



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:29 pm GMT

PDB ID : 5FTN
EMDB ID: : EMD-3299
Title : Cryo-EM structure of human p97 bound to ATPgS (Conformation III)
Authors : Banerjee, S.; Bartesaghi, A.; Merk, A.; Rao, P.; Bulfer, S.L.; Yan, Y.; Green, N.; Mroczkowski, B.; Neitz, R.J.; Wipf, P.; Falconieri, V.; Deshaies, R.J.; Milne, J.L.S.; Huryn, D.; Arkin, M.; Subramaniam, S.
Deposited on : 2016-01-14
Resolution : 3.30 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

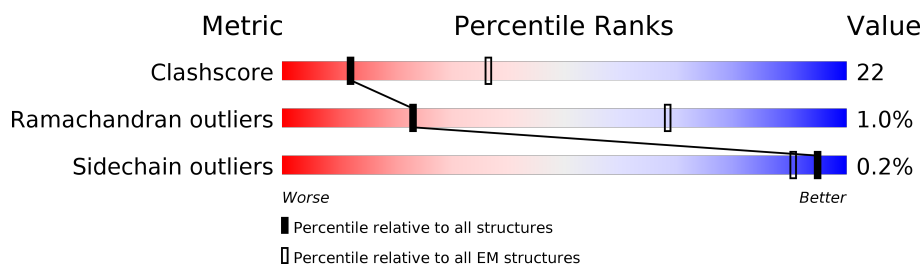
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	806	
1	B	806	
1	C	806	
1	D	806	
1	E	806	
1	F	806	

2 Entry composition [i](#)

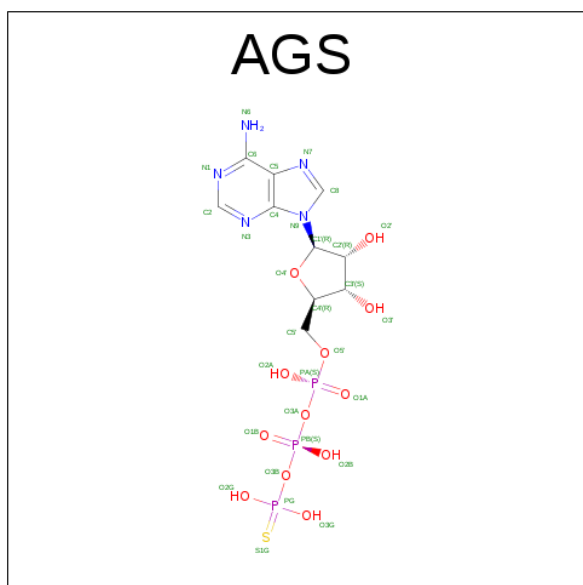
There are 3 unique types of molecules in this entry. The entry contains 34956 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	B	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	C	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	D	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	E	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		
1	F	737	Total	C	N	O	S	0	0
			5762	3627	1014	1091	30		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

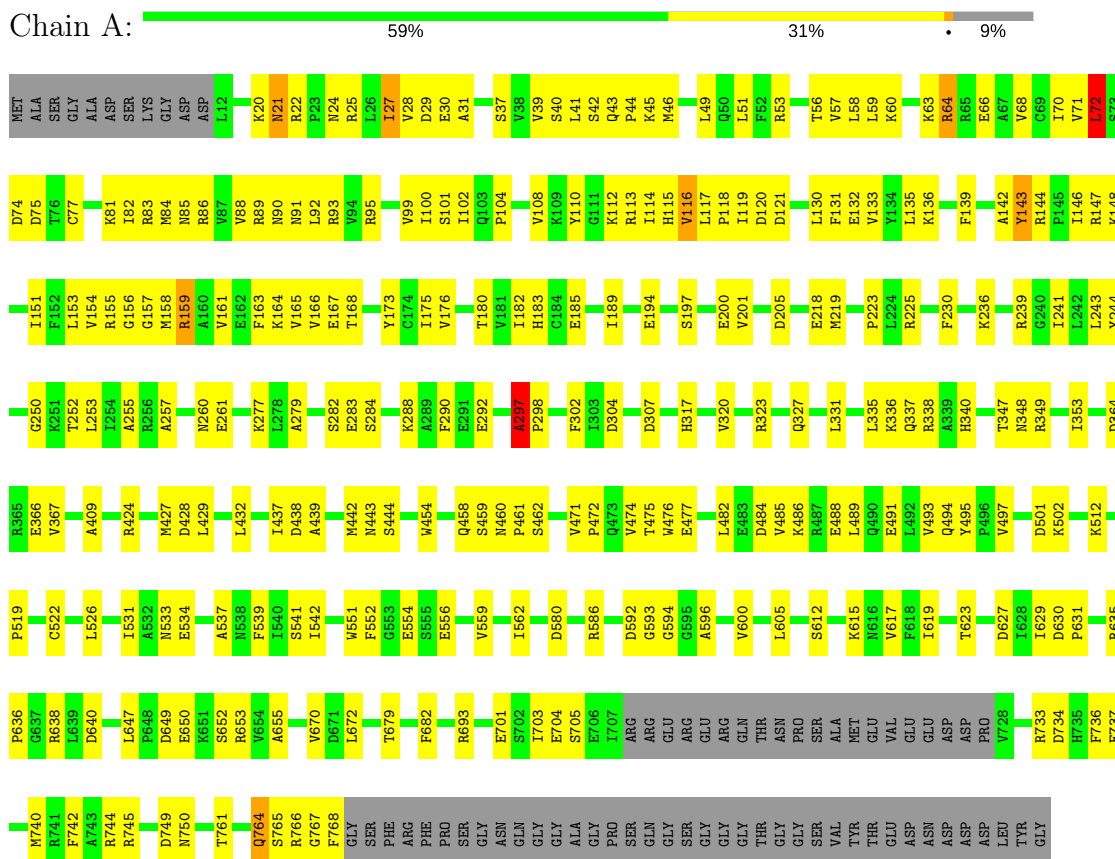
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	D	2	Total	Mg	0
			2	2	
3	E	2	Total	Mg	0
			2	2	
3	B	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	
3	A	2	Total	Mg	0
			2	2	
3	F	2	Total	Mg	0
			2	2	

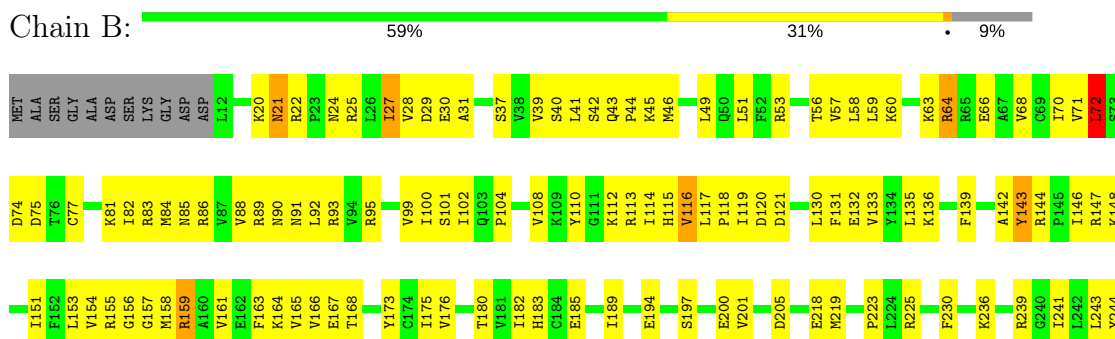
3 Residue-property plots

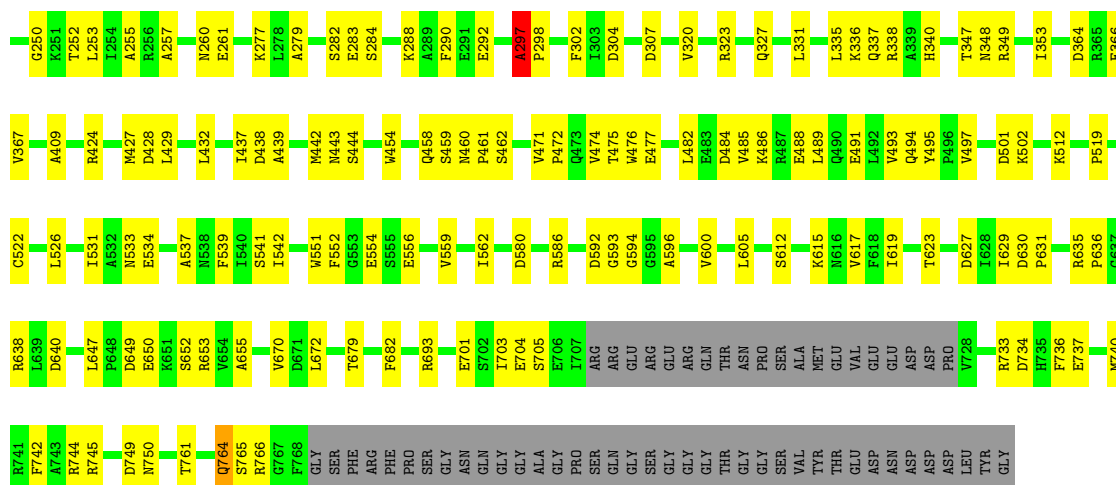
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



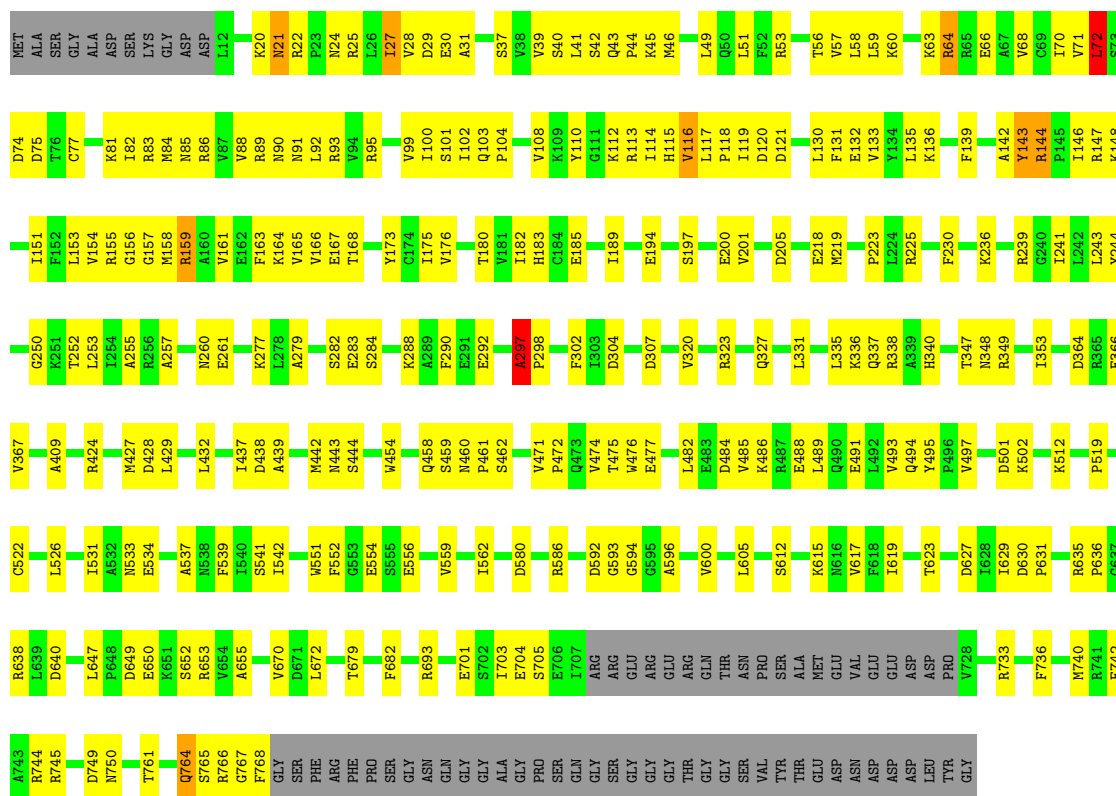
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE





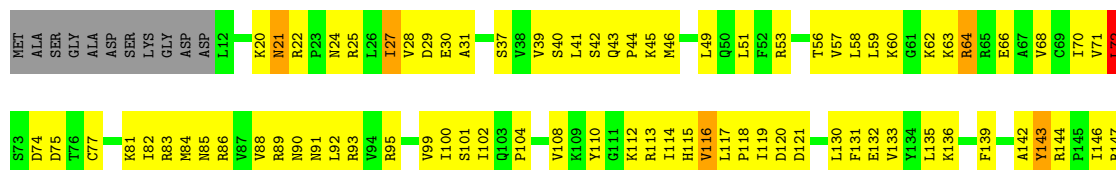
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

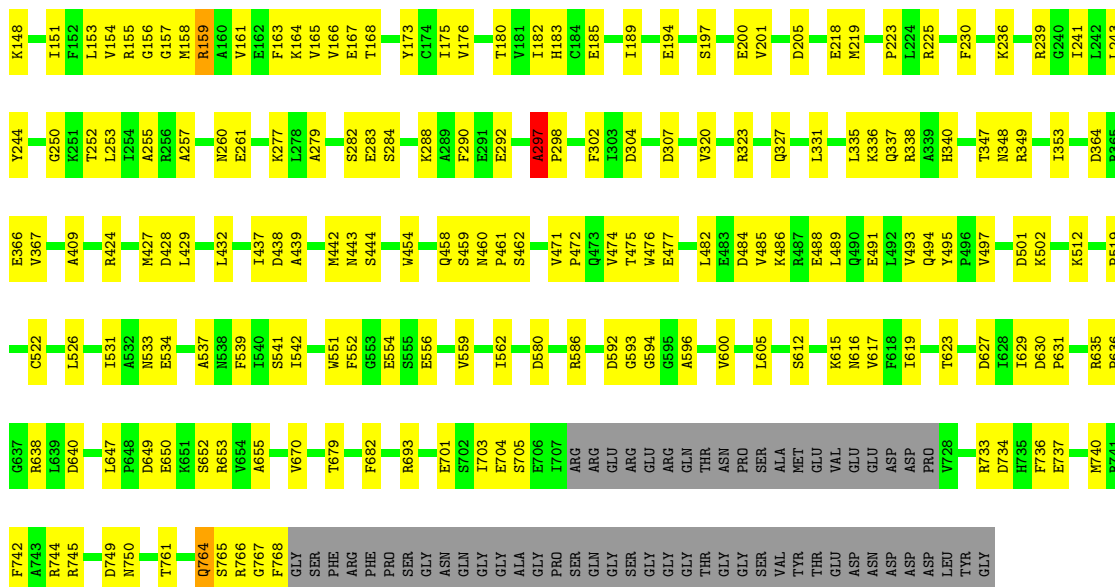
Chain C: 59% 31% 9%



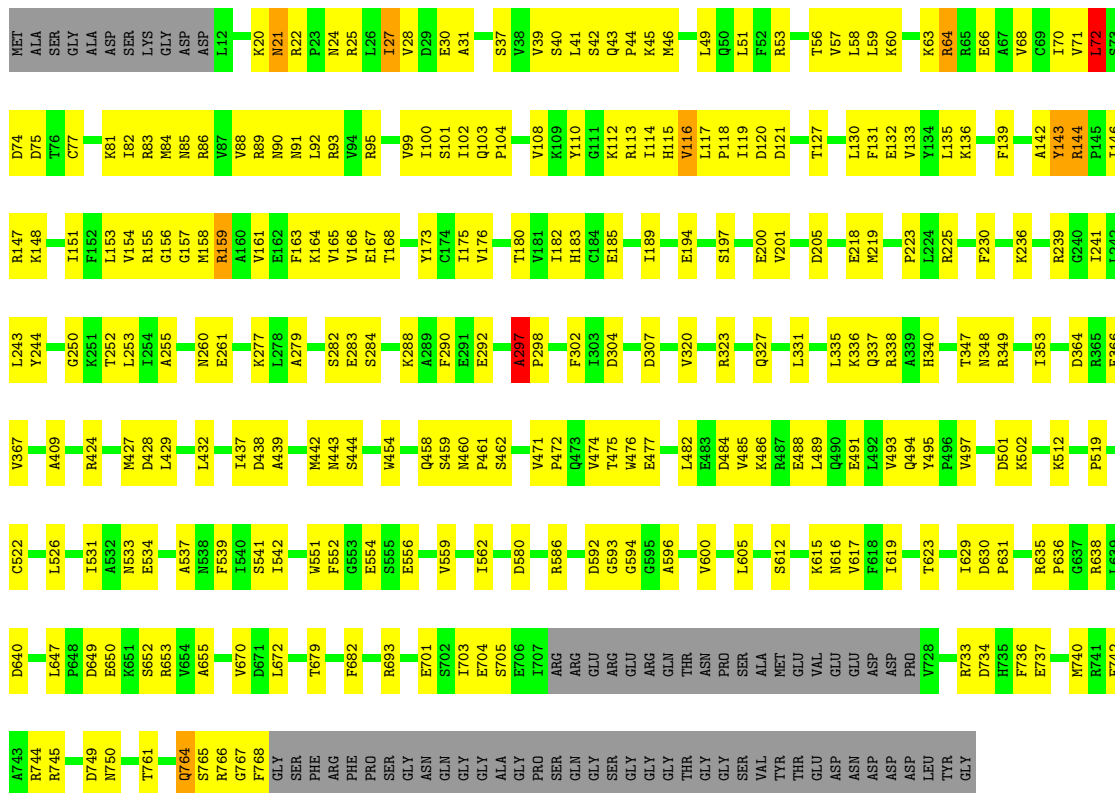
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain D: 59% 31% 9%

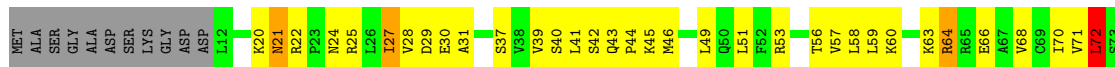




- Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



- Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE



M740	P636	P519	E366	G250	I151	D74
R741	G637	C522	V367	K251	F152	D75
F742	R638	L526	A409	T252	L153	T76
A743	L639	L531	R424	L253	V154	C77
R745	L647	A532	M427	A254	R155	K81
D749	P648	N533	D428	R256	G156	T82
N750	D649	E534	L429	A257	G157	R83
T761	S652	A537	L432	N260	M158	M84
O764	R653	N538	F539	E261	R159	N85
S765	V654	F552	I437	V261	A160	R86
R766	A655	T540	D438	K277	V161	V87
G767	V670	S541	A439	L278	F163	V88
F768	D671	I542	M442	A279	K164	R89
GLY	L672	W551	N443	S282	V166	N90
SER	T679	F553	S444	E283	E167	N91
PHE	F682	E554	W454	S284	T168	L92
ARG	PRO	S555	Q458	K288	Y173	R93
GLY	R693	E556	S459	F290	G174	V94
ASN	E701	V559	M460	E291	V176	I100
GLN	S702	I562	P461	E292	T180	S101
GLY	I703	D580	S462	A297	V181	I102
GLY	E704	R586	V471	P298	I182	Q103
ALA	S705	D592	P472	F302	H183	P104
GLY	E706	G593	Q473	I303	G184	V108
PRO	I707	G594	E477	D304	E185	K109
SER	ARG	G595	A596	L331	I189	I110
GLN	ARG	V600	L482	L335	E194	G111
GLY	GLU	L605	E483	K336	S197	K112
SER	GLU	SER	D484	Q337	E200	R113
GLY	GLY	PRO	V485	R338	V201	I114
GLY	GLY	THR	K486	R339	D205	H115
GLY	GLN	VAL	S612	Q340	E218	V116
THR	THR	GLU	K615	L331	M219	L117
GLY	ASN	VAL	N616	L335	P223	P118
GLY	PRO	GLU	V617	K336	L224	I119
SER	SER	GLU	F618	Q337	R225	D120
VAL	ALA	ASP	I619	R338	F230	D121
ASP	ASP	ASP	T623	A339	F230	L130
ASP	PRO	PRO	V495	H340	K236	F131
LEU	V728	TYR	D627	T347	R239	E132
TYR	R733	GLY	I628	N348	G240	V133
	D734		I629	R349	I241	Y134
	H735		D630	K502	L242	L135
	F736		P631	K512	L243	K136
	E737		R635		Y244	F139
						A142
						Y143
						R144
						F145
						I146
						R147
						K148

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	950	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	36980	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

5 Model quality

5.1 Standard geometry

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.50	0/5855	0.65	3/7905 (0.0%)
1	B	0.50	0/5855	0.65	3/7905 (0.0%)
1	C	0.50	0/5855	0.65	3/7905 (0.0%)
1	D	0.50	0/5855	0.65	3/7905 (0.0%)
1	E	0.50	0/5855	0.65	3/7905 (0.0%)
1	F	0.50	0/5855	0.65	3/7905 (0.0%)
All	All	0.50	0/35130	0.65	18/47430 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	6
1	D	0	6
1	E	0	6
1	F	0	6
All	All	0	36

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	143	TYR	C-N-CA	5.73	136.03	121.70
1	C	143	TYR	C-N-CA	5.73	136.02	121.70
1	A	143	TYR	C-N-CA	5.71	135.98	121.70
1	D	143	TYR	C-N-CA	5.71	135.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	143	TYR	C-N-CA	5.71	135.98	121.70
1	B	143	TYR	C-N-CA	5.70	135.96	121.70
1	C	72	LEU	CA-CB-CG	5.60	128.19	115.30
1	D	72	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	72	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	72	LEU	CA-CB-CG	5.60	128.17	115.30
1	F	72	LEU	CA-CB-CG	5.59	128.16	115.30
1	E	72	LEU	CA-CB-CG	5.58	128.14	115.30
1	C	297	ALA	C-N-CD	5.40	139.74	128.40
1	F	297	ALA	C-N-CD	5.40	139.74	128.40
1	E	297	ALA	C-N-CD	5.40	139.73	128.40
1	D	297	ALA	C-N-CD	5.39	139.73	128.40
1	B	297	ALA	C-N-CD	5.38	139.71	128.40
1	A	297	ALA	C-N-CD	5.38	139.70	128.40

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ALA	Peptide
1	A	144	ARG	Peptide
1	A	156	GLY	Peptide
1	A	159	ARG	Peptide
1	A	64	ARG	Peptide
1	A	72	LEU	Peptide
1	B	142	ALA	Peptide
1	B	144	ARG	Peptide
1	B	156	GLY	Peptide
1	B	159	ARG	Peptide
1	B	64	ARG	Peptide
1	B	72	LEU	Peptide
1	C	142	ALA	Peptide
1	C	144	ARG	Peptide
1	C	156	GLY	Peptide
1	C	159	ARG	Peptide
1	C	64	ARG	Peptide
1	C	72	LEU	Peptide
1	D	142	ALA	Peptide
1	D	144	ARG	Peptide
1	D	156	GLY	Peptide
1	D	159	ARG	Peptide
1	D	64	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	D	72	LEU	Peptide
1	E	142	ALA	Peptide
1	E	144	ARG	Peptide
1	E	156	GLY	Peptide
1	E	159	ARG	Peptide
1	E	64	ARG	Peptide
1	E	72	LEU	Peptide
1	F	142	ALA	Peptide
1	F	144	ARG	Peptide
1	F	156	GLY	Peptide
1	F	159	ARG	Peptide
1	F	64	ARG	Peptide
1	F	72	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5762	0	5841	259	0
1	B	5762	0	5841	258	0
1	C	5762	0	5841	261	0
1	D	5762	0	5841	261	0
1	E	5762	0	5841	258	0
1	F	5762	0	5841	261	0
2	A	62	0	24	10	0
2	B	62	0	24	10	0
2	C	62	0	24	10	0
2	D	62	0	24	9	0
2	E	62	0	24	10	0
2	F	62	0	24	10	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	34956	0	35190	1518	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 22.

All (1518) 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:B:113:ARG:NH2	1:B:131:PHE:CE2	2.26	1.03
1:C:113:ARG:NH2	1:C:131:PHE:CE2	2.26	1.03
1:D:113:ARG:NH2	1:D:131:PHE:CE2	2.26	1.03
1:A:113:ARG:NH2	1:A:131:PHE:CE2	2.26	1.03
1:F:113:ARG:NH2	1:F:131:PHE:CE2	2.26	1.02
1:E:113:ARG:NH2	1:E:131:PHE:CE2	2.26	1.02
1:B:596:ALA:HB3	1:B:630:ASP:HB3	1.47	0.97
1:E:596:ALA:HB3	1:E:630:ASP:HB3	1.47	0.97
1:C:113:ARG:HH22	1:C:131:PHE:HE2	1.10	0.97
1:A:596:ALA:HB3	1:A:630:ASP:HB3	1.47	0.96
1:D:596:ALA:HB3	1:D:630:ASP:HB3	1.47	0.96
1:F:596:ALA:HB3	1:F:630:ASP:HB3	1.47	0.96
1:B:113:ARG:HH22	1:B:131:PHE:HE2	1.10	0.95
1:C:113:ARG:HD3	1:C:182:ILE:CG2	1.96	0.95
1:C:596:ALA:HB3	1:C:630:ASP:HB3	1.47	0.95
1:E:113:ARG:HD3	1:E:182:ILE:CG2	1.96	0.95
1:D:113:ARG:HD3	1:D:182:ILE:CG2	1.96	0.95
1:B:113:ARG:HD3	1:B:182:ILE:CG2	1.96	0.95
1:F:113:ARG:HD3	1:F:182:ILE:CG2	1.96	0.95
1:A:113:ARG:HD3	1:A:182:ILE:CG2	1.96	0.95
1:D:113:ARG:HH22	1:D:131:PHE:HE2	1.10	0.93
1:A:113:ARG:HH22	1:A:131:PHE:HE2	1.10	0.91
1:F:113:ARG:HH22	1:F:131:PHE:HE2	1.10	0.91
1:B:113:ARG:HD3	1:B:182:ILE:HG23	1.53	0.90
1:B:297:ALA:HB1	1:B:298:PRO:HD3	1.55	0.89
1:E:113:ARG:HH22	1:E:131:PHE:HE2	1.10	0.89
1:F:113:ARG:HD3	1:F:182:ILE:HG23	1.53	0.89
1:E:113:ARG:HD3	1:E:182:ILE:HG23	1.53	0.89
1:C:297:ALA:HB1	1:C:298:PRO:HD3	1.55	0.89
1:A:113:ARG:HD3	1:A:182:ILE:HG23	1.53	0.88
1:C:113:ARG:HD3	1:C:182:ILE:HG23	1.53	0.88
1:A:297:ALA:HB1	1:A:298:PRO:HD3	1.55	0.88
1:B:250:GLY:HA2	2:B:901:AGS:O2A	1.74	0.88
1:D:297:ALA:HB1	1:D:298:PRO:HD3	1.55	0.88
1:C:250:GLY:HA2	2:C:901:AGS:O2A	1.74	0.87
1:A:250:GLY:HA2	2:A:901:AGS:O2A	1.74	0.87
1:D:113:ARG:HD3	1:D:182:ILE:HG23	1.53	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HD12	1:A:176:VAL:HG11	1.57	0.87
1:F:297:ALA:HB1	1:F:298:PRO:HD3	1.55	0.86
1:B:114:ILE:HD12	1:B:176:VAL:HG11	1.57	0.86
1:D:114:ILE:HD12	1:D:176:VAL:HG11	1.57	0.86
1:E:297:ALA:HB1	1:E:298:PRO:HD3	1.55	0.86
1:F:250:GLY:HA2	2:F:901:AGS:O2A	1.74	0.86
1:D:250:GLY:HA2	2:D:901:AGS:O2A	1.74	0.86
1:E:250:GLY:HA2	2:E:901:AGS:O2A	1.74	0.86
1:E:225:ARG:HH21	1:F:432:LEU:HD22	1.40	0.85
1:C:114:ILE:HD12	1:C:176:VAL:HG11	1.57	0.85
1:F:114:ILE:HD12	1:F:176:VAL:HG11	1.57	0.85
1:D:132:GLU:HG3	1:D:136:LYS:HD3	1.59	0.85
1:B:113:ARG:O	1:B:114:ILE:HG13	1.77	0.84
1:A:113:ARG:O	1:A:114:ILE:HG13	1.77	0.84
1:E:132:GLU:HG3	1:E:136:LYS:HD3	1.59	0.84
1:C:25:ARG:HG3	1:C:99:VAL:HG11	1.60	0.84
1:D:25:ARG:HG3	1:D:99:VAL:HG11	1.60	0.84
1:E:114:ILE:HD12	1:E:176:VAL:HG11	1.57	0.84
1:B:25:ARG:HG3	1:B:99:VAL:HG11	1.60	0.84
1:D:114:ILE:HD12	1:D:176:VAL:CG1	2.08	0.84
1:A:114:ILE:HD12	1:A:176:VAL:CG1	2.08	0.84
1:B:225:ARG:HH21	1:C:432:LEU:HD22	1.41	0.84
1:E:25:ARG:HG3	1:E:99:VAL:HG11	1.60	0.84
1:B:114:ILE:HD12	1:B:176:VAL:CG1	2.08	0.84
1:F:114:ILE:HD12	1:F:176:VAL:CG1	2.08	0.83
1:A:225:ARG:HH21	1:B:432:LEU:HD22	1.43	0.83
1:C:132:GLU:HG3	1:C:136:LYS:HD3	1.59	0.83
1:C:53:ARG:HA	1:C:72:LEU:HD11	1.60	0.83
1:F:25:ARG:HG3	1:F:99:VAL:HG11	1.60	0.83
1:D:225:ARG:HH21	1:E:432:LEU:HD22	1.42	0.83
1:D:53:ARG:HA	1:D:72:LEU:HD11	1.60	0.83
1:F:113:ARG:O	1:F:114:ILE:HG13	1.77	0.83
1:C:113:ARG:O	1:C:114:ILE:HG13	1.77	0.83
1:E:113:ARG:O	1:E:114:ILE:HG13	1.77	0.83
1:A:432:LEU:HD22	1:F:225:ARG:HH21	1.42	0.83
1:B:53:ARG:HA	1:B:72:LEU:HD11	1.60	0.83
1:A:132:GLU:HG3	1:A:136:LYS:HD3	1.59	0.83
1:A:25:ARG:HG3	1:A:99:VAL:HG11	1.60	0.83
1:C:114:ILE:HD12	1:C:176:VAL:CG1	2.08	0.83
1:D:113:ARG:O	1:D:114:ILE:HG13	1.77	0.83
1:A:53:ARG:HA	1:A:72:LEU:HD11	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ARG:HH21	1:D:432:LEU:HD22	1.42	0.82
1:E:114:ILE:HD12	1:E:176:VAL:CG1	2.08	0.82
1:E:53:ARG:HA	1:E:72:LEU:HD11	1.60	0.82
1:E:64:ARG:HH12	1:E:260:ASN:HA	1.45	0.82
1:F:53:ARG:HA	1:F:72:LEU:HD11	1.60	0.82
1:B:132:GLU:HG3	1:B:136:LYS:HD3	1.59	0.81
1:F:64:ARG:HH12	1:F:260:ASN:HA	1.44	0.81
1:B:64:ARG:HH12	1:B:260:ASN:HA	1.44	0.81
1:F:132:GLU:HG3	1:F:136:LYS:HD3	1.59	0.81
1:C:64:ARG:HH12	1:C:260:ASN:HA	1.44	0.81
1:A:64:ARG:HH12	1:A:260:ASN:HA	1.45	0.80
1:D:64:ARG:HH12	1:D:260:ASN:HA	1.45	0.80
1:D:57:VAL:HA	1:D:104:PRO:HA	1.64	0.80
1:A:22:ARG:NH1	1:A:24:ASN:HB3	1.98	0.79
1:C:57:VAL:HA	1:C:104:PRO:HA	1.64	0.79
1:B:57:VAL:HA	1:B:104:PRO:HA	1.64	0.79
1:B:22:ARG:NH1	1:B:24:ASN:HB3	1.98	0.79
1:F:22:ARG:NH1	1:F:24:ASN:HB3	1.98	0.79
1:C:22:ARG:NH1	1:C:24:ASN:HB3	1.98	0.79
1:D:22:ARG:NH1	1:D:24:ASN:HB3	1.98	0.78
1:E:586:ARG:HD3	1:E:594:GLY:HA3	1.65	0.78
2:A:901:AGS:H8	2:A:901:AGS:H5'1	1.65	0.78
1:E:57:VAL:HA	1:E:104:PRO:HA	1.64	0.78
1:F:586:ARG:HD3	1:F:594:GLY:HA3	1.65	0.78
1:E:22:ARG:NH1	1:E:24:ASN:HB3	1.98	0.78
1:A:586:ARG:HD3	1:A:594:GLY:HA3	1.65	0.78
2:E:901:AGS:H5'1	2:E:901:AGS:H8	1.65	0.78
1:A:57:VAL:HA	1:A:104:PRO:HA	1.64	0.78
1:D:586:ARG:HD3	1:D:594:GLY:HA3	1.65	0.78
1:F:57:VAL:HA	1:F:104:PRO:HA	1.64	0.78
1:B:586:ARG:HD3	1:B:594:GLY:HA3	1.65	0.78
1:C:28:VAL:HA	1:C:82:ILE:HG22	1.66	0.78
2:D:901:AGS:H8	2:D:901:AGS:H5'1	1.65	0.78
1:D:28:VAL:HA	1:D:82:ILE:HG22	1.66	0.78
2:C:901:AGS:H8	2:C:901:AGS:H5'1	1.65	0.77
1:B:28:VAL:HA	1:B:82:ILE:HG22	1.66	0.77
2:F:901:AGS:H5'1	2:F:901:AGS:H8	1.65	0.77
1:C:586:ARG:HD3	1:C:594:GLY:HA3	1.65	0.77
2:B:901:AGS:H8	2:B:901:AGS:H5'1	1.65	0.77
1:A:28:VAL:HA	1:A:82:ILE:HG22	1.66	0.76
1:D:148:LYS:HG2	1:D:165:VAL:HG11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:VAL:HA	1:E:82:ILE:HG22	1.66	0.76
1:F:28:VAL:HA	1:F:82:ILE:HG22	1.66	0.76
1:E:60:LYS:HB2	1:E:101:SER:HB3	1.68	0.76
1:F:60:LYS:HB2	1:F:101:SER:HB3	1.68	0.76
1:B:148:LYS:HG2	1:B:165:VAL:HG11	1.68	0.75
1:C:148:LYS:HG2	1:C:165:VAL:HG11	1.68	0.75
1:E:148:LYS:HG2	1:E:165:VAL:HG11	1.68	0.75
1:C:670:VAL:HA	1:C:733:ARG:HD3	1.69	0.75
1:E:670:VAL:HA	1:E:733:ARG:HD3	1.69	0.75
1:B:670:VAL:HA	1:B:733:ARG:HD3	1.69	0.74
1:D:60:LYS:HB2	1:D:101:SER:HB3	1.68	0.74
1:D:670:VAL:HA	1:D:733:ARG:HD3	1.69	0.74
1:F:670:VAL:HA	1:F:733:ARG:HD3	1.69	0.74
1:B:60:LYS:HB2	1:B:101:SER:HB3	1.68	0.74
1:C:60:LYS:HB2	1:C:101:SER:HB3	1.68	0.74
1:A:148:LYS:HG2	1:A:165:VAL:HG11	1.68	0.74
1:A:612:SER:HB3	1:A:615:LYS:HG2	1.70	0.74
1:E:113:ARG:HD3	1:E:182:ILE:HG21	1.70	0.74
1:A:670:VAL:HA	1:A:733:ARG:HD3	1.69	0.74
1:C:113:ARG:HD3	1:C:182:ILE:HG21	1.70	0.74
1:E:112:LYS:O	1:E:113:ARG:HB3	1.87	0.73
1:E:612:SER:HB3	1:E:615:LYS:HG2	1.70	0.73
1:F:612:SER:HB3	1:F:615:LYS:HG2	1.70	0.73
1:D:112:LYS:O	1:D:113:ARG:HB3	1.87	0.73
1:A:112:LYS:O	1:A:113:ARG:HB3	1.87	0.73
1:B:113:ARG:HD3	1:B:182:ILE:HG21	1.70	0.73
1:B:612:SER:HB3	1:B:615:LYS:HG2	1.70	0.73
1:F:112:LYS:O	1:F:113:ARG:HB3	1.87	0.73
1:F:148:LYS:HG2	1:F:165:VAL:HG11	1.68	0.73
1:B:112:LYS:O	1:B:113:ARG:HB3	1.87	0.73
1:C:112:LYS:O	1:C:113:ARG:HB3	1.87	0.73
1:D:612:SER:HB3	1:D:615:LYS:HG2	1.70	0.73
1:A:164:LYS:HG2	1:A:165:VAL:H	1.54	0.73
1:B:20:LYS:O	1:B:21:ASN:CG	2.28	0.73
1:C:164:LYS:HG2	1:C:165:VAL:H	1.54	0.73
1:A:113:ARG:HD3	1:A:182:ILE:HG21	1.70	0.72
1:D:164:LYS:HG2	1:D:165:VAL:H	1.54	0.72
1:A:60:LYS:HB2	1:A:101:SER:HB3	1.68	0.72
1:F:164:LYS:HG2	1:F:165:VAL:H	1.54	0.72
1:E:20:LYS:O	1:E:21:ASN:CG	2.28	0.72
1:D:20:LYS:O	1:D:21:ASN:CG	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:SER:HB3	1:C:615:LYS:HG2	1.70	0.72
1:F:113:ARG:HD3	1:F:182:ILE:HG21	1.70	0.72
1:A:20:LYS:O	1:A:21:ASN:CG	2.28	0.72
1:E:164:LYS:HG2	1:E:165:VAL:H	1.54	0.72
1:C:20:LYS:O	1:C:21:ASN:CG	2.28	0.72
1:D:113:ARG:HD3	1:D:182:ILE:HG21	1.70	0.72
1:F:20:LYS:O	1:F:21:ASN:CG	2.28	0.72
1:B:164:LYS:HG2	1:B:165:VAL:H	1.54	0.71
1:A:476:TRP:NE1	1:A:534:GLU:OE1	2.23	0.71
1:F:476:TRP:NE1	1:F:534:GLU:OE1	2.23	0.71
1:F:236:LYS:HG3	1:F:337:GLN:HE21	1.57	0.70
1:A:236:LYS:HG3	1:A:337:GLN:HE21	1.57	0.70
1:B:130:LEU:O	1:B:133:VAL:N	2.25	0.70
1:F:130:LEU:O	1:F:133:VAL:N	2.25	0.70
1:E:476:TRP:NE1	1:E:534:GLU:OE1	2.23	0.69
1:B:476:TRP:NE1	1:B:534:GLU:OE1	2.23	0.69
1:E:236:LYS:HG3	1:E:337:GLN:HE21	1.57	0.69
1:B:236:LYS:HG3	1:B:337:GLN:HE21	1.57	0.69
1:C:130:LEU:O	1:C:133:VAL:N	2.25	0.69
1:A:130:LEU:O	1:A:133:VAL:N	2.25	0.69
1:B:766:ARG:NH2	2:C:902:AGS:O3G	2.26	0.69
1:E:113:ARG:CD	1:E:182:ILE:HG21	2.23	0.69
1:A:113:ARG:CD	1:A:182:ILE:HG21	2.23	0.69
1:D:113:ARG:CD	1:D:182:ILE:HG21	2.23	0.69
1:D:236:LYS:HG3	1:D:337:GLN:HE21	1.57	0.69
1:B:113:ARG:CD	1:B:182:ILE:HG21	2.23	0.69
1:C:236:LYS:HG3	1:C:337:GLN:HE21	1.57	0.69
1:E:250:GLY:CA	2:E:901:AGS:O2A	2.41	0.69
1:A:336:LYS:HB2	1:A:338:ARG:HG2	1.75	0.69
1:C:113:ARG:CD	1:C:182:ILE:HG21	2.23	0.69
1:F:277:LYS:HB2	1:F:282:SER:HB3	1.75	0.69
1:C:277:LYS:HB2	1:C:282:SER:HB3	1.75	0.68
1:D:250:GLY:CA	2:D:901:AGS:O2A	2.41	0.68
1:B:277:LYS:HB2	1:B:282:SER:HB3	1.75	0.68
1:B:526:LEU:HD11	2:B:902:AGS:H2'	1.76	0.68
1:C:336:LYS:HB2	1:C:338:ARG:HG2	1.75	0.68
1:E:766:ARG:NH2	2:F:902:AGS:O3G	2.27	0.68
1:F:526:LEU:HD11	2:F:902:AGS:H2'	1.76	0.68
1:B:336:LYS:HB2	1:B:338:ARG:HG2	1.75	0.68
1:E:526:LEU:HD11	2:E:902:AGS:H2'	1.76	0.68
1:D:766:ARG:NH2	2:E:902:AGS:O3G	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:ARG:CD	1:F:182:ILE:HG21	2.23	0.68
1:D:277:LYS:HB2	1:D:282:SER:HB3	1.75	0.68
1:E:130:LEU:O	1:E:133:VAL:N	2.25	0.68
1:F:250:GLY:CA	2:F:901:AGS:O2A	2.41	0.68
1:A:526:LEU:HD11	2:A:902:AGS:H2'	1.76	0.68
1:C:121:ASP:HB3	1:C:161:VAL:HG22	1.76	0.68
1:C:476:TRP:NE1	1:C:534:GLU:OE1	2.23	0.68
1:F:121:ASP:HB3	1:F:161:VAL:HG22	1.76	0.68
1:F:336:LYS:HB2	1:F:338:ARG:HG2	1.75	0.68
2:A:902:AGS:O3G	1:F:766:ARG:NH2	2.26	0.68
1:A:277:LYS:HB2	1:A:282:SER:HB3	1.75	0.68
1:C:526:LEU:HD11	2:C:902:AGS:H2'	1.76	0.68
1:D:121:ASP:HB3	1:D:161:VAL:HG22	1.76	0.68
1:C:766:ARG:NH2	2:D:902:AGS:O3G	2.27	0.68
1:C:250:GLY:CA	2:C:901:AGS:O2A	2.41	0.67
1:E:121:ASP:HB3	1:E:161:VAL:HG22	1.76	0.67
1:B:250:GLY:CA	2:B:901:AGS:O2A	2.41	0.67
1:B:60:LYS:N	1:B:101:SER:O	2.27	0.67
1:D:476:TRP:NE1	1:D:534:GLU:OE1	2.23	0.67
1:E:277:LYS:HB2	1:E:282:SER:HB3	1.75	0.67
1:A:60:LYS:N	1:A:101:SER:O	2.27	0.67
1:D:526:LEU:HD11	2:D:902:AGS:H2'	1.76	0.67
1:A:250:GLY:CA	2:A:901:AGS:O2A	2.41	0.67
1:D:336:LYS:HB2	1:D:338:ARG:HG2	1.75	0.67
1:B:90:ASN:OD1	1:B:91:ASN:N	2.28	0.67
1:A:121:ASP:HB3	1:A:161:VAL:HG22	1.76	0.67
1:E:336:LYS:HB2	1:E:338:ARG:HG2	1.75	0.67
1:D:90:ASN:OD1	1:D:91:ASN:N	2.28	0.67
1:B:121:ASP:HB3	1:B:161:VAL:HG22	1.76	0.67
1:B:131:PHE:CE1	1:B:135:LEU:HD22	2.30	0.66
1:C:131:PHE:CE1	1:C:135:LEU:HD22	2.30	0.66
1:F:60:LYS:N	1:F:101:SER:O	2.27	0.66
1:F:90:ASN:OD1	1:F:91:ASN:N	2.28	0.66
1:A:766:ARG:NH2	2:B:902:AGS:O3G	2.28	0.66
1:E:90:ASN:OD1	1:E:91:ASN:N	2.28	0.66
1:F:347:THR:HG21	1:F:353:ILE:HD11	1.78	0.66
1:C:117:LEU:HD13	1:C:166:VAL:HG11	1.77	0.66
1:E:60:LYS:N	1:E:101:SER:O	2.27	0.66
1:D:117:LEU:HD13	1:D:166:VAL:HG11	1.77	0.66
1:C:472:PRO:O	1:C:533:ASN:ND2	2.29	0.66
1:C:90:ASN:OD1	1:C:91:ASN:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:THR:HG21	1:D:353:ILE:HD11	1.77	0.66
1:E:347:THR:HG21	1:E:353:ILE:HD11	1.78	0.66
1:A:117:LEU:HD13	1:A:166:VAL:HG11	1.77	0.66
1:C:60:LYS:N	1:C:101:SER:O	2.27	0.66
1:B:113:ARG:NH2	1:B:131:PHE:CZ	2.64	0.66
1:D:472:PRO:O	1:D:533:ASN:ND2	2.29	0.66
1:F:472:PRO:O	1:F:533:ASN:ND2	2.29	0.66
1:D:512:LYS:HG2	1:D:512:LYS:O	1.97	0.65
1:F:297:ALA:HB1	1:F:298:PRO:CD	2.26	0.65
1:A:472:PRO:O	1:A:533:ASN:ND2	2.29	0.65
1:B:472:PRO:O	1:B:533:ASN:ND2	2.29	0.65
1:D:409:ALA:HB2	2:D:901:AGS:H5'2	1.79	0.65
1:E:113:ARG:NH2	1:E:131:PHE:CZ	2.64	0.65
1:E:131:PHE:CE1	1:E:135:LEU:HD22	2.30	0.65
1:E:472:PRO:O	1:E:533:ASN:ND2	2.29	0.65
1:E:512:LYS:HG2	1:E:512:LYS:O	1.96	0.65
1:A:30:GLU:HA	1:A:86:ARG:NH2	2.12	0.65
1:A:90:ASN:OD1	1:A:91:ASN:N	2.28	0.65
1:B:30:GLU:HA	1:B:86:ARG:NH2	2.12	0.65
1:D:60:LYS:N	1:D:101:SER:O	2.27	0.65
1:E:117:LEU:HD13	1:E:166:VAL:HG11	1.77	0.65
1:F:131:PHE:CE1	1:F:135:LEU:HD22	2.30	0.65
1:A:347:THR:HG21	1:A:353:ILE:HD11	1.77	0.65
1:C:113:ARG:NH2	1:C:131:PHE:CZ	2.64	0.65
1:C:512:LYS:O	1:C:512:LYS:HG2	1.97	0.65
1:D:130:LEU:O	1:D:133:VAL:N	2.25	0.65
1:F:113:ARG:NH2	1:F:131:PHE:CZ	2.64	0.65
1:A:131:PHE:CE1	1:A:135:LEU:HD22	2.30	0.65
1:B:512:LYS:O	1:B:512:LYS:HG2	1.96	0.65
1:C:409:ALA:HB2	2:C:901:AGS:H5'2	1.79	0.65
1:D:113:ARG:NH2	1:D:131:PHE:CZ	2.64	0.65
1:D:491:GLU:HG2	1:D:495:TYR:CE2	2.32	0.65
1:B:117:LEU:HD13	1:B:166:VAL:HG11	1.77	0.65
1:C:347:THR:HG21	1:C:353:ILE:HD11	1.77	0.65
1:C:491:GLU:HG2	1:C:495:TYR:CE2	2.32	0.65
1:F:512:LYS:HG2	1:F:512:LYS:O	1.97	0.65
1:A:512:LYS:O	1:A:512:LYS:HG2	1.97	0.65
1:B:491:GLU:HG2	1:B:495:TYR:CE2	2.32	0.65
1:D:131:PHE:CE1	1:D:135:LEU:HD22	2.30	0.65
1:F:117:LEU:HD13	1:F:166:VAL:HG11	1.77	0.65
1:A:297:ALA:HB1	1:A:298:PRO:CD	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:NH2	1:A:131:PHE:CZ	2.64	0.65
1:B:297:ALA:HB1	1:B:298:PRO:CD	2.26	0.65
1:E:409:ALA:HB2	2:E:901:AGS:H5'2	1.79	0.65
1:E:491:GLU:HG2	1:E:495:TYR:CE2	2.32	0.64
1:F:491:GLU:HG2	1:F:495:TYR:CE2	2.32	0.64
1:A:42:SER:HB2	1:A:45:LYS:HB3	1.79	0.64
1:B:347:THR:HG21	1:B:353:ILE:HD11	1.78	0.64
1:B:409:ALA:HB2	2:B:901:AGS:H5'2	1.79	0.64
1:C:42:SER:HB2	1:C:45:LYS:HB3	1.79	0.64
1:D:42:SER:HB2	1:D:45:LYS:HB3	1.79	0.64
1:E:42:SER:HB2	1:E:45:LYS:HB3	1.79	0.64
1:C:30:GLU:HA	1:C:86:ARG:NH2	2.12	0.64
1:B:42:SER:HB2	1:B:45:LYS:HB3	1.79	0.64
1:D:22:ARG:HH11	1:D:24:ASN:HB3	1.63	0.64
1:F:42:SER:HB2	1:F:45:LYS:HB3	1.79	0.64
1:A:491:GLU:HG2	1:A:495:TYR:CE2	2.32	0.64
1:D:30:GLU:HA	1:D:86:ARG:NH2	2.12	0.64
1:E:30:GLU:HA	1:E:86:ARG:NH2	2.12	0.64
1:E:218:GLU:OE1	1:F:424:ARG:NH2	2.31	0.64
1:F:409:ALA:HB2	2:F:901:AGS:H5'2	1.79	0.64
1:F:30:GLU:HA	1:F:86:ARG:NH2	2.12	0.64
1:C:297:ALA:HB1	1:C:298:PRO:CD	2.26	0.63
1:A:409:ALA:HB2	2:A:901:AGS:H5'2	1.79	0.63
1:D:297:ALA:HB1	1:D:298:PRO:CD	2.26	0.63
1:C:239:ARG:NH1	1:C:335:LEU:O	2.32	0.63
1:F:22:ARG:HH11	1:F:24:ASN:HB3	1.63	0.63
1:B:764:GLN:N	1:B:764:GLN:OE1	2.32	0.63
1:C:764:GLN:N	1:C:764:GLN:OE1	2.32	0.63
1:A:114:ILE:CD1	1:A:176:VAL:CG1	2.77	0.63
1:B:114:ILE:O	1:B:115:HIS:CG	2.52	0.63
1:B:239:ARG:NH1	1:B:335:LEU:O	2.32	0.63
1:D:239:ARG:NH1	1:D:335:LEU:O	2.32	0.63
1:E:297:ALA:HB1	1:E:298:PRO:CD	2.26	0.63
1:F:239:ARG:NH1	1:F:335:LEU:O	2.31	0.63
1:C:114:ILE:CD1	1:C:176:VAL:CG1	2.77	0.62
1:C:114:ILE:O	1:C:115:HIS:CG	2.52	0.62
1:A:764:GLN:N	1:A:764:GLN:OE1	2.32	0.62
1:D:114:ILE:CD1	1:D:176:VAL:CG1	2.77	0.62
1:E:114:ILE:CD1	1:E:176:VAL:CG1	2.77	0.62
1:E:22:ARG:HH11	1:E:24:ASN:HB3	1.63	0.62
1:B:218:GLU:OE1	1:C:424:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:ARG:NH1	1:E:335:LEU:O	2.32	0.62
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.40	0.62
1:A:22:ARG:HH11	1:A:24:ASN:HB3	1.63	0.62
1:D:113:ARG:CD	1:D:182:ILE:CG2	2.76	0.62
1:C:218:GLU:OE1	1:D:424:ARG:NH2	2.33	0.62
1:A:114:ILE:O	1:A:115:HIS:CG	2.52	0.62
1:A:424:ARG:NH2	1:F:218:GLU:OE1	2.33	0.62
1:D:764:GLN:N	1:D:764:GLN:OE1	2.32	0.62
1:E:114:ILE:O	1:E:115:HIS:CG	2.52	0.62
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.40	0.62
1:D:40:SER:HB2	1:D:83:ARG:HB3	1.82	0.62
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.40	0.62
1:A:40:SER:HB2	1:A:83:ARG:HB3	1.82	0.62
1:C:22:ARG:HH11	1:C:24:ASN:HB3	1.63	0.62
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.40	0.62
1:F:114:ILE:O	1:F:115:HIS:CG	2.52	0.62
1:F:63:LYS:HG2	1:F:261:GLU:OE2	2.00	0.62
1:A:239:ARG:NH1	1:A:335:LEU:O	2.32	0.62
1:D:218:GLU:OE1	1:E:424:ARG:NH2	2.33	0.62
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.40	0.62
1:F:764:GLN:N	1:F:764:GLN:OE1	2.32	0.62
1:D:114:ILE:O	1:D:115:HIS:CG	2.52	0.62
1:B:40:SER:HB2	1:B:83:ARG:HB3	1.82	0.61
1:D:475:THR:HG22	1:D:476:TRP:H	1.65	0.61
1:E:113:ARG:CD	1:E:182:ILE:CG2	2.76	0.61
1:F:46:MET:HA	1:F:49:LEU:HB2	1.82	0.61
1:C:40:SER:HB2	1:C:83:ARG:HB3	1.82	0.61
1:E:63:LYS:HG2	1:E:261:GLU:OE2	2.00	0.61
1:E:764:GLN:OE1	1:E:764:GLN:N	2.32	0.61
1:F:114:ILE:CD1	1:F:176:VAL:CG1	2.77	0.61
1:F:475:THR:HG22	1:F:476:TRP:H	1.65	0.61
1:A:475:THR:HG22	1:A:476:TRP:H	1.65	0.61
1:A:74:ASP:OD2	1:A:83:ARG:HB2	2.01	0.61
1:C:556:GLU:HB3	1:D:552:PHE:CD2	2.35	0.61
1:B:22:ARG:HH11	1:B:24:ASN:HB3	1.63	0.61
1:D:84:MET:HG2	1:D:88:VAL:HG21	1.82	0.61
1:E:46:MET:HA	1:E:49:LEU:HB2	1.83	0.61
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.40	0.61
1:C:459:SER:O	1:C:462:SER:N	2.31	0.61
1:C:74:ASP:OD2	1:C:83:ARG:HB2	2.01	0.61
1:D:556:GLU:HB3	1:E:552:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:HE1	1:A:135:LEU:HD22	1.66	0.61
1:A:218:GLU:OE1	1:B:424:ARG:NH2	2.33	0.61
1:B:475:THR:HG22	1:B:476:TRP:H	1.65	0.61
1:B:63:LYS:HG2	1:B:261:GLU:OE2	2.00	0.61
1:C:586:ARG:CD	1:C:594:GLY:HA3	2.31	0.61
1:C:63:LYS:HG2	1:C:261:GLU:OE2	2.00	0.61
1:D:63:LYS:HG2	1:D:261:GLU:OE2	2.00	0.61
1:E:84:MET:HG2	1:E:88:VAL:HG21	1.82	0.61
1:D:22:ARG:NE	1:D:25:ARG:HB2	2.16	0.61
1:A:552:PHE:CD2	1:F:556:GLU:HB3	2.36	0.61
1:A:63:LYS:HG2	1:A:261:GLU:OE2	2.00	0.61
1:B:586:ARG:CD	1:B:594:GLY:HA3	2.31	0.61
1:A:22:ARG:NE	1:A:25:ARG:HB2	2.16	0.60
1:B:114:ILE:CD1	1:B:176:VAL:CG1	2.77	0.60
1:B:40:SER:HB3	1:B:82:ILE:HG13	1.83	0.60
1:F:22:ARG:NE	1:F:25:ARG:HB2	2.16	0.60
1:F:74:ASP:OD2	1:F:83:ARG:HB2	2.01	0.60
1:C:84:MET:HG2	1:C:88:VAL:HG21	1.82	0.60
1:D:119:ILE:HG23	1:D:164:LYS:HB2	1.83	0.60
1:E:119:ILE:HG23	1:E:164:LYS:HB2	1.83	0.60
1:E:22:ARG:NE	1:E:25:ARG:HB2	2.16	0.60
1:E:40:SER:HB2	1:E:83:ARG:HB3	1.82	0.60
1:F:84:MET:HG2	1:F:88:VAL:HG21	1.82	0.60
1:B:119:ILE:HG23	1:B:164:LYS:HB2	1.83	0.60
1:A:556:GLU:HB3	1:B:552:PHE:CD2	2.36	0.60
1:C:119:ILE:HG23	1:C:164:LYS:HB2	1.83	0.60
1:C:74:ASP:CG	1:C:75:ASP:H	2.05	0.60
1:D:459:SER:O	1:D:462:SER:N	2.31	0.60
1:E:74:ASP:OD2	1:E:83:ARG:HB2	2.01	0.60
1:A:519:PRO:HG3	1:A:647:LEU:HD12	1.84	0.60
1:F:586:ARG:CD	1:F:594:GLY:HA3	2.31	0.60
1:F:40:SER:HB2	1:F:83:ARG:HB3	1.82	0.60
1:B:22:ARG:NE	1:B:25:ARG:HB2	2.16	0.60
1:C:475:THR:HG22	1:C:476:TRP:H	1.65	0.60
1:C:519:PRO:HG3	1:C:647:LEU:HD12	1.84	0.60
1:D:74:ASP:OD2	1:D:83:ARG:HB2	2.01	0.60
1:E:131:PHE:HE1	1:E:135:LEU:HD22	1.66	0.60
1:B:519:PRO:HG3	1:B:647:LEU:HD12	1.84	0.60
1:B:74:ASP:OD2	1:B:83:ARG:HB2	2.01	0.60
1:C:131:PHE:HE1	1:C:135:LEU:HD22	1.66	0.60
1:C:46:MET:HA	1:C:49:LEU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:586:ARG:CD	1:E:594:GLY:HA3	2.31	0.60
1:E:74:ASP:CG	1:E:75:ASP:H	2.05	0.60
1:A:40:SER:HB3	1:A:82:ILE:HG13	1.83	0.60
1:A:46:MET:HA	1:A:49:LEU:HB2	1.83	0.60
1:D:586:ARG:CD	1:D:594:GLY:HA3	2.31	0.60
1:E:475:THR:HG22	1:E:476:TRP:H	1.65	0.60
1:C:22:ARG:NE	1:C:25:ARG:HB2	2.16	0.60
1:E:556:GLU:HB3	1:F:552:PHE:CD2	2.37	0.60
1:F:74:ASP:CG	1:F:75:ASP:H	2.05	0.60
1:B:46:MET:HA	1:B:49:LEU:HB2	1.83	0.60
1:D:519:PRO:HG3	1:D:647:LEU:HD12	1.84	0.60
1:A:586:ARG:CD	1:A:594:GLY:HA3	2.31	0.59
1:B:556:GLU:HB3	1:C:552:PHE:CD2	2.36	0.59
1:F:113:ARG:CD	1:F:182:ILE:CG2	2.76	0.59
1:F:519:PRO:HG3	1:F:647:LEU:HD12	1.84	0.59
1:C:40:SER:HB3	1:C:82:ILE:HG13	1.83	0.59
1:A:119:ILE:HG23	1:A:164:LYS:HB2	1.83	0.59
1:A:84:MET:HG2	1:A:88:VAL:HG21	1.82	0.59
1:B:84:MET:HG2	1:B:88:VAL:HG21	1.82	0.59
1:D:46:MET:HA	1:D:49:LEU:HB2	1.83	0.59
1:F:40:SER:HB3	1:F:82:ILE:HG13	1.83	0.59
1:E:519:PRO:HG3	1:E:647:LEU:HD12	1.84	0.59
1:F:119:ILE:HG23	1:F:164:LYS:HB2	1.84	0.59
1:B:74:ASP:CG	1:B:75:ASP:H	2.05	0.59
1:E:40:SER:HB3	1:E:82:ILE:HG13	1.83	0.59
1:B:66:GLU:O	1:B:147:ARG:NH2	2.36	0.59
1:D:40:SER:HB3	1:D:82:ILE:HG13	1.83	0.59
1:F:66:GLU:O	1:F:147:ARG:NH2	2.36	0.59
1:C:66:GLU:O	1:C:147:ARG:NH2	2.36	0.59
1:C:45:LYS:HE3	1:C:49:LEU:HD21	1.85	0.59
1:E:201:VAL:HG13	1:E:205:ASP:HB2	1.85	0.59
1:A:201:VAL:HG13	1:A:205:ASP:HB2	1.85	0.59
1:D:512:LYS:HZ2	1:D:619:ILE:HG13	1.68	0.59
1:F:201:VAL:HG13	1:F:205:ASP:HB2	1.85	0.59
1:D:131:PHE:HE1	1:D:135:LEU:HD22	1.66	0.58
1:D:45:LYS:HE3	1:D:49:LEU:HD21	1.85	0.58
1:E:112:LYS:O	1:E:113:ARG:CB	2.51	0.58
1:A:66:GLU:O	1:A:147:ARG:NH2	2.36	0.58
1:A:45:LYS:HE3	1:A:49:LEU:HD21	1.85	0.58
1:B:115:HIS:O	1:B:116:VAL:HB	2.04	0.58
1:B:131:PHE:HE1	1:B:135:LEU:HD22	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:HIS:O	1:D:116:VAL:HB	2.04	0.58
1:D:201:VAL:HG13	1:D:205:ASP:HB2	1.85	0.58
1:D:74:ASP:CG	1:D:75:ASP:H	2.05	0.58
1:E:66:GLU:O	1:E:147:ARG:NH2	2.36	0.58
1:F:428:ASP:OD1	1:F:429:LEU:N	2.36	0.58
1:B:45:LYS:HE3	1:B:49:LEU:HD21	1.85	0.58
1:C:59:LEU:HD13	1:C:100:ILE:HD11	1.84	0.58
1:A:59:LEU:HD13	1:A:100:ILE:HD11	1.84	0.58
1:C:132:GLU:HA	1:C:136:LYS:HB3	1.86	0.58
1:C:201:VAL:HG13	1:C:205:ASP:HB2	1.85	0.58
1:A:424:ARG:HA	1:A:427:MET:HG2	1.86	0.58
1:A:428:ASP:OD1	1:A:429:LEU:N	2.37	0.58
1:E:424:ARG:HA	1:E:427:MET:HG2	1.86	0.58
1:E:45:LYS:HE3	1:E:49:LEU:HD21	1.85	0.58
1:F:131:PHE:HE1	1:F:135:LEU:HD22	1.66	0.58
1:F:108:VAL:HG23	1:F:175:ILE:HG13	1.86	0.58
1:F:424:ARG:HA	1:F:427:MET:HG2	1.86	0.58
1:E:108:VAL:HG23	1:E:175:ILE:HG13	1.86	0.58
1:E:428:ASP:OD1	1:E:429:LEU:N	2.37	0.58
1:B:112:LYS:O	1:B:113:ARG:CB	2.51	0.58
1:C:115:HIS:O	1:C:116:VAL:HB	2.04	0.58
1:C:493:VAL:HG21	1:C:531:ILE:HG12	1.86	0.58
1:D:66:GLU:O	1:D:147:ARG:NH2	2.36	0.58
1:F:115:HIS:O	1:F:116:VAL:HB	2.04	0.58
1:F:45:LYS:HE3	1:F:49:LEU:HD21	1.85	0.58
1:F:59:LEU:HD13	1:F:100:ILE:HD11	1.84	0.58
1:B:201:VAL:HG13	1:B:205:ASP:HB2	1.85	0.58
1:B:424:ARG:HA	1:B:427:MET:HG2	1.86	0.58
1:F:132:GLU:HA	1:F:136:LYS:HB3	1.86	0.58
1:B:512:LYS:HZ2	1:B:619:ILE:HG13	1.69	0.57
1:D:59:LEU:HD13	1:D:100:ILE:HD11	1.84	0.57
1:E:493:VAL:HG21	1:E:531:ILE:HG12	1.86	0.57
1:A:108:VAL:HG23	1:A:175:ILE:HG13	1.86	0.57
1:B:493:VAL:HG21	1:B:531:ILE:HG12	1.86	0.57
1:D:424:ARG:HA	1:D:427:MET:HG2	1.86	0.57
1:E:59:LEU:HD13	1:E:100:ILE:HD11	1.84	0.57
1:A:112:LYS:O	1:A:113:ARG:CB	2.51	0.57
1:A:74:ASP:CG	1:A:75:ASP:H	2.05	0.57
1:B:59:LEU:HD13	1:B:100:ILE:HD11	1.84	0.57
1:B:223:PRO:HG3	1:B:230:PHE:CE2	2.40	0.57
1:B:428:ASP:OD1	1:B:429:LEU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ARG:HA	1:C:427:MET:HG2	1.86	0.57
1:E:132:GLU:HA	1:E:136:LYS:HB3	1.86	0.57
1:A:693:ARG:HH12	1:A:742:PHE:HD2	1.53	0.57
1:C:428:ASP:OD1	1:C:429:LEU:N	2.36	0.57
1:C:693:ARG:HH12	1:C:742:PHE:HD2	1.53	0.57
1:D:132:GLU:HA	1:D:136:LYS:HB3	1.86	0.57
1:D:693:ARG:HH12	1:D:742:PHE:HD2	1.53	0.57
1:F:693:ARG:HH12	1:F:742:PHE:HD2	1.53	0.57
1:E:223:PRO:HG3	1:E:230:PHE:CE2	2.40	0.57
1:B:132:GLU:HA	1:B:136:LYS:HB3	1.86	0.57
1:C:91:ASN:HD21	1:C:151:ILE:H	1.53	0.57
1:D:428:ASP:OD1	1:D:429:LEU:N	2.37	0.57
1:D:108:VAL:HG23	1:D:175:ILE:HG13	1.86	0.57
1:F:223:PRO:HG3	1:F:230:PHE:CE2	2.40	0.57
1:D:493:VAL:HG21	1:D:531:ILE:HG12	1.86	0.57
1:A:20:LYS:HE3	1:A:25:ARG:HH22	1.70	0.57
1:D:112:LYS:O	1:D:113:ARG:CB	2.51	0.57
1:E:115:HIS:O	1:E:116:VAL:HB	2.04	0.57
1:E:20:LYS:HE3	1:E:25:ARG:HH22	1.70	0.57
1:E:693:ARG:HH12	1:E:742:PHE:HD2	1.53	0.57
1:B:20:LYS:HE3	1:B:25:ARG:HH22	1.70	0.57
1:F:20:LYS:HE3	1:F:25:ARG:HH22	1.70	0.57
1:A:115:HIS:O	1:A:116:VAL:HB	2.04	0.56
1:A:223:PRO:HG3	1:A:230:PHE:CE2	2.40	0.56
1:B:91:ASN:HD21	1:B:151:ILE:H	1.53	0.56
1:B:693:ARG:HH12	1:B:742:PHE:HD2	1.53	0.56
1:C:112:LYS:O	1:C:113:ARG:CB	2.51	0.56
1:D:297:ALA:CB	1:D:298:PRO:HD3	2.33	0.56
1:F:297:ALA:CB	1:F:298:PRO:HD3	2.33	0.56
1:B:22:ARG:HB3	1:B:25:ARG:CB	2.36	0.56
1:C:20:LYS:HE3	1:C:25:ARG:HH22	1.70	0.56
1:E:297:ALA:CB	1:E:298:PRO:HD3	2.33	0.56
1:D:27:ILE:HG13	1:D:81:LYS:HA	1.86	0.56
1:E:27:ILE:HG13	1:E:81:LYS:HA	1.86	0.56
1:F:112:LYS:O	1:F:113:ARG:CB	2.51	0.56
1:A:297:ALA:CB	1:A:298:PRO:CD	2.84	0.56
1:A:679:THR:HB	1:A:682:PHE:CD2	2.41	0.56
1:F:679:THR:HB	1:F:682:PHE:CD2	2.41	0.56
1:A:132:GLU:HA	1:A:136:LYS:HB3	1.86	0.56
1:D:91:ASN:HD21	1:D:151:ILE:H	1.53	0.56
1:D:20:LYS:HE3	1:D:25:ARG:HH22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:ARG:HB3	1:E:25:ARG:CB	2.36	0.56
1:E:512:LYS:HZ2	1:E:619:ILE:HG13	1.70	0.56
1:E:155:ARG:HD3	1:E:161:VAL:HG23	1.88	0.56
1:A:22:ARG:HB3	1:A:25:ARG:CB	2.36	0.56
1:A:493:VAL:HG21	1:A:531:ILE:HG12	1.86	0.56
1:B:297:ALA:CB	1:B:298:PRO:CD	2.83	0.56
1:B:679:THR:HB	1:B:682:PHE:CD2	2.41	0.56
1:C:223:PRO:HG3	1:C:230:PHE:CE2	2.40	0.56
1:C:297:ALA:CB	1:C:298:PRO:CD	2.84	0.56
1:D:297:ALA:CB	1:D:298:PRO:CD	2.84	0.56
1:F:493:VAL:HG21	1:F:531:ILE:HG12	1.86	0.56
1:C:108:VAL:HG23	1:C:175:ILE:HG13	1.86	0.56
1:C:22:ARG:HB3	1:C:25:ARG:CB	2.36	0.56
1:B:108:VAL:HG23	1:B:175:ILE:HG13	1.86	0.56
1:B:27:ILE:HG13	1:B:81:LYS:HA	1.86	0.56
1:C:679:THR:HB	1:C:682:PHE:CD2	2.40	0.56
1:E:679:THR:HB	1:E:682:PHE:CD2	2.40	0.56
1:F:27:ILE:HG13	1:F:81:LYS:HA	1.86	0.56
1:A:27:ILE:HG13	1:A:81:LYS:HA	1.86	0.56
1:C:155:ARG:HD3	1:C:161:VAL:HG23	1.88	0.56
1:C:27:ILE:HG13	1:C:81:LYS:HA	1.86	0.56
1:F:64:ARG:NH1	1:F:260:ASN:O	2.39	0.56
1:A:512:LYS:HZ2	1:A:619:ILE:HG13	1.71	0.56
1:D:22:ARG:HB3	1:D:25:ARG:CB	2.36	0.56
1:A:64:ARG:NH1	1:A:260:ASN:O	2.39	0.55
1:A:91:ASN:HD21	1:A:151:ILE:H	1.53	0.55
1:D:223:PRO:HG3	1:D:230:PHE:CE2	2.40	0.55
1:F:297:ALA:CB	1:F:298:PRO:CD	2.84	0.55
1:E:91:ASN:HD21	1:E:151:ILE:H	1.53	0.55
1:F:155:ARG:HD3	1:F:161:VAL:HG23	1.88	0.55
1:F:91:ASN:HD21	1:F:151:ILE:H	1.53	0.55
1:B:39:VAL:HB	1:B:71:VAL:HG12	1.89	0.55
1:C:39:VAL:HB	1:C:71:VAL:HG12	1.89	0.55
1:D:39:VAL:HB	1:D:71:VAL:HG12	1.89	0.55
1:F:22:ARG:HB3	1:F:25:ARG:CB	2.36	0.55
1:B:155:ARG:HD3	1:B:161:VAL:HG23	1.88	0.55
1:B:459:SER:O	1:B:462:SER:N	2.31	0.55
1:B:114:ILE:HG22	1:B:115:HIS:N	2.22	0.55
1:C:201:VAL:O	1:C:260:ASN:ND2	2.32	0.55
1:D:679:THR:HB	1:D:682:PHE:CD2	2.40	0.55
1:F:114:ILE:HG22	1:F:115:HIS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:LEU:HD12	1:F:154:VAL:HG11	1.89	0.55
1:E:64:ARG:NH1	1:E:260:ASN:O	2.39	0.55
1:E:297:ALA:CB	1:E:298:PRO:CD	2.84	0.55
1:A:114:ILE:HG22	1:A:115:HIS:N	2.22	0.55
1:A:135:LEU:HD12	1:A:154:VAL:HG11	1.89	0.55
1:A:297:ALA:CB	1:A:298:PRO:HD3	2.33	0.55
1:A:155:ARG:HD3	1:A:161:VAL:HG23	1.88	0.55
1:F:146:ILE:O	1:F:173:TYR:HB2	2.07	0.55
1:B:64:ARG:NH1	1:B:260:ASN:O	2.39	0.55
1:D:155:ARG:HD3	1:D:161:VAL:HG23	1.88	0.55
1:F:459:SER:O	1:F:462:SER:N	2.31	0.55
1:B:147:ARG:NH1	1:B:148:LYS:O	2.41	0.54
1:C:114:ILE:HG22	1:C:115:HIS:N	2.22	0.54
1:E:39:VAL:HB	1:E:71:VAL:HG12	1.89	0.54
1:A:39:VAL:HB	1:A:71:VAL:HG12	1.89	0.54
1:B:201:VAL:O	1:B:260:ASN:ND2	2.32	0.54
1:D:135:LEU:HD12	1:D:154:VAL:HG11	1.89	0.54
1:D:146:ILE:O	1:D:173:TYR:HB2	2.07	0.54
1:E:114:ILE:HG22	1:E:115:HIS:N	2.21	0.54
1:A:201:VAL:O	1:A:260:ASN:ND2	2.32	0.54
1:B:113:ARG:CD	1:B:182:ILE:CG2	2.76	0.54
1:C:64:ARG:NH1	1:C:260:ASN:O	2.39	0.54
1:D:114:ILE:HG22	1:D:115:HIS:N	2.22	0.54
1:D:223:PRO:HG3	1:D:230:PHE:HE2	1.72	0.54
1:D:22:ARG:CZ	1:D:25:ARG:HB2	2.38	0.54
1:D:489:LEU:O	1:D:493:VAL:HG22	2.08	0.54
1:D:64:ARG:NH1	1:D:260:ASN:O	2.39	0.54
1:E:147:ARG:NH1	1:E:148:LYS:O	2.41	0.54
1:E:135:LEU:HD12	1:E:154:VAL:HG11	1.88	0.54
1:A:459:SER:O	1:A:462:SER:N	2.31	0.54
1:C:115:HIS:ND1	1:C:116:VAL:N	2.56	0.54
1:E:68:VAL:HG11	1:E:173:TYR:CE2	2.43	0.54
1:F:115:HIS:ND1	1:F:116:VAL:N	2.56	0.54
1:F:39:VAL:HB	1:F:71:VAL:HG12	1.89	0.54
1:C:147:ARG:NH1	1:C:148:LYS:O	2.41	0.54
1:C:489:LEU:O	1:C:493:VAL:HG22	2.08	0.54
1:A:146:ILE:O	1:A:173:TYR:HB2	2.07	0.54
1:C:512:LYS:HZ2	1:C:619:ILE:HG13	1.72	0.54
1:D:147:ARG:NH1	1:D:148:LYS:O	2.41	0.54
1:E:115:HIS:ND1	1:E:116:VAL:N	2.56	0.54
1:E:146:ILE:O	1:E:173:TYR:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:PRO:HG3	1:E:230:PHE:HE2	1.72	0.54
1:E:22:ARG:CZ	1:E:25:ARG:HB2	2.38	0.54
1:E:484:ASP:OD1	1:E:485:VAL:N	2.41	0.54
1:F:68:VAL:HG11	1:F:173:TYR:CE2	2.43	0.54
1:B:135:LEU:HD12	1:B:154:VAL:HG11	1.88	0.54
1:B:223:PRO:HG3	1:B:230:PHE:HE2	1.72	0.54
1:C:113:ARG:CD	1:C:182:ILE:CG2	2.76	0.54
1:A:147:ARG:NH1	1:A:148:LYS:O	2.41	0.54
1:A:22:ARG:CZ	1:A:25:ARG:HB2	2.38	0.54
1:B:146:ILE:O	1:B:173:TYR:HB2	2.07	0.54
1:D:559:VAL:HG21	1:D:600:VAL:HG13	1.90	0.54
1:E:108:VAL:HG11	1:E:173:TYR:CE2	2.43	0.54
1:E:489:LEU:O	1:E:493:VAL:HG22	2.08	0.54
1:E:559:VAL:HG21	1:E:600:VAL:HG13	1.90	0.54
1:F:484:ASP:OD1	1:F:485:VAL:N	2.41	0.54
1:F:512:LYS:HZ2	1:F:619:ILE:HG13	1.73	0.54
1:F:83:ARG:O	1:F:84:MET:HB2	2.08	0.54
1:B:108:VAL:HG11	1:B:173:TYR:CE2	2.43	0.54
1:C:146:ILE:O	1:C:173:TYR:HB2	2.07	0.54
1:C:223:PRO:HG3	1:C:230:PHE:HE2	1.72	0.54
1:D:83:ARG:O	1:D:84:MET:HB2	2.08	0.54
1:E:635:ARG:HE	1:E:638:ARG:NH1	2.06	0.54
1:E:83:ARG:O	1:E:84:MET:HB2	2.08	0.54
1:F:147:ARG:NH1	1:F:148:LYS:O	2.41	0.54
1:A:223:PRO:HG3	1:A:230:PHE:HE2	1.72	0.53
1:C:83:ARG:O	1:C:84:MET:HB2	2.08	0.53
1:A:539:PHE:CE2	1:A:541:SER:HB2	2.44	0.53
1:B:115:HIS:ND1	1:B:116:VAL:N	2.56	0.53
1:B:489:LEU:O	1:B:493:VAL:HG22	2.08	0.53
1:D:236:LYS:HG3	1:D:337:GLN:NE2	2.24	0.53
1:D:635:ARG:HE	1:D:638:ARG:NH1	2.06	0.53
1:F:223:PRO:HG3	1:F:230:PHE:HE2	1.72	0.53
1:F:635:ARG:HE	1:F:638:ARG:NH1	2.06	0.53
1:A:108:VAL:HG11	1:A:173:TYR:CE2	2.43	0.53
1:B:539:PHE:CE2	1:B:541:SER:HB2	2.44	0.53
1:C:135:LEU:HD12	1:C:154:VAL:HG11	1.89	0.53
1:C:22:ARG:CZ	1:C:25:ARG:HB2	2.38	0.53
1:C:635:ARG:HE	1:C:638:ARG:NH1	2.06	0.53
1:D:108:VAL:HG11	1:D:173:TYR:CE2	2.43	0.53
1:D:484:ASP:OD1	1:D:485:VAL:N	2.41	0.53
1:D:115:HIS:ND1	1:D:116:VAL:N	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:LEU:O	1:F:493:VAL:HG22	2.08	0.53
1:B:635:ARG:HE	1:B:638:ARG:NH1	2.06	0.53
1:C:108:VAL:HG11	1:C:173:TYR:CE2	2.43	0.53
1:C:559:VAL:HG21	1:C:600:VAL:HG13	1.90	0.53
1:E:636:PRO:HA	1:E:640:ASP:HB3	1.90	0.53
1:F:22:ARG:CZ	1:F:25:ARG:HB2	2.38	0.53
1:A:68:VAL:HG11	1:A:173:TYR:CE2	2.43	0.53
1:C:539:PHE:CE2	1:C:541:SER:HB2	2.44	0.53
1:C:551:TRP:CZ2	1:C:600:VAL:HG22	2.44	0.53
1:C:68:VAL:HG11	1:C:173:TYR:CE2	2.43	0.53
1:F:108:VAL:HG11	1:F:173:TYR:CE2	2.43	0.53
1:F:559:VAL:HG21	1:F:600:VAL:HG13	1.90	0.53
1:F:636:PRO:HA	1:F:640:ASP:HB3	1.90	0.53
1:A:484:ASP:OD1	1:A:485:VAL:N	2.41	0.53
1:A:489:LEU:O	1:A:493:VAL:HG22	2.08	0.53
1:B:68:VAL:HG11	1:B:173:TYR:CE2	2.43	0.53
1:B:484:ASP:OD1	1:B:485:VAL:N	2.41	0.53
1:D:68:VAL:HG11	1:D:173:TYR:CE2	2.43	0.53
1:E:482:LEU:O	1:E:486:LYS:HG3	2.09	0.53
1:E:551:TRP:CZ2	1:E:600:VAL:HG22	2.44	0.53
1:F:539:PHE:CE2	1:F:541:SER:HB2	2.44	0.53
1:A:482:LEU:O	1:A:486:LYS:HG3	2.09	0.53
1:B:22:ARG:CZ	1:B:25:ARG:HB2	2.38	0.53
1:C:113:ARG:CZ	1:C:182:ILE:HG12	2.39	0.53
1:E:113:ARG:CZ	1:E:182:ILE:HG12	2.39	0.53
1:A:113:ARG:CZ	1:A:182:ILE:HG12	2.39	0.53
1:A:115:HIS:ND1	1:A:116:VAL:N	2.56	0.53
1:A:636:PRO:HA	1:A:640:ASP:HB3	1.90	0.53
1:B:493:VAL:HG23	1:B:494:GLN:H	1.74	0.53
1:B:551:TRP:CZ2	1:B:600:VAL:HG22	2.44	0.53
1:B:83:ARG:O	1:B:84:MET:HB2	2.08	0.53
1:A:635:ARG:HE	1:A:638:ARG:NH1	2.06	0.53
1:E:113:ARG:C	1:E:114:ILE:HG13	2.30	0.53
1:A:113:ARG:C	1:A:114:ILE:HG13	2.30	0.52
1:A:493:VAL:HG23	1:A:494:GLN:H	1.74	0.52
1:A:605:LEU:HD22	1:A:638:ARG:HD3	1.91	0.52
1:B:482:LEU:O	1:B:486:LYS:HG3	2.09	0.52
1:C:484:ASP:OD1	1:C:485:VAL:N	2.41	0.52
1:D:482:LEU:O	1:D:486:LYS:HG3	2.09	0.52
1:D:551:TRP:CZ2	1:D:600:VAL:HG22	2.44	0.52
1:A:493:VAL:HG21	1:A:531:ILE:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:VAL:HG21	1:B:531:ILE:CG1	2.40	0.52
1:E:236:LYS:HG3	1:E:337:GLN:NE2	2.24	0.52
1:A:559:VAL:HG21	1:A:600:VAL:HG13	1.90	0.52
1:B:559:VAL:HG21	1:B:600:VAL:HG13	1.90	0.52
1:C:236:LYS:HG3	1:C:337:GLN:NE2	2.24	0.52
1:F:113:ARG:CZ	1:F:182:ILE:HG12	2.39	0.52
1:F:493:VAL:HG21	1:F:531:ILE:CG1	2.40	0.52
1:B:113:ARG:C	1:B:114:ILE:HG13	2.30	0.52
1:D:113:ARG:CZ	1:D:182:ILE:HG12	2.39	0.52
1:D:323:ARG:O	1:D:327:GLN:N	2.41	0.52
1:D:693:ARG:NH1	1:D:742:PHE:HB3	2.25	0.52
1:F:482:LEU:O	1:F:486:LYS:HG3	2.09	0.52
1:B:636:PRO:HA	1:B:640:ASP:HB3	1.90	0.52
1:E:539:PHE:CE2	1:E:541:SER:HB2	2.44	0.52
1:B:605:LEU:HD22	1:B:638:ARG:HD3	1.91	0.52
1:C:493:VAL:HG23	1:C:494:GLN:H	1.74	0.52
1:E:493:VAL:HG21	1:E:531:ILE:CG1	2.40	0.52
1:F:551:TRP:CZ2	1:F:600:VAL:HG22	2.44	0.52
1:F:605:LEU:HD22	1:F:638:ARG:HD3	1.91	0.52
1:A:183:HIS:HB3	1:A:185:GLU:HG2	1.92	0.52
1:A:551:TRP:CZ2	1:A:600:VAL:HG22	2.44	0.52
1:D:539:PHE:CE2	1:D:541:SER:HB2	2.44	0.52
1:B:113:ARG:CZ	1:B:182:ILE:HG12	2.39	0.52
1:B:183:HIS:HB3	1:B:185:GLU:HG2	1.92	0.52
1:D:636:PRO:HA	1:D:640:ASP:HB3	1.90	0.52
1:D:605:LEU:HD22	1:D:638:ARG:HD3	1.91	0.52
1:F:693:ARG:NH1	1:F:742:PHE:HB3	2.25	0.52
1:C:493:VAL:HG21	1:C:531:ILE:CG1	2.40	0.52
1:F:41:LEU:HD22	1:F:46:MET:SD	2.50	0.52
1:A:83:ARG:O	1:A:84:MET:HB2	2.08	0.52
1:B:323:ARG:O	1:B:327:GLN:N	2.41	0.52
1:B:92:LEU:HD21	1:B:100:ILE:HD13	1.92	0.52
1:D:74:ASP:OD2	1:D:83:ARG:CB	2.58	0.52
1:E:93:ARG:NH1	1:E:99:VAL:O	2.43	0.52
1:F:93:ARG:NH1	1:F:99:VAL:O	2.43	0.52
1:D:113:ARG:C	1:D:114:ILE:HG13	2.30	0.51
1:D:201:VAL:O	1:D:260:ASN:ND2	2.32	0.51
1:E:30:GLU:HA	1:E:86:ARG:HH22	1.75	0.51
1:E:471:VAL:HG12	1:E:537:ALA:O	2.11	0.51
1:F:113:ARG:C	1:F:114:ILE:HG13	2.30	0.51
1:F:471:VAL:HG12	1:F:537:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:ASP:OD2	1:F:83:ARG:CB	2.58	0.51
1:A:92:LEU:HD21	1:A:100:ILE:HD13	1.92	0.51
1:B:471:VAL:HG12	1:B:537:ALA:O	2.11	0.51
1:C:113:ARG:C	1:C:114:ILE:HG13	2.30	0.51
1:C:482:LEU:O	1:C:486:LYS:HG3	2.09	0.51
1:F:92:LEU:HD21	1:F:100:ILE:HD13	1.92	0.51
1:F:493:VAL:HG23	1:F:494:GLN:H	1.74	0.51
1:A:93:ARG:NH1	1:A:99:VAL:O	2.43	0.51
1:B:74:ASP:OD2	1:B:83:ARG:CB	2.58	0.51
1:C:471:VAL:HG12	1:C:537:ALA:O	2.11	0.51
1:C:636:PRO:HA	1:C:640:ASP:HB3	1.90	0.51
1:C:605:LEU:HD22	1:C:638:ARG:HD3	1.91	0.51
1:C:693:ARG:NH1	1:C:742:PHE:HB3	2.25	0.51
1:C:93:ARG:NH1	1:C:99:VAL:O	2.43	0.51
1:D:493:VAL:HG23	1:D:494:GLN:H	1.74	0.51
1:E:493:VAL:HG23	1:E:494:GLN:H	1.74	0.51
1:E:693:ARG:NH1	1:E:742:PHE:HB3	2.25	0.51
1:B:297:ALA:CB	1:B:298:PRO:HD3	2.33	0.51
1:D:93:ARG:NH1	1:D:99:VAL:O	2.43	0.51
1:E:92:LEU:HD21	1:E:100:ILE:HD13	1.92	0.51
1:E:605:LEU:HD22	1:E:638:ARG:HD3	1.91	0.51
1:F:183:HIS:HB3	1:F:185:GLU:HG2	1.92	0.51
1:F:22:ARG:HB3	1:F:25:ARG:HB2	1.93	0.51
1:A:250:GLY:N	2:A:901:AGS:O2A	2.44	0.51
1:A:471:VAL:HG12	1:A:537:ALA:O	2.11	0.51
1:A:693:ARG:NH1	1:A:742:PHE:HB3	2.25	0.51
1:A:74:ASP:OD2	1:A:83:ARG:CB	2.58	0.51
1:F:201:VAL:O	1:F:260:ASN:ND2	2.32	0.51
1:F:250:GLY:N	2:F:901:AGS:O2A	2.44	0.51
1:A:22:ARG:HB3	1:A:25:ARG:HB2	1.93	0.51
1:A:41:LEU:HD22	1:A:46:MET:SD	2.50	0.51
1:C:92:LEU:HD21	1:C:100:ILE:HD13	1.92	0.51
1:C:250:GLY:N	2:C:901:AGS:O2A	2.44	0.51
1:C:41:LEU:HD22	1:C:46:MET:SD	2.50	0.51
1:D:493:VAL:HG21	1:D:531:ILE:CG1	2.40	0.51
1:E:290:PHE:CD1	1:E:331:LEU:HD13	2.46	0.51
1:B:290:PHE:CD1	1:B:331:LEU:HD13	2.46	0.51
1:B:93:ARG:NH1	1:B:99:VAL:O	2.43	0.51
1:C:183:HIS:HB3	1:C:185:GLU:HG2	1.92	0.51
1:D:43:GLN:HB2	1:D:44:PRO:HD3	1.92	0.51
1:D:471:VAL:HG12	1:D:537:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ASP:OD2	1:E:83:ARG:CB	2.58	0.51
1:F:236:LYS:HG3	1:F:337:GLN:NE2	2.24	0.51
1:F:290:PHE:CD1	1:F:331:LEU:HD13	2.46	0.51
1:B:30:GLU:HA	1:B:86:ARG:HH22	1.75	0.51
1:A:290:PHE:CD1	1:A:331:LEU:HD13	2.46	0.51
1:A:364:ASP:OD1	1:A:364:ASP:N	2.44	0.51
1:B:236:LYS:HG3	1:B:337:GLN:NE2	2.24	0.51
1:E:459:SER:O	1:E:462:SER:N	2.31	0.51
1:F:43:GLN:HB2	1:F:44:PRO:HD3	1.92	0.51
1:B:364:ASP:N	1:B:364:ASP:OD1	2.44	0.51
1:E:323:ARG:O	1:E:327:GLN:N	2.41	0.51
1:E:41:LEU:HD22	1:E:46:MET:SD	2.50	0.51
1:E:631:PRO:HB3	1:E:766:ARG:CB	2.41	0.51
1:A:627:ASP:N	1:A:627:ASP:OD1	2.44	0.50
1:B:41:LEU:HD22	1:B:46:MET:SD	2.50	0.50
1:B:693:ARG:NH1	1:B:742:PHE:HB3	2.25	0.50
1:B:250:GLY:N	2:B:901:AGS:O2A	2.44	0.50
1:C:74:ASP:OD2	1:C:83:ARG:CB	2.58	0.50
1:D:627:ASP:OD1	1:D:627:ASP:N	2.44	0.50
1:E:183:HIS:HB3	1:E:185:GLU:HG2	1.92	0.50
1:A:43:GLN:HB2	1:A:44:PRO:HD3	1.92	0.50
1:B:85:ASN:O	1:B:88:VAL:HG22	2.12	0.50
1:C:631:PRO:HB3	1:C:766:ARG:CB	2.42	0.50
1:D:92:LEU:HD21	1:D:100:ILE:HD13	1.92	0.50
1:E:43:GLN:HB2	1:E:44:PRO:HD3	1.92	0.50
1:F:364:ASP:N	1:F:364:ASP:OD1	2.44	0.50
1:F:631:PRO:HB3	1:F:766:ARG:CB	2.41	0.50
1:A:236:LYS:HG3	1:A:337:GLN:NE2	2.24	0.50
1:C:290:PHE:CD1	1:C:331:LEU:HD13	2.46	0.50
1:C:30:GLU:HA	1:C:86:ARG:HH22	1.75	0.50
1:D:250:GLY:N	2:D:901:AGS:O2A	2.44	0.50
1:F:84:MET:CG	1:F:88:VAL:HG21	2.42	0.50
1:F:85:ASN:O	1:F:88:VAL:HG22	2.11	0.50
1:C:200:GLU:HG3	1:C:260:ASN:ND2	2.27	0.50
1:C:84:MET:CG	1:C:88:VAL:HG21	2.42	0.50
1:D:114:ILE:O	1:D:115:HIS:CD2	2.65	0.50
1:E:22:ARG:HB3	1:E:25:ARG:HB2	1.93	0.50
1:A:30:GLU:HA	1:A:86:ARG:HH22	1.75	0.50
1:B:22:ARG:HB3	1:B:25:ARG:HB2	1.93	0.50
1:B:200:GLU:HG3	1:B:260:ASN:ND2	2.27	0.50
1:B:623:THR:HG21	1:B:629:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PHE:CD1	1:D:331:LEU:HD13	2.46	0.50
1:E:85:ASN:O	1:E:88:VAL:HG22	2.12	0.50
1:B:631:PRO:HB3	1:B:766:ARG:CB	2.42	0.50
1:C:623:THR:HG21	1:C:629:ILE:HG21	1.94	0.50
1:C:85:ASN:O	1:C:88:VAL:HG22	2.12	0.50
1:D:183:HIS:HB3	1:D:185:GLU:HG2	1.92	0.50
1:E:114:ILE:O	1:E:115:HIS:CD2	2.65	0.50
1:E:250:GLY:N	2:E:901:AGS:O2A	2.44	0.50
1:A:631:PRO:HB3	1:A:766:ARG:CB	2.42	0.50
1:B:114:ILE:O	1:B:115:HIS:CD2	2.65	0.50
1:C:114:ILE:O	1:C:115:HIS:CD2	2.65	0.50
1:C:22:ARG:HB3	1:C:25:ARG:HB2	1.93	0.50
1:D:41:LEU:HD22	1:D:46:MET:SD	2.50	0.50
1:D:631:PRO:HB3	1:D:766:ARG:CB	2.42	0.50
1:B:22:ARG:NH1	1:B:24:ASN:CB	2.74	0.50
1:B:551:TRP:CD1	1:B:551:TRP:N	2.79	0.50
1:C:627:ASP:N	1:C:627:ASP:OD1	2.44	0.50
1:A:85:ASN:O	1:A:88:VAL:HG22	2.12	0.50
1:B:43:GLN:HB2	1:B:44:PRO:HD3	1.92	0.50
1:D:22:ARG:HB3	1:D:25:ARG:HB2	1.93	0.49
1:D:200:GLU:HG3	1:D:260:ASN:ND2	2.27	0.49
1:E:84:MET:CG	1:E:88:VAL:HG21	2.42	0.49
1:A:84:MET:CG	1:A:88:VAL:HG21	2.42	0.49
1:C:43:GLN:HB2	1:C:44:PRO:HD3	1.92	0.49
1:D:84:MET:CG	1:D:88:VAL:HG21	2.42	0.49
1:D:85:ASN:O	1:D:88:VAL:HG22	2.12	0.49
1:F:114:ILE:O	1:F:115:HIS:CD2	2.65	0.49
1:A:114:ILE:O	1:A:115:HIS:CD2	2.65	0.49
1:B:84:MET:CG	1:B:88:VAL:HG21	2.42	0.49
1:D:623:THR:HG21	1:D:629:ILE:HG21	1.94	0.49
1:E:201:VAL:O	1:E:260:ASN:ND2	2.32	0.49
1:A:200:GLU:HG3	1:A:260:ASN:ND2	2.27	0.49
1:A:623:THR:HG21	1:A:629:ILE:HG21	1.94	0.49
1:A:650:GLU:OE1	1:A:650:GLU:N	2.31	0.49
1:A:477:GLU:OE1	1:A:477:GLU:N	2.44	0.49
1:C:551:TRP:CD1	1:C:551:TRP:N	2.79	0.49
1:F:200:GLU:HG3	1:F:260:ASN:ND2	2.27	0.49
1:F:627:ASP:OD1	1:F:627:ASP:N	2.44	0.49
1:A:551:TRP:CD1	1:A:551:TRP:N	2.79	0.49
1:C:298:PRO:HA	1:C:340:HIS:O	2.13	0.49
1:F:551:TRP:N	1:F:551:TRP:CD1	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HG23	1:A:494:GLN:N	2.28	0.49
1:B:298:PRO:HA	1:B:340:HIS:O	2.13	0.49
1:B:477:GLU:N	1:B:477:GLU:OE1	2.44	0.49
1:F:491:GLU:HG2	1:F:495:TYR:HE2	1.78	0.49
1:F:623:THR:HG21	1:F:629:ILE:HG21	1.94	0.49
1:B:627:ASP:N	1:B:627:ASP:OD1	2.44	0.49
1:E:22:ARG:NH1	1:E:24:ASN:CB	2.74	0.49
1:F:298:PRO:HA	1:F:340:HIS:O	2.13	0.49
1:D:30:GLU:HA	1:D:86:ARG:HH22	1.75	0.49
1:E:200:GLU:HG3	1:E:260:ASN:ND2	2.27	0.49
1:C:491:GLU:HG2	1:C:495:TYR:HE2	1.78	0.48
1:D:493:VAL:HG23	1:D:494:GLN:N	2.28	0.48
1:E:554:GLU:HG3	1:F:552:PHE:CZ	2.48	0.48
1:E:551:TRP:CD1	1:E:551:TRP:N	2.79	0.48
1:E:623:THR:HG21	1:E:629:ILE:HG21	1.94	0.48
1:A:323:ARG:O	1:A:327:GLN:N	2.41	0.48
1:A:491:GLU:HG2	1:A:495:TYR:HE2	1.78	0.48
1:A:701:GLU:O	1:A:705:SER:N	2.35	0.48
1:D:551:TRP:N	1:D:551:TRP:CD1	2.79	0.48
1:D:74:ASP:OD2	1:D:83:ARG:HD3	2.14	0.48
1:E:493:VAL:HG23	1:E:494:GLN:N	2.28	0.48
1:F:30:GLU:HA	1:F:86:ARG:HH22	1.75	0.48
1:B:493:VAL:HG23	1:B:494:GLN:N	2.28	0.48
1:D:298:PRO:HA	1:D:340:HIS:O	2.13	0.48
1:E:298:PRO:HA	1:E:340:HIS:O	2.13	0.48
1:C:364:ASP:N	1:C:364:ASP:OD1	2.44	0.48
1:E:74:ASP:OD2	1:E:83:ARG:HD3	2.14	0.48
1:F:493:VAL:HG23	1:F:494:GLN:N	2.28	0.48
1:A:22:ARG:NH1	1:A:24:ASN:CB	2.74	0.48
1:A:298:PRO:HA	1:A:340:HIS:O	2.13	0.48
1:A:74:ASP:OD2	1:A:83:ARG:HD3	2.14	0.48
1:B:74:ASP:OD2	1:B:83:ARG:HD3	2.14	0.48
1:F:323:ARG:O	1:F:327:GLN:N	2.41	0.48
1:C:323:ARG:O	1:C:327:GLN:N	2.41	0.48
1:C:493:VAL:HG23	1:C:494:GLN:N	2.28	0.48
1:C:88:VAL:O	1:C:92:LEU:HB3	2.14	0.48
1:A:554:GLU:HG3	1:B:552:PHE:CZ	2.49	0.48
1:C:631:PRO:HB3	1:C:766:ARG:HB3	1.96	0.48
1:D:114:ILE:CD1	1:D:176:VAL:HG12	2.44	0.48
1:D:631:PRO:HB3	1:D:766:ARG:HB3	1.96	0.48
1:F:74:ASP:OD2	1:F:83:ARG:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:GLU:HG3	1:C:552:PHE:CZ	2.49	0.48
1:C:512:LYS:NZ	1:C:619:ILE:HG13	2.29	0.48
1:C:74:ASP:OD2	1:C:83:ARG:HD3	2.14	0.48
1:D:512:LYS:NZ	1:D:619:ILE:HG13	2.29	0.48
1:D:88:VAL:O	1:D:92:LEU:HB3	2.14	0.47
1:E:703:ILE:HG13	1:E:704:GLU:N	2.29	0.47
1:F:477:GLU:N	1:F:477:GLU:OE1	2.44	0.47
1:F:631:PRO:HB3	1:F:766:ARG:HB3	1.96	0.47
1:C:58:LEU:O	1:C:102:ILE:HA	2.15	0.47
1:D:554:GLU:HG3	1:E:552:PHE:CZ	2.49	0.47
1:A:58:LEU:O	1:A:102:ILE:HA	2.15	0.47
1:B:703:ILE:HG13	1:B:704:GLU:N	2.29	0.47
1:C:114:ILE:CD1	1:C:176:VAL:HG12	2.44	0.47
1:A:631:PRO:HB3	1:A:766:ARG:HB3	1.96	0.47
1:B:88:VAL:O	1:B:92:LEU:HB3	2.14	0.47
1:C:37:SER:O	1:C:70:ILE:HG13	2.15	0.47
1:D:443:ASN:OD1	1:D:444:SER:N	2.48	0.47
1:E:114:ILE:CD1	1:E:176:VAL:HG12	2.44	0.47
1:C:554:GLU:HG3	1:D:552:PHE:CZ	2.49	0.47
1:E:701:GLU:O	1:E:705:SER:N	2.35	0.47
1:F:703:ILE:HG13	1:F:704:GLU:N	2.29	0.47
1:A:454:TRP:O	1:A:458:GLN:HG2	2.15	0.47
1:C:454:TRP:O	1:C:458:GLN:HG2	2.15	0.47
1:C:477:GLU:OE1	1:C:477:GLU:N	2.44	0.47
1:A:37:SER:O	1:A:70:ILE:HG13	2.15	0.47
1:A:443:ASN:OD1	1:A:444:SER:N	2.48	0.47
1:A:88:VAL:O	1:A:92:LEU:HB3	2.14	0.47
1:B:114:ILE:CD1	1:B:176:VAL:HG12	2.44	0.47
1:D:37:SER:O	1:D:70:ILE:HG13	2.15	0.47
1:E:58:LEU:O	1:E:102:ILE:HA	2.15	0.47
1:E:512:LYS:NZ	1:E:619:ILE:HG13	2.29	0.47
1:A:552:PHE:CZ	1:F:554:GLU:HG3	2.49	0.47
1:A:512:LYS:NZ	1:A:619:ILE:HG13	2.29	0.47
1:B:491:GLU:HG2	1:B:495:TYR:HE2	1.78	0.47
1:B:512:LYS:NZ	1:B:619:ILE:HG13	2.29	0.47
1:B:37:SER:O	1:B:70:ILE:HG13	2.15	0.47
1:D:703:ILE:HG13	1:D:704:GLU:N	2.29	0.47
1:B:454:TRP:O	1:B:458:GLN:HG2	2.15	0.47
1:B:494:GLN:HE21	1:B:534:GLU:HG2	1.79	0.47
1:B:77:CYS:SG	1:B:83:ARG:HB2	2.55	0.47
1:C:494:GLN:HE21	1:C:534:GLU:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LEU:O	1:D:102:ILE:HA	2.15	0.47
1:E:112:LYS:O	1:E:180:THR:HB	2.15	0.47
1:E:443:ASN:OD1	1:E:444:SER:N	2.48	0.47
1:E:37:SER:O	1:E:70:ILE:HG13	2.14	0.47
1:F:37:SER:O	1:F:70:ILE:HG13	2.15	0.47
1:B:443:ASN:OD1	1:B:444:SER:N	2.48	0.47
1:E:631:PRO:HB3	1:E:766:ARG:HB3	1.96	0.47
1:F:58:LEU:O	1:F:102:ILE:HA	2.15	0.47
1:F:88:VAL:O	1:F:92:LEU:HB3	2.14	0.47
1:C:703:ILE:HG13	1:C:704:GLU:N	2.29	0.47
1:C:77:CYS:SG	1:C:83:ARG:HB2	2.55	0.47
1:E:120:ASP:OD1	1:E:120:ASP:N	2.46	0.47
1:E:454:TRP:O	1:E:458:GLN:HG2	2.15	0.47
1:F:120:ASP:OD1	1:F:120:ASP:N	2.46	0.47
1:F:114:ILE:CD1	1:F:176:VAL:HG12	2.44	0.47
1:F:443:ASN:OD1	1:F:444:SER:N	2.48	0.47
1:F:512:LYS:NZ	1:F:619:ILE:HG13	2.29	0.47
1:A:114:ILE:CD1	1:A:176:VAL:HG12	2.44	0.46
1:A:77:CYS:SG	1:A:83:ARG:HB2	2.55	0.46
1:E:364:ASP:N	1:E:364:ASP:OD1	2.44	0.46
1:E:88:VAL:O	1:E:92:LEU:HB3	2.14	0.46
1:F:454:TRP:O	1:F:458:GLN:HG2	2.15	0.46
1:E:652:SER:O	1:E:655:ALA:N	2.49	0.46
1:F:494:GLN:HE21	1:F:534:GLU:HG2	1.79	0.46
1:C:443:ASN:OD1	1:C:444:SER:N	2.48	0.46
1:D:364:ASP:OD1	1:D:364:ASP:N	2.44	0.46
1:F:649:ASP:O	1:F:653:ARG:HG3	2.16	0.46
1:A:112:LYS:O	1:A:180:THR:HB	2.15	0.46
1:A:494:GLN:HE21	1:A:534:GLU:HG2	1.79	0.46
1:A:649:ASP:O	1:A:653:ARG:HG3	2.16	0.46
1:B:112:LYS:O	1:B:180:THR:HB	2.15	0.46
1:C:649:ASP:O	1:C:653:ARG:HG3	2.16	0.46
1:D:244:TYR:HE1	1:D:366:GLU:HB3	1.81	0.46
1:E:494:GLN:HE21	1:E:534:GLU:HG2	1.79	0.46
1:A:244:TYR:HE1	1:A:366:GLU:HB3	1.81	0.46
1:A:288:LYS:O	1:A:292:GLU:HG2	2.16	0.46
1:B:475:THR:HG22	1:B:476:TRP:N	2.31	0.46
1:B:494:GLN:O	1:B:497:VAL:HG12	2.16	0.46
1:B:512:LYS:HE2	1:B:617:VAL:O	2.16	0.46
1:B:649:ASP:O	1:B:653:ARG:HG3	2.16	0.46
1:C:112:LYS:O	1:C:180:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:CYS:SG	1:D:83:ARG:HB2	2.55	0.46
1:F:112:LYS:O	1:F:180:THR:HB	2.15	0.46
1:F:494:GLN:O	1:F:497:VAL:HG12	2.16	0.46
1:B:58:LEU:O	1:B:102:ILE:HA	2.15	0.46
1:B:252:THR:O	1:B:255:ALA:HB3	2.16	0.46
1:B:244:TYR:HE1	1:B:366:GLU:HB3	1.81	0.46
1:D:284:SER:O	1:D:288:LYS:HG2	2.16	0.46
1:E:77:CYS:SG	1:E:83:ARG:HB2	2.55	0.46
1:F:244:TYR:HE1	1:F:366:GLU:HB3	1.81	0.46
1:F:252:THR:O	1:F:255:ALA:HB3	2.16	0.46
1:A:652:SER:O	1:A:655:ALA:N	2.49	0.46
1:B:288:LYS:O	1:B:292:GLU:HG2	2.16	0.46
1:C:243:LEU:HD23	1:C:367:VAL:HB	1.98	0.46
1:D:243:LEU:HD23	1:D:367:VAL:HB	1.98	0.46
1:D:454:TRP:O	1:D:458:GLN:HG2	2.15	0.46
1:D:494:GLN:HE21	1:D:534:GLU:HG2	1.79	0.46
1:D:652:SER:O	1:D:655:ALA:N	2.49	0.46
1:E:252:THR:O	1:E:255:ALA:HB3	2.16	0.46
1:E:243:LEU:HD23	1:E:367:VAL:HB	1.98	0.46
1:B:652:SER:O	1:B:655:ALA:N	2.49	0.46
1:B:631:PRO:HB3	1:B:766:ARG:HB3	1.96	0.46
1:C:749:ASP:OD1	1:C:750:ASN:N	2.49	0.46
1:C:84:MET:SD	1:C:88:VAL:HG21	2.56	0.46
1:E:288:LYS:O	1:E:292:GLU:HG2	2.16	0.46
1:E:302:PHE:CE2	1:E:304:ASP:HB2	2.51	0.46
1:B:749:ASP:OD1	1:B:750:ASN:N	2.49	0.46
1:C:302:PHE:CE2	1:C:304:ASP:HB2	2.51	0.46
1:C:244:TYR:HE1	1:C:366:GLU:HB3	1.81	0.46
1:C:744:ARG:HD2	1:C:744:ARG:HA	1.76	0.46
1:D:22:ARG:NH1	1:D:24:ASN:CB	2.74	0.46
1:D:288:LYS:O	1:D:292:GLU:HG2	2.16	0.46
1:D:302:PHE:CE2	1:D:304:ASP:HB2	2.51	0.46
1:D:749:ASP:OD1	1:D:750:ASN:N	2.49	0.46
1:E:284:SER:O	1:E:288:LYS:HG2	2.16	0.46
1:E:244:TYR:HE1	1:E:366:GLU:HB3	1.81	0.46
1:E:649:ASP:O	1:E:653:ARG:HG3	2.16	0.46
1:F:22:ARG:NH2	1:F:25:ARG:HA	2.31	0.46
1:F:302:PHE:CE2	1:F:304:ASP:HB2	2.51	0.46
1:F:652:SER:O	1:F:655:ALA:N	2.49	0.46
1:A:302:PHE:CE2	1:A:304:ASP:HB2	2.51	0.46
1:A:703:ILE:HG13	1:A:704:GLU:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:MET:SD	1:B:88:VAL:HG21	2.56	0.46
1:C:284:SER:O	1:C:288:LYS:HG2	2.16	0.46
1:C:494:GLN:O	1:C:497:VAL:HG12	2.16	0.46
1:D:252:THR:O	1:D:255:ALA:HB3	2.16	0.46
1:A:252:THR:O	1:A:255:ALA:HB3	2.16	0.45
1:B:22:ARG:NH2	1:B:25:ARG:HA	2.31	0.45
1:C:288:LYS:O	1:C:292:GLU:HG2	2.16	0.45
1:C:74:ASP:OD1	1:C:75:ASP:N	2.49	0.45
1:C:82:ILE:HA	1:C:82:ILE:HD12	1.88	0.45
1:D:512:LYS:HE2	1:D:617:VAL:O	2.16	0.45
1:D:84:MET:SD	1:D:88:VAL:HG21	2.56	0.45
1:E:157:GLY:O	1:E:159:ARG:N	2.50	0.45
1:E:494:GLN:O	1:E:497:VAL:HG12	2.16	0.45
1:F:135:LEU:HD23	1:F:135:LEU:O	2.17	0.45
1:F:749:ASP:OD1	1:F:750:ASN:N	2.49	0.45
1:A:512:LYS:HE2	1:A:617:VAL:O	2.16	0.45
1:C:22:ARG:NH2	1:C:25:ARG:HA	2.31	0.45
1:C:475:THR:HG22	1:C:476:TRP:N	2.31	0.45
1:C:512:LYS:HE2	1:C:617:VAL:O	2.16	0.45
1:D:157:GLY:O	1:D:159:ARG:N	2.49	0.45
1:D:112:LYS:O	1:D:180:THR:HB	2.15	0.45
1:D:494:GLN:O	1:D:497:VAL:HG12	2.16	0.45
1:D:616:ASN:OD1	1:D:616:ASN:N	2.37	0.45
1:A:494:GLN:O	1:A:497:VAL:HG12	2.16	0.45
1:B:116:VAL:HA	1:B:163:PHE:HZ	1.81	0.45
1:C:652:SER:O	1:C:655:ALA:N	2.49	0.45
1:D:74:ASP:OD1	1:D:75:ASP:N	2.49	0.45
1:E:477:GLU:N	1:E:477:GLU:OE1	2.44	0.45
1:E:749:ASP:OD1	1:E:750:ASN:N	2.49	0.45
1:F:288:LYS:O	1:F:292:GLU:HG2	2.16	0.45
1:F:77:CYS:SG	1:F:83:ARG:HB2	2.55	0.45
1:A:284:SER:O	1:A:288:LYS:HG2	2.16	0.45
1:B:302:PHE:CE2	1:B:304:ASP:HB2	2.51	0.45
1:D:116:VAL:HA	1:D:163:PHE:HZ	1.81	0.45
1:D:485:VAL:HA	1:D:488:GLU:HB3	1.99	0.45
1:E:119:ILE:HG13	1:E:120:ASP:H	1.82	0.45
1:E:22:ARG:NH2	1:E:25:ARG:HA	2.31	0.45
1:F:157:GLY:O	1:F:159:ARG:N	2.49	0.45
1:D:119:ILE:HG13	1:D:120:ASP:H	1.82	0.45
1:D:649:ASP:O	1:D:653:ARG:HG3	2.16	0.45
1:E:458:GLN:C	1:E:461:PRO:HD2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:MET:SD	1:E:88:VAL:HG21	2.56	0.45
1:B:135:LEU:O	1:B:135:LEU:HD23	2.17	0.45
1:C:135:LEU:HD23	1:C:135:LEU:O	2.17	0.45
1:D:139:PHE:HD2	1:D:143:TYR:HE1	1.64	0.45
1:E:475:THR:HG22	1:E:476:TRP:N	2.31	0.45
1:F:117:LEU:HA	1:F:118:PRO:HD3	1.82	0.45
1:F:512:LYS:HE2	1:F:617:VAL:O	2.16	0.45
1:F:74:ASP:OD1	1:F:75:ASP:N	2.49	0.45
1:A:22:ARG:NH2	1:A:25:ARG:HA	2.31	0.45
1:A:744:ARG:HD2	1:A:744:ARG:HA	1.76	0.45
1:A:749:ASP:OD1	1:A:750:ASN:N	2.49	0.45
1:A:74:ASP:OD1	1:A:75:ASP:N	2.49	0.45
1:B:243:LEU:HD23	1:B:367:VAL:HB	1.98	0.45
1:B:284:SER:O	1:B:288:LYS:HG2	2.16	0.45
1:B:458:GLN:C	1:B:461:PRO:HD2	2.37	0.45
1:C:458:GLN:C	1:C:461:PRO:HD2	2.37	0.45
1:B:764:GLN:NE2	1:C:745:ARG:O	2.50	0.45
1:D:114:ILE:CG2	1:D:115:HIS:N	2.80	0.45
1:D:458:GLN:C	1:D:461:PRO:HD2	2.37	0.45
1:E:116:VAL:HA	1:E:163:PHE:HZ	1.81	0.45
1:F:243:LEU:HD23	1:F:367:VAL:HB	1.98	0.45
1:F:84:MET:SD	1:F:88:VAL:HG21	2.56	0.45
1:A:139:PHE:HD2	1:A:143:TYR:HE1	1.64	0.45
1:C:114:ILE:CG2	1:C:115:HIS:N	2.80	0.45
1:C:166:VAL:HG23	1:C:167:GLU:H	1.82	0.45
1:E:512:LYS:HE2	1:E:617:VAL:O	2.16	0.45
1:A:243:LEU:HD23	1:A:367:VAL:HB	1.98	0.45
1:A:84:MET:SD	1:A:88:VAL:HG21	2.56	0.45
1:C:157:GLY:O	1:C:159:ARG:N	2.49	0.45
1:C:252:THR:O	1:C:255:ALA:HB3	2.16	0.45
1:D:135:LEU:O	1:D:135:LEU:HD23	2.17	0.45
1:D:22:ARG:NH2	1:D:25:ARG:HA	2.31	0.45
1:D:74:ASP:HB2	1:D:83:ARG:CZ	2.47	0.45
1:E:114:ILE:HD12	1:E:176:VAL:HG12	1.96	0.45
1:F:22:ARG:NH1	1:F:24:ASN:CB	2.74	0.45
1:A:157:GLY:O	1:A:159:ARG:N	2.49	0.45
1:D:119:ILE:HG13	1:D:120:ASP:OD1	2.17	0.45
1:E:139:PHE:HD2	1:E:143:TYR:HE1	1.64	0.45
1:F:284:SER:O	1:F:288:LYS:HG2	2.16	0.45
1:F:439:ALA:HA	1:F:442:MET:HB2	1.99	0.45
1:F:31:ALA:HB2	1:F:83:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:GLN:C	1:A:461:PRO:HD2	2.37	0.44
1:A:605:LEU:HD22	1:A:638:ARG:CD	2.48	0.44
1:A:31:ALA:HB2	1:A:83:ARG:HG2	1.99	0.44
1:B:501:ASP:OD1	1:B:502:LYS:N	2.51	0.44
1:C:139:PHE:HD2	1:C:143:TYR:HE1	1.64	0.44
1:C:22:ARG:HB3	1:C:25:ARG:HB3	1.99	0.44
1:C:437:ILE:HG13	1:C:438:ASP:OD1	2.18	0.44
1:D:501:ASP:OD1	1:D:502:LYS:N	2.51	0.44
1:C:593:GLY:HA3	1:D:592:ASP:HA	1.99	0.44
1:F:139:PHE:HD2	1:F:143:TYR:HE1	1.64	0.44
1:F:458:GLN:C	1:F:461:PRO:HD2	2.37	0.44
1:F:605:LEU:HD22	1:F:638:ARG:CD	2.48	0.44
1:A:119:ILE:HG13	1:A:120:ASP:OD1	2.17	0.44
1:A:56:THR:HB	1:A:68:VAL:HG13	2.00	0.44
1:B:119:ILE:HG13	1:B:120:ASP:OD1	2.17	0.44
1:B:31:ALA:HB2	1:B:83:ARG:HG2	1.99	0.44
1:B:701:GLU:O	1:B:705:SER:N	2.35	0.44
1:B:74:ASP:HB2	1:B:83:ARG:CZ	2.47	0.44
1:C:116:VAL:HA	1:C:163:PHE:HZ	1.81	0.44
1:C:439:ALA:HA	1:C:442:MET:HB2	1.99	0.44
1:C:501:ASP:OD1	1:C:502:LYS:N	2.51	0.44
1:C:736:PHE:O	1:C:740:MET:HG2	2.18	0.44
1:D:166:VAL:HG23	1:D:167:GLU:H	1.82	0.44
1:D:701:GLU:O	1:D:705:SER:N	2.35	0.44
1:E:279:ALA:HB1	1:E:320:VAL:HG21	1.99	0.44
1:F:116:VAL:HA	1:F:163:PHE:HZ	1.81	0.44
1:A:135:LEU:HD23	1:A:135:LEU:O	2.17	0.44
1:A:166:VAL:HG23	1:A:167:GLU:H	1.82	0.44
1:B:22:ARG:HB3	1:B:25:ARG:HB3	1.99	0.44
1:B:485:VAL:HA	1:B:488:GLU:HB3	1.99	0.44
1:C:485:VAL:HA	1:C:488:GLU:HB3	1.99	0.44
1:E:119:ILE:HG13	1:E:120:ASP:OD1	2.17	0.44
1:F:119:ILE:HG13	1:F:120:ASP:H	1.82	0.44
1:F:501:ASP:OD1	1:F:502:LYS:N	2.51	0.44
1:F:82:ILE:HD12	1:F:82:ILE:HA	1.88	0.44
1:A:116:VAL:HA	1:A:163:PHE:HZ	1.81	0.44
1:A:437:ILE:HG13	1:A:438:ASP:OD1	2.18	0.44
1:A:580:ASP:N	1:A:580:ASP:OD1	2.51	0.44
1:A:672:LEU:HD23	1:A:672:LEU:HA	1.78	0.44
1:B:119:ILE:HG13	1:B:120:ASP:H	1.82	0.44
1:B:157:GLY:O	1:B:159:ARG:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:GLY:HA3	1:C:592:ASP:HA	1.99	0.44
1:C:119:ILE:HG13	1:C:120:ASP:H	1.82	0.44
1:D:736:PHE:O	1:D:740:MET:HG2	2.18	0.44
1:E:135:LEU:O	1:E:135:LEU:HD23	2.17	0.44
1:F:279:ALA:HB1	1:F:320:VAL:HG21	2.00	0.44
1:F:437:ILE:HG13	1:F:438:ASP:OD1	2.18	0.44
1:F:701:GLU:O	1:F:705:SER:N	2.35	0.44
1:F:74:ASP:HB2	1:F:83:ARG:CZ	2.47	0.44
1:A:745:ARG:O	1:F:764:GLN:NE2	2.50	0.44
1:A:501:ASP:OD1	1:A:502:LYS:N	2.51	0.44
1:B:74:ASP:OD1	1:B:75:ASP:N	2.49	0.44
1:C:114:ILE:HD12	1:C:176:VAL:HG12	1.96	0.44
1:C:29:ASP:N	1:C:82:ILE:O	2.34	0.44
1:D:439:ALA:HA	1:D:442:MET:HB2	1.99	0.44
1:D:477:GLU:OE1	1:D:477:GLU:N	2.44	0.44
1:D:605:LEU:HD22	1:D:638:ARG:CD	2.48	0.44
1:F:119:ILE:HG13	1:F:120:ASP:OD1	2.17	0.44
1:F:166:VAL:HG23	1:F:167:GLU:H	1.82	0.44
1:A:117:LEU:HA	1:A:118:PRO:HD3	1.82	0.44
1:A:29:ASP:N	1:A:82:ILE:O	2.34	0.44
1:B:166:VAL:HG23	1:B:167:GLU:H	1.82	0.44
1:A:593:GLY:HA3	1:B:592:ASP:HA	1.99	0.44
1:B:650:GLU:OE1	1:B:650:GLU:N	2.31	0.44
1:D:22:ARG:HB3	1:D:25:ARG:HB3	1.99	0.44
1:D:764:GLN:NE2	1:E:745:ARG:O	2.51	0.44
1:E:74:ASP:OD1	1:E:75:ASP:N	2.49	0.44
1:E:764:GLN:NE2	1:F:745:ARG:O	2.51	0.44
1:E:74:ASP:HB2	1:E:83:ARG:CZ	2.47	0.44
1:F:475:THR:HG22	1:F:476:TRP:N	2.31	0.44
1:A:119:ILE:HG13	1:A:120:ASP:H	1.82	0.44
1:A:74:ASP:HB2	1:A:83:ARG:CZ	2.47	0.44
1:B:114:ILE:HD12	1:B:176:VAL:HG12	1.96	0.44
1:B:139:PHE:HD2	1:B:143:TYR:HE1	1.64	0.44
1:B:437:ILE:HG13	1:B:438:ASP:OD1	2.17	0.44
1:C:74:ASP:HB2	1:C:83:ARG:CZ	2.47	0.44
1:E:119:ILE:HG22	1:E:189:ILE:HG12	2.00	0.44
1:E:31:ALA:HB2	1:E:83:ARG:HG2	1.99	0.44
1:F:653:ARG:NE	1:F:679:THR:O	2.51	0.44
1:A:653:ARG:NE	1:A:679:THR:O	2.51	0.44
1:B:460:ASN:OD1	1:B:460:ASN:N	2.51	0.44
1:B:46:MET:HG2	1:B:51:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:LEU:HD22	1:B:638:ARG:CD	2.48	0.44
1:B:56:THR:HB	1:B:68:VAL:HG13	2.00	0.44
1:C:764:GLN:NE2	1:D:745:ARG:O	2.51	0.44
1:D:110:TYR:HA	1:D:175:ILE:O	2.18	0.44
1:E:650:GLU:OE1	1:E:650:GLU:N	2.31	0.44
1:F:110:TYR:HA	1:F:175:ILE:O	2.18	0.44
1:F:580:ASP:N	1:F:580:ASP:OD1	2.51	0.44
1:F:736:PHE:O	1:F:740:MET:HG2	2.18	0.44
1:A:485:VAL:HA	1:A:488:GLU:HB3	1.99	0.44
1:A:253:LEU:HD22	2:A:901:AGS:H2'	2.00	0.44
1:C:119:ILE:HG13	1:C:120:ASP:OD1	2.17	0.44
1:C:653:ARG:NE	1:C:679:THR:O	2.51	0.44
1:D:119:ILE:HG22	1:D:189:ILE:HG12	2.00	0.44
1:E:114:ILE:CG2	1:E:115:HIS:N	2.80	0.44
1:E:117:LEU:HA	1:E:118:PRO:HD3	1.82	0.44
1:E:605:LEU:HD22	1:E:638:ARG:CD	2.48	0.44
1:E:653:ARG:NE	1:E:679:THR:O	2.51	0.44
1:F:56:THR:HB	1:F:68:VAL:HG13	2.00	0.44
1:F:253:LEU:HD22	2:F:901:AGS:H2'	2.00	0.44
1:A:592:ASP:HA	1:F:593:GLY:HA3	1.99	0.43
1:B:114:ILE:CG2	1:B:115:HIS:N	2.80	0.43
1:B:253:LEU:HD22	2:B:901:AGS:H2'	2.00	0.43
1:B:672:LEU:HD23	1:B:672:LEU:HA	1.78	0.43
1:B:736:PHE:O	1:B:740:MET:HG2	2.18	0.43
1:C:307:ASP:OD1	1:C:307:ASP:N	2.51	0.43
1:C:580:ASP:N	1:C:580:ASP:OD1	2.51	0.43
1:D:114:ILE:HD12	1:D:176:VAL:HG12	1.96	0.43
1:D:46:MET:HG2	1:D:51:LEU:HB3	2.00	0.43
1:E:485:VAL:HA	1:E:488:GLU:HB3	1.99	0.43
1:E:580:ASP:OD1	1:E:580:ASP:N	2.51	0.43
1:E:40:SER:CB	1:E:83:ARG:HB3	2.48	0.43
1:E:253:LEU:HD22	2:E:901:AGS:H2'	2.00	0.43
1:F:307:ASP:OD1	1:F:307:ASP:N	2.51	0.43
1:A:59:LEU:HB3	1:A:102:ILE:HG22	2.01	0.43
1:A:279:ALA:HB1	1:A:320:VAL:HG21	1.99	0.43
1:B:115:HIS:O	1:B:116:VAL:CB	2.66	0.43
1:B:41:LEU:HB3	1:B:72:LEU:HA	2.00	0.43
1:C:476:TRP:CZ3	1:C:486:LYS:HG2	2.54	0.43
1:C:253:LEU:HD22	2:C:901:AGS:H2'	2.00	0.43
1:D:253:LEU:HD22	2:D:901:AGS:H2'	2.00	0.43
1:D:650:GLU:OE1	1:D:650:GLU:N	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:VAL:HG23	1:E:167:GLU:H	1.82	0.43
1:E:437:ILE:HG13	1:E:438:ASP:OD1	2.17	0.43
1:E:616:ASN:N	1:E:616:ASN:OD1	2.37	0.43
1:F:114:ILE:CG2	1:F:115:HIS:N	2.80	0.43
1:F:59:LEU:HB3	1:F:102:ILE:HG22	2.00	0.43
1:A:114:ILE:CG2	1:A:115:HIS:N	2.80	0.43
1:A:439:ALA:HA	1:A:442:MET:HB2	1.99	0.43
1:A:764:GLN:NE2	1:B:745:ARG:O	2.52	0.43
1:B:110:TYR:HA	1:B:175:ILE:O	2.18	0.43
1:B:119:ILE:HG22	1:B:189:ILE:HG12	2.00	0.43
1:C:64:ARG:HH12	1:C:260:ASN:CA	2.25	0.43
1:C:672:LEU:HD23	1:C:672:LEU:HA	1.78	0.43
1:D:279:ALA:HB1	1:D:320:VAL:HG21	2.00	0.43
1:D:653:ARG:NE	1:D:679:THR:O	2.51	0.43
1:E:110:TYR:HA	1:E:175:ILE:O	2.18	0.43
1:E:167:GLU:HG2	1:E:168:THR:N	2.33	0.43
1:F:58:LEU:N	1:F:103:GLN:O	2.38	0.43
1:F:485:VAL:HA	1:F:488:GLU:HB3	1.99	0.43
1:A:307:ASP:N	1:A:307:ASP:OD1	2.51	0.43
1:B:279:ALA:HB1	1:B:320:VAL:HG21	1.99	0.43
1:B:476:TRP:CZ3	1:B:486:LYS:HG2	2.54	0.43
1:B:653:ARG:NE	1:B:679:THR:O	2.51	0.43
1:C:31:ALA:HB2	1:C:83:ARG:HG2	1.99	0.43
1:C:542:ILE:HG12	1:C:562:ILE:HD13	2.01	0.43
1:D:167:GLU:HG2	1:D:168:THR:N	2.33	0.43
1:D:437:ILE:HG13	1:D:438:ASP:OD1	2.18	0.43
1:D:476:TRP:CZ3	1:D:486:LYS:HG2	2.54	0.43
1:D:491:GLU:HG2	1:D:495:TYR:HE2	1.78	0.43
1:B:59:LEU:HB3	1:B:102:ILE:HG22	2.01	0.43
1:B:307:ASP:OD1	1:B:307:ASP:N	2.51	0.43
1:B:542:ILE:HG12	1:B:562:ILE:HD13	2.00	0.43
1:C:119:ILE:HG22	1:C:189:ILE:HG12	2.00	0.43
1:D:307:ASP:N	1:D:307:ASP:OD1	2.51	0.43
1:D:593:GLY:HA3	1:E:592:ASP:HA	1.99	0.43
1:D:62:LYS:HE3	1:D:62:LYS:HB3	1.82	0.43
1:D:56:THR:HB	1:D:68:VAL:HG13	2.00	0.43
1:D:31:ALA:HB2	1:D:83:ARG:HG2	1.99	0.43
1:E:58:LEU:N	1:E:103:GLN:O	2.38	0.43
1:E:439:ALA:HA	1:E:442:MET:HB2	1.99	0.43
1:A:194:GLU:O	1:A:197:SER:HB3	2.19	0.43
1:A:41:LEU:HB3	1:A:72:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLY:O	1:B:592:ASP:N	2.52	0.43
1:C:279:ALA:HB1	1:C:320:VAL:HG21	1.99	0.43
1:D:82:ILE:HA	1:D:82:ILE:HD12	1.88	0.43
1:E:501:ASP:OD1	1:E:502:LYS:N	2.51	0.43
1:E:736:PHE:O	1:E:740:MET:HG2	2.18	0.43
1:E:250:GLY:N	2:E:901:AGS:O2B	2.51	0.43
1:F:194:GLU:O	1:F:197:SER:HB3	2.19	0.43
1:A:110:TYR:HA	1:A:175:ILE:O	2.18	0.43
1:A:46:MET:HG2	1:A:51:LEU:HB3	2.00	0.43
2:A:901:AGS:C8	2:A:901:AGS:H5'1	2.44	0.43
1:C:110:TYR:HA	1:C:175:ILE:O	2.18	0.43
1:C:56:THR:HB	1:C:68:VAL:HG13	2.00	0.43
1:C:593:GLY:O	1:D:592:ASP:N	2.52	0.43
1:E:22:ARG:HB3	1:E:25:ARG:HB3	1.99	0.43
1:E:460:ASN:N	1:E:460:ASN:OD1	2.51	0.43
1:E:491:GLU:HG2	1:E:495:TYR:HE2	1.78	0.43
1:F:250:GLY:N	2:F:901:AGS:O2B	2.51	0.43
1:A:167:GLU:HG2	1:A:168:THR:N	2.33	0.43
1:A:113:ARG:CD	1:A:182:ILE:CG2	2.76	0.43
1:A:460:ASN:N	1:A:460:ASN:OD1	2.51	0.43
1:B:439:ALA:HA	1:B:442:MET:HB2	1.99	0.43
1:B:250:GLY:N	2:B:901:AGS:O2B	2.51	0.43
1:C:167:GLU:HG2	1:C:168:THR:N	2.33	0.43
1:C:41:LEU:HB3	1:C:72:LEU:HA	2.00	0.43
1:E:115:HIS:O	1:E:116:VAL:CB	2.66	0.43
1:A:736:PHE:O	1:A:740:MET:HG2	2.18	0.43
1:B:580:ASP:OD1	1:B:580:ASP:N	2.51	0.43
1:B:40:SER:CB	1:B:83:ARG:HB3	2.48	0.43
1:C:22:ARG:NH1	1:C:24:ASN:CB	2.74	0.43
1:C:460:ASN:N	1:C:460:ASN:OD1	2.51	0.43
1:C:701:GLU:O	1:C:705:SER:N	2.35	0.43
1:D:460:ASN:OD1	1:D:460:ASN:N	2.51	0.43
1:E:46:MET:HG2	1:E:51:LEU:HB3	2.00	0.43
1:E:744:ARG:HD2	1:E:744:ARG:HA	1.76	0.43
1:A:476:TRP:CZ3	1:A:486:LYS:HG2	2.54	0.43
1:B:167:GLU:HG2	1:B:168:THR:N	2.33	0.43
1:B:631:PRO:HB3	1:B:766:ARG:HA	2.01	0.43
2:B:901:AGS:C8	2:B:901:AGS:H5'1	2.44	0.43
1:E:59:LEU:HB3	1:E:102:ILE:HG22	2.00	0.43
1:E:56:THR:HB	1:E:68:VAL:HG13	2.00	0.43
1:B:194:GLU:O	1:B:197:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HB3	1:C:102:ILE:HG22	2.00	0.42
1:C:605:LEU:HD22	1:C:638:ARG:CD	2.48	0.42
1:D:153:LEU:O	1:D:153:LEU:HD12	2.19	0.42
1:D:542:ILE:HG12	1:D:562:ILE:HD13	2.01	0.42
1:D:580:ASP:OD1	1:D:580:ASP:N	2.51	0.42
1:E:194:GLU:O	1:E:197:SER:HB3	2.19	0.42
1:E:476:TRP:CZ3	1:E:486:LYS:HG2	2.54	0.42
1:F:167:GLU:HG2	1:F:168:THR:N	2.33	0.42
1:F:22:ARG:HB3	1:F:25:ARG:HB3	2.00	0.42
1:F:41:LEU:HB3	1:F:72:LEU:HA	2.00	0.42
1:A:115:HIS:O	1:A:116:VAL:CB	2.66	0.42
1:B:761:THR:HG22	1:C:744:ARG:HE	1.84	0.42
1:C:46:MET:HG2	1:C:51:LEU:HB3	2.00	0.42
1:D:475:THR:HG22	1:D:476:TRP:N	2.31	0.42
1:E:41:LEU:HB3	1:E:72:LEU:HA	2.00	0.42
1:E:593:GLY:HA3	1:F:592:ASP:HA	2.00	0.42
1:F:115:HIS:O	1:F:116:VAL:CB	2.66	0.42
1:F:119:ILE:HG22	1:F:189:ILE:CG1	2.50	0.42
1:F:119:ILE:HG22	1:F:189:ILE:HG12	2.00	0.42
1:F:460:ASN:N	1:F:460:ASN:OD1	2.51	0.42
1:F:616:ASN:OD1	1:F:616:ASN:N	2.37	0.42
1:F:672:LEU:HD23	1:F:672:LEU:HA	1.78	0.42
1:D:631:PRO:HB3	1:D:766:ARG:HA	2.01	0.42
1:F:64:ARG:HH12	1:F:260:ASN:CA	2.25	0.42
1:A:153:LEU:HD12	1:A:153:LEU:O	2.19	0.42
1:A:542:ILE:HG12	1:A:562:ILE:HD13	2.01	0.42
1:C:40:SER:CB	1:C:83:ARG:HB3	2.48	0.42
1:A:155:ARG:HH21	1:A:157:GLY:HA3	1.84	0.42
1:B:593:GLY:O	1:C:592:ASP:N	2.52	0.42
1:C:119:ILE:HG22	1:C:189:ILE:CG1	2.50	0.42
1:E:476:TRP:HE3	1:E:486:LYS:HE2	1.84	0.42
1:F:476:TRP:CZ3	1:F:486:LYS:HG2	2.54	0.42
1:A:119:ILE:HG22	1:A:189:ILE:HG12	2.00	0.42
1:A:475:THR:HG22	1:A:476:TRP:N	2.31	0.42
1:C:115:HIS:O	1:C:116:VAL:CB	2.66	0.42
1:D:59:LEU:HB3	1:D:102:ILE:HG22	2.01	0.42
1:D:194:GLU:O	1:D:197:SER:HB3	2.19	0.42
1:D:40:SER:CB	1:D:83:ARG:HB3	2.48	0.42
1:E:119:ILE:HG22	1:E:189:ILE:CG1	2.50	0.42
1:F:46:MET:HG2	1:F:51:LEU:HB3	2.00	0.42
1:A:40:SER:CB	1:A:83:ARG:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:PRO:HB3	1:C:766:ARG:HA	2.01	0.42
1:D:115:HIS:O	1:D:116:VAL:CB	2.66	0.42
1:E:28:VAL:HG13	1:E:89:ARG:HH22	1.84	0.42
1:F:28:VAL:HG13	1:F:89:ARG:HH22	1.84	0.42
1:B:119:ILE:HG22	1:B:189:ILE:CG1	2.50	0.42
1:C:155:ARG:HH21	1:C:157:GLY:HA3	1.84	0.42
1:C:650:GLU:OE1	1:C:650:GLU:N	2.31	0.42
2:C:901:AGS:C8	2:C:901:AGS:H5'1	2.44	0.42
1:D:155:ARG:HH21	1:D:157:GLY:HA3	1.84	0.42
1:D:476:TRP:HE3	1:D:486:LYS:HE2	1.84	0.42
1:E:153:LEU:O	1:E:153:LEU:HD12	2.19	0.42
1:E:761:THR:HG22	1:F:744:ARG:HE	1.84	0.42
1:A:476:TRP:HE3	1:A:486:LYS:HE2	1.84	0.42
1:A:592:ASP:N	1:F:593:GLY:O	2.52	0.42
1:A:631:PRO:HB3	1:A:766:ARG:HA	2.01	0.42
1:B:153:LEU:O	1:B:153:LEU:HD12	2.20	0.42
1:C:153:LEU:O	1:C:153:LEU:HD12	2.19	0.42
1:C:194:GLU:O	1:C:197:SER:HB3	2.19	0.42
1:D:593:GLY:O	1:E:592:ASP:N	2.52	0.42
1:D:250:GLY:N	2:D:901:AGS:O2B	2.51	0.42
1:E:307:ASP:N	1:E:307:ASP:OD1	2.51	0.42
1:F:336:LYS:CB	1:F:338:ARG:HG2	2.49	0.42
1:F:542:ILE:HG12	1:F:562:ILE:HD13	2.00	0.42
1:F:29:ASP:N	1:F:82:ILE:O	2.34	0.42
1:A:119:ILE:HG22	1:A:189:ILE:CG1	2.50	0.42
1:D:119:ILE:HG22	1:D:189:ILE:CG1	2.50	0.42
1:E:542:ILE:HG12	1:E:562:ILE:HD13	2.01	0.42
1:E:631:PRO:HB3	1:E:766:ARG:HA	2.00	0.42
1:B:24:ASN:HA	1:B:45:LYS:NZ	2.35	0.41
1:D:41:LEU:HB3	1:D:72:LEU:HA	2.00	0.41
1:D:28:VAL:HG13	1:D:89:ARG:HH22	1.84	0.41
1:A:117:LEU:HD23	1:A:118:PRO:O	2.20	0.41
1:B:117:LEU:HD23	1:B:118:PRO:O	2.21	0.41
1:B:164:LYS:HG2	1:B:165:VAL:N	2.30	0.41
1:B:476:TRP:HE3	1:B:486:LYS:HE2	1.84	0.41
1:A:164:LYS:HG2	1:A:165:VAL:N	2.30	0.41
1:A:22:ARG:HB3	1:A:25:ARG:HB3	1.99	0.41
1:A:24:ASN:HA	1:A:45:LYS:NZ	2.35	0.41
1:B:29:ASP:N	1:B:82:ILE:O	2.34	0.41
1:C:113:ARG:HG2	1:C:114:ILE:N	2.36	0.41
1:C:132:GLU:O	1:C:136:LYS:NZ	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:734:ASP:O	1:F:737:GLU:HB2	2.21	0.41
1:A:734:ASP:O	1:A:737:GLU:HB2	2.21	0.41
1:D:117:LEU:HD23	1:D:118:PRO:O	2.20	0.41
1:D:64:ARG:HH12	1:D:260:ASN:CA	2.25	0.41
1:F:153:LEU:HD12	1:F:153:LEU:O	2.19	0.41
1:B:120:ASP:OD1	1:B:120:ASP:N	2.46	0.41
1:B:155:ARG:HH21	1:B:157:GLY:HA3	1.84	0.41
1:C:117:LEU:HD23	1:C:118:PRO:O	2.21	0.41
1:C:348:ASN:OD1	1:C:349:ARG:HG3	2.21	0.41
1:D:113:ARG:HG2	1:D:114:ILE:N	2.35	0.41
1:E:494:GLN:NE2	1:E:534:GLU:HG2	2.36	0.41
1:F:155:ARG:HH21	1:F:157:GLY:HA3	1.84	0.41
1:F:283:GLU:OE2	1:F:320:VAL:HG13	2.21	0.41
1:F:476:TRP:HE3	1:F:486:LYS:HE2	1.84	0.41
1:F:494:GLN:NE2	1:F:534:GLU:HG2	2.36	0.41
1:E:593:GLY:O	1:F:592:ASP:N	2.53	0.41
1:A:744:ARG:HE	1:F:761:THR:HG22	1.84	0.41
1:D:744:ARG:HA	1:D:744:ARG:HD2	1.76	0.41
1:D:761:THR:HG22	1:E:744:ARG:HE	1.84	0.41
1:E:155:ARG:HH21	1:E:157:GLY:HA3	1.84	0.41
1:E:348:ASN:OD1	1:E:349:ARG:HG3	2.21	0.41
1:F:219:MET:SD	1:F:241:ILE:HD12	2.61	0.41
1:F:631:PRO:HB3	1:F:766:ARG:HA	2.01	0.41
1:A:219:MET:SD	1:A:241:ILE:HD12	2.61	0.41
1:A:82:ILE:HD12	1:A:82:ILE:HA	1.88	0.41
1:B:121:ASP:HB3	1:B:161:VAL:CG2	2.49	0.41
1:B:28:VAL:HG13	1:B:89:ARG:HH22	1.84	0.41
1:C:336:LYS:CB	1:C:338:ARG:HG2	2.49	0.41
1:D:219:MET:SD	1:D:241:ILE:HD12	2.61	0.41
1:E:59:LEU:HA	1:E:101:SER:O	2.21	0.41
1:E:734:ASP:O	1:E:737:GLU:HB2	2.21	0.41
1:A:257:ALA:O	1:A:261:GLU:HG2	2.21	0.41
1:A:494:GLN:NE2	1:A:534:GLU:HG2	2.36	0.41
1:A:28:VAL:HG13	1:A:89:ARG:HH22	1.84	0.41
1:B:113:ARG:CG	1:B:182:ILE:HG21	2.51	0.41
1:B:283:GLU:OE2	1:B:320:VAL:HG13	2.21	0.41
1:B:494:GLN:NE2	1:B:534:GLU:HG2	2.36	0.41
1:B:670:VAL:HG13	1:B:733:ARG:HH11	1.86	0.41
1:C:257:ALA:O	1:C:261:GLU:HG2	2.21	0.41
1:D:24:ASN:HA	1:D:45:LYS:NZ	2.35	0.41
1:D:494:GLN:NE2	1:D:534:GLU:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:LEU:HA	1:D:101:SER:O	2.21	0.41
1:E:117:LEU:HD23	1:E:118:PRO:O	2.20	0.41
1:F:348:ASN:OD1	1:F:349:ARG:HG3	2.21	0.41
1:A:113:ARG:CG	1:A:182:ILE:HG21	2.51	0.41
1:A:761:THR:HG22	1:B:744:ARG:HE	1.85	0.41
1:C:219:MET:SD	1:C:241:ILE:HD12	2.61	0.41
1:C:283:GLU:OE2	1:C:320:VAL:HG13	2.21	0.41
1:C:28:VAL:HG13	1:C:89:ARG:HH22	1.84	0.41
1:C:24:ASN:HA	1:C:45:LYS:NZ	2.35	0.41
1:D:670:VAL:HG13	1:D:733:ARG:HH11	1.86	0.41
1:E:283:GLU:OE2	1:E:320:VAL:HG13	2.20	0.41
1:E:64:ARG:HH12	1:E:260:ASN:CA	2.25	0.41
1:F:59:LEU:HA	1:F:101:SER:O	2.21	0.41
1:F:115:HIS:CG	1:F:116:VAL:H	2.38	0.41
1:A:592:ASP:CA	1:F:593:GLY:HA3	2.51	0.41
1:A:512:LYS:O	1:A:512:LYS:CG	2.68	0.41
1:A:764:GLN:O	1:A:765:SER:C	2.60	0.41
1:B:113:ARG:HG2	1:B:114:ILE:N	2.35	0.41
1:B:257:ALA:O	1:B:261:GLU:HG2	2.21	0.41
1:B:59:LEU:HA	1:B:101:SER:O	2.21	0.41
1:C:164:LYS:HG2	1:C:165:VAL:N	2.30	0.41
1:C:113:ARG:CG	1:C:182:ILE:HG21	2.51	0.41
1:C:59:LEU:HA	1:C:101:SER:O	2.21	0.41
1:D:348:ASN:OD1	1:D:349:ARG:HG3	2.21	0.41
1:C:761:THR:HG22	1:D:744:ARG:HE	1.85	0.41
1:E:24:ASN:HA	1:E:45:LYS:NZ	2.35	0.41
1:E:512:LYS:CG	1:E:512:LYS:O	2.68	0.41
1:D:593:GLY:HA3	1:E:592:ASP:CA	2.51	0.41
1:F:113:ARG:CG	1:F:182:ILE:HG21	2.51	0.41
2:F:901:AGS:H5'1	2:F:901:AGS:C8	2.44	0.41
1:A:348:ASN:OD1	1:A:349:ARG:HG3	2.21	0.41
1:B:166:VAL:HG23	1:B:167:GLU:N	2.36	0.41
1:B:734:ASP:O	1:B:737:GLU:HB2	2.21	0.41
1:C:121:ASP:HB3	1:C:161:VAL:CG2	2.49	0.41
1:C:476:TRP:HE3	1:C:486:LYS:HE2	1.84	0.41
1:E:144:ARG:HB2	1:E:176:VAL:HG22	2.03	0.41
1:E:166:VAL:HG23	1:E:167:GLU:N	2.36	0.41
1:E:219:MET:SD	1:E:241:ILE:HD12	2.61	0.41
1:F:60:LYS:O	1:F:100:ILE:HD12	2.21	0.41
1:A:250:GLY:N	2:A:901:AGS:O2B	2.51	0.40
1:C:593:GLY:HA3	1:D:592:ASP:CA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ALA:O	1:D:261:GLU:HG2	2.21	0.40
1:D:283:GLU:OE2	1:D:320:VAL:HG13	2.21	0.40
1:D:767:GLY:O	1:D:768:PHE:CG	2.75	0.40
1:E:672:LEU:HA	1:E:672:LEU:HD23	1.78	0.40
1:F:144:ARG:HB2	1:F:176:VAL:HG22	2.03	0.40
1:F:512:LYS:CG	1:F:512:LYS:O	2.68	0.40
1:A:60:LYS:O	1:A:100:ILE:HD12	2.21	0.40
1:A:41:LEU:HD23	1:A:72:LEU:CA	2.51	0.40
1:B:117:LEU:HA	1:B:118:PRO:HD3	1.82	0.40
1:B:348:ASN:OD1	1:B:349:ARG:HG3	2.21	0.40
1:C:58:LEU:N	1:C:103:GLN:O	2.38	0.40
1:C:670:VAL:HG13	1:C:733:ARG:HH11	1.86	0.40
1:D:734:ASP:O	1:D:737:GLU:HB2	2.21	0.40
1:D:764:GLN:O	1:D:765:SER:C	2.60	0.40
1:D:29:ASP:N	1:D:82:ILE:O	2.34	0.40
1:E:767:GLY:O	1:E:768:PHE:CG	2.75	0.40
1:A:283:GLU:OE2	1:A:320:VAL:HG13	2.21	0.40
1:B:219:MET:SD	1:B:241:ILE:HD12	2.61	0.40
1:B:41:LEU:HD23	1:B:72:LEU:CA	2.51	0.40
1:C:41:LEU:HD23	1:C:72:LEU:CA	2.51	0.40
1:C:767:GLY:O	1:C:768:PHE:CG	2.75	0.40
2:C:902:AGS:O2G	2:C:902:AGS:O1B	2.39	0.40
1:D:60:LYS:O	1:D:100:ILE:HD12	2.21	0.40
1:D:166:VAL:HG23	1:D:167:GLU:N	2.36	0.40
1:D:22:ARG:O	1:D:25:ARG:HB3	2.21	0.40
1:E:127:THR:O	1:E:133:VAL:HG21	2.22	0.40
1:E:30:GLU:O	1:E:83:ARG:HG3	2.21	0.40
1:F:117:LEU:HD23	1:F:118:PRO:O	2.21	0.40
1:F:257:ALA:O	1:F:261:GLU:HG2	2.21	0.40
1:A:166:VAL:HG23	1:A:167:GLU:N	2.36	0.40
1:A:670:VAL:HG13	1:A:733:ARG:HH11	1.86	0.40
1:A:767:GLY:O	1:A:768:PHE:CG	2.75	0.40
1:B:764:GLN:O	1:B:765:SER:C	2.60	0.40
1:C:22:ARG:O	1:C:25:ARG:HB3	2.21	0.40
1:C:764:GLN:O	1:C:765:SER:C	2.60	0.40
1:D:164:LYS:HB3	1:D:164:LYS:HE3	1.93	0.40
1:E:764:GLN:O	1:E:765:SER:C	2.60	0.40
2:E:902:AGS:O1B	2:E:902:AGS:O2G	2.39	0.40
1:A:317:HIS:NE2	1:F:317:HIS:CE1	2.89	0.40
1:F:41:LEU:HD23	1:F:72:LEU:CA	2.51	0.40
1:B:42:SER:HB2	1:B:45:LYS:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ARG:HB2	1:C:176:VAL:HG22	2.03	0.40
1:C:494:GLN:NE2	1:C:534:GLU:HG2	2.36	0.40
1:F:113:ARG:HG2	1:F:114:ILE:N	2.35	0.40
1:F:40:SER:CB	1:F:83:ARG:HB3	2.48	0.40
1:F:30:GLU:O	1:F:83:ARG:HG3	2.21	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 PDB entries followed by that with respect to all EM entries.

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	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	18	53
1	B	733/806 (91%)	671 (92%)	55 (8%)	7 (1%)	18	53
1	C	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	18	53
1	D	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	18	53
1	E	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	18	53
1	F	733/806 (91%)	672 (92%)	54 (7%)	7 (1%)	18	53
All	All	4398/4836 (91%)	4031 (92%)	325 (7%)	42 (1%)	23	53

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ALA
1	B	297	ALA
1	C	297	ALA
1	D	297	ALA
1	E	297	ALA
1	F	297	ALA
1	A	95	ARG

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Mol	Chain	Res	Type
1	A	116	VAL
1	B	95	ARG
1	B	116	VAL
1	C	95	ARG
1	C	116	VAL
1	D	95	ARG
1	D	116	VAL
1	E	95	ARG
1	E	116	VAL
1	F	95	ARG
1	F	116	VAL
1	A	158	MET
1	B	158	MET
1	C	158	MET
1	D	158	MET
1	E	158	MET
1	F	158	MET
1	A	764	GLN
1	B	764	GLN
1	C	764	GLN
1	D	764	GLN
1	E	764	GLN
1	F	764	GLN
1	A	21	ASN
1	B	21	ASN
1	C	21	ASN
1	D	21	ASN
1	E	21	ASN
1	F	21	ASN
1	A	27	ILE
1	B	27	ILE
1	C	27	ILE
1	D	27	ILE
1	E	27	ILE
1	F	27	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	626/678 (92%)	625 (100%)	1 (0%)	94	98
1	B	626/678 (92%)	625 (100%)	1 (0%)	94	98
1	C	626/678 (92%)	625 (100%)	1 (0%)	94	98
1	D	626/678 (92%)	625 (100%)	1 (0%)	94	98
1	E	626/678 (92%)	625 (100%)	1 (0%)	94	98
1	F	626/678 (92%)	625 (100%)	1 (0%)	94	98
All	All	3756/4068 (92%)	3750 (100%)	6 (0%)	95	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	VAL
1	B	474	VAL
1	C	474	VAL
1	D	474	VAL
1	E	474	VAL
1	F	474	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	317	HIS
1	A	327	GLN
1	A	337	GLN
1	A	494	GLN
1	B	91	ASN
1	B	317	HIS
1	B	327	GLN
1	B	337	GLN
1	B	494	GLN
1	C	91	ASN
1	C	317	HIS
1	C	327	GLN
1	C	337	GLN
1	C	494	GLN
1	D	91	ASN
1	D	317	HIS

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Mol	Chain	Res	Type
1	D	327	GLN
1	D	337	GLN
1	D	494	GLN
1	E	91	ASN
1	E	317	HIS
1	E	327	GLN
1	E	337	GLN
1	E	494	GLN
1	F	91	ASN
1	F	317	HIS
1	F	327	GLN
1	F	337	GLN
1	F	494	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AGS	A	901	-	26,33,33	2.04	3 (11%)	22,52,52	1.80	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AGS	A	902	-	26,33,33	2.04	2 (7%)	22,52,52	1.85	3 (13%)
2	AGS	B	901	-	26,33,33	2.03	3 (11%)	22,52,52	1.80	3 (13%)
2	AGS	B	902	-	26,33,33	2.03	2 (7%)	22,52,52	1.87	3 (13%)
2	AGS	C	901	-	26,33,33	2.04	3 (11%)	22,52,52	1.80	3 (13%)
2	AGS	C	902	-	26,33,33	2.04	2 (7%)	22,52,52	1.86	3 (13%)
2	AGS	D	901	-	26,33,33	2.04	3 (11%)	22,52,52	1.80	3 (13%)
2	AGS	D	902	-	26,33,33	2.04	3 (11%)	22,52,52	1.85	3 (13%)
2	AGS	E	901	-	26,33,33	2.04	3 (11%)	22,52,52	1.80	3 (13%)
2	AGS	E	902	-	26,33,33	2.04	2 (7%)	22,52,52	1.85	3 (13%)
2	AGS	F	901	-	26,33,33	2.04	3 (11%)	22,52,52	1.80	3 (13%)
2	AGS	F	902	-	26,33,33	2.03	3 (11%)	22,52,52	1.85	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	A	901	-	-	0/17/38/38	0/3/3/3
2	AGS	A	902	-	-	0/17/38/38	0/3/3/3
2	AGS	B	901	-	-	0/17/38/38	0/3/3/3
2	AGS	B	902	-	-	0/17/38/38	0/3/3/3
2	AGS	C	901	-	-	0/17/38/38	0/3/3/3
2	AGS	C	902	-	-	0/17/38/38	0/3/3/3
2	AGS	D	901	-	-	0/17/38/38	0/3/3/3
2	AGS	D	902	-	-	0/17/38/38	0/3/3/3
2	AGS	E	901	-	-	0/17/38/38	0/3/3/3
2	AGS	E	902	-	-	0/17/38/38	0/3/3/3
2	AGS	F	901	-	-	0/17/38/38	0/3/3/3
2	AGS	F	902	-	-	0/17/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	AGS	PG-O3G	-2.04	1.48	1.55
2	E	901	AGS	PG-O3G	-2.03	1.48	1.55
2	A	901	AGS	PG-O3G	-2.03	1.48	1.55
2	D	901	AGS	PG-O3G	-2.03	1.48	1.55
2	F	901	AGS	PG-O3G	-2.03	1.48	1.55
2	B	901	AGS	PG-O3G	-2.03	1.48	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	902	AGS	PG-O3G	-2.01	1.48	1.55
2	D	902	AGS	PG-O3G	-2.00	1.48	1.55
2	B	901	AGS	C5-C4	2.97	1.47	1.40
2	C	901	AGS	C5-C4	2.99	1.47	1.40
2	A	901	AGS	C5-C4	3.01	1.47	1.40
2	D	901	AGS	C5-C4	3.01	1.47	1.40
2	B	902	AGS	C5-C4	3.02	1.47	1.40
2	E	902	AGS	C5-C4	3.02	1.47	1.40
2	A	902	AGS	C5-C4	3.03	1.47	1.40
2	D	902	AGS	C5-C4	3.03	1.47	1.40
2	F	902	AGS	C5-C4	3.03	1.47	1.40
2	C	902	AGS	C5-C4	3.04	1.47	1.40
2	E	901	AGS	C5-C4	3.05	1.47	1.40
2	F	901	AGS	C5-C4	3.06	1.47	1.40
2	B	902	AGS	PG-S1G	8.87	2.07	1.90
2	B	901	AGS	PG-S1G	8.87	2.07	1.90
2	F	902	AGS	PG-S1G	8.87	2.07	1.90
2	F	901	AGS	PG-S1G	8.89	2.07	1.90
2	A	902	AGS	PG-S1G	8.89	2.07	1.90
2	A	901	AGS	PG-S1G	8.90	2.07	1.90
2	D	901	AGS	PG-S1G	8.90	2.07	1.90
2	E	901	AGS	PG-S1G	8.91	2.07	1.90
2	C	902	AGS	PG-S1G	8.92	2.07	1.90
2	C	901	AGS	PG-S1G	8.94	2.07	1.90
2	D	902	AGS	PG-S1G	8.94	2.07	1.90
2	E	902	AGS	PG-S1G	8.95	2.07	1.90

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	AGS	N3-C2-N1	-5.94	123.68	128.86
2	C	902	AGS	N3-C2-N1	-5.89	123.73	128.86
2	F	902	AGS	N3-C2-N1	-5.89	123.73	128.86
2	A	902	AGS	N3-C2-N1	-5.88	123.74	128.86
2	D	902	AGS	N3-C2-N1	-5.88	123.74	128.86
2	E	902	AGS	N3-C2-N1	-5.85	123.77	128.86
2	A	901	AGS	N3-C2-N1	-5.80	123.81	128.86
2	D	901	AGS	N3-C2-N1	-5.80	123.81	128.86
2	C	901	AGS	N3-C2-N1	-5.79	123.82	128.86
2	E	901	AGS	N3-C2-N1	-5.78	123.82	128.86
2	B	901	AGS	N3-C2-N1	-5.78	123.82	128.86
2	F	901	AGS	N3-C2-N1	-5.76	123.84	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	AGS	PB-O3B-PG	-3.61	120.67	132.35
2	E	902	AGS	PB-O3B-PG	-3.61	120.69	132.35
2	A	902	AGS	PB-O3B-PG	-3.60	120.71	132.35
2	D	902	AGS	PB-O3B-PG	-3.60	120.71	132.35
2	C	902	AGS	PB-O3B-PG	-3.60	120.72	132.35
2	F	902	AGS	PB-O3B-PG	-3.60	120.72	132.35
2	B	901	AGS	PB-O3B-PG	-3.11	122.29	132.35
2	F	901	AGS	PB-O3B-PG	-3.11	122.31	132.35
2	A	901	AGS	PB-O3B-PG	-3.10	122.33	132.35
2	D	901	AGS	PB-O3B-PG	-3.10	122.33	132.35
2	E	901	AGS	PB-O3B-PG	-3.09	122.35	132.35
2	C	901	AGS	PB-O3B-PG	-3.09	122.35	132.35
2	F	901	AGS	C4-C5-N7	-2.97	106.54	109.41
2	C	902	AGS	C4-C5-N7	-2.96	106.55	109.41
2	B	901	AGS	C4-C5-N7	-2.92	106.59	109.41
2	A	902	AGS	C4-C5-N7	-2.91	106.60	109.41
2	B	902	AGS	C4-C5-N7	-2.91	106.60	109.41
2	D	902	AGS	C4-C5-N7	-2.91	106.60	109.41
2	E	902	AGS	C4-C5-N7	-2.91	106.60	109.41
2	A	901	AGS	C4-C5-N7	-2.91	106.60	109.41
2	D	901	AGS	C4-C5-N7	-2.91	106.60	109.41
2	C	901	AGS	C4-C5-N7	-2.91	106.60	109.41
2	E	901	AGS	C4-C5-N7	-2.90	106.61	109.41
2	F	902	AGS	C4-C5-N7	-2.89	106.61	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AGS	8	0
2	A	902	AGS	2	0
2	B	901	AGS	8	0
2	B	902	AGS	2	0
2	C	901	AGS	7	0
2	C	902	AGS	3	0
2	D	901	AGS	7	0
2	D	902	AGS	2	0
2	E	901	AGS	7	0
2	E	902	AGS	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	901	AGS	8	0
2	F	902	AGS	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.