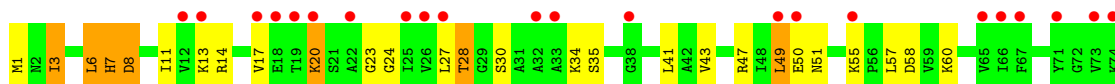
- Molecule 2: groES protein



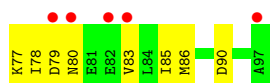
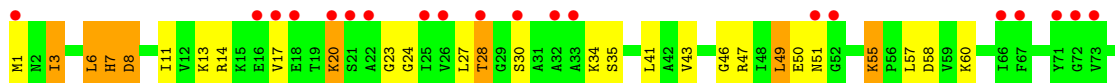
- Molecule 2: groES protein



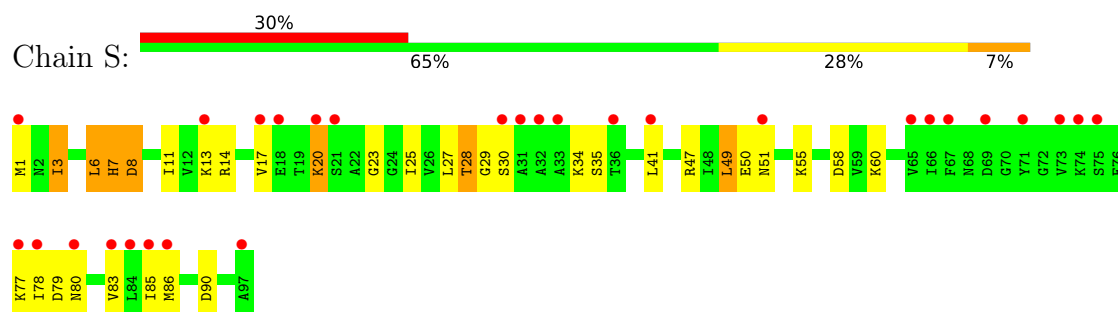
- Molecule 2: groES protein



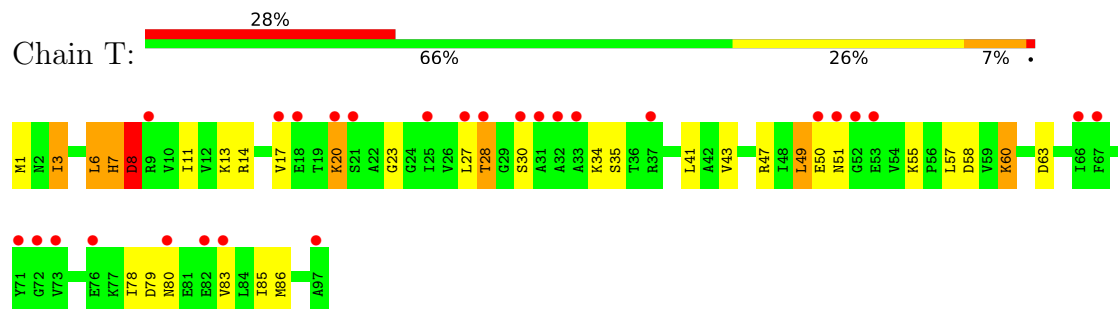
- Molecule 2: groES protein



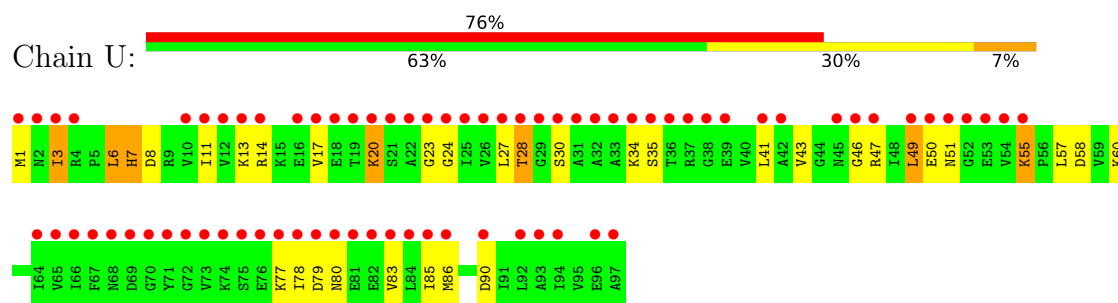
- Molecule 2: groES protein



- Molecule 2: groES protein



- Molecule 2: groES protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtrriage
Refinement program	REFMAC refinac_5.1.24 24/04/2001	Depositor
R, R_{free}	0.269 , 0.287 0.272 , 0.289	Depositor DCC
R_{free} test set	12081 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtrriage
Anisotropy	0.614	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.003 for k,h,-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	59283	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3976	105	0
1	B	3856	0	3976	99	0
1	C	3856	0	3976	109	0
1	D	3856	0	3976	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1567) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:MET:SD	1:E:114:MET:CE	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:HG2	1:G:18:ARG:HH11	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:HG2	1:E:18:ARG:HH11	1.11	1.11
1:A:18:ARG:HH11	1:A:18:ARG:HG2	1.14	1.11
1:B:18:ARG:HG2	1:B:18:ARG:HH11	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:HH11	1:B:18:ARG:CG	1.71	1.03
1:B:432:GLN:NE2	1:B:436:GLN:HE22	1.56	1.02
1:D:414:GLY:O	1:D:417:VAL:HG12	1.58	1.02
1:F:414:GLY:O	1:F:417:VAL:HG12	1.59	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:HG2	1:D:18:ARG:HH11	1.24	1.01
1:D:432:GLN:HE21	1:D:436:GLN:NE2	1.58	1.00
1:F:18:ARG:HH11	1:F:18:ARG:CG	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:HH11	1:G:18:ARG:CG	1.77	0.97
1:C:18:ARG:HH11	1:C:18:ARG:CG	1.76	0.97
1:L:426:LEU:HD12	1:L:444:LEU:HD21	1.48	0.95
1:E:44:PHE:HD1	1:E:44:PHE:H	1.06	0.95
1:B:204:PHE:HE2	1:B:266:THR:HG21	1.32	0.95
1:F:18:ARG:HG2	1:F:18:ARG:NH1	1.76	0.95
1:B:18:ARG:HG2	1:B:18:ARG:NH1	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:HH11	1:D:18:ARG:CG	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:HG2	1:I:404:ARG:HH11	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:HH11	1:A:18:ARG:CG	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:E:432:GLN:HE21	1:E:436:GLN:HE22	0.96	0.91
1:G:18:ARG:HG2	1:G:18:ARG:NH1	1.81	0.91
1:D:430:ARG:HG2	1:D:430:ARG:HH11	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:A:44:PHE:HD1	1:A:44:PHE:H	1.07	0.91
1:H:65:LYS:O	1:H:66:PHE:HB2	1.66	0.91
1:J:426:LEU:HD12	1:J:444:LEU:HD21	1.53	0.90
1:L:69:MET:HE1	1:L:522:THR:HB	1.52	0.90
1:G:432:GLN:HE21	1:G:436:GLN:NE2	1.70	0.90
1:C:18:ARG:HG2	1:C:18:ARG:NH1	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:B:44:PHE:HD1	1:B:44:PHE:H	1.00	0.89
1:M:426:LEU:HD12	1:M:444:LEU:HD21	1.54	0.89
1:G:44:PHE:HD1	1:G:44:PHE:H	1.08	0.88
1:A:430:ARG:HH11	1:A:430:ARG:HG2	1.36	0.88
1:B:432:GLN:HE21	1:B:436:GLN:NE2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:426:LEU:HD12	1:H:444:LEU:HD21	1.57	0.85
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:C:430:ARG:HH11	1:C:430:ARG:HG2	1.43	0.84
1:H:69:MET:HE1	1:H:522:THR:HB	1.58	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:CD1	1:E:44:PHE:N	2.47	0.83
1:D:74:VAL:O	1:D:77:VAL:HG13	1.79	0.82
1:E:430:ARG:HG2	1:E:430:ARG:HH11	1.43	0.82
1:C:100:ILE:HD11	1:C:514:MET:HE1	1.60	0.82
1:F:44:PHE:CD1	1:F:44:PHE:N	2.48	0.81
1:D:44:PHE:CD1	1:D:44:PHE:N	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:HH11	1:L:404:ARG:HG2	1.46	0.81
1:C:204:PHE:CE2	1:C:266:THR:HG21	2.17	0.80
1:F:430:ARG:HG2	1:F:430:ARG:HH11	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:B:44:PHE:CD1	1:B:44:PHE:N	2.46	0.78
1:D:18:ARG:HG2	1:D:18:ARG:NH1	1.91	0.78
1:G:44:PHE:CD1	1:G:44:PHE:N	2.48	0.78
1:G:204:PHE:CE2	1:G:266:THR:HG21	2.18	0.78
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.66	0.77
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: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:C:74:VAL:O	1:C:77:VAL:HG13	1.85	0.77
1:D:432:GLN:HE21	1:D:436:GLN:HE22	0.79	0.77
1:A:409:GLU:OE2	1:A:501:ARG:NH2	2.17	0.77
1:M:131:LEU:HD13	1:M:422:VAL:HG11	1.66	0.76
1:M:421:ARG:HD2	1:M:474:GLY:O	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:PRO:HA	1:E:153:ASN:HD21	1.50	0.76
1:L:38:VAL:HG22	1:M:519:CYS:HB3	1.67	0.76
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:100:ILE:O	1:K:104:LEU:HB2	1.86	0.75
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.51	0.75
1:A:44:PHE:CD1	1:A:44:PHE:N	2.46	0.75
1:H:69:MET:CE	1:H:522:THR:HB	2.16	0.75
1:C:33:PRO:HA	1:C:153:ASN:HD21	1.51	0.75
1:C:44:PHE:HD1	1:C:44:PHE:N	1.81	0.75
1:D:204:PHE:CE2	1:D:266:THR:HG21	2.18	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:HG2	1:J:404:ARG:HH11	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: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:M:69:MET:CE	1:M:522:THR:HB	2.17	0.74
1:I:421:ARG:HD2	1:I:474:GLY:O	1.86	0.74
1:K:419:LEU:CD2	1:K:500:THR:CG2	2.65	0.74
1:A:100:ILE:HD11	1:A:514:MET:HE1	1.70	0.74
1:B:44:PHE:HD1	1:B:44:PHE:N	1.82	0.74
1:N:65:LYS:O	1:N:66:PHE:CB	2.36	0.74
1:A:385:THR:HG21	1:G:510:VAL:HG12	1.71	0.73
1:M:100:ILE:O	1:M:104:LEU:HB2	1.88	0.73
1:N:419:LEU:CD2	1:N:500:THR:HG23	2.18	0.73
1:I:149:THR:HG23	1:I:159:GLY:HA3	1.70	0.73
1:J:421:ARG:HD2	1:J:474:GLY:O	1.87	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:HD1	1:E:44:PHE:N	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:H:149:THR:HG23	1:H:159:GLY:HA3	1.71	0.73
1:M:232:GLU:HB3	1:M:309:LEU:HB2	1.71	0.73
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232:GLU:HB3	1:H:309:LEU:HB2	1.69	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
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:H:421:ARG:HD2	1:H:474:GLY:O	1.89	0.72
1:J:232:GLU:HB3	1:J:309:LEU:HB2	1.70	0.72
1:M:419:LEU:CD2	1:M:500:THR:HG23	2.20	0.72
1:N:421:ARG:HD2	1:N:474:GLY:O	1.89	0.72
1:H:100:ILE:O	1:H:104:LEU:HB2	1.90	0.72
1:K:149:THR:HG23	1:K:159:GLY:HA3	1.70	0.72
1:N:100:ILE:O	1:N:104:LEU:HB2	1.90	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:D:409:GLU:OE2	1:D:501:ARG:NH2	2.22	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:J:100:ILE:O	1:J:104:LEU:HB2	1.90	0.71
1:G:44:PHE:HD1	1:G:44:PHE:N	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:K:32:GLY:HA2	1:K:454:ILE:HD13	1.71	0.71
1:L:227:ILE:HD12	1:L:309:LEU:HD11	1.73	0.71
1:I:227:ILE:HD12	1:I:309:LEU:HD11	1.72	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: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:N:227:ILE:HD12	1:N:309:LEU:HD11	1.72	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:H:419:LEU:CD2	1:H:500:THR:CG2	2.69	0.70
1:K:69:MET:CE	1:K:522:THR:HB	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:100:ILE:O	1:L:104:LEU:HB2	1.92	0.70
1:A:430:ARG:HG2	1:A:430:ARG:NH1	2.07	0.70
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.73	0.70
1:I:419:LEU:CD2	1:I:500:THR:CG2	2.69	0.70
1:A:20:VAL:HG13	1:A:74:VAL:HG11	1.73	0.69
1:H:27:VAL:HG11	1:H:93:THR:HG21	1.73	0.69
1:M:419:LEU:CD2	1:M:500:THR:CG2	2.69	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:F:33:PRO:HA	1:F:153:ASN:HD21	1.57	0.69
1:I:419:LEU:CD2	1:I:500:THR:HG23	2.23	0.69
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.08	0.69
1:J:200:LEU:HD12	1:J:276:VAL:HA	1.75	0.69
1:D:44:PHE:HD1	1:D:44:PHE:N	1.84	0.68
1:A:44:PHE:HD1	1:A:44:PHE:N	1.85	0.68
1:K:200:LEU:HD12	1:K:276:VAL:HA	1.74	0.68
1:M:173:GLY:O	1:M:404:ARG:NH2	2.25	0.68
1:H:200:LEU:HD12	1:H:276:VAL:HA	1.75	0.68
1:H:452:ARG:HG2	1:H:452:ARG:HH11	1.58	0.68
1:M:32:GLY:HA2	1:M:454:ILE:HD13	1.75	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:J:131:LEU:CD1	1:J:422:VAL:HG11	2.25	0.67
1:K:65:LYS:O	1:K:66:PHE:CB	2.38	0.67
1:M:131:LEU:CD1	1:M:422:VAL:HG11	2.23	0.67
1:D:430:ARG:HG2	1:D:430:ARG:NH1	2.05	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:I:65:LYS:O	1:I:66:PHE:CB	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:13:ARG:HD2	1:F:104:LEU:HD22	1.77	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
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:A:13:ARG:HD2	1:A:104:LEU:HD22	1.78	0.66
1:G:100:ILE:HD11	1:G:514:MET:HE1	1.78	0.66
1:I:452:ARG:HG2	1:I:452:ARG:HH11	1.60	0.66
1:J:452:ARG:HG2	1:J:452:ARG:HH11	1.59	0.66
1:L:419:LEU:CD2	1:L:500:THR:CG2	2.74	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:G:13:ARG:HD2	1:G:104:LEU:HD22	1.78	0.65
1:I:194:GLN:HB2	1:I:331:THR:HB	1.78	0.65
1:M:452:ARG:HG2	1:M:452:ARG:HH11	1.59	0.65
1:N:32:GLY:HA2	1:N:454:ILE:HD13	1.77	0.65
2:U:7:HIS:O	2:U:8:ASP:HB3	1.97	0.65
4:B:701:ADP:O3B	5:B:801:HOH:O	2.13	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
1:I:32:GLY:HA2	1:I:454:ILE:HD13	1.77	0.65
2:S:7:HIS:O	2:S:8:ASP:HB3	1.95	0.65
1:L:27:VAL:HG11	1:L:93:THR:HG21	1.78	0.65
1:A:39:VAL:HG23	1:G:517:THR:HG23	1.78	0.65
1:H:65:LYS:O	1:H:66:PHE:CB	2.37	0.65
1:M:385:THR:HG23	1:M:388:GLU:HB2	1.79	0.64
1:F:44:PHE:HD1	1:F:44:PHE:N	1.87	0.64
1:C:430:ARG:HG2	1:C:430:ARG:NH1	2.10	0.64
1:M:65:LYS:O	1:M:66:PHE:CB	2.34	0.64
1:C:516:THR:OG1	1:D:37:ASN:ND2	2.29	0.64
1:K:452:ARG:HG2	1:K:452:ARG:HH11	1.62	0.64
1:E:417:VAL:HG11	1:E:488:MET:HG3	1.79	0.64
1:G:288:MET:HG2	1:G:368:ARG:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:LEU:CD1	1:L:422:VAL:HG11	2.28	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
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:H:194:GLN:HB2	1:H:331:THR:HB	1.81	0.63
1:J:27:VAL:HG11	1:J:93:THR:HG21	1.81	0.63
1:I:30:THR:HB	1:I:51:LYS:O	1.99	0.63
1:J:65:LYS:O	1:J:66:PHE:CB	2.40	0.63
1:H:96:ALA:O	1:H:100:ILE:HG13	1.98	0.62
1:C:13:ARG:HD2	1:C:104:LEU:HD22	1.79	0.62
1:D:18:ARG:HH11	1:D:18:ARG:CB	2.11	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:HG2	1:F:430:ARG:NH1	2.12	0.62
1:B:64:ASP:HB3	1:B:67:GLU:HB2	1.81	0.62
1:J:194:GLN:HB2	1:J:331:THR:HB	1.82	0.62
1:L:173:GLY:O	1:L:404:ARG:NH2	2.32	0.62
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.82	0.62
1:B:111:MET:HG2	1:B:435:ASP:OD1	1.99	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ASP:HB3	1:D:67:GLU:HB2	1.83	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:N:173:GLY:O	1:N:404:ARG:NH2	2.33	0.61
1:I:2:ALA:O	1:I:4:LYS:HE3	1.99	0.61
1:J:426:LEU:CD1	1:J:444:LEU:HD21	2.30	0.61
1:A:414:GLY:O	1:A:417:VAL:CG1	2.40	0.61
2:P:20:LYS:HB3	2:P:27:LEU:HG	1.83	0.61
2:S:20:LYS:HB3	2:S:27:LEU:HG	1.83	0.61
1:N:131:LEU:HD13	1:N:422:VAL:HG11	1.82	0.61
1:F:409:GLU:OE2	1:F:501:ARG:NH2	2.31	0.61
1:K:199:TYR:HA	1:K:276:VAL:HG12	1.83	0.61
1:L:426:LEU:CD1	1:L:444:LEU:HD21	2.27	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:B:419:LEU:HG	1:B:447:MET:HG2	1.83	0.60
1:F:419:LEU:HG	1:F:447:MET:HG2	1.82	0.60
1:K:419:LEU:HD21	1:K:500:THR:HG23	1.82	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:J:449:ALA:HB3	1:J:450:PRO:HD3	1.83	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:N:385:THR:HG23	1:N:388:GLU:HB2	1.83	0.60
1:F:193:MET:HG3	1:F:371:LYS:HB3	1.84	0.60
1:G:33:PRO:HA	1:G:153:ASN:ND2	2.17	0.60
1:L:452:ARG:HH11	1:L:452:ARG:HG2	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:G:302:SER:H	1:G:307:MET:HE3	1.66	0.60
1:L:404:ARG:HG2	1:L:404:ARG:NH1	2.11	0.60
1:L:24:ALA:HA	1:L:27:VAL:HG12	1.84	0.59
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.83	0.59
1:B:510:VAL:HG12	1:C:385:THR:HG21	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:ILE:HG12	1:F:330:THR:HG23	1.83	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: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:L:149:THR:CG2	1:L:159:GLY:HA3	2.32	0.59
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.83	0.59
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.84	0.59
1:M:149:THR:CG2	1:M:159:GLY:HA3	2.31	0.59
1:M:426:LEU:CD1	1:M:444:LEU:HD21	2.30	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: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:C:520:MET:HG2	1:D:39:VAL:HB	1.84	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:A:325:ILE:HG12	1:A:330:THR:HG23	1.85	0.58
1:A:419:LEU:HG	1:A:447:MET:HG2	1.85	0.58
1:I:411:VAL:HG21	1:I:494:LEU:HD12	1.86	0.58
1:M:449:ALA:HB3	1:M:450:PRO:HD3	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:B:325:ILE:HG12	1:B:330:THR:HG23	1.86	0.58
1:J:174:VAL:HG21	1:J:194:GLN:HB3	1.86	0.58
1:E:268:ARG:HH21	2:S:27:LEU:CD2	2.16	0.58
1:L:64:ASP:HB3	1:L:67:GLU:HB2	1.85	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:D:325:ILE:HG12	1:D:330:THR:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:VAL:HB	1:M:520:MET:HG2	1.86	0.57
1:L:313:THR:HG22	1:L:314:LEU:H	1.69	0.57
1:N:426:LEU:CD1	1:N:444:LEU:HD21	2.31	0.57
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.87	0.57
1:J:199:TYR:HA	1:J:276:VAL:HG12	1.87	0.57
1:L:146:GLN:HE21	1:L:150:ILE:HD11	1.69	0.57
1:A:39:VAL:HB	1:G:520:MET:HG2	1.86	0.57
1:C:20:VAL:HG13	1:C:74:VAL:HG11	1.86	0.57
1:N:404:ARG:HG2	1:N:404:ARG:NH1	2.20	0.57
1:A:33:PRO:HA	1:A:153:ASN:HD21	1.70	0.57
1:A:37:ASN:ND2	1:G:516:THR:OG1	2.31	0.57
1:B:193:MET:HG3	1:B:371:LYS:HB3	1.87	0.57
1:M:270:ILE:HA	1:N:257:GLU:OE2	2.04	0.57
2:P:3:ILE:HD13	2:P:11:ILE:HG21	1.87	0.57
1:E:419:LEU:HG	1:E:447:MET:HG2	1.86	0.57
1:J:24:ALA:HA	1:J:27:VAL:HG12	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:H:223:ALA:HB3	1:H:251:ALA:HB2	1.87	0.57
1:K:385:THR:HG23	1:K:388:GLU:HB2	1.86	0.57
1:K:426:LEU:CD1	1:K:444:LEU:HD21	2.33	0.57
1:N:223:ALA:HB3	1:N:251:ALA:HB2	1.87	0.57
1:G:111:MET:HG2	1:G:435:ASP:OD1	2.05	0.56
1:L:19:GLY:HA3	1:L:67:GLU:O	2.04	0.56
1:H:16:MET:HG3	1:H:520:MET:SD	2.44	0.56
1:B:124:VAL:HG13	1:B:504:LEU:HD13	1.87	0.56
1:F:18:ARG:CG	1:F:18:ARG:NH1	2.45	0.56
1:G:419:LEU:HG	1:G:447:MET:HG2	1.88	0.56
1:I:419:LEU:HD21	1:I:500:THR:HG23	1.87	0.56
1:J:145:ALA:O	1:J:149:THR:HG23	2.05	0.56
1:J:313:THR:HG22	1:J:314:LEU:H	1.69	0.56
1:K:404:ARG:HG2	1:K:404:ARG:NH1	2.15	0.56
1:D:288:MET:HG2	1:D:368:ARG:HD2	1.86	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: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:E:430:ARG:HG2	1:E:430:ARG:NH1	2.13	0.56
1:F:33:PRO:HA	1:F:153:ASN:ND2	2.21	0.56
1:K:96:ALA:O	1:K:100:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:24:ALA:HA	1:M:27:VAL:HG12	1.88	0.56
1:N:19:GLY:HA3	1:N:67:GLU:O	2.05	0.56
1:F:64:ASP:HB3	1:F:67:GLU:HB2	1.88	0.56
1:H:313:THR:HG22	1:H:314:LEU:H	1.70	0.56
1:J:385:THR:HG23	1:J:388:GLU:HB2	1.86	0.56
1:L:199:TYR:HA	1:L:276:VAL:HG12	1.87	0.56
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.86	0.56
1:C:268:ARG:HD2	2:Q:27:LEU:CD2	2.34	0.56
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.87	0.56
1:H:426:LEU:CD1	1:H:444:LEU:HD21	2.34	0.56
1:N:146:GLN:HE21	1:N:150:ILE:HD11	1.69	0.56
1:J:123:ALA:HB2	1:J:440:ILE:HG23	1.88	0.56
1:A:111:MET:HG2	1:A:435:ASP:OD1	2.05	0.56
1:C:419:LEU:HG	1:C:447:MET:HG2	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:H:404:ARG:HG2	1:H:404:ARG:NH1	2.20	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:M:47:PRO:HG2	1:N:73:MET:HG3	1.88	0.56
1:M:69:MET:HE2	1:M:522:THR:HB	1.88	0.56
1:M:199:TYR:HA	1:M:276:VAL:HG12	1.86	0.56
2:T:3:ILE:HD13	2:T:11:ILE:HG21	1.87	0.56
1:H:199:TYR:HA	1:H:276:VAL:HG12	1.87	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:M:90:THR:O	1:M:94:VAL:HG23	2.05	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
1:K:2:ALA:O	1:K:4:LYS:HE3	2.05	0.55
2:O:3:ILE:HD13	2:O:11:ILE:HG21	1.88	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:H:146:GLN:HE21	1:H:150:ILE:HD11	1.70	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:F:124:VAL:HG13	1:F:504:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:413:ALA:HB1	1:M:417:VAL:HB	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:HH11	1:C:18:ARG:CB	2.18	0.55
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.88	0.55
1:N:77:VAL:HG22	1:N:506:TYR:HD1	1.71	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:F:74:VAL:HG13	1:F:514:MET:HE3	1.88	0.55
1:G:238:GLU:OE2	1:G:238:GLU:HA	2.07	0.55
1:I:426:LEU:CD1	1:I:444:LEU:HD21	2.31	0.55
1:K:313:THR:HG22	1:K:314:LEU:H	1.72	0.55
1:M:346:VAL:HG21	1:M:373:ALA:HB2	1.89	0.55
1:A:238:GLU:HA	1:A:238:GLU:OE2	2.07	0.55
1:D:409:GLU:CD	1:D:501:ARG:HH21	2.07	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:N:149:THR:CG2	1:N:159:GLY:HA3	2.36	0.55
1:N:419:LEU:HD21	1:N:500:THR:HG23	1.89	0.55
1:N:452:ARG:HG2	1:N:452:ARG:NH1	2.22	0.55
1:H:24:ALA:HA	1:H:27:VAL:HG12	1.88	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
2:R:13:LYS:HB3	2:R:41:LEU:HD11	1.89	0.54
1:C:238:GLU:OE2	1:C:238:GLU:HA	2.07	0.54
1:D:487:ASN:O	1:D:491:MET:HG3	2.08	0.54
1:E:64:ASP:HB3	1:E:67:GLU:HB2	1.90	0.54
1:I:27:VAL:HG11	1:I:93:THR:HG21	1.88	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:M:419:LEU:HD21	1:M:500:THR:HG23	1.89	0.54
2:Q:3:ILE:HD13	2:Q:11:ILE:HG21	1.88	0.54
1:G:18:ARG:CG	1:G:18:ARG:NH1	2.49	0.54
1:J:404:ARG:HG2	1:J:404:ARG:NH1	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: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:N:419:LEU:HD11	1:N:504:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:510:VAL:HG23	1:D:514:MET:CE	2.38	0.54
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.89	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: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:D:353:ILE:HG12	1:D:365:LEU:HB3	1.89	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
2:R:23:GLY:H	2:S:80:ASN:HD21	1.56	0.54
1:C:153:ASN:O	1:C:154:SER:HB2	2.07	0.54
1:J:77:VAL:HG22	1:J:506:TYR:HD1	1.73	0.54
1:J:346:VAL:HG21	1:J:373:ALA:HB2	1.88	0.54
1:A:18:ARG:HH11	1:A:18:ARG:CB	2.21	0.53
1:D:452:ARG:HG2	1:D:452:ARG:HH11	1.73	0.53
1:J:16:MET:O	1:J:20:VAL:HG12	2.08	0.53
1:J:223:ALA:HB3	1:J:251:ALA:HB2	1.90	0.53
1:J:419:LEU:HD11	1:J:504:LEU:HG	1.89	0.53
2:Q:13:LYS:HB3	2:Q:41:LEU:HD11	1.90	0.53
1:D:150:ILE:HD13	1:D:493:ILE:HA	1.90	0.53
1:G:510:VAL:CG2	1:G:514:MET:HE2	2.38	0.53
1:H:130:GLU:HG3	1:H:426:LEU:HD23	1.91	0.53
1:I:313:THR:HG22	1:I:314:LEU:H	1.74	0.53
1:L:218:PRO:HB3	1:L:246:PRO:HB2	1.91	0.53
1:B:238:GLU:OE2	1:B:238:GLU:HA	2.09	0.53
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.89	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:218:PRO:HB3	1:M:246:PRO:HB2	1.91	0.53
1:M:223:ALA:HB3	1:M:251:ALA:HB2	1.90	0.53
1:A:238:GLU:OE1	2:O:24:GLY:HA3	2.09	0.53
1:G:162:ILE:HG21	1:G:403:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:403:THR:O	1:K:407:VAL:HG23	2.09	0.53
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.90	0.53
1:J:419:LEU:HD21	1:J:500: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:B:302:SER:H	1:B:307:MET:HE3	1.74	0.53
1:C:18:ARG:CG	1:C:18:ARG:NH1	2.46	0.53
1:D:302:SER:H	1:D:307:MET:HE3	1.73	0.53
1:E:20:VAL:HG13	1:E:74:VAL:HG11	1.90	0.53
1:J:161:LEU:HD21	1:J:185:ASP:HB3	1.91	0.53
1:L:161:LEU:HD21	1:L:185:ASP:HB3	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:D:162:ILE:HG12	1:D:400:LEU:HD23	1.90	0.52
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:K:161:LEU:HD21	1:K:185:ASP:HB3	1.90	0.52
1:N:123:ALA:HB2	1:N:440:ILE:HG23	1.91	0.52
1:B:18:ARG:HH11	1:B:18:ARG:CB	2.20	0.52
1:C:409:GLU:OE2	1:C:501:ARG:NH2	2.33	0.52
1:E:238:GLU:OE2	1:E:238:GLU:HA	2.09	0.52
1:H:123:ALA:HB2	1:H:440:ILE:HG23	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
1:K:419:LEU:HD11	1:K:504:LEU:HG	1.92	0.52
2:Q:47:ARG:HD2	2:Q:49:LEU:HB2	1.91	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:N:66:PHE:H	1:N:69:MET:HG3	1.75	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:H:235:PRO:HG3	1:H:310:GLU:HA	1.92	0.52
1:K:145:ALA:O	1:K:149:THR:HG23	2.10	0.52
1:L:145:ALA:O	1:L:149:THR:HG23	2.09	0.52
1:B:162:ILE:HG12	1:B:400:LEU:HD23	1.91	0.52
1:F:77:VAL:HG23	1:F:92:ALA:HB1	1.91	0.52
1:M:326:ASN:ND2	1:M:328:ASP:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.90	0.52
2:O:23:GLY:H	2:P: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
2:Q:23:GLY:H	2:R:80:ASN:HD21	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:F:452:ARG:HG2	1:F:452:ARG:HH11	1.74	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:L:326:ASN:ND2	1:L:328:ASP:H	2.08	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
1:F:238:GLU:HA	1:F:238:GLU:OE2	2.08	0.52
1:H:161:LEU:HD21	1:H:185:ASP:HB3	1.92	0.52
1:H:443:ALA:O	1:H:447:MET:HG3	2.10	0.52
1:N:411:VAL:HG21	1:N:494:LEU:HD12	1.92	0.52
2:T:47:ARG:HD2	2:T:49:LEU:HB2	1.92	0.52
1:H:102:GLU:OE2	1:H:445:ARG:NH1	2.43	0.52
1:H:130:GLU:HG3	1:H:426:LEU:CD2	2.40	0.52
1:K:19:GLY:HA3	1:K:67:GLU:O	2.09	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:C:381:VAL:CG1	1:C:392:LYS:HG2	2.40	0.51
1:C:501:ARG:HD3	1:C:505:GLN:OE1	2.11	0.51
1:D:6:VAL:O	1:D:6:VAL:HG23	2.11	0.51
1:E:162:ILE:HG12	1:E:400:LEU:HD23	1.91	0.51
1:K:346:VAL:HG21	1:K:373:ALA:HB2	1.91	0.51
1:M:2:ALA:O	1:M:4:LYS:HE3	2.11	0.51
1:M:145:ALA:O	1:M:149:THR:HG23	2.10	0.51
1:M:161:LEU:HD21	1:M:185:ASP:HB3	1.91	0.51
1:N:131:LEU:CD1	1:N:422:VAL:HG11	2.40	0.51
2:P:23:GLY:H	2:Q:80:ASN:HD21	1.58	0.51
1:A:487:ASN:O	1:A:491:MET:HG3	2.10	0.51
1:C:302:SER:H	1:C:307:MET:HE3	1.75	0.51
1:D:32:GLY:HA2	4:D:703:ADP:H5'1	1.91	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:C:449:ALA:HB3	1:C:450:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:ARG:HG2	1:C:452:ARG:HH11	1.74	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:J:16:MET:O	1:J:20:VAL:CG1	2.59	0.51
1:K:149:THR:CG2	1:K:156:GLU:HA	2.41	0.51
1:M:64:ASP:HB3	1:M:67:GLU:HB2	1.91	0.51
2:T:47:ARG:HD3	2:T:49:LEU:HD12	1.93	0.51
1:E:432:GLN:NE2	1:E:436:GLN:NE2	2.39	0.51
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.91	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:C:268:ARG:HH21	2:Q:27:LEU:HD23	1.74	0.51
1:F:162:ILE:HG12	1:F:400:LEU:HD23	1.92	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:L:346:VAL:HG21	1:L:373:ALA:HB2	1.92	0.51
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.93	0.51
1:N:419:LEU:HD22	1:N:500:THR:CG2	2.41	0.51
1:E:224:ASP:HB3	1:E:302:SER:HA	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:L:77:VAL:HG22	1:L:506:TYR:HD1	1.75	0.51
1:E:153:ASN:O	1:E:154:SER:HB2	2.11	0.51
1:F:18:ARG:HH11	1:F:18:ARG:CB	2.21	0.51
1:I:161:LEU:HD21	1:I:185:ASP:HB3	1.92	0.51
1:J:218:PRO:HB3	1:J:246:PRO:HB2	1.93	0.51
1:N:476:TYR:HA	1:N:486:GLY:O	2.10	0.51
2:U:11:ILE:HG12	2:U:85:ILE:HG12	1.93	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:146:GLN:HE21	1:I:150:ILE:HD11	1.74	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
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:A:28:LYS:HD2	1:A:453:GLN:CD	2.31	0.50
1:B:420:ILE:HD13	1:B:451:LEU:HD13	1.93	0.50
1:D:238:GLU:HA	1:D:238:GLU:OE2	2.11	0.50
1:G:238:GLU:OE1	2:U:24:GLY:HA3	2.11	0.50
1:L:64:ASP:C	1:L:65:LYS:O	2.46	0.50
1:L:228:SER:O	1:L:257:GLU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:409:GLU:CD	1:A:501:ARG:HH21	2.10	0.50
1:B:381:VAL:HG21	1:B:393:LYS:HA	1.93	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:J:66:PHE:H	1:J:69:MET:HG3	1.77	0.50
1:A:300:VAL:O	1:A:307:MET:HE3	2.11	0.50
1:C:42:LYS:HE2	1:C:48:THR:OG1	2.11	0.50
1:D:204:PHE:HE1	1:D:274:ALA:HB2	1.77	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:K:102:GLU:OE2	1:K:445:ARG:NH1	2.44	0.50
2:O:50:GLU:HA	2:U:50:GLU:OE1	2.11	0.50
2:P:47:ARG:HD2	2:P:49:LEU:HB2	1.94	0.50
1:B:237:LEU:HD21	1:B:271:VAL:HG21	1.93	0.50
1:H:417:VAL:HG21	1:H:488:MET:HG3	1.92	0.50
1:L:96:ALA:O	1:L:100:ILE:HG13	2.11	0.50
1:N:2:ALA:O	1:N:4:LYS:HE3	2.11	0.50
1:N:145:ALA:O	1:N:149:THR:HG23	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: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
1:J:413:ALA:HB1	1:J:417:VAL:HB	1.92	0.50
1:K:218:PRO:HB3	1:K:246:PRO:HB2	1.93	0.50
1:N:193:MET:HG3	1:N:371:LYS:HB3	1.93	0.50
2:O:47:ARG:HD2	2:O:49:LEU:HB2	1.94	0.50
2:T:6:LEU:O	2:T:7:HIS:O	2.29	0.50
1:B:452:ARG:HH11	1:B:452:ARG:HG2	1.75	0.50
1:C:28:LYS:HD2	1:C:453:GLN:CD	2.32	0.50
1:F:356:ALA:HB3	1:F:362:ARG:HG3	1.94	0.50
1:I:346:VAL:HG21	1:I:373:ALA:HB2	1.93	0.50
1:J:135:SER:HA	1:J:412:VAL:HG12	1.94	0.50
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.94	0.50
1:A:356:ALA:HB3	1:A:362:ARG:HG3	1.94	0.50
1:B:224:ASP:HB3	1:B:302:SER:HA	1.93	0.50
1:D:28:LYS:HD2	1:D:453:GLN:CD	2.32	0.50
1:E:381:VAL:HG21	1:E:393:LYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ASP:HB3	1:F:302:SER:HA	1.93	0.50
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.92	0.50
1:M:102:GLU:OE2	1:M:445:ARG:NH1	2.45	0.50
1:N:30:THR:HB	1:N:51:LYS:O	2.12	0.50
1:N:161:LEU:HD21	1:N:185:ASP:HB3	1.93	0.50
2:U:47:ARG:HD3	2:U:49:LEU:HD12	1.94	0.50
1:A:124:VAL:HG13	1:A:504:LEU:HD13	1.94	0.50
1:B:34:LYS:HD2	1:B:458:CYS:SG	2.52	0.50
1:B:381:VAL:CG1	1:B:392:LYS:HG2	2.42	0.50
1:C:77:VAL:HG23	1:C:92:ALA:HB1	1.93	0.50
1:C:162:ILE:HG12	1:C:400:LEU:HD23	1.93	0.50
1:C:381:VAL:HG21	1:C:393:LYS:HA	1.93	0.50
1:E:111:MET:HG2	1:E:435:ASP:OD1	2.12	0.50
1:I:19:GLY:HA3	1:I:67:GLU:O	2.11	0.50
1:M:149:THR:CG2	1:M:156:GLU:HA	2.42	0.50
1:C:237:LEU:HD21	1:C:271:VAL:HG21	1.93	0.49
1:D:501:ARG:HD3	1:D:505:GLN:OE1	2.12	0.49
1:H:419:LEU:HD11	1:H:504:LEU:HG	1.94	0.49
1:M:19:GLY:HA3	1:M:67:GLU:O	2.12	0.49
1:A:42:LYS:HG2	1:A:44:PHE:CE2	2.47	0.49
1:D:224:ASP:HB3	1:D:302:SER:HA	1.93	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:G:237:LEU:HD21	1:G:271:VAL:HG21	1.93	0.49
1:C:124:VAL:HG13	1:C:504:LEU:HD13	1.93	0.49
1:E:356:ALA:HB3	1:E:362:ARG:HG3	1.94	0.49
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.94	0.49
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.94	0.49
2:R:47:ARG:HD2	2:R:49:LEU:HB2	1.94	0.49
1:K:228:SER:O	1:K:257:GLU:HB3	2.12	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:D:522:THR:OG1	1:D:523:ASP:N	2.46	0.49
1:F:237:LEU:HD21	1:F:271:VAL:HG21	1.93	0.49
1:H:259:LEU:O	1:H:263:VAL:HG23	2.13	0.49
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.94	0.49
1:N:218:PRO:HB3	1:N:246:PRO:HB2	1.95	0.49
1:G:74:VAL:HG13	1:G:514:MET:HE1	1.95	0.49
1:H:77:VAL:HG22	1:H:506:TYR:HD1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:ALA:O	1:L:4:LYS:HE3	2.13	0.49
1:L:163:ALA:O	1:L:167:ASP:HB2	2.12	0.49
2:Q:47:ARG:HD3	2:Q:49:LEU:HD12	1.94	0.49
1:C:224:ASP:HB3	1:C:302:SER:HA	1.94	0.49
1:K:193:MET:HG3	1:K:371:LYS:HB3	1.94	0.49
1:K:449:ALA:HB3	1:K:450:PRO:HD3	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: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:J:193:MET:HG3	1:J:371:LYS:HB3	1.93	0.49
1:M:135:SER:HA	1:M:412:VAL:HG12	1.95	0.49
1:G:28:LYS:C	1:G:30:THR:N	2.66	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
2:O:80:ASN:ND2	2:U:23:GLY:H	2.09	0.49
1:H:360:TYR:O	1:H:364:LYS:HB2	2.12	0.49
1:J:360:TYR:O	1:J:364:LYS:HB2	2.13	0.49
2:T:11:ILE:HG12	2:T:85:ILE:HG12	1.95	0.49
1:A:237:LEU:HD21	1:A:271:VAL:HG21	1.95	0.48
1:E:204:PHE:HE1	1:E:274:ALA:HB2	1.77	0.48
1:G:356:ALA:HB3	1:G:362:ARG:HG3	1.95	0.48
1:G:414:GLY:O	1:G:417:VAL:CG1	2.45	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:18:ARG:HB2	1:A:67:GLU:HG2	1.95	0.48
1:B:356:ALA:HB3	1:B:362:ARG:HG3	1.95	0.48
1:C:95:LEU:O	1:C:99:ILE:HG13	2.12	0.48
1:E:18:ARG:HH11	1:E:18:ARG:CB	2.25	0.48
1:H:419:LEU:HD21	1:H:500:THR:CG2	2.40	0.48
1:H:452:ARG:HG2	1:H:452:ARG:NH1	2.27	0.48
1:I:66:PHE:H	1:I:69:MET:HG3	1.78	0.48
1:J:38:VAL:HG22	1:K:519:CYS:HB3	1.94	0.48
1:L:411:VAL:HG21	1:L:494:LEU:HD12	1.94	0.48
1:C:247:LEU:HB3	1:C:273:VAL:HG12	1.94	0.48
1:C:517:THR:HG23	1:D:39:VAL:HG23	1.95	0.48
1:N:15:LYS:HB3	1:N:66:PHE:HB3	1.95	0.48
1:H:403:THR:O	1:H:407:VAL:HG23	2.13	0.48
1:I:179:ASP:OD1	1:I:393:LYS:HD2	2.13	0.48
1:M:130:GLU:HG3	1:M:426:LEU:HD23	1.94	0.48
1:M:443:ALA:O	1:M:447:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.95	0.48
1:N:266:THR:CG2	1:N:273:VAL:H	2.26	0.48
2:O:47:ARG:HD3	2:O:49:LEU:HD12	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:K:413:ALA:HB1	1:K:417:VAL:HB	1.95	0.48
1:I:80:LYS:HA	1:I:83:ASP:HB2	1.94	0.48
1:L:428:ASP:O	1:L:430:ARG:HG2	2.13	0.48
1:N:130:GLU:HG3	1:N:426:LEU:CD2	2.44	0.48
2:O:11:ILE:HG12	2:O:85:ILE:HG12	1.95	0.48
2:P:11:ILE:HG12	2:P:85:ILE:HG12	1.94	0.48
1:A:257:GLU:O	1:A:261:THR:HG23	2.13	0.48
1:C:204:PHE:HE1	1:C:274:ALA:HB2	1.77	0.48
1:D:356:ALA:HB3	1:D:362:ARG:HG3	1.95	0.48
1:D:420:ILE:HD13	1:D:451:LEU:HD13	1.95	0.48
1:H:193:MET:HG3	1:H:371:LYS:HB3	1.94	0.48
1:M:130:GLU:HG3	1:M:426:LEU:CD2	2.43	0.48
1:N:455:VAL:HG13	1:N:460:GLU:HB2	1.95	0.48
1:B:381:VAL:CG1	1:B:392:LYS:CG	2.91	0.48
1:D:102:GLU:HB3	1:D:442:VAL:HG22	1.96	0.48
1:E:18:ARG:CG	1:E:18:ARG:NH1	2.51	0.48
1:E:95:LEU:O	1:E:99:ILE:HG13	2.13	0.48
1:G:162:ILE:HG12	1:G:400:LEU:HD23	1.95	0.48
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:J:102:GLU:HB3	1:J:442:VAL:HG22	1.96	0.48
1:J:321:LYS:HB2	1:J:334:ASP:HB3	1.96	0.48
1:K:30:THR:HB	1:K:51:LYS:O	2.13	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: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:H:519:CYS:HB3	1:N:38:VAL:HG22	1.96	0.48
1:I:15:LYS:HB3	1:I:66:PHE:HB3	1.96	0.48
1:I:34:LYS:HB2	1:I:458:CYS:SG	2.54	0.48
1:I:77:VAL:HG22	1:I:506:TYR:HD1	1.78	0.48
1:K:102:GLU:HB3	1:K:442:VAL:HG22	1.96	0.48
1:L:179:ASP:OD1	1:L:393:LYS:HD2	2.14	0.48
2:R:34:LYS:HG3	2:R:35:SER:H	1.79	0.48
1:C:356:ALA:HB3	1:C:362:ARG:HG3	1.95	0.48
1:D:237:LEU:HD21	1:D:271:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:LEU:HB3	1:E:273:VAL:HG12	1.96	0.48
1:K:123:ALA:HB2	1:K:440:ILE:HG23	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:A:32:GLY:HA2	4:A:700:ADP:H5'1	1.96	0.47
1:A:510:VAL:HG23	1:A:514:MET:HE2	1.96	0.47
1:B:206:ASN:O	1:B:207:LYS:HG2	2.14	0.47
1:B:257:GLU:O	1:B:261:THR:HG23	2.14	0.47
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.95	0.47
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: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:N:11:ASP:O	1:N:12:ALA:C	2.50	0.47
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.96	0.47
1:H:226:LYS:HG3	1:H:252:GLU:HB3	1.96	0.47
1:K:16:MET:HG3	1:K:520:MET:SD	2.54	0.47
1:K:259:LEU:O	1:K:263:VAL: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:F:197:ARG:HA	1:F:197:ARG:HD3	1.62	0.47
1:F:204:PHE:HE1	1:F:274:ALA:HB2	1.79	0.47
1:H:455:VAL:HG11	1:H:461:GLU:O	2.13	0.47
1:I:163:ALA:O	1:I:167:ASP:HB2	2.14	0.47
1:I:259:LEU:O	1:I:263:VAL:HG23	2.14	0.47
1:J:266:THR:CG2	1:J:273:VAL:H	2.27	0.47
2:S:47:ARG:HD3	2:S:49:LEU:HD12	1.95	0.47
1:A:80:LYS:HD2	1:A:506:TYR:CE1	2.50	0.47
1:A:204:PHE:HE1	1:A:274:ALA:HB2	1.78	0.47
1:B:232:GLU:HB3	1:B:309:LEU:HB3	1.96	0.47
1:C:74:VAL:HG13	1:C:514:MET:HE1	1.95	0.47
1:F:461:GLU:HA	1:F:462:PRO:HD3	1.79	0.47
1:I:103:GLY:O	1:I:106:ALA:HB3	2.14	0.47
1:I:266:THR:CG2	1:I:273:VAL:H	2.27	0.47
1:J:138:CYS:SG	1:J:144:ILE:HD13	2.54	0.47
1:J:417:VAL:HG21	1:J:488:MET:HG3	1.96	0.47
1:N:69:MET:HE2	1:N:522:THR:HB	1.93	0.47
2:P:47:ARG:HD3	2:P:49:LEU:HD12	1.95	0.47
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.97	0.47
1:F:381:VAL:HG21	1:F:393:LYS:HA	1.96	0.47
1:H:135:SER:HA	1:H:412:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:ASP:OD1	1:J:393:LYS:HD2	2.15	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:N:163:ALA:O	1:N:167:ASP:HB2	2.14	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:G:42:LYS:HG2	1:G:44:PHE:CE2	2.50	0.47
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.96	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
1:F:381:VAL:CG1	1:F:392:LYS:HG2	2.45	0.47
1:F:432:GLN:NE2	1:F:436:GLN:NE2	2.41	0.47
1:G:455:VAL:HG21	1:G:465:VAL:HG11	1.96	0.47
1:G:510:VAL:CG2	1:G:514:MET:CE	2.92	0.47
1:I:123:ALA:HB2	1:I:440:ILE:HG23	1.97	0.47
1:N:15:LYS:HA	1:N:15:LYS:HD3	1.70	0.47
2:O:78:ILE:HD13	2:O:83:VAL:HG21	1.96	0.47
2:R:47:ARG:HD3	2:R:49:LEU:HD12	1.95	0.47
2:S:11:ILE:HG12	2:S:85:ILE:HG12	1.95	0.47
1:B:234:LEU:HD22	2:P:23:GLY:HA3	1.96	0.47
1:B:268:ARG:HH21	2:P:27:LEU:CD2	2.27	0.47
1:E:232:GLU:HB3	1:E:309:LEU:HB3	1.96	0.47
1:E:510:VAL:HG23	1:E:514:MET:CE	2.45	0.47
1:F:232:GLU:HB3	1:F:309:LEU:HB3	1.96	0.47
1:G:18:ARG:HH11	1:G:18:ARG:CB	2.26	0.47
1:G:232:GLU:HB3	1:G:309:LEU:HB3	1.97	0.47
1:G:247:LEU:HB3	1:G:273:VAL:HG12	1.97	0.47
1:I:365:LEU:O	1:I:369:VAL:HG23	2.15	0.47
1:J:15:LYS:HB3	1:J:66:PHE:HB3	1.97	0.47
1:J:228:SER:O	1:J:257:GLU:HB3	2.15	0.47
1:K:179:ASP:OD1	1:K:393:LYS:HD2	2.14	0.47
1:K:443:ALA:O	1:K:447:MET:HG3	2.14	0.47
1:L:130:GLU:HG3	1:L:426:LEU:CD2	2.44	0.47
1:L:360:TYR:O	1:L:364:LYS:HB2	2.15	0.47
1:L:413:ALA:HB1	1:L:417:VAL:HB	1.97	0.47
1:A:247:LEU:HB3	1:A:273:VAL:HG12	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
1:F:18:ARG:HB2	1:F:67:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.96	0.47
1:I:130:GLU:HG3	1:I:426:LEU:HD23	1.97	0.47
1:I:360:TYR:O	1:I:364:LYS:HB2	2.15	0.47
1:L:30:THR:HB	1:L:51:LYS:O	2.14	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:L:266:THR:CG2	1:L:273:VAL:H	2.27	0.47
1:M:444:LEU:HD23	1:M:444:LEU:HA	1.72	0.47
2:Q:50:GLU:OE1	2:R:50:GLU:HA	2.15	0.47
1:D:233:MET:HB3	1:D:237:LEU:HD12	1.96	0.47
1:G:206:ASN:O	1:G:207:LYS:HG2	2.15	0.47
1:I:135:SER:HA	1:I:412:VAL:HG12	1.96	0.47
1:I:321:LYS:HB2	1:I:334:ASP:HB3	1.97	0.47
1:K:411:VAL:HG21	1:K:494:LEU:HD12	1.97	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:B:247:LEU:HB3	1:B:273:VAL:HG12	1.96	0.46
1:C:73:MET:CE	1:C:73:MET:CG	2.92	0.46
1:D:247:LEU:HB3	1:D:273:VAL:HG12	1.97	0.46
1:G:257:GLU:O	1:G:261:THR:HG23	2.15	0.46
1:H:228:SER:O	1:H:257:GLU:HB3	2.15	0.46
1:H:326:ASN:ND2	1:H:328:ASP:H	2.12	0.46
1:I:428:ASP:O	1:I:430:ARG:HG2	2.14	0.46
1:L:11:ASP:O	1:L:12:ALA:C	2.51	0.46
1:M:77:VAL:HG11	1:M:510:VAL:HB	1.97	0.46
1:N:360:TYR:O	1:N:364:LYS:HB2	2.15	0.46
1:B:414:GLY:O	1:B:417:VAL:CG1	2.43	0.46
1:J:259:LEU:O	1:J:263:VAL:HG23	2.15	0.46
1:L:16:MET:HG3	1:L:520:MET:SD	2.56	0.46
1:L:476:TYR:HA	1:L:486:GLY:O	2.15	0.46
1:M:266:THR:CG2	1:M:273:VAL:H	2.28	0.46
1:A:206:ASN:O	1:A:207:LYS:HG2	2.15	0.46
1:C:233:MET:HB3	1:C:237:LEU:HD12	1.96	0.46
1:E:18:ARG:HB2	1:E:67:GLU:HG2	1.97	0.46
1:E:420:ILE:HD13	1:E:451:LEU:HD13	1.97	0.46
1:F:302:SER:H	1:F:307:MET:HE3	1.79	0.46
1:G:351:GLN:O	1:G:351:GLN:HG2	2.15	0.46
1:K:40:LEU:HD12	1:L:521:VAL:HB	1.96	0.46
1:K:262:LEU:O	1:K:266:THR:HG23	2.15	0.46
1:K:433:ASN:OD1	1:K:435:ASP:HB2	2.16	0.46
1:M:13:ARG:HD2	1:M:104:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:232:GLU:HB3	1:C:309:LEU:HB3	1.98	0.46
1:C:351:GLN:O	1:C:351:GLN:HG2	2.16	0.46
1:D:232:GLU:HB3	1:D:309:LEU:HB3	1.98	0.46
1:G:233:MET:HB3	1:G:237:LEU:HD12	1.98	0.46
1:B:254:VAL:HG12	1:B:259:LEU:HB2	1.97	0.46
1:J:100:ILE:HG23	1:J:104:LEU:HD22	1.97	0.46
1:L:135:SER:HA	1:L:412:VAL:HG12	1.98	0.46
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.98	0.46
1:A:430:ARG:NH1	1:A:430:ARG:CG	2.78	0.46
1:A:510:VAL:CG2	1:A:514:MET:HE2	2.45	0.46
1:B:204:PHE:HE1	1:B:274:ALA:HB2	1.80	0.46
1:E:461:GLU:HA	1:E:462:PRO:HD3	1.82	0.46
1:H:85:ALA:HA	1:H:498:LYS:HD3	1.98	0.46
1:I:403:THR:O	1:I:407:VAL:HG23	2.15	0.46
1:M:77:VAL:HG22	1:M:506:TYR:HD1	1.81	0.46
1:M:259:LEU:O	1:M:263:VAL:HG23	2.15	0.46
1:N:321:LYS:HB2	1:N:334:ASP:HB3	1.98	0.46
1:N:413:ALA:HB1	1:N:417:VAL:HB	1.98	0.46
1:C:248:LEU:HD22	1:C:323:VAL:HG11	1.97	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:D:455:VAL:HG21	1:D:465:VAL:HG11	1.98	0.46
1:E:381:VAL:CG1	1:E:392:LYS:CG	2.94	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:A:351:GLN:HG2	1:A:351:GLN:O	2.15	0.46
1:A:381:VAL:HG21	1:A:393:LYS:HA	1.98	0.46
1:E:501:ARG:HD3	1:E:505:GLN:OE1	2.16	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: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:E:91:THR:O	1:E:92:ALA:C	2.53	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:J:411:VAL:HG21	1:J:494:LEU:HD12	1.97	0.46
1:N:130:GLU:HG3	1:N:426:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:HA2	4:B:701:ADP:H5'1	1.98	0.46
1:C:206:ASN:O	1:C:207:LYS:HG2	2.16	0.46
1:D:254:VAL:HG12	1:D:259:LEU:HB2	1.97	0.46
1:E:124:VAL:HG13	1:E:504:LEU:HD13	1.96	0.46
1:F:28:LYS:HD2	1:F:453:GLN:CD	2.36	0.46
1:M:38:VAL:HG12	1:M:40:LEU:HD13	1.96	0.46
2:T:78:ILE:HD13	2:T:83:VAL:HG21	1.98	0.46
1:A:381:VAL:CG1	1:A:392:LYS:CG	2.94	0.45
1:B:351:GLN:O	1:B:351:GLN:HG2	2.16	0.45
1:G:501:ARG:HD3	1:G:505:GLN:OE1	2.15	0.45
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.56	0.45
1:K:426:LEU:O	1:K:444:LEU:HD11	2.16	0.45
1:A:501:ARG:HD3	1:A:505:GLN:OE1	2.16	0.45
1:F:351:GLN:O	1:F:351:GLN:HG2	2.16	0.45
1:G:225:LYS:HG2	1:G:303:GLU:HB2	1.99	0.45
1:G:381:VAL:HG21	1:G:393:LYS:HA	1.98	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:L:433:ASN:OD1	1:L:435:ASP:HB2	2.17	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
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:A:49:ILE:HD13	1:G:513:LEU:HB3	1.97	0.45
1:D:381:VAL:CG1	1:D:392:LYS:HG2	2.47	0.45
1:D:381:VAL:HG21	1:D:393:LYS:HA	1.97	0.45
1:E:261:THR:HG22	2:S:29:GLY:HA3	1.97	0.45
1:I:270:ILE:HA	1:J:257:GLU:OE2	2.16	0.45
2:S:78:ILE:HD13	2:S:83:VAL:HG21	1.99	0.45
1:A:384:ALA:O	1:G:506:TYR:HE1	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:D:225:LYS:HG2	1:D:303:GLU:HB2	1.98	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:I:104:LEU:HD12	1:I:104:LEU:HA	1.75	0.45
1:M:179:ASP:OD1	1:M:393:LYS:HD2	2.17	0.45
2:R:78:ILE:HD13	2:R:83:VAL:HG21	1.98	0.45
1:C:23:LEU:CD1	1:C:23:LEU:C	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:270:ILE:HG23	1:L:229:ASN:HD21	1.82	0.45
1:M:138:CYS:SG	1:M:144:ILE:HD13	2.56	0.45
1:M:321:LYS:HB2	1:M:334:ASP:HB3	1.99	0.45
1:A:77:VAL:HG23	1:A:92:ALA:HB1	1.99	0.45
1:B:300:VAL:O	1:B:307:MET:HE3	2.17	0.45
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.57	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
1:N:228:SER:O	1:N:257:GLU:HB3	2.17	0.45
2:S:23:GLY:H	2:T:80:ASN:HD21	1.64	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:G:197:ARG:HG2	1:G:277:LYS:O	2.17	0.45
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.57	0.45
1:L:365:LEU:O	1:L:369:VAL:HG23	2.16	0.45
1:L:433:ASN:HD22	1:L:433:ASN:HA	1.59	0.45
1:L:444:LEU:HD23	1:L:444:LEU:HA	1.74	0.45
1:M:270:ILE:HG23	1:N:229:ASN:ND2	2.32	0.45
1:A:28:LYS:HD2	1:A:453:GLN:NE2	2.31	0.45
1:C:257:GLU:O	1:C:261:THR:HG23	2.17	0.45
1:D:105:LYS:HB2	1:D:105:LYS:HE3	1.74	0.45
1:E:351:GLN:O	1:E:351:GLN:HG2	2.16	0.45
1:F:233:MET:HB3	1:F:237:LEU:HD12	1.98	0.45
1:F:413:ALA:CB	1:F:417:VAL:HG13	2.47	0.45
1:I:417:VAL:HG21	1:I:488:MET:HG3	1.98	0.45
1:M:16:MET:HG3	1:M:520:MET:SD	2.57	0.45
1:D:351:GLN:O	1:D:351:GLN:HG2	2.16	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:L:16:MET:O	1:L:20:VAL:HG12	2.17	0.45
1:L:47:PRO:CG	1:M:73:MET:HG3	2.44	0.45
1:L:419:LEU:HD11	1:L:504:LEU:HG	1.99	0.45
1:J:64:ASP:OD1	1:J:65:LYS:O	2.34	0.44
1:J:365:LEU:O	1:J:369:VAL:HG23	2.17	0.44
1:L:259:LEU:O	1:L:263:VAL:HG23	2.18	0.44
2:Q:11:ILE:HG12	2:Q:85:ILE:HG12	1.98	0.44
1:C:32:GLY:HA2	4:C:702:ADP:H5'1	1.98	0.44
1:D:28:LYS:C	1:D:30:THR:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:LYS:HB3	1:H:66:PHE:HB3	1.99	0.44
1:I:213:VAL:O	1:I:324:VAL:HA	2.17	0.44
1:K:444:LEU:HD23	1:K:444:LEU:HA	1.69	0.44
1:N:262:LEU:O	1:N:266:THR:HG23	2.17	0.44
1:N:429:LEU:HB3	1:N:440:ILE:HG21	2.00	0.44
2:P:34:LYS:HG3	2:P:35:SER:H	1.82	0.44
1:B:153:ASN:O	1:B:154:SER:HB2	2.17	0.44
1:E:28:LYS:HD2	1:E:453:GLN:CD	2.38	0.44
1:E:257:GLU:O	1:E:261:THR:HG23	2.17	0.44
1:F:510:VAL:HG23	1:F:514:MET:CE	2.47	0.44
1:K:16:MET:O	1:K:20:VAL:HG12	2.17	0.44
1:M:417:VAL:HG21	1:M:488:MET:HG3	1.99	0.44
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.57	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:B:18:ARG:HB2	1:B:67:GLU:HG2	1.99	0.44
1:C:420:ILE:HD13	1:C:451:LEU:HD13	1.99	0.44
1:F:254:VAL:HG12	1:F:259:LEU:HB2	2.00	0.44
1:J:163:ALA:O	1:J:167:ASP:HB2	2.17	0.44
1:N:16:MET:HG3	1:N:520:MET:SD	2.57	0.44
1:N:77:VAL:HG11	1:N:510:VAL:HB	1.99	0.44
2:Q:43:VAL:HG13	2:Q:57:LEU:HD12	2.00	0.44
1:A:461:GLU:HA	1:A:462:PRO:HD3	1.89	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:E:233:MET:HB3	1:E:237:LEU:HD12	1.98	0.44
1:G:16:MET:O	1:G:20:VAL:HG23	2.18	0.44
1:G:18:ARG:HB2	1:G:67:GLU:HG2	1.99	0.44
1:G:24:ALA:O	1:G:28:LYS:HG3	2.17	0.44
1:G:197:ARG:HA	1:G:197:ARG:HD3	1.64	0.44
1:H:15:LYS:HA	1:H:15:LYS:HD3	1.72	0.44
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.58	0.44
1:J:69:MET:HE2	1:J:522:THR:HB	1.95	0.44
1:J:444:LEU:HA	1:J:444:LEU:HD23	1.71	0.44
1:K:38:VAL:HG12	1:K:40:LEU:HD13	1.98	0.44
1:K:126:ALA:HB1	1:K:426:LEU:HD22	2.00	0.44
1:L:226:LYS:HG3	1:L:252:GLU:HB3	1.99	0.44
1:L:342:ILE:O	1:L:346:VAL:HG23	2.17	0.44
1:M:419:LEU:HD21	1:M:500:THR:CG2	2.42	0.44
1:C:413:ALA:CB	1:C:417:VAL:HG13	2.47	0.44
1:E:150:ILE:HD13	1:E:493:ILE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:PRO:HG3	4:F:705:ADP:C6	2.53	0.44
4:G:706:ADP:O3B	5:G:806:HOH:O	2.21	0.44
1:J:90:THR:O	1:J:94:VAL:HG23	2.17	0.44
1:N:513:LEU:HD12	1:N:513:LEU:HA	1.90	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:A:233:MET:HB3	1:A:237:LEU:HD12	2.00	0.44
1:C:28:LYS:HD2	1:C:453:GLN:NE2	2.33	0.44
1:C:225:LYS:HG2	1:C:303:GLU:HB2	2.00	0.44
1:C:365:LEU:O	1:C:369:VAL:HG13	2.18	0.44
1:E:31:LEU:HD23	1:E:453:GLN:HB3	2.00	0.44
1:E:225:LYS:HG2	1:E:303:GLU:HB2	1.99	0.44
1:E:421:ARG:HA	1:E:421:ARG:HD3	1.72	0.44
1:H:34:LYS:HB2	1:H:458:CYS:SG	2.58	0.44
1:A:130:GLU:HB3	1:A:422:VAL:HB	1.99	0.44
1:D:42:LYS:HG2	1:D:44:PHE:CE2	2.52	0.44
1:D:100:ILE:HD11	1:D:514:MET:CE	2.46	0.44
1:D:300:VAL:O	1:D:307:MET:HE3	2.18	0.44
1:D:301:ILE:HG22	1:D:301:ILE:O	2.18	0.44
1:F:162:ILE:HG21	1:F:403:THR:HG21	2.00	0.44
1:G:80:LYS:HD2	1:G:506:TYR:CE1	2.53	0.44
1:G:451:LEU:HD21	1:G:465:VAL:HG12	1.99	0.44
1:G:495:ASP:CG	4:G:706:ADP:HO2'	2.21	0.44
1:J:126:ALA:HB1	1:J:426:LEU:HD22	2.00	0.44
1:K:270:ILE:HG23	1:L:229:ASN:ND2	2.33	0.44
1:M:85:ALA:HA	1:M:498:LYS:HD3	2.00	0.44
1:I:228:SER:O	1:I:257:GLU:HB3	2.18	0.44
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:M:15:LYS:HB3	1:M:66:PHE:HB3	2.00	0.44
1:A:254:VAL:HG12	1:A:259:LEU:HB2	2.00	0.43
1:D:28:LYS:C	1:D:30:THR:N	2.68	0.43
1:D:327:LYS:O	1:D:327:LYS:HG2	2.18	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
1:F:451:LEU:HD21	1:F:465:VAL:HG12	1.98	0.43
1:G:28:LYS:HD2	1:G:453:GLN:NE2	2.32	0.43
1:I:285:ARG:HA	1:I:288:MET:HB2	1.99	0.43
1:I:296:THR:HB	1:I:319:GLN:H	1.82	0.43
1:I:326:ASN:HD22	1:I:328:ASP:H	1.65	0.43
1:J:64:ASP:C	1:J:65:LYS:O	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:455:VAL:HG11	1:L:461:GLU:O	2.17	0.43
1:M:15:LYS:HA	1:M:15:LYS:HD3	1.73	0.43
1:M:262:LEU:O	1:M:266:THR:HG23	2.17	0.43
2:T:43:VAL:HG13	2:T:57:LEU:HD12	2.00	0.43
1:A:349:ILE:HG23	1:A:365:LEU:HD12	2.00	0.43
1:A:361:ASP:O	1:A:365:LEU:HD23	2.18	0.43
1:E:234:LEU:HD22	2:S:23:GLY:HA3	1.99	0.43
1:J:104:LEU:HD12	1:J:104:LEU:HA	1.66	0.43
1:K:130:GLU:HG3	1:K:426:LEU:CD2	2.48	0.43
1:M:87:ASP:HB3	1:M:499:VAL:HG21	2.00	0.43
1:M:227:ILE:CD1	1:M:309:LEU:HD11	2.47	0.43
1:N:38:VAL:HG12	1:N:40:LEU:HD13	1.99	0.43
2:O:96:GLU:O	2:P:1:MET:HB2	2.18	0.43
1:A:102:GLU:HB3	1:A:442:VAL:HG22	2.01	0.43
1:A:381:VAL:HG11	1:A:392:LYS:HG3	2.01	0.43
1:B:413:ALA:CB	1:B:417:VAL:HG13	2.48	0.43
1:B:519:CYS:HB3	1:C:38:VAL:HG22	2.01	0.43
1:C:254:VAL:HG12	1:C:259:LEU:HB2	2.00	0.43
1:D:414:GLY:O	1:D:417:VAL:CG1	2.48	0.43
1:I:476:TYR:HA	1:I:486:GLY:O	2.18	0.43
2:T:34:LYS:HG3	2:T:35:SER:H	1.82	0.43
1:A:421:ARG:HD3	1:A:421:ARG:HA	1.68	0.43
1:D:6:VAL:O	1:D:6:VAL:CG2	2.66	0.43
1:D:18:ARG:HH11	1:D:18:ARG:HB3	1.83	0.43
1:H:30:THR:HB	1:H:51:LYS:O	2.18	0.43
1:H:365:LEU:O	1:H:369:VAL:HG23	2.19	0.43
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.90	0.43
1:K:452:ARG:HG2	1:K:452:ARG:NH1	2.32	0.43
1:N:102:GLU:OE2	1:N:445:ARG:NH1	2.50	0.43
1:N:104:LEU:HD12	1:N:104:LEU:HA	1.71	0.43
2:O:50:GLU:OE1	2:P:50:GLU:HA	2.18	0.43
1:G:175:ILE:HG21	1:G:400:LEU:HD21	2.01	0.43
1:J:80:LYS:HA	1:J:83:ASP:HB2	2.00	0.43
1:K:77:VAL:HG22	1:K:506:TYR:HD1	1.82	0.43
1:K:77:VAL:HG11	1:K:510:VAL:HB	1.98	0.43
1:K:130:GLU:HG3	1:K:426:LEU:HD23	1.99	0.43
1:K:226:LYS:HG3	1:K:252:GLU:HB3	2.00	0.43
1:N:213:VAL:O	1:N:324:VAL:HA	2.18	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:B:225:LYS:HG2	1:B:303:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:VAL:O	1:C:307:MET:HE3	2.19	0.43
1:F:197:ARG:HG2	1:F:277:LYS:O	2.18	0.43
1:L:102:GLU:HB3	1:L:442:VAL:HG22	2.01	0.43
1:N:77:VAL:HG22	1:N:506:TYR:CD1	2.53	0.43
1:C:510:VAL:HG23	1:C:514:MET:CE	2.49	0.43
1:D:18:ARG:CG	1:D:18:ARG:NH1	2.52	0.43
1:D:257:GLU:O	1:D:261:THR:HG23	2.18	0.43
1:H:409:GLU:OE2	1:H:501:ARG:NH2	2.47	0.43
1:I:443:ALA:O	1:I:447:MET:HG3	2.19	0.43
1:N:34:LYS:HB2	1:N:458:CYS:SG	2.58	0.43
2:P:50:GLU:OE1	2:Q:50:GLU:HA	2.19	0.43
2:Q:34:LYS:HG3	2:Q:35:SER:H	1.83	0.43
2:T:23:GLY:H	2:U:80:ASN:HD21	1.66	0.43
1:D:452:ARG:HG2	1:D:452:ARG:NH1	2.33	0.43
1:E:248:LEU:HD22	1:E:323:VAL:HG11	2.00	0.43
1:G:254:VAL:HG12	1:G:259:LEU:HB2	2.00	0.43
1:G:421:ARG:HD3	1:G:421:ARG:HA	1.69	0.43
1:K:524:LEU:HD23	1:K:524:LEU:HA	1.87	0.43
1:N:126:ALA:HB1	1:N:426:LEU:HD22	2.00	0.43
2:R:46:GLY:HA3	2:R:55:LYS:O	2.19	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:381:VAL:CG1	1:G:392:LYS:CG	2.97	0.43
1:G:524:LEU:HD23	1:G:524:LEU:HA	1.84	0.43
1:K:66:PHE:H	1:K:69:MET:HG3	1.83	0.43
1:L:34:LYS:HB2	1:L:458:CYS:SG	2.58	0.43
1:L:72:GLN:HA	1:L:72:GLN:NE2	2.33	0.43
1:M:80:LYS:HA	1:M:83:ASP:HB2	2.00	0.43
1:N:69:MET:CE	1:N:522:THR:CB	2.93	0.43
1:B:130:GLU:HB3	1:B:422:VAL:HB	2.01	0.43
1:E:42:LYS:HG2	1:E:44:PHE:CE2	2.53	0.43
1:E:409:GLU:OE2	1:E:501:ARG:NH2	2.42	0.43
1:F:248:LEU:HD22	1:F:323:VAL:HG11	1.99	0.43
1:G:19:GLY:HA3	1:G:67:GLU:O	2.19	0.43
1:G:28:LYS:HD2	1:G:453:GLN:CD	2.39	0.43
1:G:77:VAL:HG23	1:G:92:ALA:HB1	2.01	0.43
1:H:7:LYS:HD2	1:H:66:PHE:CE2	2.54	0.43
1:H:433:ASN:OD1	1:H:435:ASP:HB2	2.18	0.43
1:J:262:LEU:O	1:J:266:THR:HG23	2.18	0.43
1:M:419:LEU:HD22	1:M:500:THR:CG2	2.47	0.43
1:N:7:LYS:HD2	1:N:66:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ILE:O	1:B:301:ILE:HG22	2.19	0.42
1:F:257:GLU:O	1:F:261:THR:HG23	2.19	0.42
1:H:444:LEU:HD23	1:H:444:LEU:HA	1.72	0.42
1:I:96:ALA:O	1:I:100:ILE:HG13	2.18	0.42
1:K:64:ASP:OD1	1:K:65:LYS:O	2.37	0.42
1:K:270:ILE:HA	1:L:257:GLU:OE2	2.19	0.42
1:M:64:ASP:C	1:M:65:LYS:O	2.56	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:102:GLU:HB3	1:B:442:VAL:HG22	2.01	0.42
1:B:432:GLN:NE2	1:B:436:GLN:NE2	2.39	0.42
1:F:520:MET:HG2	1:G:39:VAL:HB	2.00	0.42
1:J:226:LYS:HG3	1:J:252:GLU:HB3	2.01	0.42
1:K:285:ARG:HA	1:K:288:MET:HB2	2.01	0.42
1:A:365:LEU:O	1:A:369:VAL:HG13	2.19	0.42
1:A:477:GLY:HA3	1:A:488:MET:SD	2.59	0.42
1:D:349:ILE:HG23	1:D:365:LEU:HD12	2.01	0.42
1:D:421:ARG:HA	1:D:421:ARG:HD3	1.73	0.42
1:G:349:ILE:HG23	1:G:365:LEU:HD12	2.01	0.42
1:G:455:VAL:HG11	1:G:462:PRO:HA	2.02	0.42
1:K:429:LEU:HB3	1:K:440:ILE:HG21	2.01	0.42
2:U:34:LYS:HG3	2:U:35:SER:H	1.84	0.42
2:U:43:VAL:HG13	2:U:57:LEU:HD12	2.01	0.42
1:A:286:LYS:HE2	1:A:304:GLU:OE1	2.19	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:D:105:LYS:HD3	1:K:110:GLY:O	2.19	0.42
1:D:248:LEU:HD22	1:D:323:VAL:HG11	2.01	0.42
1:D:451:LEU:HD21	1:D:465:VAL:HG12	2.01	0.42
1:G:288:MET:O	1:G:291:ASP:HB2	2.19	0.42
1:J:32:GLY:HA2	1:J:454:ILE:CD1	2.46	0.42
1:J:77:VAL:HG22	1:J:506:TYR:CD1	2.54	0.42
1:J:477:GLY:O	1:J:485:TYR:HA	2.19	0.42
1:L:524:LEU:HD23	1:L:524:LEU:HA	1.82	0.42
1:M:426:LEU:H	1:M:426:LEU:HG	1.67	0.42
1:M:441:LYS:O	1:M:442:VAL:C	2.58	0.42
1:N:215:LEU:HB3	1:N:218:PRO:HG3	2.01	0.42
1:N:285:ARG:HA	1:N:288:MET:HB2	2.01	0.42
1:D:77:VAL:HG23	1:D:92:ALA:HB1	2.01	0.42
1:E:80:LYS:HD2	1:E:506:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:LYS:HA	1:I:15:LYS:HD3	1.73	0.42
1:M:22:VAL:HG11	1:M:62:LEU:HD21	2.02	0.42
1:A:90:THR:O	1:A:94:VAL:HG23	2.19	0.42
1:A:381:VAL:CG1	1:A:392:LYS:HG2	2.49	0.42
1:B:510:VAL:HG23	1:B:514:MET:CE	2.49	0.42
1:D:28:LYS:O	1:D:30:THR:N	2.52	0.42
1:F:42:LYS:HG2	1:F:44:PHE:CE2	2.54	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:H:419:LEU:HD22	1:H:500:THR:CG2	2.47	0.42
1:K:15:LYS:HD3	1:K:15:LYS:HA	1.74	0.42
1:L:138:CYS:SG	1:L:144:ILE:HD13	2.60	0.42
1:L:213:VAL:O	1:L:324:VAL:HA	2.20	0.42
1:A:301:ILE:HG21	1:A:309:LEU:HD12	2.02	0.42
1:D:430:ARG:NH1	1:D:430:ARG:CG	2.75	0.42
1:F:34:LYS:HD2	1:F:458:CYS:SG	2.60	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:I:262:LEU:O	1:I:266:THR:HG23	2.19	0.42
1:J:8:PHE:O	1:J:9:GLY:C	2.57	0.42
1:J:419:LEU:HD22	1:J:500:THR:CG2	2.47	0.42
1:L:126:ALA:HB1	1:L:426:LEU:HD22	2.02	0.42
1:M:104:LEU:HA	1:M:104:LEU:HD12	1.72	0.42
1:M:413:ALA:CB	1:M:417:VAL:HB	2.50	0.42
1:N:87:ASP:HB3	1:N:499:VAL:HG21	2.02	0.42
1:A:150:ILE:HD13	1:A:493:ILE:HA	2.02	0.42
1:B:42:LYS:HG2	1:B:44:PHE:CE2	2.55	0.42
1:B:381:VAL:HG11	1:B:392:LYS:HG3	2.02	0.42
1:C:455:VAL:HG21	1:C:465:VAL:HG11	2.01	0.42
1:D:33:PRO:HG3	4:D:703:ADP:C6	2.55	0.42
1:D:41:ASP:O	1:D:42:LYS:HG3	2.20	0.42
1:E:286:LYS:HE2	1:E:304:GLU:OE1	2.20	0.42
1:F:204:PHE:O	1:F:204:PHE:CG	2.73	0.42
1:H:285:ARG:HA	1:H:288:MET:HB2	2.01	0.42
1:I:130:GLU:HG3	1:I:426:LEU:CD2	2.49	0.42
1:J:215:LEU:HB3	1:J:218:PRO:HG3	2.02	0.42
1:K:213:VAL:O	1:K:324:VAL:HA	2.20	0.42
1:M:215:LEU:HB3	1:M:218:PRO:HG3	2.01	0.42
1:M:234:LEU:N	1:M:235:PRO:HD2	2.34	0.42
1:N:444:LEU:HA	1:N:444:LEU:HD23	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:CG	1:A:368:ARG:HD2	2.50	0.42
1:E:455:VAL:HG21	1:E:465:VAL:HG11	2.02	0.42
1:F:219:PHE:HB3	1:F:317:LEU:HD13	2.01	0.42
1:F:301:ILE:O	1:F:301:ILE:HG22	2.20	0.42
1:F:501:ARG:HD3	1:F:505:GLN:OE1	2.19	0.42
1:K:11:ASP:O	1:K:12:ALA:C	2.59	0.42
1:K:342:ILE:O	1:K:346:VAL:HG23	2.20	0.42
1:L:15:LYS:HB3	1:L:66:PHE:HB3	2.02	0.42
1:L:80:LYS:HA	1:L:83:ASP:HB2	2.02	0.42
1:M:455:VAL:HG13	1:M:460:GLU:HB2	2.01	0.42
1:B:23:LEU:CD1	1:B:23:LEU:C	2.88	0.41
1:B:381:VAL:HG12	1:B:392:LYS:HG2	2.02	0.41
1:F:413:ALA:HB3	1:F:417:VAL:HG13	2.02	0.41
1:G:28:LYS:C	1:G:30:THR:H	2.22	0.41
1:H:234:LEU:N	1:H:235:PRO:HD2	2.35	0.41
1:J:213:VAL:O	1:J:324:VAL:HA	2.19	0.41
1:L:15:LYS:HA	1:L:15:LYS:HD3	1.76	0.41
1:L:285:ARG:HA	1:L:288:MET:HB2	2.02	0.41
1:L:443:ALA:O	1:L:447:MET:HG3	2.20	0.41
1:M:39:VAL:HB	1:N:520:MET:HG2	2.02	0.41
1:N:149:THR:HG22	1:N:156:GLU:HA	2.02	0.41
1:A:381:VAL:CG1	1:A:392:LYS:HG3	2.50	0.41
1:C:130:GLU:HB3	1:C:422:VAL:HB	2.03	0.41
1:G:301:ILE:HG21	1:G:309:LEU:HD12	2.02	0.41
1:K:296:THR:HB	1:K:319:GLN:H	1.84	0.41
1:L:104:LEU:HD12	1:L:104:LEU:HA	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:N:64:ASP:OD1	1:N:65:LYS:O	2.37	0.41
1:N:85:ALA:HA	1:N:498:LYS:HD3	2.02	0.41
2:S:34:LYS:HG3	2:S:35:SER:H	1.84	0.41
1:A:24:ALA:O	1:A:28:LYS:HG3	2.20	0.41
1:B:44:PHE:HB2	1:B:45:GLY:H	1.76	0.41
1:B:286:LYS:HE2	1:B:304:GLU:OE1	2.20	0.41
1:C:197:ARG:HD3	1:C:197:ARG:HA	1.66	0.41
1:E:130:GLU:HB3	1:E:422:VAL:HB	2.01	0.41
1:F:28:LYS:O	1:F:30:THR:N	2.53	0.41
1:H:342:ILE:O	1:H:346:VAL:HG23	2.20	0.41
1:H:524:LEU:HD23	1:H:524:LEU:HA	1.84	0.41
1:I:524:LEU:HA	1:I:524:LEU:HD23	1.85	0.41
1:J:2:ALA:O	1:J:4:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:VAL:HB	1:L:520:MET:HG2	2.02	0.41
1:K:428:ASP:O	1:K:429:LEU:C	2.58	0.41
1:M:226:LYS:HG3	1:M:252:GLU:HB3	2.01	0.41
1:M:476:TYR:HA	1:M:486:GLY:O	2.20	0.41
1:B:501:ARG:HD3	1:B:505:GLN:OE1	2.20	0.41
1:C:114:MET:O	1:C:114:MET:HE3	2.20	0.41
1:C:286:LYS:HE2	1:C:304:GLU:OE1	2.21	0.41
1:D:28:LYS:HD2	1:D:453:GLN:NE2	2.36	0.41
1:E:102:GLU:HB3	1:E:442:VAL:HG22	2.03	0.41
1:E:270:ILE:HG23	2:S:25:ILE:HG22	2.03	0.41
1:H:104:LEU:HA	1:H:104:LEU:HD12	1.74	0.41
1:I:64:ASP:C	1:I:65:LYS:O	2.58	0.41
1:K:16:MET:O	1:K:20:VAL:CG1	2.69	0.41
1:K:104:LEU:HD12	1:K:104:LEU:HA	1.80	0.41
1:N:100:ILE:HG23	1:N:104:LEU:HD22	2.01	0.41
2:T:60:LYS:HG2	2:T:63:ASP:OD2	2.20	0.41
1:C:197:ARG:H	1:C:329:THR:HA	1.84	0.41
1:C:204:PHE:O	1:C:204:PHE:CG	2.73	0.41
1:D:69:MET:O	1:D:73:MET:HG3	2.21	0.41
1:D:238:GLU:OE1	2:R:24:GLY:HA3	2.20	0.41
1:E:150:ILE:CD1	1:E:493:ILE:HA	2.50	0.41
1:F:349:ILE:HG23	1:F:365:LEU:HD12	2.01	0.41
1:F:421:ARG:HD3	1:F:421:ARG:HA	1.74	0.41
1:G:289:LEU:HA	1:G:292:ILE:HD12	2.02	0.41
1:H:428:ASP:O	1:H:429:LEU:C	2.58	0.41
1:L:16:MET:O	1:L:20:VAL:CG1	2.69	0.41
1:N:13:ARG:HD2	1:N:104:LEU:HD11	2.03	0.41
1:B:261:THR:HG22	2:P:29:GLY:HA3	2.01	0.41
1:E:365:LEU:O	1:E:369:VAL:HG13	2.20	0.41
1:F:301:ILE:HG21	1:F:309:LEU:HD12	2.03	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: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:K:215:LEU:HB3	1:K:218:PRO:HG3	2.02	0.41
1:M:66:PHE:HD1	1:M:520:MET:HE2	1.85	0.41
1:A:248:LEU:HD22	1:A:323:VAL:HG11	2.02	0.41
1:B:95:LEU:O	1:B:99:ILE:HG13	2.21	0.41
1:C:421:ARG:HD3	1:C:421:ARG:HA	1.74	0.41
1:E:288:MET:CG	1:E:368:ARG:HD2	2.49	0.41
1:F:28:LYS:C	1:F:30:THR:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:MET:HE1	1:G:514:MET:HB3	2.03	0.41
1:G:248:LEU:HD22	1:G:323:VAL:HG11	2.02	0.41
1:H:10:ASN:O	1:H:11:ASP:C	2.59	0.41
1:H:69:MET:HE2	1:H:522:THR:HB	2.00	0.41
1:I:11:ASP:O	1:I:12:ALA:C	2.58	0.41
1:J:101:THR:HG22	1:J:105:LYS:HE3	2.02	0.41
1:J:437:ASN:HA	1:J:440:ILE:HD12	2.01	0.41
1:M:461:GLU:HA	1:M:462:PRO:HD3	1.89	0.41
1:N:296:THR:HB	1:N:319:GLN:H	1.85	0.41
1:A:204:PHE:O	1:A:204:PHE:CG	2.74	0.41
1:B:248:LEU:HD22	1:B:323:VAL:HG11	2.01	0.41
1:C:30:THR:HB	1:C:51:LYS:HG2	2.03	0.41
1:C:162:ILE:HG21	1:C:403:THR:HG21	2.03	0.41
1:C:452:ARG:HH12	1:C:463:SER:HB3	1.85	0.41
1:D:240:VAL:HG11	1:D:247:LEU:HB2	2.03	0.41
1:D:456:LEU:HD13	1:D:462:PRO:CG	2.51	0.41
1:D:524:LEU:HD23	1:D:524:LEU:HA	1.99	0.41
1:E:198:GLY:HA2	1:E:326:ASN:O	2.21	0.41
1:E:451:LEU:HD21	1:E:465:VAL:HG12	2.02	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:H:433:ASN:HD22	1:H:433:ASN:HA	1.54	0.41
1:I:221:LEU:HD12	1:I:249:ILE:HG23	2.02	0.41
1:L:198:GLY:HA3	1:L:328:ASP:HA	2.03	0.41
1:M:270:ILE:HG23	1:N:229:ASN:HD21	1.86	0.41
1:A:6:VAL:O	1:A:6:VAL:HG23	2.20	0.41
1:A:39:VAL:HG12	1:G:69:MET:CE	2.51	0.41
1:A:348:GLN:HE21	1:A:348:GLN:HB3	1.68	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:B:247:LEU:O	1:B:273:VAL:HA	2.21	0.41
1:B:365:LEU:O	1:B:369:VAL:HG13	2.21	0.41
1:B:444:LEU:O	1:B:447:MET:HB2	2.20	0.41
1:C:238:GLU:OE1	2:Q:24:GLY:HA3	2.21	0.41
1:D:19:GLY:HA3	1:D:67:GLU:O	2.20	0.41
1:D:150:ILE:CD1	1:D:493:ILE:HA	2.51	0.41
1:D:286:LYS:HE2	1:D:304:GLU:OE1	2.20	0.41
1:D:288:MET:O	1:D:291:ASP:HB2	2.21	0.41
1:D:413:ALA:CB	1:D:417:VAL:HG13	2.51	0.41
1:E:16:MET:HE1	1:E:514:MET:HB3	2.03	0.41
1:E:288:MET:O	1:E:291:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:GLU:HB3	1:F:442:VAL:HG22	2.03	0.41
1:F:259:LEU:O	1:F:263:VAL:HG23	2.21	0.41
1:F:288:MET:CG	1:F:368:ARG:HD2	2.49	0.41
1:F:361:ASP:O	1:F:365:LEU:HD23	2.21	0.41
1:F:519:CYS:HB3	1:G:38:VAL:HG22	2.03	0.41
1:H:200:LEU:CD1	1:H:276:VAL:HA	2.49	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:I:421:ARG:NH2	1:I:469:VAL:O	2.51	0.41
1:J:43:SER:HB2	1:J:44:PHE:CD1	2.55	0.41
1:J:234:LEU:N	1:J:235:PRO:HD2	2.36	0.41
1:J:342:ILE:O	1:J:346:VAL:HG23	2.21	0.41
1:K:15:LYS:HB3	1:K:66:PHE:HB3	2.03	0.41
1:K:234:LEU:N	1:K:235:PRO:HD2	2.36	0.41
1:K:455:VAL:HG13	1:K:460:GLU:HB2	2.02	0.41
1:L:266:THR:HG22	1:L:273:VAL:H	1.85	0.41
1:M:213:VAL:O	1:M:324:VAL:HA	2.21	0.41
1:M:452:ARG:HG2	1:M:452:ARG:NH1	2.29	0.41
1:N:138:CYS:SG	1:N:144:ILE:HD13	2.61	0.41
1:C:288:MET:CG	1:C:368:ARG:HD2	2.49	0.41
1:E:19:GLY:HA3	1:E:67:GLU:O	2.21	0.41
1:G:95:LEU:O	1:G:99:ILE:HG13	2.21	0.41
1:I:100:ILE:HG23	1:I:104:LEU:HD22	2.02	0.41
1:I:513:LEU:HD12	1:I:513:LEU:HA	1.94	0.41
1:J:22:VAL:HG11	1:J:62:LEU:HD21	2.02	0.41
1:J:34:LYS:HB2	1:J:458:CYS:SG	2.61	0.41
1:L:221:LEU:HD12	1:L:249:ILE:HG23	2.02	0.41
1:N:461:GLU:HA	1:N:462:PRO:HD3	1.93	0.41
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.92	0.40
1:B:204:PHE:O	1:B:204:PHE:CG	2.74	0.40
1:E:349:ILE:HG23	1:E:365:LEU:HD12	2.01	0.40
1:F:19:GLY:HA3	1:F:67:GLU:O	2.21	0.40
1:F:288:MET:O	1:F:291:ASP:HB2	2.21	0.40
1:H:381:VAL:HG21	1:H:393:LYS:HA	2.03	0.40
1:I:444:LEU:HD23	1:I:444:LEU:HA	1.67	0.40
1:I:452:ARG:HG2	1:I:452:ARG:NH1	2.31	0.40
1:M:428:ASP:O	1:M:429:LEU:C	2.59	0.40
1:M:437:ASN:HA	1:M:440:ILE:HD12	2.03	0.40
2:U:46:GLY:HA3	2:U:55:LYS:O	2.21	0.40
1:C:301:ILE:O	1:C:301:ILE:HG22	2.22	0.40
1:C:361:ASP:O	1:C:365:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ARG:O	1:C:408:GLU:HG2	2.21	0.40
1:E:327:LYS:O	1:E:327:LYS:HG2	2.20	0.40
1:F:42:LYS:HE2	1:F:48:THR:OG1	2.22	0.40
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.84	0.40
1:H:521:VAL:HB	1:N:40:LEU:HD12	2.04	0.40
1:J:11:ASP:O	1:J:12:ALA:C	2.59	0.40
1:J:433:ASN:HD22	1:J:433:ASN:HA	1.57	0.40
1:L:419:LEU:HD22	1:L:500:THR:CG2	2.50	0.40
2:R:43:VAL:HG13	2:R:57:LEU:HD12	2.04	0.40
1:A:452:ARG:HG2	1:A:452:ARG:HH11	1.86	0.40
1:B:16:MET:CE	1:B:514:MET:HB3	2.51	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:B:461:GLU:HA	1:B:462:PRO:HD3	1.83	0.40
1:C:413:ALA:HB3	1:C:417:VAL:HG13	2.02	0.40
1:D:301:ILE:HG21	1:D:309:LEU:HD12	2.04	0.40
1:E:301:ILE:HG21	1:E:309:LEU:HD12	2.04	0.40
1:G:288:MET:CG	1:G:368:ARG:HD2	2.48	0.40
1:H:38:VAL:HG12	1:H:40:LEU:HD13	2.03	0.40
1:H:496:PRO:HB2	1:H:499:VAL:HG13	2.04	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:I:433:ASN:OD1	1:I:435:ASP:HB2	2.22	0.40
1:L:350:ARG:HA	1:L:353:ILE:HD12	2.04	0.40
1:L:429:LEU:HB3	1:L:440:ILE:HG21	2.04	0.40
1:M:201:SER:HA	1:M:202:PRO:HD3	1.95	0.40
1:A:301:ILE:O	1:A:301:ILE:HG22	2.21	0.40
1:D:204:PHE:O	1:D:204:PHE:CG	2.74	0.40
1:D:219:PHE:HB3	1:D:317:LEU:HD13	2.02	0.40
1:E:33:PRO:HG3	4:E:704:ADP:C6	2.56	0.40
1:E:247:LEU:O	1:E:273:VAL:HA	2.21	0.40
1:E:452:ARG:HH11	1:E:452:ARG:HG2	1.86	0.40
1:F:286:LYS:HE2	1:F:304:GLU:OE1	2.22	0.40
1:G:381:VAL:CG1	1:G:392:LYS:HG3	2.52	0.40
1:H:201:SER:HA	1:H:202:PRO:HD3	1.95	0.40
1:M:266:THR:HG22	1:M:273:VAL:H	1.86	0.40
1:N:32:GLY:CA	1:N:454:ILE:HG23	2.52	0.40
2:O:55:LYS:H	2:O:55:LYS:HE2	1.87	0.40
1:B:301:ILE:HG21	1:B:309:LEU:HD12	2.04	0.40
1:B:404:ARG:O	1:B:408:GLU:HG2	2.21	0.40
1:D:90:THR:O	1:D:94:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:449:ALA:HB3	1:D:450:PRO:HD3	2.04	0.40
1:E:90:THR:O	1:E:94:VAL:HG23	2.21	0.40
1:E:413:ALA:HB3	1:E:417:VAL:HG13	2.04	0.40
1:G:28:LYS:O	1:G:29:VAL:C	2.59	0.40
1:G:197:ARG:H	1:G:329:THR:HA	1.87	0.40
1:H:149:THR:HG22	1:H:156:GLU:HA	2.04	0.40
1:H:461:GLU:HA	1:H:462:PRO:HD3	1.90	0.40
1:J:198:GLY:HA3	1:J:328:ASP:HA	2.03	0.40
1:K:72:GLN:HE22	1:K:75:LYS:NZ	2.20	0.40
2:P:46:GLY:HA3	2:P:55:LYS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/524 (100%)	485 (93%)	33 (6%)	4 (1%)	19	57
1	B	522/524 (100%)	484 (93%)	33 (6%)	5 (1%)	15	53
1	C	522/524 (100%)	484 (93%)	34 (6%)	4 (1%)	19	57
1	D	522/524 (100%)	485 (93%)	32 (6%)	5 (1%)	15	53
1	E	522/524 (100%)	489 (94%)	29 (6%)	4 (1%)	19	57
1	F	522/524 (100%)	490 (94%)	27 (5%)	5 (1%)	15	53
1	G	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	15	53
1	H	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	15	53
1	I	522/524 (100%)	483 (92%)	32 (6%)	7 (1%)	12	45
1	J	522/524 (100%)	480 (92%)	38 (7%)	4 (1%)	19	57
1	K	522/524 (100%)	479 (92%)	38 (7%)	5 (1%)	15	53
1	L	522/524 (100%)	483 (92%)	34 (6%)	5 (1%)	15	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	522/524 (100%)	480 (92%)	37 (7%)	5 (1%)	15	53
1	N	522/524 (100%)	483 (92%)	35 (7%)	4 (1%)	19	57
2	O	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	11
2	P	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	11
2	Q	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	1	7
2	R	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	11
2	S	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	11
2	T	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	1	7
2	U	95/97 (98%)	76 (80%)	14 (15%)	5 (5%)	2	11
All	All	7973/8015 (100%)	7303 (92%)	566 (7%)	104 (1%)	12	45

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
1	H	270	ILE
1	I	66	PHE
1	I	270	ILE

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Mol	Chain	Res	Type
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
2	T	51	ASN
2	U	49	LEU
2	U	51	ASN

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Mol	Chain	Res	Type
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 [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	359 (89%)	45 (11%)	6	25
1	B	404/404 (100%)	358 (89%)	46 (11%)	5	24
1	C	404/404 (100%)	356 (88%)	48 (12%)	5	22
1	D	404/404 (100%)	357 (88%)	47 (12%)	5	23
1	E	404/404 (100%)	358 (89%)	46 (11%)	5	24
1	F	404/404 (100%)	357 (88%)	47 (12%)	5	23
1	G	404/404 (100%)	354 (88%)	50 (12%)	4	20
1	H	404/404 (100%)	347 (86%)	57 (14%)	3	16
1	I	404/404 (100%)	349 (86%)	55 (14%)	3	17
1	J	404/404 (100%)	349 (86%)	55 (14%)	3	17
1	K	404/404 (100%)	347 (86%)	57 (14%)	3	16
1	L	404/404 (100%)	348 (86%)	56 (14%)	3	16
1	M	404/404 (100%)	347 (86%)	57 (14%)	3	16
1	N	404/404 (100%)	349 (86%)	55 (14%)	3	17
2	O	80/80 (100%)	70 (88%)	10 (12%)	4	20
2	P	80/80 (100%)	70 (88%)	10 (12%)	4	20
2	Q	80/80 (100%)	70 (88%)	10 (12%)	4	20
2	R	80/80 (100%)	69 (86%)	11 (14%)	3	17
2	S	80/80 (100%)	69 (86%)	11 (14%)	3	17
2	T	80/80 (100%)	70 (88%)	10 (12%)	4	20
2	U	80/80 (100%)	69 (86%)	11 (14%)	3	17
All	All	6216/6216 (100%)	5422 (87%)	794 (13%)	4	19

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
1	A	44	PHE
1	A	48	THR

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Mol	Chain	Res	Type
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
1	B	18	ARG
1	B	23	LEU

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Mol	Chain	Res	Type
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
1	B	461	GLU
1	B	483	GLU

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Mol	Chain	Res	Type
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
1	C	419	LEU
1	C	420	ILE

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Mol	Chain	Res	Type
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
1	D	387	VAL
1	D	391	GLU

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Mol	Chain	Res	Type
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
1	E	348	GLN
1	E	350	ARG

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Mol	Chain	Res	Type
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
1	F	281	PHE
1	F	284	ARG

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Mol	Chain	Res	Type
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
1	G	183	LEU
1	G	184	GLN

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Mol	Chain	Res	Type
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
1	H	104	LEU
1	H	114	MET

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Mol	Chain	Res	Type
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
1	H	468	THR
1	H	483	GLU

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Mol	Chain	Res	Type
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
1	I	357	THR
1	I	385	THR

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Mol	Chain	Res	Type
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
1	J	272	LYS
1	J	284	ARG

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Mol	Chain	Res	Type
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
1	K	107	VAL
1	K	114	MET

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Mol	Chain	Res	Type
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
1	K	494	LEU
1	K	504	LEU

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Mol	Chain	Res	Type
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
1	L	357	THR
1	L	385	THR

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Mol	Chain	Res	Type
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
1	M	255	GLU
1	M	272	LYS

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Mol	Chain	Res	Type
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
1	N	89	THR
1	N	104	LEU

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Mol	Chain	Res	Type
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
1	N	494	LEU
1	N	504	LEU

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Mol	Chain	Res	Type
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
2	R	60	LYS
2	R	77	LYS

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Mol	Chain	Res	Type
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

Sometimes 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
1	A	146	GLN
1	A	153	ASN

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Mol	Chain	Res	Type
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
1	E	457	ASN
1	E	475	ASN

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Mol	Chain	Res	Type
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
1	J	146	GLN
1	J	326	ASN

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	F	705	3	24,29,29	1.16	2 (8%)	29,45,45	2.02	7 (24%)
4	ADP	D	703	3	24,29,29	1.53	5 (20%)	29,45,45	2.27	11 (37%)
4	ADP	B	701	3	24,29,29	1.44	4 (16%)	29,45,45	2.20	8 (27%)
4	ADP	G	706	3	24,29,29	1.28	1 (4%)	29,45,45	2.20	8 (27%)
4	ADP	C	702	3	24,29,29	1.25	3 (12%)	29,45,45	2.37	10 (34%)
4	ADP	E	704	3	24,29,29	1.31	3 (12%)	29,45,45	2.12	8 (27%)
4	ADP	A	700	3	24,29,29	1.30	4 (16%)	29,45,45	2.23	10 (34%)

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	F	705	3	-	4/12/32/32	0/3/3/3
4	ADP	D	703	3	-	4/12/32/32	0/3/3/3
4	ADP	B	701	3	-	4/12/32/32	0/3/3/3
4	ADP	G	706	3	-	4/12/32/32	0/3/3/3
4	ADP	C	702	3	-	4/12/32/32	0/3/3/3
4	ADP	E	704	3	-	4/12/32/32	0/3/3/3
4	ADP	A	700	3	-	4/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	706	ADP	C2-N3	4.43	1.39	1.32
4	B	701	ADP	C2-N3	4.17	1.38	1.32
4	D	703	ADP	C2-N3	3.88	1.38	1.32
4	A	700	ADP	C2-N3	3.77	1.38	1.32
4	E	704	ADP	C2-N3	3.74	1.38	1.32
4	C	702	ADP	C2-N3	3.54	1.37	1.32
4	F	705	ADP	C2-N3	3.49	1.37	1.32
4	B	701	ADP	C2-N1	3.13	1.39	1.33
4	D	703	ADP	C2-N1	3.03	1.39	1.33
4	D	703	ADP	C2'-C1'	-2.90	1.49	1.53
4	C	702	ADP	C2-N1	2.68	1.38	1.33
4	D	703	ADP	O4'-C1'	-2.66	1.37	1.41
4	F	705	ADP	C2-N1	2.58	1.38	1.33
4	E	704	ADP	C2-N1	2.55	1.38	1.33
4	B	701	ADP	C2'-C1'	-2.41	1.50	1.53
4	A	700	ADP	O4'-C4'	-2.33	1.39	1.45
4	A	700	ADP	C2-N1	2.29	1.38	1.33
4	D	703	ADP	O4'-C4'	-2.19	1.40	1.45
4	C	702	ADP	C2'-C1'	-2.15	1.50	1.53
4	E	704	ADP	C2'-C1'	-2.12	1.50	1.53
4	A	700	ADP	C2'-C1'	-2.05	1.50	1.53
4	B	701	ADP	O4'-C4'	-2.03	1.40	1.45

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	ADP	N3-C2-N1	-6.41	118.65	128.68
4	A	700	ADP	N3-C2-N1	-6.04	119.24	128.68
4	F	705	ADP	N3-C2-N1	-5.75	119.69	128.68
4	C	702	ADP	N3-C2-N1	-5.56	119.99	128.68
4	E	704	ADP	N3-C2-N1	-5.54	120.02	128.68
4	B	701	ADP	N3-C2-N1	-5.46	120.14	128.68
4	G	706	ADP	N3-C2-N1	-5.29	120.42	128.68
4	C	702	ADP	PA-O3A-PB	-4.86	116.14	132.83
4	E	704	ADP	PA-O3A-PB	-4.75	116.52	132.83
4	G	706	ADP	PA-O3A-PB	-4.70	116.71	132.83
4	F	705	ADP	PA-O3A-PB	-4.62	116.96	132.83
4	A	700	ADP	PA-O3A-PB	-4.61	117.00	132.83
4	D	703	ADP	PA-O3A-PB	-4.61	117.01	132.83
4	C	702	ADP	O3'-C3'-C4'	-4.58	97.82	111.05
4	B	701	ADP	PA-O3A-PB	-4.48	117.47	132.83
4	G	706	ADP	O3'-C3'-C4'	-4.14	99.09	111.05
4	B	701	ADP	O3'-C3'-C4'	-4.06	99.31	111.05
4	A	700	ADP	C1'-N9-C4	-3.69	120.16	126.64
4	E	704	ADP	C1'-N9-C4	-3.67	120.20	126.64
4	G	706	ADP	C4-C5-N7	-3.66	105.58	109.40
4	B	701	ADP	C1'-N9-C4	-3.57	120.37	126.64
4	B	701	ADP	C4-C5-N7	-3.55	105.70	109.40
4	D	703	ADP	C1'-N9-C4	-3.42	120.64	126.64
4	D	703	ADP	O3'-C3'-C4'	-3.40	101.23	111.05
4	C	702	ADP	C4-C5-N7	-3.33	105.93	109.40
4	E	704	ADP	O5'-C5'-C4'	3.30	120.35	108.99
4	C	702	ADP	O3B-PB-O3A	3.18	115.28	104.64
4	E	704	ADP	C4-C5-N7	-3.15	106.11	109.40
4	D	703	ADP	O5'-C5'-C4'	3.13	119.78	108.99
4	F	705	ADP	O5'-C5'-C4'	3.05	119.50	108.99
4	A	700	ADP	O3'-C3'-C4'	-3.04	102.27	111.05
4	B	701	ADP	O5'-C5'-C4'	3.01	119.36	108.99
4	C	702	ADP	C1'-N9-C4	-3.01	121.35	126.64
4	A	700	ADP	O5'-C5'-C4'	2.94	119.11	108.99
4	G	706	ADP	C2'-C3'-C4'	2.91	108.29	102.64
4	C	702	ADP	O5'-C5'-C4'	2.91	119.00	108.99
4	A	700	ADP	C4-C5-N7	-2.90	106.37	109.40
4	F	705	ADP	C1'-N9-C4	-2.84	121.65	126.64
4	G	706	ADP	O5'-C5'-C4'	2.83	118.75	108.99
4	G	706	ADP	C1'-N9-C4	-2.78	121.76	126.64
4	F	705	ADP	O3'-C3'-C4'	-2.76	103.07	111.05
4	F	705	ADP	C4-C5-N7	-2.73	106.55	109.40
4	E	704	ADP	O3'-C3'-C4'	-2.61	103.51	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	ADP	C2'-C3'-C4'	2.55	107.59	102.64
4	B	701	ADP	O3B-PB-O3A	2.52	113.10	104.64
4	C	702	ADP	C5-C6-N6	2.50	124.16	120.35
4	D	703	ADP	O2'-C2'-C1'	-2.45	101.80	110.85
4	C	702	ADP	C2'-C3'-C4'	2.41	107.33	102.64
4	D	703	ADP	C4-C5-N7	-2.39	106.91	109.40
4	C	702	ADP	O2'-C2'-C1'	-2.33	102.25	110.85
4	G	706	ADP	O3'-C3'-C2'	-2.29	104.43	111.82
4	D	703	ADP	O2B-PB-O3A	-2.28	96.99	104.64
4	D	703	ADP	O3B-PB-O3A	2.21	112.03	104.64
4	E	704	ADP	C2'-C3'-C4'	2.19	106.90	102.64
4	A	700	ADP	O3B-PB-O3A	2.19	111.98	104.64
4	D	703	ADP	C3'-C2'-C1'	2.16	104.23	100.98
4	B	701	ADP	C2'-C3'-C4'	2.15	106.83	102.64
4	E	704	ADP	O2'-C2'-C1'	-2.13	102.98	110.85
4	A	700	ADP	O3'-C3'-C2'	-2.07	105.11	111.82
4	F	705	ADP	C3'-C2'-C1'	2.03	104.03	100.98
4	D	703	ADP	C2'-C3'-C4'	2.02	106.56	102.64
4	A	700	ADP	N6-C6-N1	-2.01	114.40	118.57

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	ADP	O4'-C4'-C5'-O5'
4	A	700	ADP	O4'-C4'-C5'-O5'
4	C	702	ADP	O4'-C4'-C5'-O5'
4	D	703	ADP	O4'-C4'-C5'-O5'
4	E	704	ADP	O4'-C4'-C5'-O5'
4	F	705	ADP	O4'-C4'-C5'-O5'
4	G	706	ADP	O4'-C4'-C5'-O5'
4	G	706	ADP	C3'-C4'-C5'-O5'
4	A	700	ADP	C3'-C4'-C5'-O5'
4	B	701	ADP	C3'-C4'-C5'-O5'
4	C	702	ADP	C3'-C4'-C5'-O5'
4	D	703	ADP	C3'-C4'-C5'-O5'
4	E	704	ADP	C3'-C4'-C5'-O5'
4	F	705	ADP	C3'-C4'-C5'-O5'
4	A	700	ADP	PB-O3A-PA-O1A
4	B	701	ADP	PB-O3A-PA-O1A
4	C	702	ADP	PB-O3A-PA-O1A
4	D	703	ADP	PB-O3A-PA-O1A

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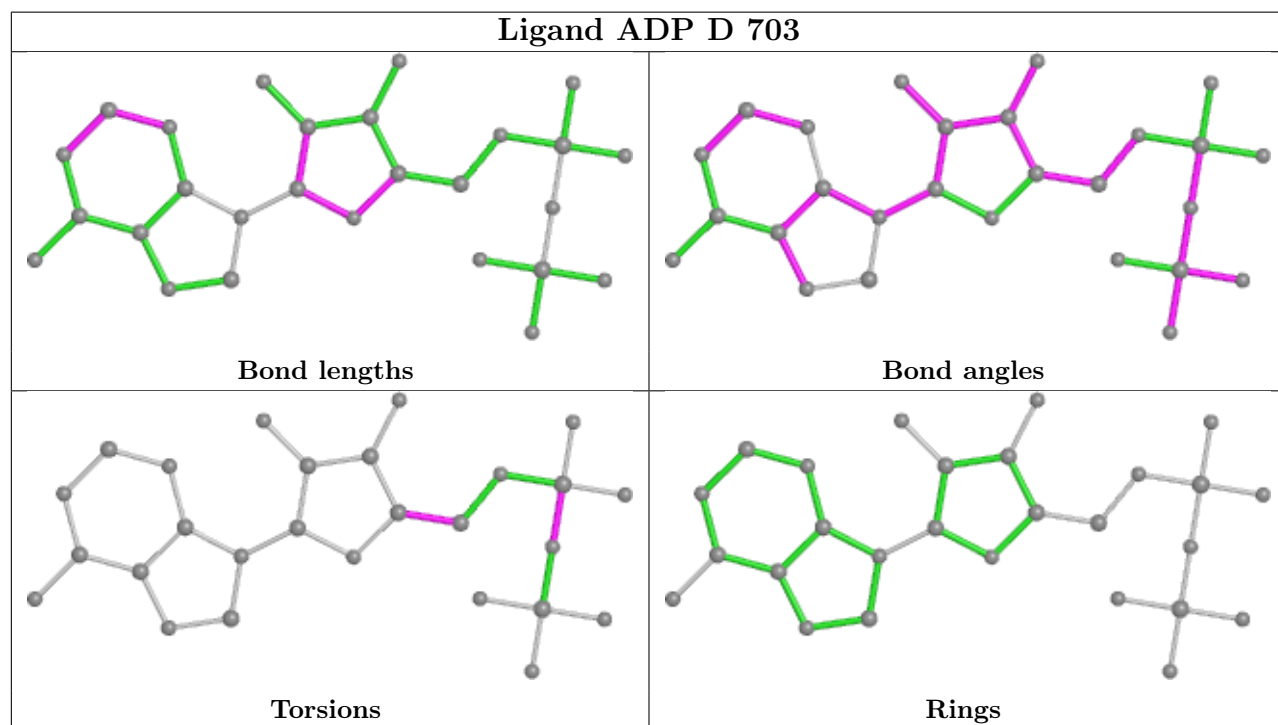
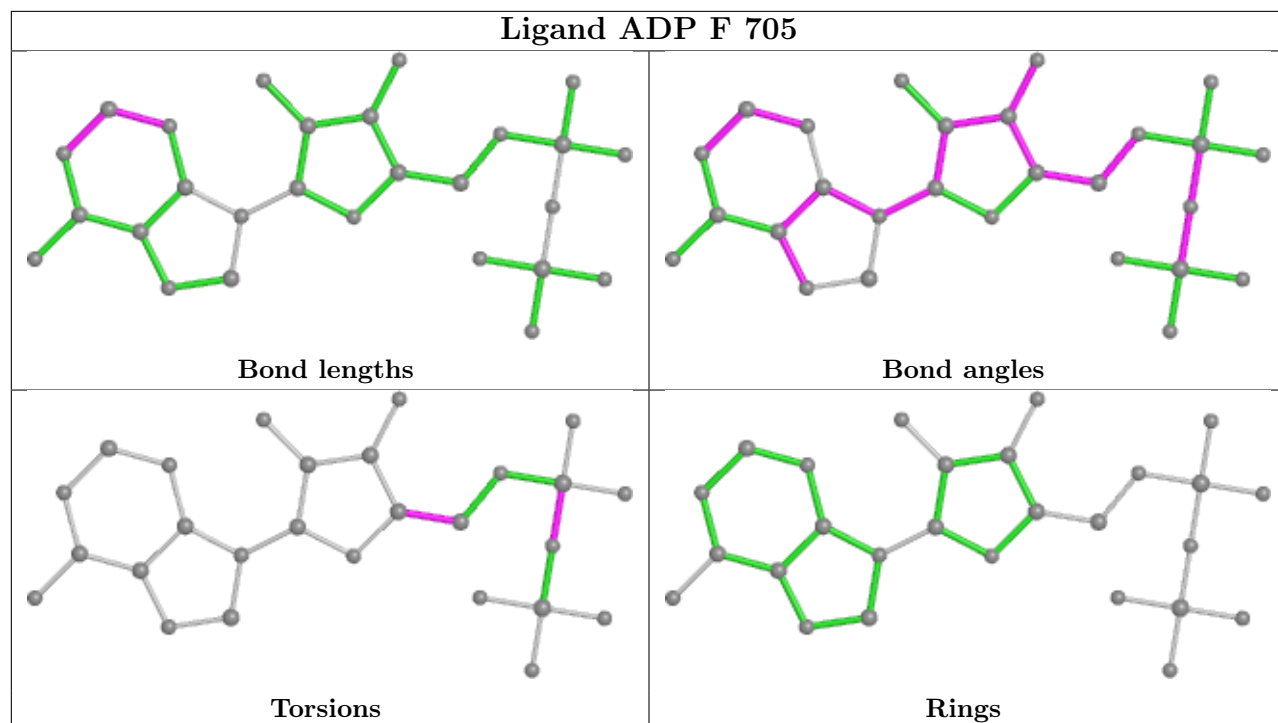
Mol	Chain	Res	Type	Atoms
4	E	704	ADP	PB-O3A-PA-O1A
4	F	705	ADP	PB-O3A-PA-O1A
4	A	700	ADP	PB-O3A-PA-O2A
4	B	701	ADP	PB-O3A-PA-O2A
4	G	706	ADP	PB-O3A-PA-O1A
4	C	702	ADP	PB-O3A-PA-O2A
4	D	703	ADP	PB-O3A-PA-O2A
4	E	704	ADP	PB-O3A-PA-O2A
4	F	705	ADP	PB-O3A-PA-O2A
4	G	706	ADP	PB-O3A-PA-O2A

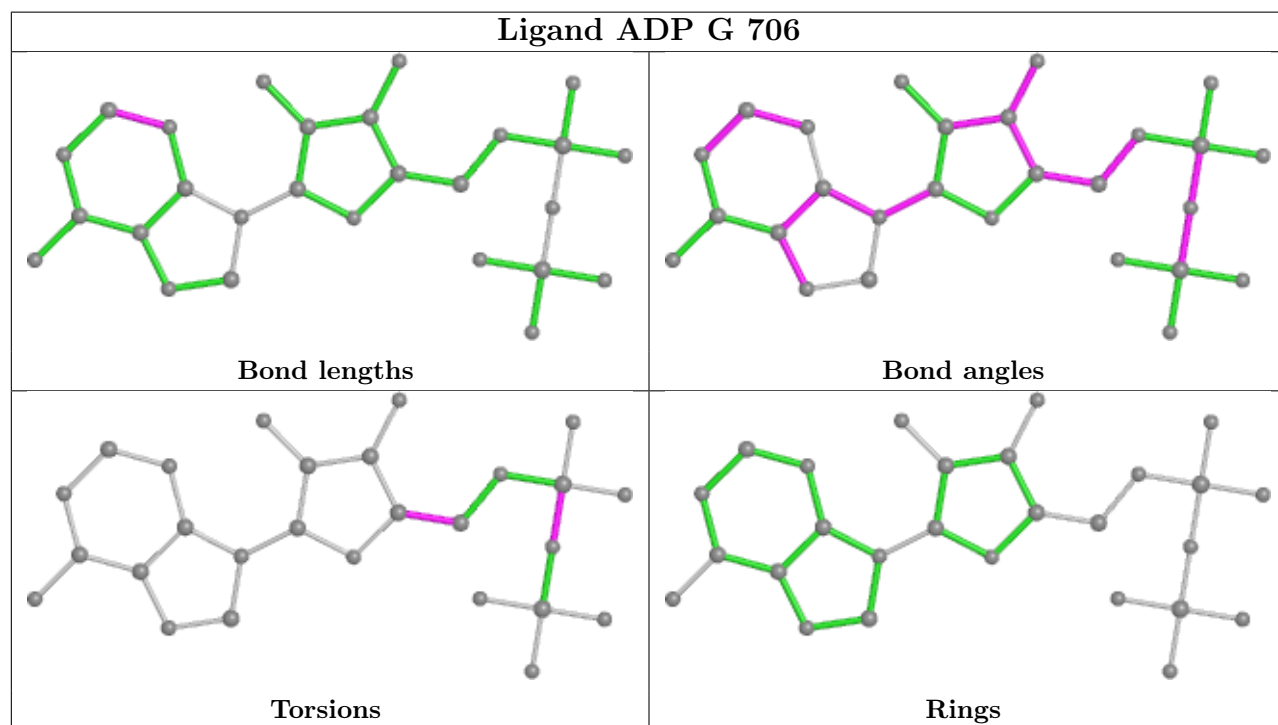
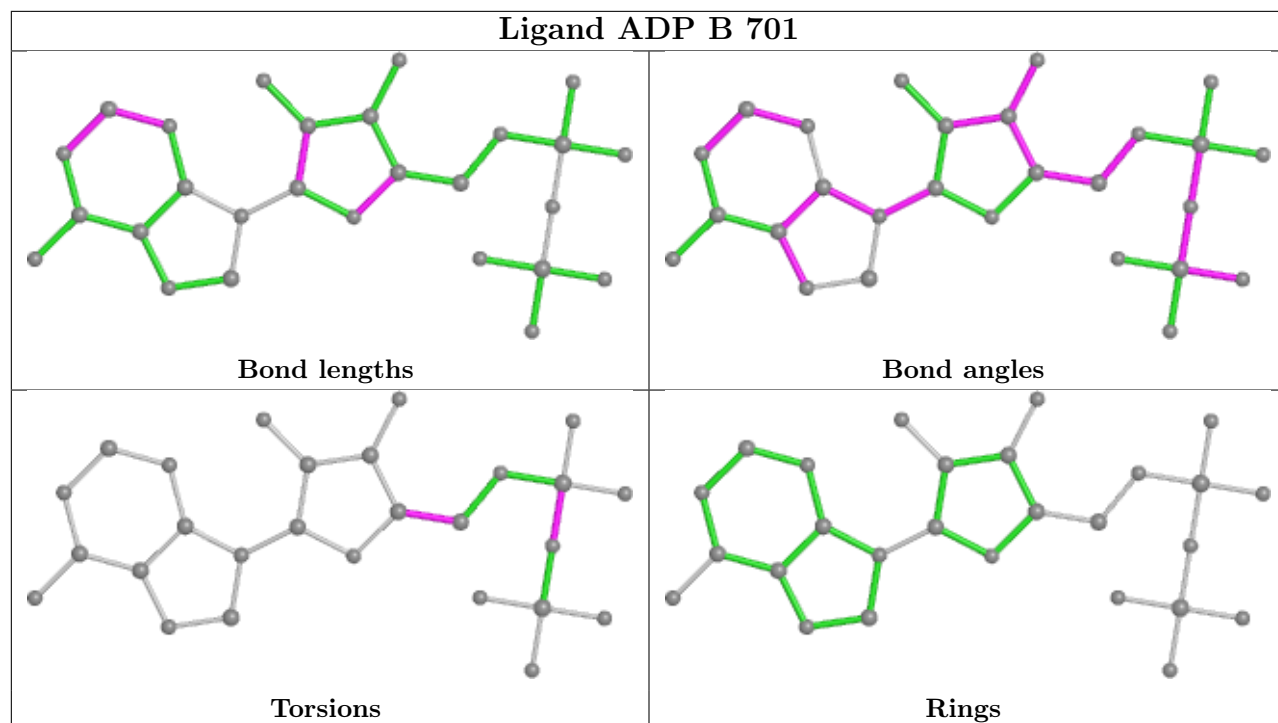
There are no ring outliers.

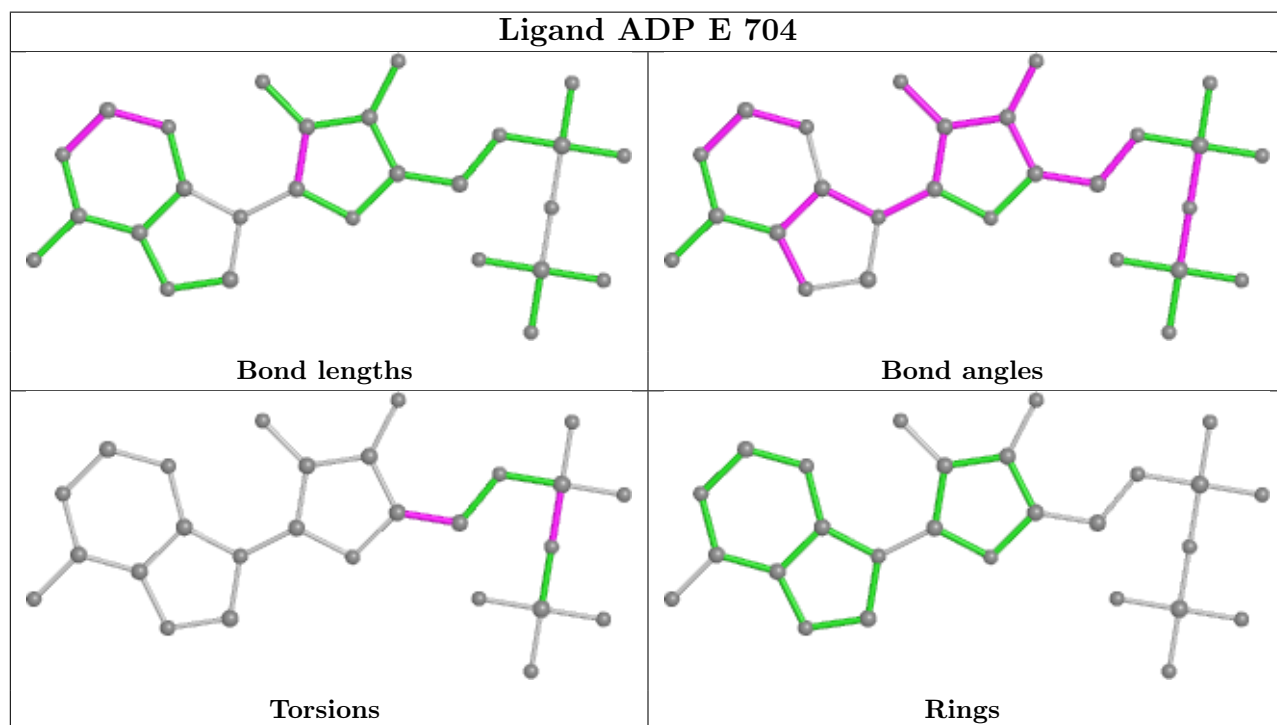
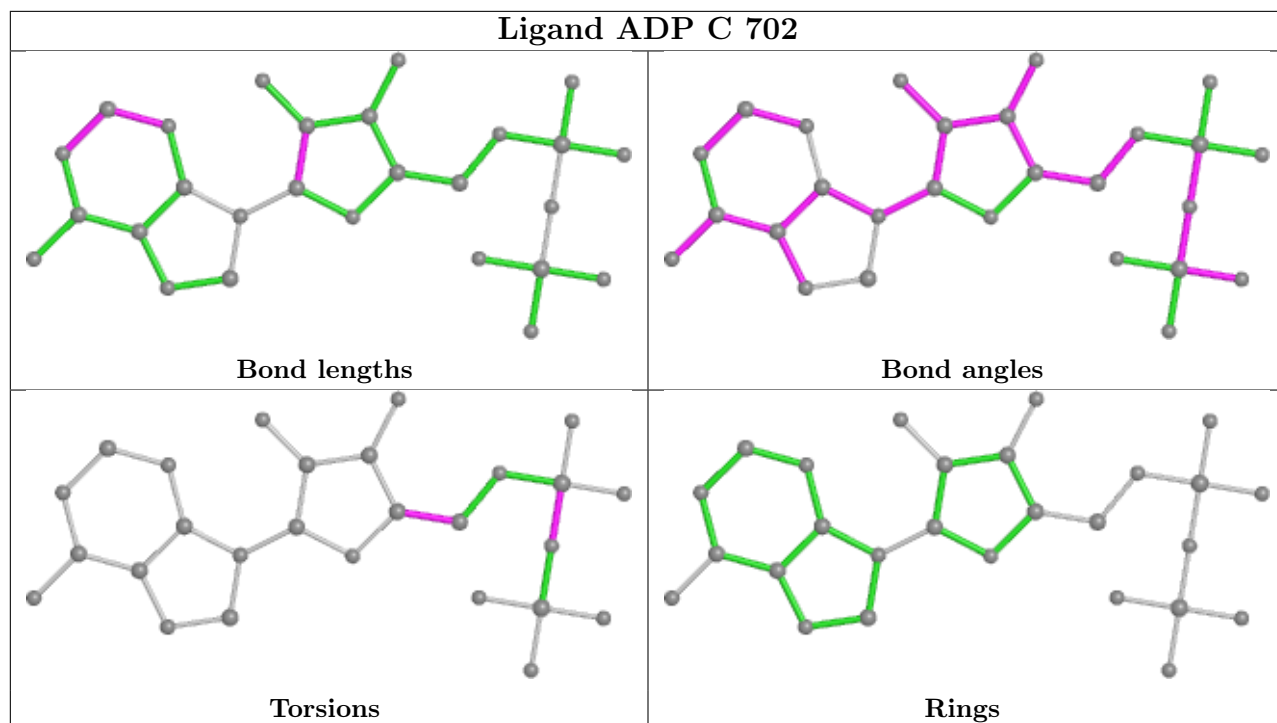
7 monomers are involved in 14 short contacts:

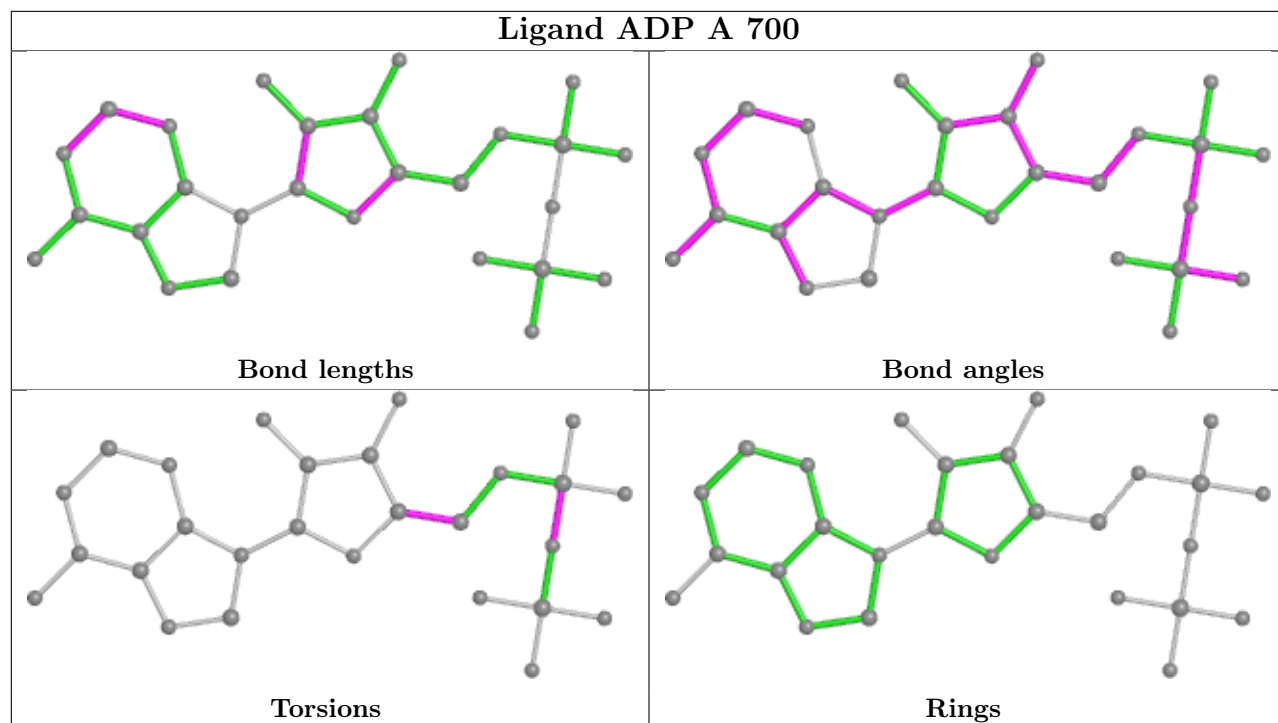
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	705	ADP	1	0
4	D	703	ADP	3	0
4	B	701	ADP	2	0
4	G	706	ADP	3	0
4	C	702	ADP	2	0
4	E	704	ADP	1	0
4	A	700	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/524 (100%)	0.60	58 (11%) 5 1	5, 7, 9, 10	0
1	B	524/524 (100%)	0.70	62 (11%) 4 1	5, 7, 9, 10	0
1	C	524/524 (100%)	0.49	49 (9%) 8 3	5, 7, 9, 10	0
1	D	524/524 (100%)	0.53	54 (10%) 6 2	5, 7, 9, 10	0
1	E	524/524 (100%)	0.79	62 (11%) 4 1	5, 7, 9, 10	0
1	F	524/524 (100%)	0.85	72 (13%) 3 1	5, 7, 9, 10	0
1	G	524/524 (100%)	0.68	65 (12%) 4 1	5, 7, 9, 10	0
1	H	524/524 (100%)	0.33	19 (3%) 42 17	6, 7, 9, 10	0
1	I	524/524 (100%)	0.30	12 (2%) 60 31	5, 7, 9, 10	0
1	J	524/524 (100%)	0.42	28 (5%) 26 10	5, 7, 9, 10	0
1	K	524/524 (100%)	0.58	44 (8%) 11 3	5, 7, 9, 10	0
1	L	524/524 (100%)	0.63	42 (8%) 12 4	5, 7, 9, 10	0
1	M	524/524 (100%)	0.48	35 (6%) 17 5	5, 7, 9, 10	0
1	N	524/524 (100%)	0.52	31 (5%) 22 7	5, 7, 9, 10	0
2	O	97/97 (100%)	1.73	34 (35%) 0 0	7, 7, 8, 8	0
2	P	97/97 (100%)	1.60	27 (27%) 0 0	7, 7, 8, 8	0
2	Q	97/97 (100%)	1.40	29 (29%) 0 0	7, 7, 8, 8	0
2	R	97/97 (100%)	1.50	25 (25%) 0 0	7, 7, 8, 8	0
2	S	97/97 (100%)	1.72	29 (29%) 0 0	7, 7, 8, 8	0
2	T	97/97 (100%)	1.55	27 (27%) 0 0	7, 7, 8, 8	0
2	U	97/97 (100%)	3.19	74 (76%) 0 0	7, 7, 8, 8	0
All	All	8015/8015 (100%)	0.67	878 (10%) 5 2	5, 7, 9, 10	0

All (878) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361	ASP	16.6
1	F	361	ASP	10.5
1	E	361	ASP	10.2
1	A	361	ASP	9.9
1	G	199	TYR	9.5
1	G	361	ASP	8.9
1	G	208	PRO	8.6
1	A	353	ILE	8.5
1	E	353	ILE	8.3
2	U	32	ALA	8.3
1	B	361	ASP	8.1
1	F	357	THR	7.8
1	D	361	ASP	7.7
1	D	212	ALA	7.6
1	B	353	ILE	7.4
1	F	353	ILE	7.4
1	B	355	GLU	7.2
1	A	357	THR	7.2
1	L	264	VAL	7.1
1	F	355	GLU	7.1
1	A	321	LYS	7.1
1	C	212	ALA	7.1
1	E	281	PHE	7.1
1	L	357	THR	7.1
2	U	33	ALA	7.0
2	P	23	GLY	6.9
1	I	264	VAL	6.8
2	T	97	ALA	6.8
2	R	17	VAL	6.8
1	D	365	LEU	6.7
2	S	32	ALA	6.7
2	P	32	ALA	6.7
1	B	365	LEU	6.7
1	B	357	THR	6.7
1	D	357	THR	6.6
2	U	30	SER	6.6
1	A	365	LEU	6.6
1	C	357	THR	6.6
1	I	268	ARG	6.6
2	O	25	ILE	6.6
1	G	362	ARG	6.5
2	U	17	VAL	6.4
1	F	172	GLU	6.4

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Mol	Chain	Res	Type	RSRZ
2	O	97	ALA	6.4
2	U	31	ALA	6.4
1	A	208	PRO	6.3
1	C	353	ILE	6.3
1	F	210	THR	6.3
1	F	349	ILE	6.2
1	G	353	ILE	6.2
1	E	357	THR	6.2
1	A	349	ILE	6.2
2	U	22	ALA	6.1
1	K	356	ALA	6.1
1	G	357	THR	6.1
2	S	31	ALA	6.1
2	T	18	GLU	6.0
2	R	18	GLU	6.0
1	E	338	GLU	5.9
1	G	251	ALA	5.9
1	A	360	TYR	5.9
2	S	51	ASN	5.9
1	D	353	ILE	5.8
2	U	18	GLU	5.8
1	E	365	LEU	5.8
2	S	33	ALA	5.8
1	E	280	GLY	5.7
2	U	51	ASN	5.7
2	R	51	ASN	5.6
1	E	340	ALA	5.6
2	T	25	ILE	5.6
2	P	18	GLU	5.6
1	G	214	GLU	5.6
1	M	358	SER	5.6
1	C	267	MET	5.6
1	C	360	TYR	5.5
2	O	72	GLY	5.5
1	M	360	TYR	5.5
1	K	360	TYR	5.5
2	U	97	ALA	5.4
1	C	270	ILE	5.4
1	F	171	LYS	5.4
2	Q	18	GLU	5.4
1	G	212	ALA	5.4
2	U	28	THR	5.4

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Mol	Chain	Res	Type	RSRZ
1	K	186	GLU	5.4
1	N	183	LEU	5.4
2	T	52	GLY	5.3
1	M	357	THR	5.3
1	E	364	LYS	5.3
1	E	354	GLU	5.2
1	B	348	GLN	5.2
1	F	212	ALA	5.2
1	B	349	ILE	5.2
1	H	360	TYR	5.2
1	B	284	ARG	5.2
2	R	25	ILE	5.1
1	C	199	TYR	5.1
2	U	19	THR	5.1
2	U	71	TYR	5.1
1	A	284	ARG	5.0
1	G	195	PHE	5.0
2	O	17	VAL	5.0
1	A	203	TYR	5.0
2	P	1	MET	5.0
2	Q	25	ILE	5.0
1	B	279	PRO	4.9
2	R	80	ASN	4.9
1	B	364	LYS	4.9
2	O	83	VAL	4.9
2	S	18	GLU	4.9
1	F	375	GLY	4.9
1	D	284	ARG	4.9
1	G	349	ILE	4.9
2	S	97	ALA	4.9
1	A	355	GLU	4.8
1	F	267	MET	4.9
2	O	1	MET	4.9
1	D	349	ILE	4.8
1	E	279	PRO	4.8
1	L	353	ILE	4.8
2	P	51	ASN	4.8
2	S	80	ASN	4.8
2	U	26	VAL	4.8
2	U	1	MET	4.8
1	G	350	ARG	4.8
2	U	21	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	355	GLU	4.8
1	G	210	THR	4.8
2	S	17	VAL	4.7
1	C	210	THR	4.7
2	U	25	ILE	4.7
1	L	268	ARG	4.7
1	L	177	VAL	4.7
2	S	30	SER	4.7
1	E	321	LYS	4.7
1	E	360	TYR	4.7
1	G	256	GLY	4.6
1	E	284	ARG	4.6
1	E	209	GLU	4.6
1	N	360	TYR	4.6
1	F	352	GLN	4.6
1	J	365	LEU	4.6
2	U	23	GLY	4.6
1	B	192	GLY	4.5
1	D	209	GLU	4.5
1	D	199	TYR	4.5
1	J	353	ILE	4.5
1	E	341	ALA	4.5
1	D	268	ARG	4.5
1	A	364	LYS	4.5
1	G	354	GLU	4.5
2	Q	32	ALA	4.5
1	B	346	VAL	4.5
2	U	78	ILE	4.4
2	R	1	MET	4.4
1	N	266	THR	4.4
2	T	82	GLU	4.4
1	G	360	TYR	4.4
2	U	69	ASP	4.4
1	G	365	LEU	4.4
2	S	1	MET	4.4
1	K	188	ASP	4.4
2	P	20	LYS	4.4
2	P	31	ALA	4.4
2	U	16	GLU	4.3
1	E	210	THR	4.3
1	F	331	THR	4.3
1	G	198	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	N	357	THR	4.3
1	L	349	ILE	4.3
1	D	338	GLU	4.3
2	P	33	ALA	4.3
1	M	284	ARG	4.3
2	P	67	PHE	4.3
1	C	362	ARG	4.2
1	F	364	LYS	4.2
1	I	357	THR	4.2
2	S	21	SER	4.2
2	U	20	LYS	4.2
1	F	251	ALA	4.2
2	Q	27	LEU	4.2
2	Q	71	TYR	4.2
2	U	27	LEU	4.2
1	B	352	GLN	4.2
2	U	65	VAL	4.2
1	M	264	VAL	4.2
1	D	321	LYS	4.2
1	F	350	ARG	4.2
1	F	374	GLY	4.2
1	D	360	TYR	4.2
2	P	49	LEU	4.1
2	U	52	GLY	4.1
1	B	354	GLU	4.1
2	O	21	SER	4.1
1	M	268	ARG	4.1
2	U	80	ASN	4.1
1	B	350	ARG	4.1
2	S	83	VAL	4.1
1	C	349	ILE	4.1
2	O	31	ALA	4.0
2	O	32	ALA	4.0
1	E	346	VAL	4.0
2	O	66	ILE	4.0
1	L	362	ARG	4.0
1	E	349	ILE	4.0
2	Q	78	ILE	4.0
2	O	22	ALA	4.0
1	C	251	ALA	4.0
2	S	36	THR	4.0
1	G	279	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
2	R	20	LYS	4.0
2	U	35	SER	4.0
1	K	295	LEU	4.0
2	T	17	VAL	3.9
2	U	79	ASP	3.9
1	A	338	GLU	3.9
1	J	356	ALA	3.9
2	P	85	ILE	3.9
2	U	72	GLY	3.9
2	P	25	ILE	3.9
2	R	21	SER	3.9
2	R	30	SER	3.9
2	T	71	TYR	3.9
2	U	83	VAL	3.9
1	K	187	LEU	3.9
1	E	195	PHE	3.9
2	U	49	LEU	3.9
2	O	36	THR	3.9
2	U	75	SER	3.9
2	R	79	ASP	3.9
2	S	66	ILE	3.9
2	U	38	GLY	3.9
2	T	80	ASN	3.9
1	C	271	VAL	3.8
2	P	71	TYR	3.8
1	A	320	ALA	3.8
1	E	352	GLN	3.8
1	F	273	VAL	3.8
1	G	222	LEU	3.8
1	B	360	TYR	3.8
1	B	351	GLN	3.8
1	A	238	GLU	3.8
1	C	350	ARG	3.8
1	F	365	LEU	3.7
1	F	203	TYR	3.7
2	T	33	ALA	3.7
2	R	83	VAL	3.7
1	D	172	GLU	3.7
1	F	323	VAL	3.7
1	I	270	ILE	3.7
1	I	360	TYR	3.7
1	F	214	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	T	72	GLY	3.7
1	C	365	LEU	3.7
1	B	208	PRO	3.6
2	O	51	ASN	3.6
2	P	97	ALA	3.6
2	Q	80	ASN	3.6
2	U	84	LEU	3.6
1	G	364	LYS	3.6
2	T	51	ASN	3.6
2	R	33	ALA	3.6
2	O	80	ASN	3.6
1	E	371	LYS	3.6
1	J	181	THR	3.6
2	U	2	ASN	3.6
2	U	67	PHE	3.6
1	F	377	ALA	3.6
1	N	186	GLU	3.6
2	U	53	GLU	3.6
1	F	360	TYR	3.5
1	N	350	ARG	3.5
1	A	352	GLN	3.5
1	C	284	ARG	3.5
1	C	279	PRO	3.5
1	E	334	ASP	3.5
2	T	53	GLU	3.5
2	T	32	ALA	3.5
1	A	281	PHE	3.5
2	P	17	VAL	3.5
2	P	21	SER	3.5
2	S	67	PHE	3.5
1	G	203	TYR	3.5
2	Q	26	VAL	3.5
2	U	10	VAL	3.5
1	J	223	ALA	3.5
2	O	18	GLU	3.5
2	P	30	SER	3.5
1	E	362	ARG	3.5
1	M	349	ILE	3.5
1	D	362	ARG	3.4
1	G	284	ARG	3.4
1	F	174	VAL	3.4
1	K	349	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	U	82	GLU	3.4
2	O	27	LEU	3.4
2	T	27	LEU	3.4
1	H	356	ALA	3.4
1	J	330	THR	3.4
1	J	268	ARG	3.4
1	J	372	LEU	3.4
1	J	267	MET	3.4
1	J	366	GLN	3.4
1	B	203	TYR	3.4
1	K	372	LEU	3.4
1	C	358	SER	3.4
1	B	224	ASP	3.4
2	R	97	ALA	3.4
1	D	251	ALA	3.4
1	E	256	GLY	3.3
1	F	230	ILE	3.3
1	B	199	TYR	3.3
2	T	67	PHE	3.3
1	K	185	ASP	3.3
1	N	184	GLN	3.3
1	D	195	PHE	3.3
1	F	356	ALA	3.3
2	R	22	ALA	3.3
1	L	267	MET	3.3
2	O	38	GLY	3.3
2	O	67	PHE	3.3
1	E	368	ARG	3.3
1	L	356	ALA	3.3
2	U	93	ALA	3.3
1	A	322	ARG	3.3
2	U	96	GLU	3.2
1	D	355	GLU	3.2
1	L	270	ILE	3.2
1	J	396	VAL	3.2
1	E	350	ARG	3.2
1	E	332	ILE	3.2
1	G	209	GLU	3.2
1	A	271	VAL	3.2
1	G	376	VAL	3.2
2	P	80	ASN	3.2
1	A	193	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	ILE	3.2
2	Q	13	LYS	3.2
1	A	358	SER	3.2
1	G	267	MET	3.2
1	E	270	ILE	3.2
2	O	82	GLU	3.2
1	B	278	ALA	3.2
1	K	384	ALA	3.2
1	F	283	ASP	3.1
1	G	172	GLU	3.1
1	F	281	PHE	3.1
2	U	85	ILE	3.1
2	U	36	THR	3.1
1	B	238	GLU	3.1
2	U	66	ILE	3.1
1	B	212	ALA	3.1
1	L	352	GLN	3.1
2	U	92	LEU	3.1
1	M	233	MET	3.1
2	S	71	TYR	3.1
1	A	251	ALA	3.1
1	G	271	VAL	3.1
1	A	172	GLU	3.1
2	Q	82	GLU	3.1
1	B	267	MET	3.1
2	Q	66	ILE	3.1
1	G	207	LYS	3.1
2	P	52	GLY	3.1
1	G	321	LYS	3.1
1	G	332	ILE	3.1
2	U	29	GLY	3.1
1	D	203	TYR	3.1
2	Q	20	LYS	3.1
2	S	20	LYS	3.1
1	A	376	VAL	3.1
1	G	371	LYS	3.1
1	K	352	GLN	3.1
2	O	33	ALA	3.0
2	T	83	VAL	3.0
1	B	200	LEU	3.0
1	B	347	ALA	3.0
1	D	309	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	322	ARG	3.0
1	E	196	ASP	3.0
1	F	213	VAL	3.0
2	O	30	SER	3.0
2	O	37	ARG	3.0
1	F	170	GLY	3.0
1	H	342	ILE	3.0
1	J	193	MET	3.0
2	U	39	GLU	3.0
1	G	229	ASN	3.0
1	M	243	ALA	3.0
1	F	284	ARG	3.0
2	T	28	THR	3.0
1	F	288	MET	3.0
1	N	525	PRO	3.0
1	B	362	ARG	3.0
1	L	354	GLU	3.0
2	O	26	VAL	3.0
2	U	12	VAL	3.0
1	G	281	PHE	2.9
2	S	74	LYS	2.9
1	B	44	PHE	2.9
2	P	84	LEU	2.9
2	U	41	LEU	2.9
1	B	367	GLU	2.9
1	D	352	GLN	2.9
1	M	186	GLU	2.9
2	R	82	GLU	2.9
1	F	376	VAL	2.9
1	L	271	VAL	2.9
1	G	280	GLY	2.9
1	M	208	PRO	2.9
2	O	23	GLY	2.9
1	F	351	GLN	2.9
1	E	44	PHE	2.9
1	M	372	LEU	2.9
1	A	279	PRO	2.9
2	U	68	ASN	2.9
2	Q	65	VAL	2.9
1	B	223	ALA	2.9
1	D	314	LEU	2.9
1	G	309	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	340	ALA	2.9
1	H	186	GLU	2.9
2	U	81	GLU	2.9
1	B	193	MET	2.9
2	R	52	GLY	2.9
1	A	210	THR	2.9
1	C	223	ALA	2.9
1	D	279	PRO	2.9
1	E	322	ARG	2.9
1	C	242	LYS	2.9
1	K	44	PHE	2.9
2	U	13	LYS	2.9
2	U	24	GLY	2.9
1	E	231	ARG	2.9
1	F	338	GLU	2.9
1	G	211	GLY	2.9
1	I	267	MET	2.8
1	N	267	MET	2.8
1	F	195	PHE	2.8
1	L	180	GLY	2.8
1	A	209	GLU	2.8
1	C	214	GLU	2.8
1	E	303	GLU	2.8
1	E	203	TYR	2.8
2	S	73	VAL	2.8
1	E	216	GLU	2.8
1	K	144	ILE	2.8
1	M	176	THR	2.8
2	S	85	ILE	2.8
1	N	369	VAL	2.8
1	D	267	MET	2.8
1	K	350	ARG	2.8
1	N	242	LYS	2.8
2	O	19	THR	2.8
1	C	203	TYR	2.8
1	E	336	VAL	2.8
2	Q	12	VAL	2.8
2	R	73	VAL	2.8
2	S	65	VAL	2.8
1	A	356	ALA	2.8
1	A	270	ILE	2.8
1	F	358	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	294	THR	2.8
2	U	77	LYS	2.8
1	B	230	ILE	2.8
2	R	72	GLY	2.8
1	F	209	GLU	2.8
2	O	95	VAL	2.8
1	L	360	TYR	2.8
2	P	93	ALA	2.8
2	U	76	GLU	2.8
2	Q	73	VAL	2.8
2	U	70	GLY	2.7
1	B	214	GLU	2.7
1	C	195	PHE	2.7
1	E	172	GLU	2.7
1	N	342	ILE	2.7
2	U	3	ILE	2.7
1	G	359	ASP	2.7
1	L	215	LEU	2.7
1	B	322	ARG	2.7
1	F	322	ARG	2.7
1	K	268	ARG	2.7
2	S	13	LYS	2.7
1	A	195	PHE	2.7
1	B	338	GLU	2.7
1	D	204	PHE	2.7
1	D	237	LEU	2.7
1	B	321	LYS	2.7
1	G	277	LYS	2.7
1	N	165	ALA	2.7
2	U	34	LYS	2.7
1	A	256	GLY	2.7
1	B	209	GLU	2.7
2	Q	50	GLU	2.7
1	G	346	VAL	2.7
1	A	345	ARG	2.7
1	C	172	GLU	2.7
1	K	193	MET	2.7
1	A	214	GLU	2.7
1	F	341	ALA	2.7
1	F	386	GLU	2.7
1	F	44	PHE	2.7
1	H	44	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	192	GLY	2.7
2	Q	33	ALA	2.7
1	B	277	LYS	2.7
1	E	331	THR	2.7
1	K	381	VAL	2.7
1	M	185	ASP	2.7
2	T	73	VAL	2.7
1	B	340	ALA	2.7
1	K	171	LYS	2.7
1	M	361	ASP	2.7
1	B	327	LYS	2.6
2	Q	49	LEU	2.6
2	S	84	LEU	2.6
1	E	324	VAL	2.6
1	I	44	PHE	2.6
1	F	333	ILE	2.6
1	F	319	GLN	2.6
1	G	247	LEU	2.6
1	N	361	ASP	2.6
1	D	364	LYS	2.6
1	F	304	GLU	2.6
1	G	171	LYS	2.6
1	C	288	MET	2.6
1	H	372	LEU	2.6
1	J	183	LEU	2.6
1	B	382	GLY	2.6
1	M	244	GLY	2.6
2	P	72	GLY	2.6
1	A	223	ALA	2.6
2	Q	67	PHE	2.6
1	M	175	ILE	2.6
2	S	69	ASP	2.6
1	B	320	ALA	2.6
1	D	257	GLU	2.6
1	J	352	GLN	2.6
2	O	78	ILE	2.6
2	R	66	ILE	2.6
2	S	78	ILE	2.6
1	A	373	ALA	2.6
1	C	209	GLU	2.6
1	G	320	ALA	2.6
1	J	357	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	233	MET	2.6
2	U	86	MET	2.6
1	B	237	LEU	2.6
1	L	221	LEU	2.6
1	D	214	GLU	2.6
1	N	238	GLU	2.6
2	U	50	GLU	2.6
1	M	44	PHE	2.6
1	G	351	GLN	2.6
1	C	211	GLY	2.6
2	R	16	GLU	2.6
2	T	21	SER	2.6
1	B	368	ARG	2.6
1	C	278	ALA	2.6
1	C	347	ALA	2.6
1	F	362	ARG	2.6
1	H	368	ARG	2.6
1	J	44	PHE	2.6
2	T	20	LYS	2.6
1	H	193	MET	2.6
1	J	381	VAL	2.6
1	L	156	GLU	2.6
2	O	65	VAL	2.6
2	P	2	ASN	2.6
1	C	355	GLU	2.5
2	Q	38	GLY	2.5
2	R	28	THR	2.5
1	C	364	LYS	2.5
1	D	376	VAL	2.5
2	Q	55	LYS	2.5
2	U	54	VAL	2.5
2	T	30	SER	2.5
1	F	373	ALA	2.5
1	A	229	ASN	2.5
1	B	171	LYS	2.5
1	K	368	ARG	2.5
1	K	196	ASP	2.5
1	C	338	GLU	2.5
1	A	362	ARG	2.5
1	K	346	VAL	2.5
1	D	358	SER	2.5
1	B	280	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	322	ARG	2.5
1	L	305	ILE	2.5
1	G	215	LEU	2.5
1	F	359	ASP	2.5
1	B	275	ALA	2.5
1	C	356	ALA	2.5
2	O	71	TYR	2.5
1	A	368	ARG	2.5
1	F	173	GLY	2.5
2	Q	84	LEU	2.5
1	N	396	VAL	2.5
2	U	73	VAL	2.5
1	K	291	ASP	2.5
1	L	364	LYS	2.5
1	G	355	GLU	2.5
1	I	340	ALA	2.5
1	K	373	ALA	2.5
1	I	349	ILE	2.5
1	M	138	CYS	2.5
2	R	26	VAL	2.5
1	M	340	ALA	2.5
1	E	286	LYS	2.5
1	J	311	LYS	2.5
1	C	138	CYS	2.5
1	L	195	PHE	2.5
1	B	358	SER	2.5
1	C	208	PRO	2.5
1	E	309	LEU	2.5
1	E	214	GLU	2.5
1	A	212	ALA	2.5
1	E	372	LEU	2.5
1	H	525	PRO	2.4
1	M	365	LEU	2.5
2	U	4	ARG	2.4
1	N	189	VAL	2.4
1	B	283	ASP	2.4
2	U	74	LYS	2.4
1	A	274	ALA	2.4
1	G	223	ALA	2.4
1	G	347	ALA	2.4
2	S	41	LEU	2.4
1	A	346	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	2.4
1	B	309	LEU	2.4
1	F	181	THR	2.4
1	D	208	PRO	2.4
1	E	174	VAL	2.4
1	K	158	VAL	2.4
1	K	297	GLY	2.4
1	C	268	ARG	2.4
1	E	285	ARG	2.4
1	H	268	ARG	2.4
1	B	331	THR	2.4
1	M	275	ALA	2.4
1	M	161	LEU	2.4
1	N	365	LEU	2.4
1	N	372	LEU	2.4
2	O	49	LEU	2.4
1	D	196	ASP	2.4
1	H	364	LYS	2.4
1	D	320	ALA	2.4
1	M	152	ALA	2.4
1	K	183	LEU	2.4
1	F	138	CYS	2.4
1	F	280	GLY	2.4
1	L	63	GLU	2.4
1	J	175	ILE	2.4
1	K	379	ILE	2.4
1	N	349	ILE	2.4
2	U	55	LYS	2.4
1	C	354	GLU	2.4
1	H	357	THR	2.4
1	D	325	ILE	2.4
1	F	309	LEU	2.4
1	K	270	ILE	2.4
2	Q	85	ILE	2.4
1	G	252	GLU	2.3
1	G	334	ASP	2.3
1	F	193	MET	2.3
1	L	313	THR	2.3
1	K	494	LEU	2.3
1	N	270	ILE	2.3
1	L	263	VAL	2.3
2	O	73	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	272	LYS	2.3
2	T	9	ARG	2.3
1	L	266	THR	2.3
1	G	270	ILE	2.3
1	K	234	LEU	2.3
1	N	187	LEU	2.3
2	O	48	ILE	2.3
1	B	281	PHE	2.3
1	N	180	GLY	2.3
1	A	348	GLN	2.3
1	F	348	GLN	2.3
1	L	381	VAL	2.3
1	E	359	ASP	2.3
1	D	238	GLU	2.3
1	D	256	GLY	2.3
1	D	297	GLY	2.3
2	P	74	LYS	2.3
2	S	77	LYS	2.3
1	M	236	VAL	2.3
2	Q	17	VAL	2.3
2	U	47	ARG	2.3
1	G	291	ASP	2.3
1	E	175	ILE	2.3
1	E	524	LEU	2.3
1	F	234	LEU	2.3
1	E	330	THR	2.3
1	L	160	LYS	2.3
1	G	204	PHE	2.3
1	G	196	ASP	2.3
1	G	227	ILE	2.3
1	M	362	ARG	2.3
1	B	217	SER	2.3
1	A	324	VAL	2.3
1	A	351	GLN	2.3
1	D	356	ALA	2.3
1	K	127	ALA	2.3
2	R	71	TYR	2.3
2	U	46	GLY	2.3
1	J	266	THR	2.3
1	L	369	VAL	2.3
1	D	171	LYS	2.3
1	A	334	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	U	90	ASP	2.3
1	D	340	ALA	2.3
2	U	11	ILE	2.3
1	L	484	GLU	2.3
1	N	381	VAL	2.3
2	T	76	GLU	2.3
2	U	45	ASN	2.3
1	A	359	ASP	2.3
1	A	248	LEU	2.3
1	A	267	MET	2.3
1	L	269	GLY	2.3
1	C	308	GLU	2.3
1	G	324	VAL	2.2
2	U	14	ARG	2.2
1	C	224	ASP	2.2
1	A	237	LEU	2.2
1	L	127	ALA	2.2
2	T	31	ALA	2.2
1	E	219	PHE	2.2
1	K	366	GLN	2.2
1	F	494	LEU	2.2
1	K	480	ALA	2.2
1	L	384	ALA	2.2
1	K	203	TYR	2.2
1	N	172	GLU	2.2
1	B	377	ALA	2.2
1	C	238	GLU	2.2
1	M	367	GLU	2.2
1	E	348	GLN	2.2
1	D	245	LYS	2.2
1	N	177	VAL	2.2
1	G	326	ASN	2.2
2	O	75	SER	2.2
2	T	50	GLU	2.2
1	E	375	GLY	2.2
1	C	322	ARG	2.2
1	F	162	ILE	2.2
1	I	266	THR	2.2
2	R	67	PHE	2.2
1	J	184	GLN	2.2
1	A	273	VAL	2.2
1	D	303	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	339	GLU	2.2
1	C	372	LEU	2.2
1	F	185	ASP	2.2
1	B	195	PHE	2.2
1	M	364	LYS	2.2
1	E	194	GLN	2.2
2	Q	19	THR	2.2
1	E	267	MET	2.2
1	G	194	GLN	2.2
1	K	284	ARG	2.2
1	M	431	GLY	2.2
1	C	359	ASP	2.2
1	G	372	LEU	2.2
1	F	390	LYS	2.2
1	M	199	TYR	2.2
2	T	37	ARG	2.2
1	F	215	LEU	2.2
1	F	308	GLU	2.2
1	B	381	VAL	2.2
1	D	200	LEU	2.1
1	H	283	ASP	2.1
1	J	289	LEU	2.1
1	K	134	LEU	2.1
1	D	275	ALA	2.1
1	M	356	ALA	2.1
2	T	66	ILE	2.1
1	D	371	LYS	2.1
1	H	284	ARG	2.1
1	L	261	THR	2.1
1	C	192	GLY	2.1
1	C	324	VAL	2.1
1	D	336	VAL	2.1
1	E	477	GLY	2.1
1	L	494	LEU	2.1
1	H	270	ILE	2.1
1	K	175	ILE	2.1
2	O	64	ILE	2.1
2	Q	22	ALA	2.1
1	H	350	ARG	2.1
1	H	369	VAL	2.1
1	I	263	VAL	2.1
1	L	378	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	234	LEU	2.1
1	J	242	LYS	2.1
1	G	275	ALA	2.1
1	I	343	GLN	2.1
1	N	384	ALA	2.1
2	U	42	ALA	2.1
2	S	86	MET	2.1
1	F	346	VAL	2.1
1	G	358	SER	2.1
1	N	431	GLY	2.1
1	E	237	LEU	2.1
1	H	524	LEU	2.1
1	A	354	GLU	2.1
1	F	220	ILE	2.1
1	L	373	ALA	2.1
2	U	64	ILE	2.1
1	D	213	VAL	2.1
1	K	524	LEU	2.1
2	P	82	GLU	2.1
1	E	212	ALA	2.1
1	F	175	ILE	2.1
1	G	175	ILE	2.1
1	B	268	ARG	2.1
1	J	350	ARG	2.1
2	U	94	ILE	2.1
1	E	192	GLY	2.1
1	D	271	VAL	2.1
1	N	271	VAL	2.1
1	M	238	GLU	2.1
1	A	314	LEU	2.1
1	B	234	LEU	2.1
2	S	75	SER	2.1
1	E	294	THR	2.1
1	H	343	GLN	2.1
1	J	313	THR	2.1
1	L	175	ILE	2.1
1	L	203	TYR	2.1
1	A	268	ARG	2.1
2	U	37	ARG	2.1
1	B	324	VAL	2.1
1	M	240	VAL	2.1
1	A	249	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	357	THR	2.1
1	M	285	ARG	2.1
1	B	172	GLU	2.1
2	Q	74	LYS	2.1
1	E	204	PHE	2.1
1	F	200	LEU	2.0
1	C	228	SER	2.0
2	Q	79	ASP	2.0
1	C	373	ALA	2.0
1	L	147	VAL	2.0
1	C	250	ILE	2.0
2	P	22	ALA	2.0
2	Q	97	ALA	2.0
2	R	32	ALA	2.0
1	C	346	VAL	2.0
1	D	288	MET	2.0
1	K	138	CYS	2.0
1	F	229	ASN	2.0
1	G	348	GLN	2.0
1	M	168	LYS	2.0
1	B	251	ALA	2.0
1	D	304	GLU	2.0
1	N	358	SER	2.0
2	P	66	ILE	2.0
1	D	525	PRO	2.0
1	L	265	ASN	2.0
1	A	347	ALA	2.0
1	F	211	GLY	2.0
1	J	382	GLY	2.0
1	K	172	GLU	2.0
1	K	388	GLU	2.0
1	L	325	ILE	2.0
1	N	353	ILE	2.0
1	F	371	LYS	2.0
1	J	222	LEU	2.0
1	K	200	LEU	2.0
1	L	365	LEU	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

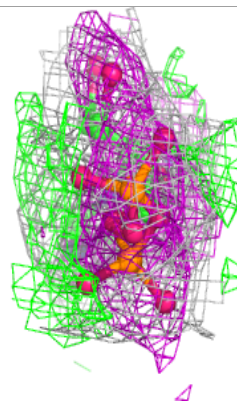
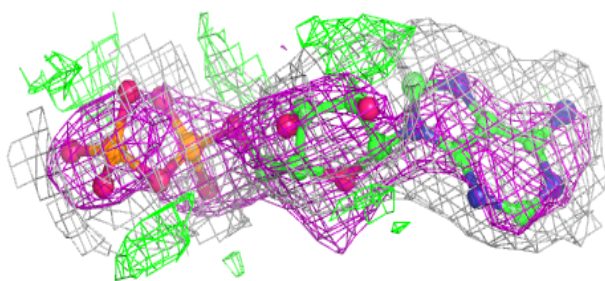
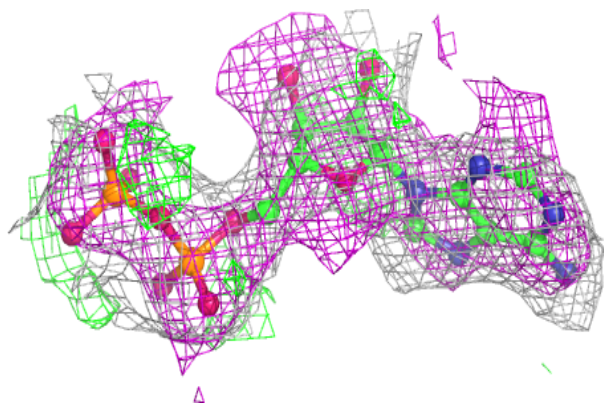
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ADP	E	704	27/27	0.89	0.19	6,8,9,10	0
4	ADP	B	701	27/27	0.90	0.20	6,8,9,10	0
4	ADP	F	705	27/27	0.91	0.21	6,8,9,10	0
4	ADP	A	700	27/27	0.92	0.18	6,8,9,11	0
4	ADP	D	703	27/27	0.93	0.17	6,8,9,10	0
3	MG	B	602	1/1	0.94	0.21	2,2,2,2	0
4	ADP	G	706	27/27	0.94	0.15	6,8,9,10	0
3	MG	C	603	1/1	0.95	0.18	2,2,2,2	0
4	ADP	C	702	27/27	0.95	0.13	6,8,9,10	0
3	MG	F	606	1/1	0.96	0.27	2,2,2,2	0
3	MG	A	601	1/1	0.96	0.28	2,2,2,2	0
3	MG	D	604	1/1	0.97	0.32	2,2,2,2	0
3	MG	E	605	1/1	0.97	0.18	2,2,2,2	0
3	MG	G	607	1/1	0.98	0.20	2,2,2,2	0

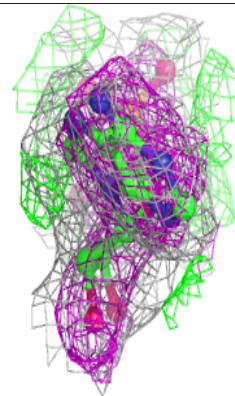
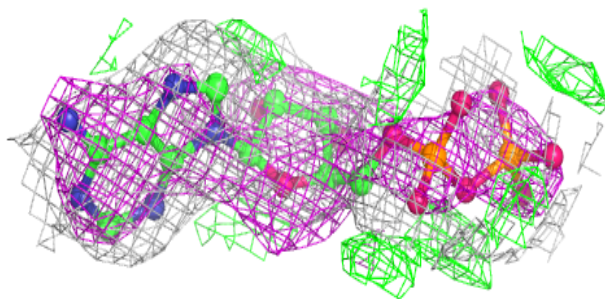
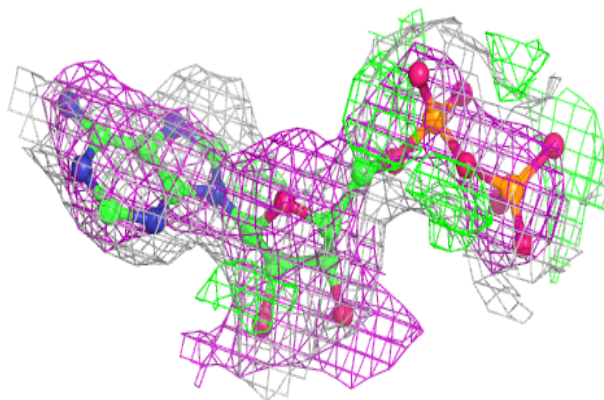
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP E 704:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

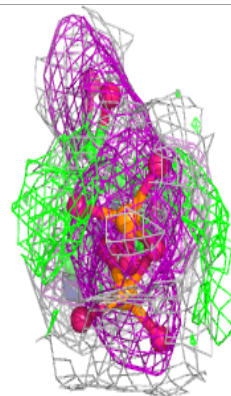
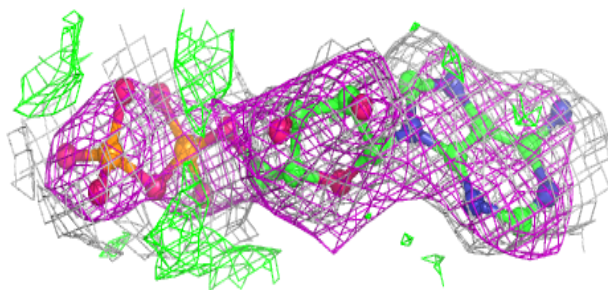
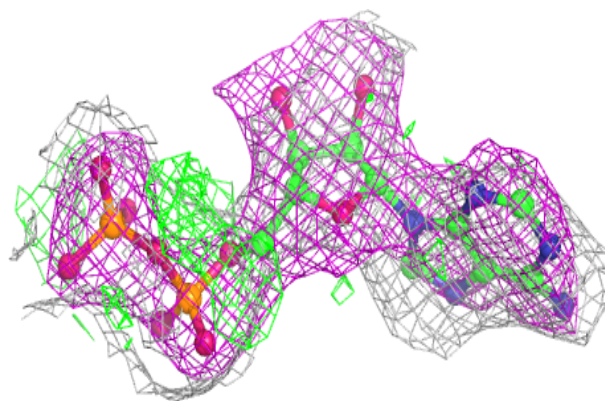
**Electron density around ADP B 701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

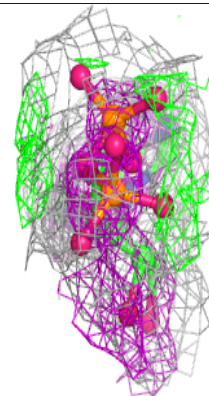
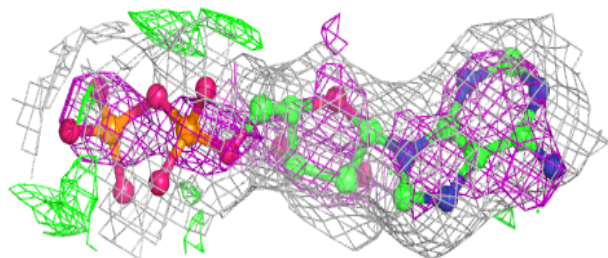
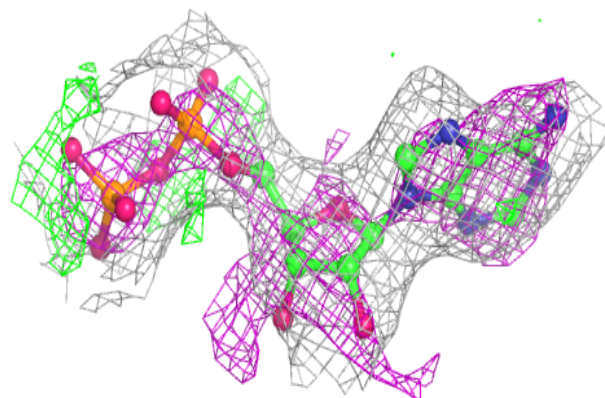


Electron density around ADP F 705:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

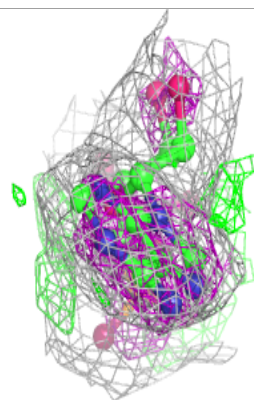
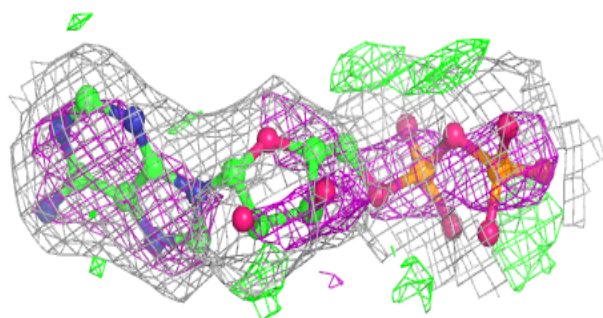
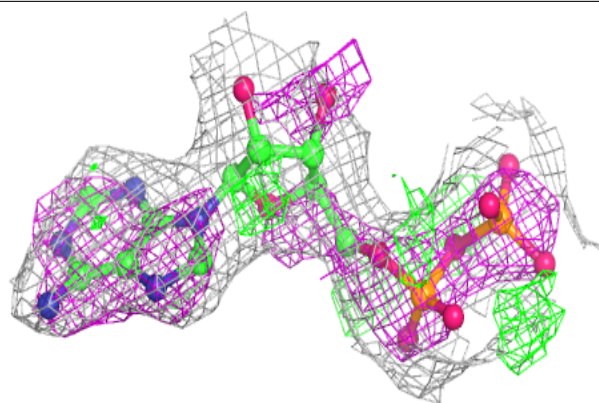
**Electron density around ADP A 700:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

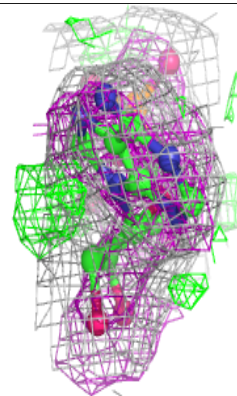
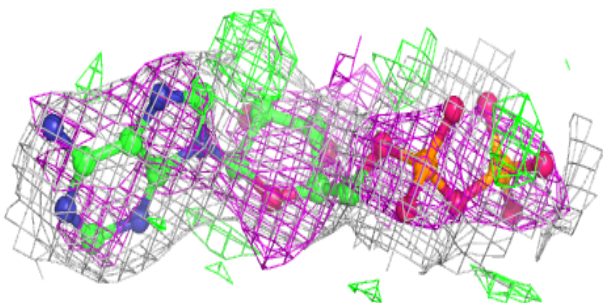
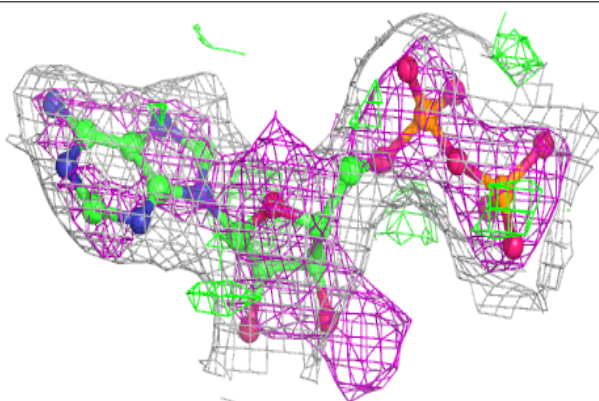


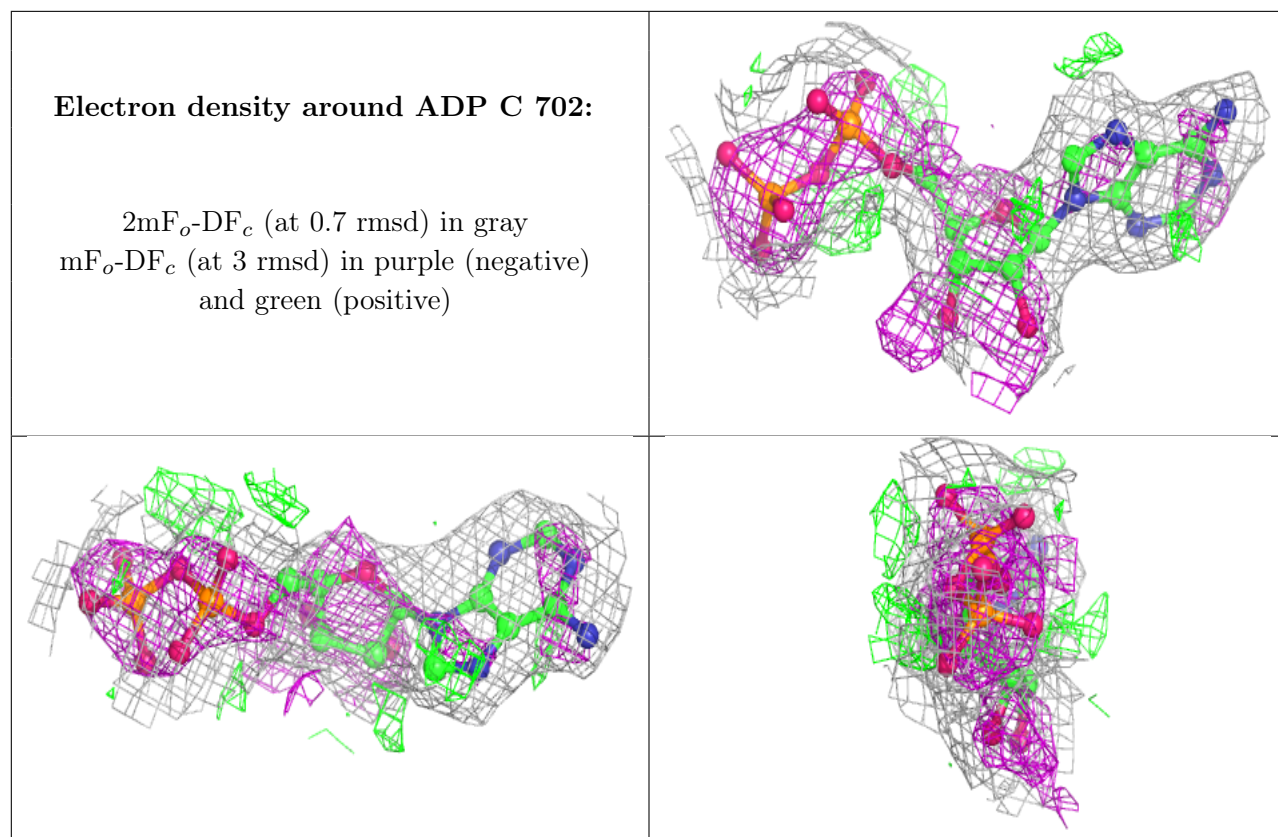
Electron density around ADP D 703:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP G 706:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.