



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:21 PM BST

PDB ID : 5FTL
EMDB ID: : EMD-3297
Title : Cryo-EM structure of human p97 bound to ATPgS (Conformation I)
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.; Hury, D.; Arkin, M.; Subramaniam, S.
Deposited on : 2016-01-14
Resolution : 3.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

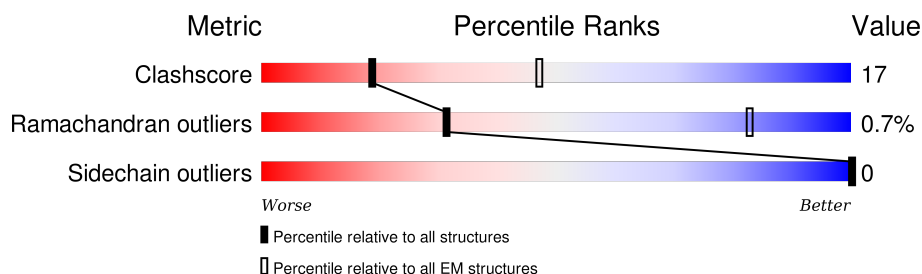
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	59% 30% 10%
1	B	806	59% 30% 10%
1	C	806	60% 29% 10%
1	D	806	59% 30% 10%
1	E	806	59% 30% 10%
1	F	806	59% 30% 10%

2 Entry composition [i](#)

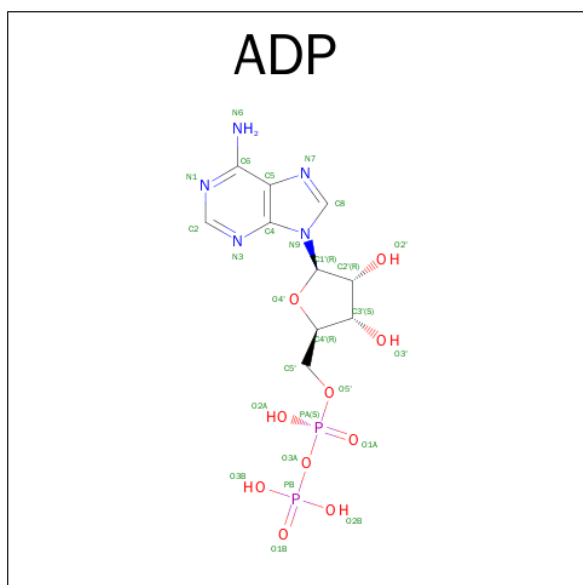
There are 2 unique types of molecules in this entry. The entry contains 34278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	B	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	C	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	D	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	E	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		
1	F	723	Total	C	N	O	S	0	0
			5659	3561	996	1072	30		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

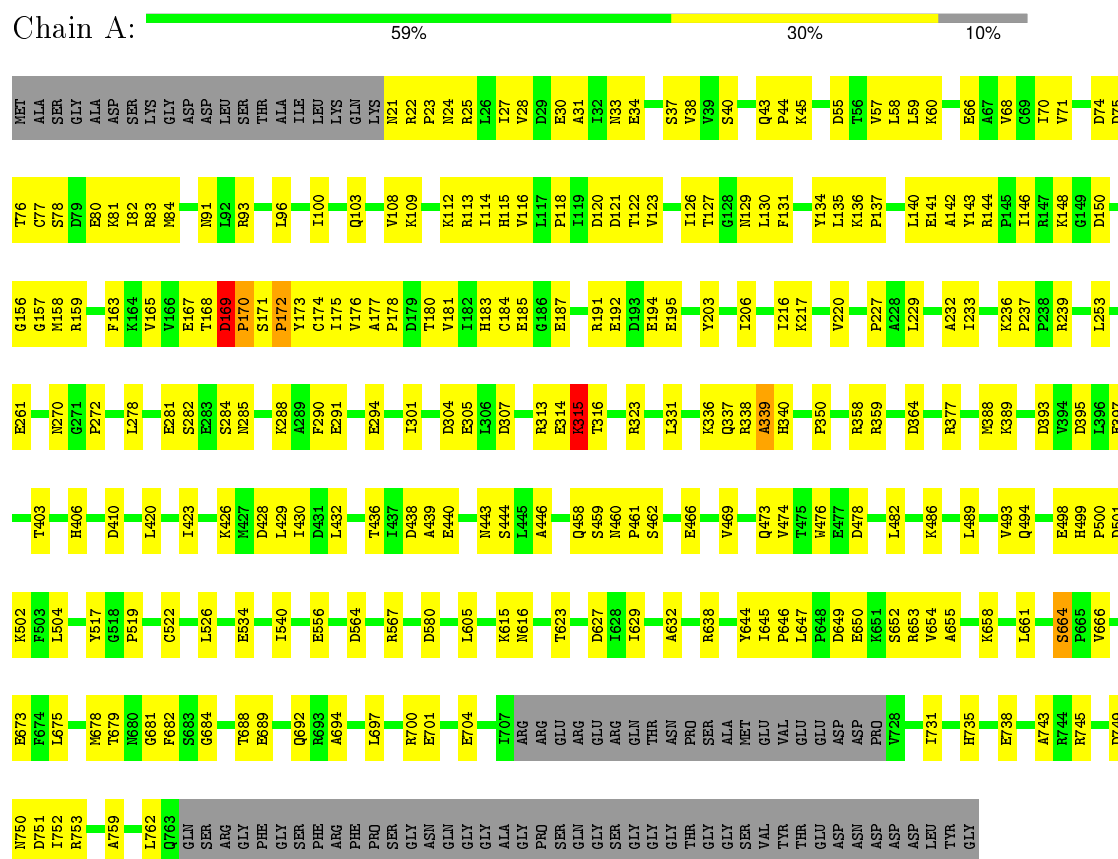


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 54	C 20	N 10	O 20	P 4	0
2	A	1	Total 54	C 20	N 10	O 20	P 4	0
2	B	1	Total 54	C 20	N 10	O 20	P 4	0
2	B	1	Total 54	C 20	N 10	O 20	P 4	0
2	C	1	Total 54	C 20	N 10	O 20	P 4	0
2	C	1	Total 54	C 20	N 10	O 20	P 4	0
2	D	1	Total 54	C 20	N 10	O 20	P 4	0
2	D	1	Total 54	C 20	N 10	O 20	P 4	0
2	E	1	Total 54	C 20	N 10	O 20	P 4	0
2	E	1	Total 54	C 20	N 10	O 20	P 4	0
2	F	1	Total 54	C 20	N 10	O 20	P 4	0
2	F	1	Total 54	C 20	N 10	O 20	P 4	0

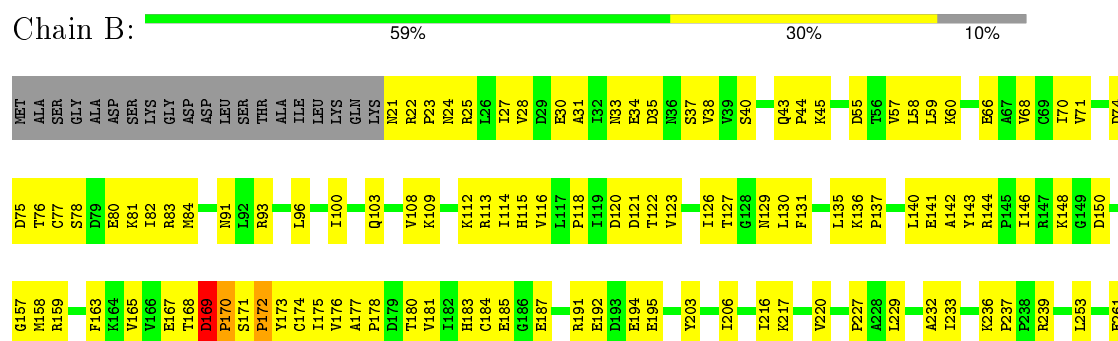
3 Residue-property plots

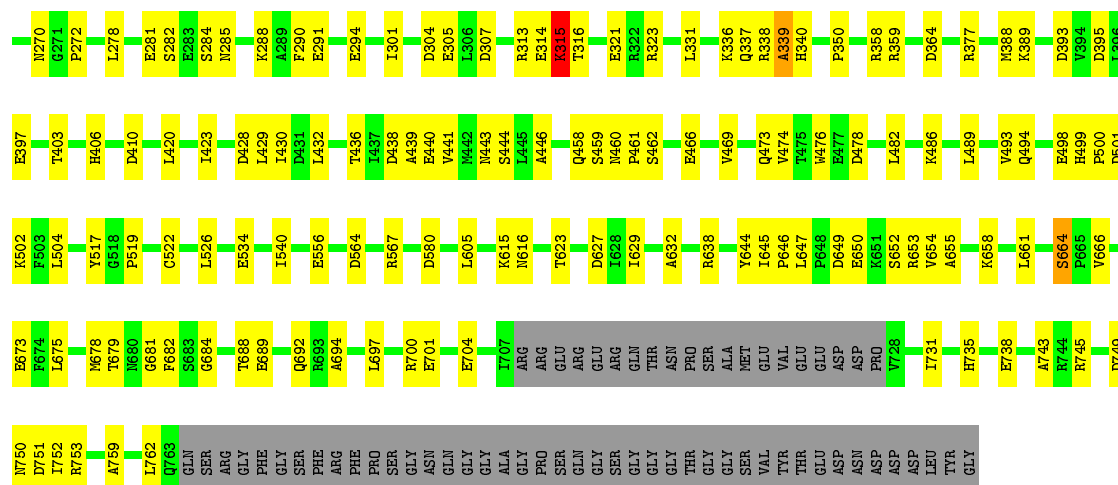
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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



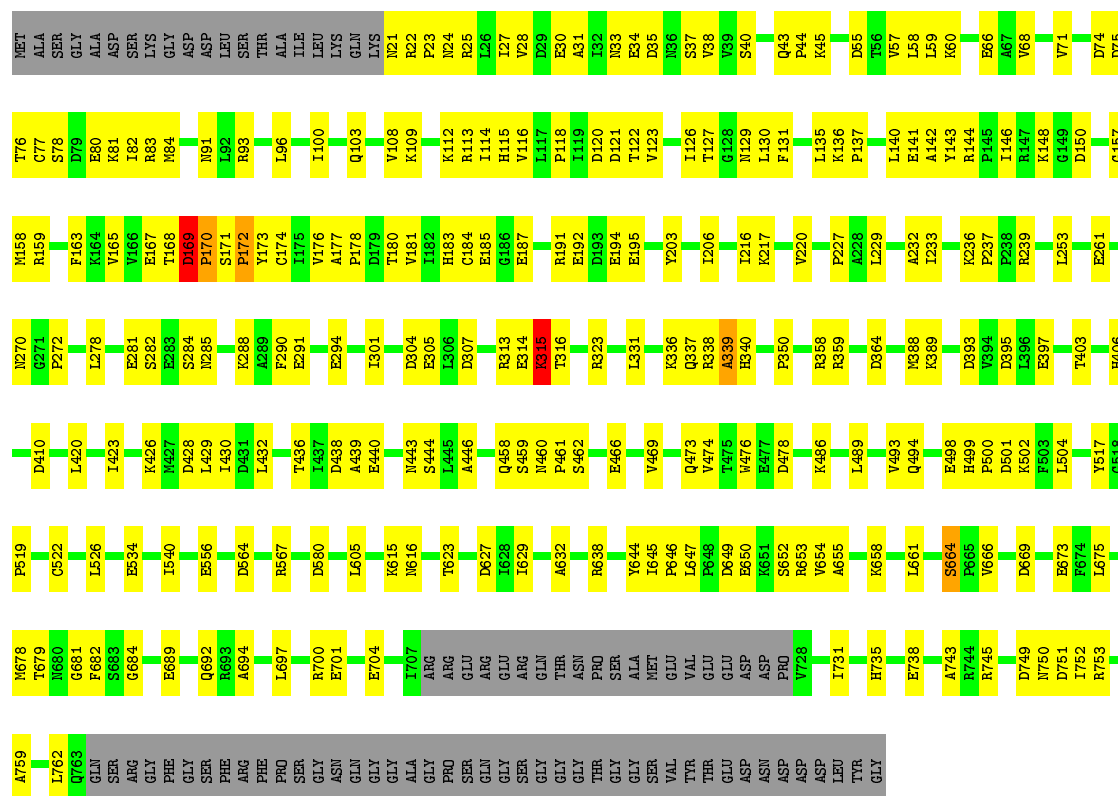
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE





• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

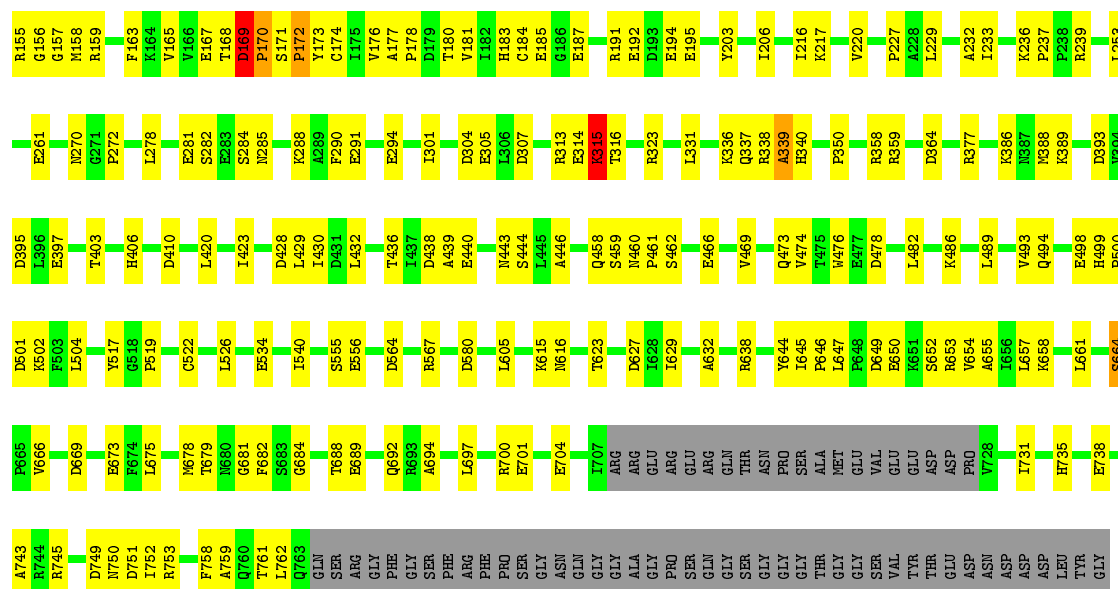
Chain C: 60% 29% 10%



• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

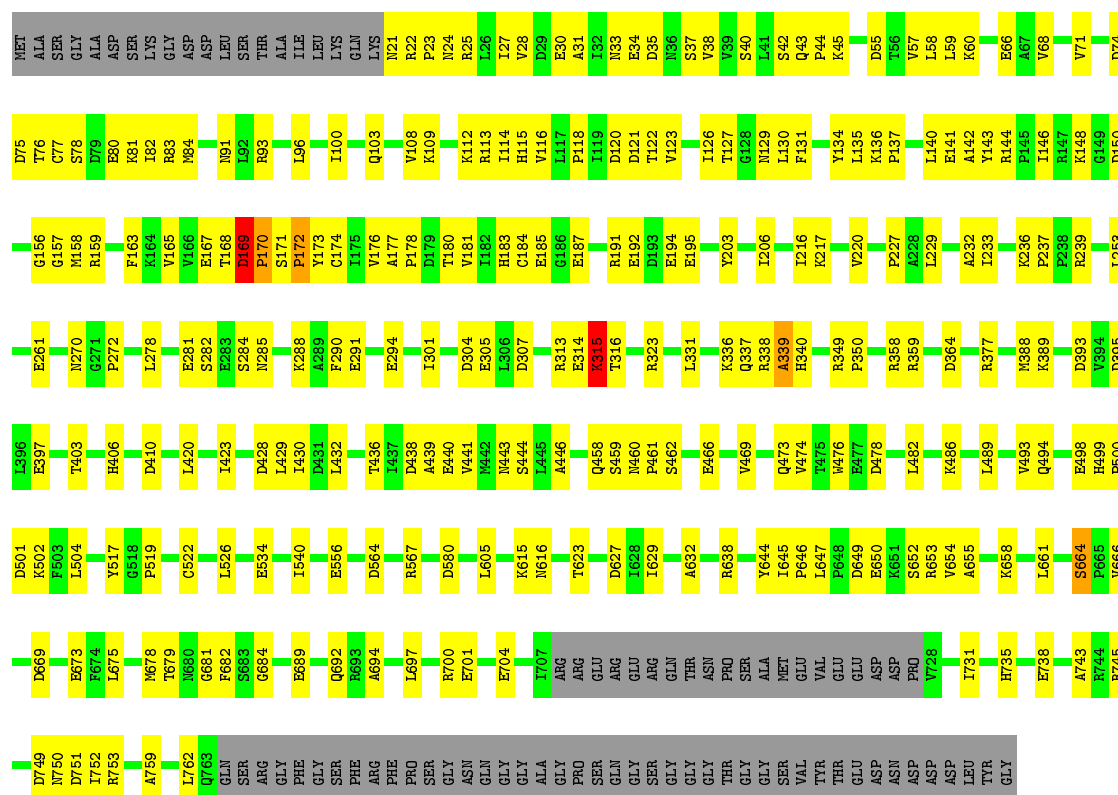
Chain D: 59% 30% 10%





• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain E: 59% 30% 10%



• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain F: 59% 30% 10%



S	A743	S664	E498	D393	E261	G156	T76
	R744	V666	P500	V394	N270	M158	C77
	R745		D501	D395	G271	R159	S78
		D669	K502	L396	P272		D79
	D749		F503	E397		F163	E80
	R750	E673	L504	N401	L278	K164	K81
	D751	F674	Y517	E402	E281	V165	R82
	I752	L675	G518	T403	S282	R83	R83
	R753		P519	H406	E283	E167	M84
	A759	K678	C522	H406	S284	T168	N91
T		R680		D410	N285	D169	L92
	I762	F682	L526	L420	K288	P170	R93
	GLN	S683	E534	L423	E289	S171	
	SER	G684			F290	P172	L96
	ARG		I540	D428	E291	Y173	I100
		T688	E556	L429		A177	
	PHE	E689	D564	I430	E294	P178	Q103
	GLY		R567	D431	I301	D179	V108
	SER	Q692	D680	L432	D304	T180	K109
	PHE	S693			E305	V181	
C	A694	A694	R57	T436	D307	H181	K112
		L697	D680	D438		H182	R113
	R700		L605	A439	A310	C184	I114
	ASN	E701		A440		E185	H115
	GLN		K615			G186	V116
	GLY	E704	N616	N443	R313	E187	I117
	GLY			S444	E314		P118
	ALA	I707	T623	L445	T316	D191	I119
	GLY	ARG		A446		E192	D120
	PRO	ARG	D627		E321	D193	T121
G	GLU	GLN	I628	Q458	R322	E194	V123
	GLN	ARG	I629	S459	R323	Y203	I126
	GLY	GLU	S460	N460	I324	G128	T127
	GLY	ARG	A632	P461	V325	I206	N129
	GLY	GLN		S462		L130	L130
	THR	THR	R638		L331	I216	F131
	ASN	ASN		E466		K217	
	PRO	PRO	Y644		R336		Y134
	GLY	GLY	I645	V469	Q337	V220	L135
	GLY	GLY	P646		R338		K136
V	VAL	GLU	L647	Q473	A339	P227	P137
	THR	VAL	F648	V474	H340	E228	
	THR	THR	D649	T475		I229	L140
	GLU	GLU	B650	N476	P350	A232	A141
	GLU	GLU	F651	E477		I233	A142
	ASP	ASP	S652	D478	R358		Y143
	ASN	ASN	R653		R359		R144
	ASP	PRO	V654	K486	D364	K236	F145
	ASP		A655		R377	P237	I146
	LEU	ASP	I731	L489		P238	I147
L	THR		K658		R239	K148	
	THR	H735		V493		L253	F149
	GLY			Q494	K388		D150
		E738		V380			

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	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	105000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

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: 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 >2	RMSZ	# Z >2
1	A	0.47	0/5751	0.59	1/7767 (0.0%)
1	B	0.47	0/5751	0.59	1/7767 (0.0%)
1	C	0.47	0/5751	0.59	1/7767 (0.0%)
1	D	0.47	0/5751	0.59	1/7767 (0.0%)
1	E	0.47	0/5751	0.59	1/7767 (0.0%)
1	F	0.47	0/5751	0.59	1/7767 (0.0%)
All	All	0.47	0/34506	0.59	6/46602 (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	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	4
All	All	0	24

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	664	SER	C-N-CD	5.22	139.37	128.40
1	A	664	SER	C-N-CD	5.21	139.33	128.40
1	B	664	SER	C-N-CD	5.20	139.32	128.40
1	C	664	SER	C-N-CD	5.20	139.31	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	664	SER	C-N-CD	5.19	139.29	128.40
1	E	664	SER	C-N-CD	5.19	139.29	128.40

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ASP	Peptide
1	A	172	PRO	Peptide
1	A	23	PRO	Peptide
1	A	315	LYS	Peptide
1	B	169	ASP	Peptide
1	B	172	PRO	Peptide
1	B	23	PRO	Peptide
1	B	315	LYS	Peptide
1	C	169	ASP	Peptide
1	C	172	PRO	Peptide
1	C	23	PRO	Peptide
1	C	315	LYS	Peptide
1	D	169	ASP	Peptide
1	D	172	PRO	Peptide
1	D	23	PRO	Peptide
1	D	315	LYS	Peptide
1	E	169	ASP	Peptide
1	E	172	PRO	Peptide
1	E	23	PRO	Peptide
1	E	315	LYS	Peptide
1	F	169	ASP	Peptide
1	F	172	PRO	Peptide
1	F	23	PRO	Peptide
1	F	315	LYS	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	5659	0	5731	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5659	0	5731	200	0
1	C	5659	0	5731	195	0
1	D	5659	0	5731	201	0
1	E	5659	0	5731	199	0
1	F	5659	0	5731	199	0
2	A	54	0	24	3	0
2	B	54	0	24	3	0
2	C	54	0	24	3	0
2	D	54	0	24	3	0
2	E	54	0	24	3	0
2	F	54	0	24	3	0
All	All	34278	0	34530	1163	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 17.

All (1163) 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:C:294:GLU:OE2	1:C:338:ARG:HG3	1.53	1.08
1:A:294:GLU:OE2	1:A:338:ARG:HG3	1.53	1.07
1:E:294:GLU:OE2	1:E:338:ARG:HG3	1.53	1.07
1:D:294:GLU:OE2	1:D:338:ARG:HG3	1.53	1.06
1:F:294:GLU:OE2	1:F:338:ARG:HG3	1.53	1.06
1:B:294:GLU:OE2	1:B:338:ARG:HG3	1.53	1.06
1:B:294:GLU:CD	1:B:338:ARG:HG3	1.81	1.01
1:E:294:GLU:CD	1:E:338:ARG:HG3	1.81	1.01
1:F:294:GLU:CD	1:F:338:ARG:HG3	1.81	1.01
1:C:294:GLU:CD	1:C:338:ARG:HG3	1.81	1.00
1:A:294:GLU:CD	1:A:338:ARG:HG3	1.81	1.00
1:D:294:GLU:CD	1:D:338:ARG:HG3	1.81	1.00
1:F:127:THR:HB	1:F:438:ASP:HA	1.56	0.88
1:E:127:THR:HB	1:E:438:ASP:HA	1.56	0.87
1:B:127:THR:HB	1:B:438:ASP:HA	1.56	0.87
1:C:127:THR:HB	1:C:438:ASP:HA	1.56	0.87
1:A:127:THR:HB	1:A:438:ASP:HA	1.56	0.87
1:D:127:THR:HB	1:D:438:ASP:HA	1.56	0.86
1:F:701:GLU:HA	1:F:704:GLU:HB3	1.68	0.76
1:A:701:GLU:HA	1:A:704:GLU:HB3	1.68	0.76
1:B:701:GLU:HA	1:B:704:GLU:HB3	1.68	0.75
1:E:701:GLU:HA	1:E:704:GLU:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:701:GLU:HA	1:C:704:GLU:HB3	1.68	0.75
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.69	0.74
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.69	0.74
1:D:701:GLU:HA	1:D:704:GLU:HB3	1.68	0.74
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.69	0.74
1:E:294:GLU:OE1	1:E:338:ARG:NE	2.21	0.73
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.69	0.73
1:F:294:GLU:OE1	1:F:338:ARG:NE	2.21	0.73
1:E:519:PRO:HG3	1:E:647:LEU:HD12	1.71	0.73
1:E:157:GLY:HA2	1:E:443:ASN:HA	1.71	0.73
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.69	0.73
1:D:519:PRO:HG3	1:D:647:LEU:HD12	1.71	0.73
1:B:519:PRO:HG3	1:B:647:LEU:HD12	1.71	0.73
1:B:157:GLY:HA2	1:B:443:ASN:HA	1.71	0.73
1:F:519:PRO:HG3	1:F:647:LEU:HD12	1.71	0.73
1:F:439:ALA:O	1:F:443:ASN:ND2	2.22	0.72
1:A:294:GLU:OE1	1:A:338:ARG:NE	2.21	0.72
1:D:294:GLU:OE1	1:D:338:ARG:NE	2.21	0.72
1:E:439:ALA:O	1:E:443:ASN:ND2	2.22	0.72
1:C:294:GLU:OE1	1:C:338:ARG:NE	2.21	0.72
1:C:439:ALA:O	1:C:443:ASN:ND2	2.22	0.72
1:F:157:GLY:HA2	1:F:443:ASN:HA	1.71	0.72
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.69	0.72
1:A:439:ALA:O	1:A:443:ASN:ND2	2.22	0.72
1:B:439:ALA:O	1:B:443:ASN:ND2	2.22	0.72
1:A:157:GLY:HA2	1:A:443:ASN:HA	1.71	0.72
1:D:157:GLY:HA2	1:D:443:ASN:HA	1.71	0.72
1:C:519:PRO:HG3	1:C:647:LEU:HD12	1.71	0.72
1:D:439:ALA:O	1:D:443:ASN:ND2	2.22	0.72
1:E:337:GLN:HA	1:E:337:GLN:NE2	2.05	0.71
1:B:294:GLU:OE1	1:B:338:ARG:NE	2.21	0.71
1:C:157:GLY:HA2	1:C:443:ASN:HA	1.71	0.71
1:D:337:GLN:HA	1:D:337:GLN:NE2	2.05	0.71
1:A:519:PRO:HG3	1:A:647:LEU:HD12	1.71	0.71
1:F:337:GLN:HA	1:F:337:GLN:NE2	2.05	0.71
1:B:337:GLN:HA	1:B:337:GLN:NE2	2.05	0.71
1:A:294:GLU:CD	1:A:338:ARG:CG	2.59	0.71
1:A:337:GLN:HA	1:A:337:GLN:NE2	2.05	0.70
1:D:294:GLU:CD	1:D:338:ARG:CG	2.59	0.70
1:C:337:GLN:NE2	1:C:337:GLN:HA	2.05	0.70
1:A:294:GLU:CD	1:A:338:ARG:HE	1.95	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLU:CD	1:B:338:ARG:HE	1.95	0.70
1:D:142:ALA:HB1	1:D:144:ARG:HG3	1.74	0.70
1:E:294:GLU:CD	1:E:338:ARG:CG	2.59	0.69
1:C:294:GLU:CD	1:C:338:ARG:HE	1.95	0.69
1:F:294:GLU:CD	1:F:338:ARG:CG	2.59	0.69
1:B:142:ALA:HB1	1:B:144:ARG:HG3	1.74	0.69
1:D:77:CYS:SG	1:D:78:SER:N	2.66	0.69
1:E:142:ALA:HB1	1:E:144:ARG:HG3	1.74	0.69
1:C:294:GLU:CD	1:C:338:ARG:CG	2.59	0.69
1:D:294:GLU:CD	1:D:338:ARG:HE	1.95	0.69
1:E:294:GLU:CD	1:E:338:ARG:HE	1.94	0.69
1:F:294:GLU:CD	1:F:338:ARG:HE	1.95	0.69
1:C:142:ALA:HB1	1:C:144:ARG:HG3	1.74	0.69
1:C:77:CYS:SG	1:C:78:SER:N	2.66	0.69
1:E:77:CYS:SG	1:E:78:SER:N	2.66	0.69
1:B:443:ASN:OD1	1:B:444:SER:N	2.26	0.69
1:D:443:ASN:OD1	1:D:444:SER:N	2.26	0.69
1:C:443:ASN:OD1	1:C:444:SER:N	2.26	0.68
1:F:77:CYS:SG	1:F:78:SER:N	2.66	0.68
1:B:77:CYS:SG	1:B:78:SER:N	2.66	0.68
1:E:443:ASN:OD1	1:E:444:SER:N	2.26	0.68
1:A:77:CYS:SG	1:A:78:SER:N	2.66	0.68
1:A:142:ALA:HB1	1:A:144:ARG:HG3	1.74	0.68
1:B:294:GLU:CD	1:B:338:ARG:CG	2.59	0.68
1:F:443:ASN:OD1	1:F:444:SER:N	2.26	0.68
1:A:443:ASN:OD1	1:A:444:SER:N	2.26	0.68
1:F:476:TRP:NE1	1:F:534:GLU:OE1	2.26	0.68
1:D:281:GLU:O	1:D:285:ASN:ND2	2.28	0.67
1:C:281:GLU:O	1:C:285:ASN:ND2	2.28	0.67
1:B:59:LEU:HB3	1:B:100:ILE:HD11	1.76	0.67
1:F:281:GLU:O	1:F:285:ASN:ND2	2.28	0.67
1:B:281:GLU:O	1:B:285:ASN:ND2	2.28	0.67
1:A:281:GLU:O	1:A:285:ASN:ND2	2.28	0.67
1:C:59:LEU:HB3	1:C:100:ILE:HD11	1.76	0.67
1:F:142:ALA:HB1	1:F:144:ARG:HG3	1.74	0.67
1:E:59:LEU:HB3	1:E:100:ILE:HD11	1.76	0.67
1:C:476:TRP:NE1	1:C:534:GLU:OE1	2.26	0.67
1:A:476:TRP:NE1	1:A:534:GLU:OE1	2.26	0.66
1:E:694:ALA:HB1	1:E:731:ILE:HD11	1.78	0.66
1:F:59:LEU:HB3	1:F:100:ILE:HD11	1.76	0.66
1:E:281:GLU:O	1:E:285:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:ND2	1:A:150:ASP:OD1	2.29	0.66
1:E:316:THR:HG21	1:F:315:LYS:HE2	1.78	0.66
1:C:430:ILE:HG22	1:C:432:LEU:HG	1.78	0.66
1:E:430:ILE:HG22	1:E:432:LEU:HG	1.78	0.66
1:B:430:ILE:HG22	1:B:432:LEU:HG	1.78	0.66
1:A:694:ALA:HB1	1:A:731:ILE:HD11	1.77	0.66
1:D:91:ASN:ND2	1:D:150:ASP:OD1	2.29	0.66
1:A:59:LEU:HB3	1:A:100:ILE:HD11	1.76	0.66
1:E:91:ASN:ND2	1:E:150:ASP:OD1	2.29	0.66
1:A:316:THR:HG21	1:B:315:LYS:HE2	1.78	0.66
1:F:649:ASP:OD1	1:F:650:GLU:N	2.29	0.66
1:B:694:ALA:HB1	1:B:731:ILE:HD11	1.77	0.66
1:C:694:ALA:HB1	1:C:731:ILE:HD11	1.78	0.66
1:A:430:ILE:HG22	1:A:432:LEU:HG	1.78	0.66
1:B:476:TRP:NE1	1:B:534:GLU:OE1	2.26	0.66
1:D:430:ILE:HG22	1:D:432:LEU:HG	1.78	0.66
1:B:91:ASN:ND2	1:B:150:ASP:OD1	2.29	0.65
1:D:476:TRP:NE1	1:D:534:GLU:OE1	2.26	0.65
1:F:430:ILE:HG22	1:F:432:LEU:HG	1.78	0.65
1:B:316:THR:HG21	1:C:315:LYS:HE2	1.78	0.65
1:F:313:ARG:HG3	1:F:314:GLU:H	1.61	0.65
1:D:694:ALA:HB1	1:D:731:ILE:HD11	1.77	0.65
1:D:59:LEU:HB3	1:D:100:ILE:HD11	1.76	0.65
1:A:313:ARG:HG3	1:A:314:GLU:H	1.62	0.65
1:A:232:ALA:O	1:B:159:ARG:NH2	2.30	0.65
1:B:232:ALA:O	1:C:159:ARG:NH2	2.30	0.65
1:A:315:LYS:HE2	1:F:316:THR:HG21	1.79	0.65
1:B:313:ARG:HG3	1:B:314:GLU:H	1.61	0.65
1:A:143:TYR:HE1	1:A:178:PRO:HD3	1.62	0.65
1:E:313:ARG:HG3	1:E:314:GLU:H	1.61	0.65
1:F:143:TYR:HE1	1:F:178:PRO:HD3	1.62	0.65
1:C:313:ARG:HG3	1:C:314:GLU:H	1.61	0.65
1:D:313:ARG:HG3	1:D:314:GLU:H	1.62	0.65
1:A:159:ARG:NH2	1:F:232:ALA:O	2.30	0.65
1:D:316:THR:HG21	1:E:315:LYS:HE2	1.79	0.65
1:F:694:ALA:HB1	1:F:731:ILE:HD11	1.77	0.65
1:F:91:ASN:ND2	1:F:150:ASP:OD1	2.29	0.65
1:A:649:ASP:OD1	1:A:650:GLU:N	2.29	0.64
1:D:338:ARG:O	1:D:338:ARG:HG2	1.98	0.64
1:A:21:ASN:O	1:A:25:ARG:NH2	2.31	0.64
1:B:21:ASN:O	1:B:25:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ASN:ND2	1:C:150:ASP:OD1	2.29	0.64
1:C:21:ASN:O	1:C:25:ARG:NH2	2.31	0.64
1:C:316:THR:HG21	1:D:315:LYS:HE2	1.79	0.64
1:E:232:ALA:O	1:F:159:ARG:NH2	2.30	0.64
1:C:338:ARG:O	1:C:338:ARG:HG2	1.97	0.64
1:A:338:ARG:HG2	1:A:338:ARG:O	1.97	0.64
1:D:232:ALA:O	1:E:159:ARG:NH2	2.30	0.64
1:B:143:TYR:HE1	1:B:178:PRO:HD3	1.62	0.64
1:F:338:ARG:O	1:F:338:ARG:HG2	1.97	0.64
1:F:21:ASN:O	1:F:25:ARG:NH2	2.31	0.64
1:E:338:ARG:HG2	1:E:338:ARG:O	1.97	0.64
1:E:143:TYR:HE1	1:E:178:PRO:HD3	1.62	0.64
1:A:440:GLU:HA	1:A:443:ASN:HD21	1.63	0.63
1:E:476:TRP:NE1	1:E:534:GLU:OE1	2.26	0.63
1:B:440:GLU:HA	1:B:443:ASN:HD21	1.64	0.63
1:C:143:TYR:HE1	1:C:178:PRO:HD3	1.61	0.63
1:B:338:ARG:O	1:B:338:ARG:HG2	1.97	0.63
1:D:21:ASN:O	1:D:25:ARG:NH2	2.31	0.63
1:A:749:ASP:OD1	1:A:750:ASN:N	2.32	0.63
1:F:440:GLU:HA	1:F:443:ASN:HD21	1.64	0.63
1:D:749:ASP:OD1	1:D:750:ASN:N	2.32	0.63
1:E:440:GLU:HA	1:E:443:ASN:HD21	1.63	0.63
1:D:143:TYR:HE1	1:D:178:PRO:HD3	1.62	0.63
1:E:350:PRO:O	1:E:358:ARG:NH2	2.32	0.63
1:E:647:LEU:HD13	1:E:752:ILE:HD13	1.80	0.63
1:F:116:VAL:HG12	1:F:165:VAL:HA	1.81	0.63
1:C:440:GLU:HA	1:C:443:ASN:HD21	1.63	0.63
1:E:649:ASP:OD1	1:E:650:GLU:N	2.29	0.63
1:D:440:GLU:HA	1:D:443:ASN:HD21	1.63	0.63
1:F:45:LYS:NZ	1:F:77:CYS:SG	2.72	0.63
1:C:647:LEU:HD13	1:C:752:ILE:HD13	1.81	0.62
1:C:45:LYS:NZ	1:C:77:CYS:SG	2.72	0.62
1:F:350:PRO:O	1:F:358:ARG:NH2	2.32	0.62
1:B:749:ASP:OD1	1:B:750:ASN:N	2.32	0.62
1:B:45:LYS:NZ	1:B:77:CYS:SG	2.72	0.62
1:B:116:VAL:HG12	1:B:165:VAL:HA	1.81	0.62
1:E:116:VAL:HG12	1:E:165:VAL:HA	1.81	0.62
1:B:350:PRO:O	1:B:358:ARG:NH2	2.32	0.62
1:A:116:VAL:HG12	1:A:165:VAL:HA	1.81	0.62
1:A:337:GLN:O	1:A:338:ARG:HB3	1.99	0.62
1:F:647:LEU:HD13	1:F:752:ILE:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LYS:NZ	1:D:77:CYS:SG	2.72	0.62
1:A:45:LYS:NZ	1:A:77:CYS:SG	2.72	0.62
1:E:749:ASP:OD1	1:E:750:ASN:N	2.32	0.62
1:F:749:ASP:OD1	1:F:750:ASN:N	2.32	0.62
1:C:232:ALA:O	1:D:159:ARG:NH2	2.31	0.62
1:D:350:PRO:O	1:D:358:ARG:NH2	2.32	0.62
1:E:21:ASN:O	1:E:25:ARG:NH2	2.31	0.62
1:C:749:ASP:OD1	1:C:750:ASN:N	2.32	0.62
1:C:350:PRO:O	1:C:358:ARG:NH2	2.32	0.62
1:C:649:ASP:OD1	1:C:650:GLU:N	2.29	0.62
1:A:350:PRO:O	1:A:358:ARG:NH2	2.32	0.62
1:D:116:VAL:HG12	1:D:165:VAL:HA	1.81	0.62
1:B:647:LEU:HD13	1:B:752:ILE:HD13	1.81	0.62
1:A:406:HIS:CE1	1:A:461:PRO:HA	2.35	0.62
1:E:337:GLN:HA	1:E:337:GLN:HE21	1.65	0.62
1:D:337:GLN:O	1:D:338:ARG:HB3	1.99	0.62
1:D:647:LEU:HD13	1:D:752:ILE:HD13	1.80	0.62
1:C:116:VAL:HG12	1:C:165:VAL:HA	1.81	0.62
1:B:406:HIS:CE1	1:B:461:PRO:HA	2.35	0.62
1:F:337:GLN:HA	1:F:337:GLN:HE21	1.65	0.61
1:E:45:LYS:NZ	1:E:77:CYS:SG	2.72	0.61
1:E:337:GLN:O	1:E:338:ARG:HB3	1.99	0.61
1:D:649:ASP:OD1	1:D:650:GLU:N	2.29	0.61
1:F:406:HIS:CE1	1:F:461:PRO:HA	2.35	0.61
1:C:337:GLN:O	1:C:338:ARG:HB3	1.99	0.61
1:B:337:GLN:O	1:B:338:ARG:HB3	1.99	0.61
1:B:649:ASP:OD1	1:B:650:GLU:N	2.29	0.61
1:D:337:GLN:HA	1:D:337:GLN:HE21	1.65	0.61
1:A:337:GLN:HA	1:A:337:GLN:HE21	1.65	0.61
1:A:647:LEU:HD13	1:A:752:ILE:HD13	1.81	0.61
1:F:337:GLN:O	1:F:338:ARG:HB3	1.99	0.60
1:C:406:HIS:CE1	1:C:461:PRO:HA	2.35	0.60
1:E:501:ASP:OD1	1:E:502:LYS:N	2.35	0.60
1:C:337:GLN:HE21	1:C:337:GLN:HA	1.65	0.60
1:A:501:ASP:OD1	1:A:502:LYS:N	2.35	0.60
1:A:112:LYS:N	1:A:169:ASP:OD2	2.31	0.60
1:E:673:GLU:N	1:E:673:GLU:OE1	2.34	0.60
1:B:337:GLN:HA	1:B:337:GLN:HE21	1.65	0.60
1:E:406:HIS:CE1	1:E:461:PRO:HA	2.35	0.60
1:D:406:HIS:CE1	1:D:461:PRO:HA	2.35	0.60
1:F:673:GLU:OE1	1:F:673:GLU:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:501:ASP:OD1	1:F:502:LYS:N	2.35	0.59
1:C:501:ASP:OD1	1:C:502:LYS:N	2.35	0.59
1:B:130:LEU:HD21	1:B:163:PHE:CE1	2.38	0.59
1:A:130:LEU:HD21	1:A:163:PHE:CE1	2.38	0.59
1:E:130:LEU:HD21	1:E:163:PHE:CE1	2.38	0.59
1:D:130:LEU:HD21	1:D:163:PHE:CE1	2.38	0.59
1:D:112:LYS:N	1:D:169:ASP:OD2	2.31	0.59
1:B:389:LYS:HZ2	1:B:446:ALA:HB2	1.68	0.59
1:C:130:LEU:HD21	1:C:163:PHE:CE1	2.38	0.59
1:F:130:LEU:HD21	1:F:163:PHE:CE1	2.38	0.59
1:B:458:GLN:O	1:B:461:PRO:HD2	2.03	0.59
1:F:458:GLN:O	1:F:461:PRO:HD2	2.03	0.59
1:D:458:GLN:O	1:D:461:PRO:HD2	2.03	0.58
1:D:501:ASP:OD1	1:D:502:LYS:N	2.35	0.58
1:C:458:GLN:O	1:C:461:PRO:HD2	2.03	0.58
1:E:458:GLN:O	1:E:461:PRO:HD2	2.03	0.58
1:B:501:ASP:OD1	1:B:502:LYS:N	2.35	0.58
1:F:112:LYS:N	1:F:169:ASP:OD2	2.31	0.58
1:A:750:ASN:OD1	1:A:751:ASP:N	2.37	0.58
1:A:108:VAL:HG22	1:A:109:LYS:H	1.69	0.58
1:F:750:ASN:OD1	1:F:751:ASP:N	2.37	0.58
1:B:108:VAL:HG22	1:B:109:LYS:H	1.69	0.58
1:F:476:TRP:HE1	1:F:534:GLU:CD	2.07	0.57
1:A:476:TRP:HE1	1:A:534:GLU:CD	2.07	0.57
1:B:750:ASN:OD1	1:B:751:ASP:N	2.37	0.57
1:E:112:LYS:N	1:E:169:ASP:OD2	2.31	0.57
1:C:750:ASN:OD1	1:C:751:ASP:N	2.37	0.57
1:A:458:GLN:O	1:A:461:PRO:HD2	2.03	0.57
1:A:673:GLU:OE1	1:A:673:GLU:N	2.34	0.57
1:C:476:TRP:HE1	1:C:534:GLU:CD	2.07	0.57
1:A:143:TYR:HA	1:A:176:VAL:O	2.05	0.57
1:C:108:VAL:HG22	1:C:109:LYS:H	1.69	0.57
1:F:108:VAL:HG22	1:F:109:LYS:H	1.69	0.57
1:C:564:ASP:OD1	1:C:567:ARG:NH1	2.37	0.57
1:B:143:TYR:HA	1:B:176:VAL:O	2.05	0.57
1:D:143:TYR:HA	1:D:176:VAL:O	2.05	0.57
1:E:750:ASN:OD1	1:E:751:ASP:N	2.37	0.57
1:C:143:TYR:HA	1:C:176:VAL:O	2.05	0.57
1:D:750:ASN:OD1	1:D:751:ASP:N	2.37	0.57
1:B:203:TYR:CZ	1:B:261:GLU:HG2	2.40	0.57
1:A:294:GLU:HG3	1:A:338:ARG:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:615:LYS:HG2	1:F:616:ASN:H	1.70	0.57
1:A:564:ASP:OD1	1:A:567:ARG:NH1	2.37	0.57
1:F:294:GLU:HG3	1:F:338:ARG:HG2	1.87	0.57
1:D:476:TRP:HE1	1:D:534:GLU:CD	2.07	0.57
1:E:294:GLU:HG3	1:E:338:ARG:HG2	1.87	0.56
1:B:476:TRP:HE1	1:B:534:GLU:CD	2.07	0.56
1:B:615:LYS:HG2	1:B:616:ASN:H	1.70	0.56
1:C:203:TYR:CZ	1:C:261:GLU:HG2	2.40	0.56
1:D:615:LYS:HG2	1:D:616:ASN:H	1.70	0.56
1:D:108:VAL:HG22	1:D:109:LYS:H	1.69	0.56
1:F:143:TYR:HA	1:F:176:VAL:O	2.05	0.56
1:E:476:TRP:HE1	1:E:534:GLU:CD	2.07	0.56
1:B:146:ILE:HG23	1:B:165:VAL:HG21	1.88	0.56
1:A:146:ILE:HG23	1:A:165:VAL:HG21	1.88	0.56
1:C:146:ILE:HG23	1:C:165:VAL:HG21	1.87	0.56
1:A:203:TYR:CZ	1:A:261:GLU:HG2	2.40	0.56
1:B:556:GLU:N	1:B:556:GLU:OE1	2.38	0.56
1:C:364:ASP:OD1	1:C:364:ASP:N	2.35	0.56
1:F:564:ASP:OD1	1:F:567:ARG:NH1	2.37	0.56
1:B:112:LYS:N	1:B:169:ASP:OD2	2.31	0.56
1:E:108:VAL:HG22	1:E:109:LYS:H	1.69	0.56
1:B:75:ASP:OD1	1:B:76:THR:N	2.37	0.56
1:C:294:GLU:HG3	1:C:338:ARG:HG2	1.87	0.56
1:D:203:TYR:CZ	1:D:261:GLU:HG2	2.40	0.56
1:F:146:ILE:HG23	1:F:165:VAL:HG21	1.88	0.56
1:E:564:ASP:OD1	1:E:567:ARG:NH1	2.37	0.56
1:E:203:TYR:CZ	1:E:261:GLU:HG2	2.40	0.56
1:C:615:LYS:HG2	1:C:616:ASN:H	1.70	0.56
1:B:129:ASN:OD1	1:B:131:PHE:N	2.39	0.56
1:F:129:ASN:OD1	1:F:131:PHE:N	2.39	0.56
1:E:143:TYR:HA	1:E:176:VAL:O	2.05	0.56
1:A:170:PRO:O	1:A:173:TYR:HB3	2.06	0.56
1:E:129:ASN:OD1	1:E:131:PHE:N	2.39	0.56
1:C:556:GLU:N	1:C:556:GLU:OE1	2.38	0.56
1:D:294:GLU:HG3	1:D:338:ARG:HG2	1.87	0.56
1:A:650:GLU:HG3	1:A:653:ARG:NH2	2.21	0.56
1:E:146:ILE:HG23	1:E:165:VAL:HG21	1.88	0.56
1:A:129:ASN:OD1	1:A:131:PHE:N	2.39	0.56
1:D:239:ARG:NH2	1:D:337:GLN:H	2.04	0.55
1:F:650:GLU:HG3	1:F:653:ARG:NH2	2.21	0.55
1:B:170:PRO:O	1:B:173:TYR:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:PRO:O	1:E:173:TYR:HB3	2.06	0.55
1:B:564:ASP:OD1	1:B:567:ARG:NH1	2.37	0.55
1:F:170:PRO:O	1:F:173:TYR:HB3	2.06	0.55
1:F:203:TYR:CZ	1:F:261:GLU:HG2	2.40	0.55
1:D:146:ILE:HG23	1:D:165:VAL:HG21	1.88	0.55
1:B:650:GLU:HG3	1:B:653:ARG:NH2	2.21	0.55
1:D:290:PHE:CD1	1:D:301:ILE:HD13	2.42	0.55
1:D:129:ASN:OD1	1:D:131:PHE:N	2.39	0.55
1:F:389:LYS:HZ2	1:F:446:ALA:HB2	1.70	0.55
1:E:290:PHE:CD1	1:E:301:ILE:HD13	2.42	0.55
1:B:294:GLU:HG3	1:B:338:ARG:HG2	1.87	0.55
1:C:650:GLU:HG3	1:C:653:ARG:NH2	2.21	0.55
1:E:615:LYS:HG2	1:E:616:ASN:H	1.70	0.55
1:B:673:GLU:OE1	1:B:673:GLU:N	2.34	0.55
1:A:239:ARG:NH2	1:A:337:GLN:H	2.04	0.55
1:E:359:ARG:HH12	1:F:305:GLU:CD	2.10	0.55
1:E:650:GLU:HG3	1:E:653:ARG:NH2	2.21	0.55
1:D:170:PRO:O	1:D:173:TYR:HB3	2.06	0.55
1:A:615:LYS:HG2	1:A:616:ASN:H	1.70	0.55
1:C:129:ASN:OD1	1:C:131:PHE:N	2.39	0.55
1:C:239:ARG:NH2	1:C:337:GLN:H	2.04	0.55
1:B:239:ARG:NH2	1:B:337:GLN:H	2.04	0.55
1:D:75:ASP:OD1	1:D:76:THR:N	2.37	0.55
1:A:290:PHE:CD1	1:A:301:ILE:HD13	2.42	0.55
1:B:364:ASP:N	1:B:364:ASP:OD1	2.35	0.55
1:C:290:PHE:CD1	1:C:301:ILE:HD13	2.42	0.55
1:E:389:LYS:HZ2	1:E:446:ALA:HB2	1.71	0.55
1:C:389:LYS:HZ2	1:C:446:ALA:HB2	1.72	0.54
1:A:305:GLU:CD	1:F:359:ARG:HH12	2.10	0.54
1:A:632:ALA:O	1:A:638:ARG:NH1	2.40	0.54
1:B:290:PHE:CD1	1:B:301:ILE:HD13	2.42	0.54
1:F:239:ARG:NH2	1:F:337:GLN:H	2.04	0.54
1:C:76:THR:OG1	1:C:83:ARG:NH1	2.39	0.54
1:C:170:PRO:O	1:C:173:TYR:HB3	2.06	0.54
1:D:556:GLU:OE1	1:D:556:GLU:N	2.38	0.54
1:D:650:GLU:HG3	1:D:653:ARG:NH2	2.21	0.54
1:E:632:ALA:O	1:E:638:ARG:NH1	2.40	0.54
1:E:498:GLU:OE1	1:E:499:HIS:NE2	2.41	0.54
1:E:112:LYS:HG2	1:E:113:ARG:HG3	1.90	0.54
1:D:498:GLU:OE1	1:D:499:HIS:NE2	2.41	0.54
1:A:359:ARG:HH12	1:B:305:GLU:CD	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:PHE:CD1	1:F:301:ILE:HD13	2.42	0.54
1:E:127:THR:OG1	1:E:436:THR:O	2.26	0.54
1:E:654:VAL:O	1:E:658:LYS:HG2	2.08	0.54
1:A:338:ARG:O	1:A:339:ALA:HB3	2.08	0.54
1:E:428:ASP:OD1	1:E:429:LEU:N	2.41	0.54
1:F:498:GLU:OE1	1:F:499:HIS:NE2	2.41	0.54
1:F:632:ALA:O	1:F:638:ARG:NH1	2.40	0.54
1:B:498:GLU:OE1	1:B:499:HIS:NE2	2.41	0.54
1:C:294:GLU:CD	1:C:338:ARG:NE	2.61	0.54
1:F:294:GLU:CD	1:F:338:ARG:NE	2.61	0.54
1:C:359:ARG:HH12	1:D:305:GLU:CD	2.11	0.54
1:E:239:ARG:NH2	1:E:337:GLN:H	2.04	0.54
1:E:76:THR:OG1	1:E:83:ARG:NH1	2.39	0.54
1:D:76:THR:OG1	1:D:83:ARG:NH1	2.39	0.54
1:F:428:ASP:OD1	1:F:429:LEU:N	2.41	0.54
1:D:564:ASP:OD1	1:D:567:ARG:NH1	2.37	0.54
1:A:498:GLU:OE1	1:A:499:HIS:NE2	2.41	0.54
1:C:338:ARG:O	1:C:339:ALA:HB3	2.08	0.54
1:F:112:LYS:HG2	1:F:113:ARG:HG3	1.90	0.54
1:F:654:VAL:O	1:F:658:LYS:HG2	2.08	0.54
1:C:112:LYS:N	1:C:169:ASP:OD2	2.31	0.54
1:B:654:VAL:O	1:B:658:LYS:HG2	2.08	0.53
1:D:389:LYS:HZ2	1:D:446:ALA:HB2	1.73	0.53
1:E:78:SER:OG	1:E:81:LYS:HG2	2.09	0.53
1:D:428:ASP:OD1	1:D:429:LEU:N	2.41	0.53
1:B:109:LYS:HD3	1:B:173:TYR:CE1	2.44	0.53
1:F:109:LYS:HD3	1:F:173:TYR:CE1	2.44	0.53
1:B:112:LYS:HG2	1:B:113:ARG:HG3	1.90	0.53
1:A:654:VAL:O	1:A:658:LYS:HG2	2.08	0.53
1:D:338:ARG:O	1:D:339:ALA:HB3	2.08	0.53
1:A:109:LYS:HD3	1:A:173:TYR:CE1	2.44	0.53
1:B:338:ARG:O	1:B:339:ALA:HB3	2.08	0.53
1:F:127:THR:OG1	1:F:436:THR:O	2.26	0.53
1:B:76:THR:OG1	1:B:83:ARG:NH1	2.39	0.53
1:B:282:SER:O	1:B:285:ASN:N	2.40	0.53
1:A:428:ASP:OD1	1:A:429:LEU:N	2.41	0.53
1:B:359:ARG:HH12	1:C:305:GLU:CD	2.10	0.53
1:D:127:THR:OG1	1:D:436:THR:O	2.26	0.53
1:D:78:SER:OG	1:D:81:LYS:HG2	2.09	0.53
1:A:282:SER:O	1:A:285:ASN:N	2.40	0.53
1:E:282:SER:O	1:E:285:ASN:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ASP:OD1	1:B:429:LEU:N	2.41	0.53
1:D:112:LYS:HG2	1:D:113:ARG:HG3	1.90	0.53
1:C:112:LYS:HG2	1:C:113:ARG:HG3	1.90	0.53
1:C:127:THR:OG1	1:C:436:THR:O	2.26	0.53
1:A:75:ASP:OD1	1:A:76:THR:N	2.37	0.53
1:F:78:SER:OG	1:F:81:LYS:HG2	2.09	0.53
1:C:498:GLU:OE1	1:C:499:HIS:NE2	2.41	0.53
1:E:233:ILE:HD11	1:F:158:MET:HB2	1.91	0.53
1:D:359:ARG:HH12	1:E:305:GLU:CD	2.11	0.53
1:D:294:GLU:CD	1:D:338:ARG:NE	2.61	0.53
1:F:177:ALA:O	1:F:180:THR:HG22	2.09	0.53
1:D:177:ALA:O	1:D:180:THR:HG22	2.09	0.53
1:D:526:LEU:HD11	2:D:900:ADP:H2'	1.91	0.53
1:D:673:GLU:N	1:D:673:GLU:OE1	2.34	0.53
1:F:338:ARG:O	1:F:339:ALA:HB3	2.08	0.53
1:C:109:LYS:HD3	1:C:173:TYR:CE1	2.44	0.53
1:C:526:LEU:HD11	2:C:900:ADP:H2'	1.91	0.53
1:C:428:ASP:OD1	1:C:429:LEU:N	2.41	0.53
1:A:177:ALA:O	1:A:180:THR:HG22	2.09	0.53
1:C:203:TYR:CE2	1:C:217:LYS:HE2	2.44	0.53
1:D:203:TYR:CE2	1:D:217:LYS:HE2	2.44	0.53
1:B:233:ILE:HD11	1:C:158:MET:HB2	1.91	0.53
1:E:556:GLU:OE1	1:E:556:GLU:N	2.38	0.53
1:C:654:VAL:O	1:C:658:LYS:HG2	2.08	0.53
1:A:233:ILE:HD11	1:B:158:MET:HB2	1.91	0.53
1:B:127:THR:OG1	1:B:436:THR:O	2.26	0.53
1:A:78:SER:OG	1:A:81:LYS:HG2	2.09	0.53
1:C:282:SER:O	1:C:285:ASN:N	2.40	0.53
1:E:177:ALA:O	1:E:180:THR:HG22	2.09	0.53
1:E:203:TYR:CE2	1:E:217:LYS:HE2	2.44	0.53
1:E:526:LEU:HD11	2:E:900:ADP:H2'	1.91	0.53
1:F:701:GLU:OE2	1:F:735:HIS:NE2	2.42	0.52
1:D:282:SER:O	1:D:285:ASN:N	2.40	0.52
1:B:203:TYR:CE2	1:B:217:LYS:HE2	2.44	0.52
1:D:654:VAL:O	1:D:658:LYS:HG2	2.08	0.52
1:E:338:ARG:O	1:E:339:ALA:HB3	2.08	0.52
1:E:701:GLU:OE2	1:E:735:HIS:NE2	2.42	0.52
1:F:526:LEU:HD11	2:F:900:ADP:H2'	1.91	0.52
1:E:294:GLU:CD	1:E:338:ARG:NE	2.61	0.52
1:C:78:SER:OG	1:C:81:LYS:HG2	2.09	0.52
1:B:78:SER:OG	1:B:81:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:THR:HB	1:F:406:HIS:ND1	2.24	0.52
1:C:403:THR:HB	1:C:406:HIS:ND1	2.25	0.52
1:F:605:LEU:HD22	1:F:638:ARG:HD3	1.92	0.52
1:C:177:ALA:O	1:C:180:THR:HG22	2.09	0.52
1:D:109:LYS:HD3	1:D:173:TYR:CE1	2.44	0.52
1:A:526:LEU:HD11	2:A:900:ADP:H2'	1.91	0.52
1:B:526:LEU:HD11	2:B:900:ADP:H2'	1.91	0.52
1:B:93:ARG:HH21	1:B:194:GLU:HG3	1.75	0.52
1:E:239:ARG:HH22	1:E:337:GLN:H	1.58	0.52
1:D:239:ARG:HH22	1:D:337:GLN:H	1.58	0.52
1:A:112:LYS:HG2	1:A:113:ARG:HG3	1.90	0.52
1:F:203:TYR:CE2	1:F:217:LYS:HE2	2.44	0.52
1:A:605:LEU:HD22	1:A:638:ARG:HD3	1.92	0.52
1:F:556:GLU:N	1:F:556:GLU:OE1	2.38	0.52
1:A:556:GLU:N	1:A:556:GLU:OE1	2.38	0.52
1:A:701:GLU:OE2	1:A:735:HIS:NE2	2.42	0.52
1:B:177:ALA:O	1:B:180:THR:HG22	2.09	0.52
1:B:403:THR:HB	1:B:406:HIS:ND1	2.24	0.52
1:E:109:LYS:HD3	1:E:173:TYR:CE1	2.44	0.52
1:A:158:MET:HB2	1:F:233:ILE:HD11	1.92	0.52
1:D:233:ILE:HD11	1:E:158:MET:HB2	1.91	0.52
1:C:673:GLU:N	1:C:673:GLU:OE1	2.34	0.52
1:F:76:THR:OG1	1:F:83:ARG:NH1	2.39	0.52
1:D:93:ARG:HH21	1:D:194:GLU:HG3	1.75	0.52
1:C:605:LEU:HD22	1:C:638:ARG:HD3	1.92	0.52
1:C:632:ALA:O	1:C:638:ARG:NH1	2.40	0.52
1:C:239:ARG:HH22	1:C:337:GLN:H	1.58	0.52
1:A:127:THR:OG1	1:A:436:THR:O	2.26	0.52
1:A:403:THR:HB	1:A:406:HIS:ND1	2.25	0.52
1:D:158:MET:HG2	1:D:388:MET:HB3	1.92	0.52
1:C:236:LYS:HD2	1:C:237:PRO:HD2	1.92	0.52
1:B:605:LEU:HD22	1:B:638:ARG:HD3	1.92	0.52
1:B:460:ASN:OD1	1:B:460:ASN:N	2.43	0.52
1:B:473:GLN:OE1	1:B:473:GLN:N	2.32	0.52
1:F:239:ARG:HH22	1:F:337:GLN:H	1.58	0.52
1:C:158:MET:HG2	1:C:388:MET:HB3	1.92	0.52
1:F:697:LEU:HD11	1:F:738:GLU:OE1	2.10	0.52
1:A:364:ASP:N	1:A:364:ASP:OD1	2.35	0.52
1:E:75:ASP:OD1	1:E:76:THR:N	2.37	0.52
1:D:701:GLU:OE2	1:D:735:HIS:NE2	2.42	0.52
1:C:233:ILE:HD11	1:D:158:MET:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:TYR:CE2	1:A:217:LYS:HE2	2.44	0.51
1:B:33:ASN:OD1	1:B:34:GLU:N	2.44	0.51
1:E:460:ASN:N	1:E:460:ASN:OD1	2.43	0.51
1:A:76:THR:OG1	1:A:83:ARG:NH1	2.39	0.51
1:E:403:THR:HB	1:E:406:HIS:ND1	2.24	0.51
1:E:605:LEU:HD22	1:E:638:ARG:HD3	1.92	0.51
1:B:236:LYS:HD2	1:B:237:PRO:HD2	1.92	0.51
1:C:697:LEU:HD11	1:C:738:GLU:OE1	2.10	0.51
1:B:697:LEU:HD11	1:B:738:GLU:OE1	2.10	0.51
1:A:697:LEU:HD11	1:A:738:GLU:OE1	2.10	0.51
1:F:389:LYS:NZ	1:F:446:ALA:HB2	2.25	0.51
1:D:389:LYS:NZ	1:D:446:ALA:HB2	2.25	0.51
1:A:33:ASN:OD1	1:A:34:GLU:N	2.43	0.51
1:E:93:ARG:HH21	1:E:194:GLU:HG3	1.75	0.51
1:D:605:LEU:HD22	1:D:638:ARG:HD3	1.92	0.51
1:B:337:GLN:NE2	1:B:337:GLN:CA	2.73	0.51
1:C:75:ASP:OD1	1:C:76:THR:N	2.37	0.51
1:C:644:TYR:CZ	1:C:646:PRO:HB3	2.46	0.51
1:B:644:TYR:CZ	1:B:646:PRO:HB3	2.46	0.51
1:A:460:ASN:N	1:A:460:ASN:OD1	2.43	0.51
1:E:700:ARG:O	1:E:704:GLU:N	2.32	0.51
1:E:131:PHE:HA	1:E:135:LEU:HD13	1.93	0.51
1:A:131:PHE:HA	1:A:135:LEU:HD13	1.93	0.51
1:D:236:LYS:HD2	1:D:237:PRO:HD2	1.92	0.51
1:F:93:ARG:HH21	1:F:194:GLU:HG3	1.75	0.51
1:F:282:SER:O	1:F:285:ASN:N	2.40	0.51
1:D:403:THR:HB	1:D:406:HIS:ND1	2.25	0.51
1:F:131:PHE:HA	1:F:135:LEU:HD13	1.93	0.51
1:C:33:ASN:OD1	1:C:34:GLU:N	2.43	0.51
1:D:460:ASN:OD1	1:D:460:ASN:N	2.43	0.51
1:D:644:TYR:CZ	1:D:646:PRO:HB3	2.46	0.51
1:D:30:GLU:HB3	1:D:96:LEU:HD21	1.93	0.51
1:A:236:LYS:HD2	1:A:237:PRO:HD2	1.92	0.51
1:E:697:LEU:HD11	1:E:738:GLU:OE1	2.10	0.51
1:B:239:ARG:HH22	1:B:337:GLN:H	1.58	0.51
1:E:389:LYS:NZ	1:E:446:ALA:HB2	2.26	0.51
1:D:473:GLN:OE1	1:D:473:GLN:N	2.32	0.51
1:A:239:ARG:HH22	1:A:337:GLN:H	1.58	0.51
1:B:30:GLU:HB3	1:B:96:LEU:HD21	1.93	0.51
1:A:30:GLU:HB3	1:A:96:LEU:HD21	1.93	0.51
1:C:93:ARG:HH21	1:C:194:GLU:HG3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD13	2:D:807:ADP:H2'	1.93	0.51
1:C:460:ASN:N	1:C:460:ASN:OD1	2.43	0.51
1:C:701:GLU:OE2	1:C:735:HIS:NE2	2.42	0.50
1:D:697:LEU:HD11	1:D:738:GLU:OE1	2.10	0.50
1:D:33:ASN:OD1	1:D:34:GLU:N	2.44	0.50
1:A:337:GLN:CA	1:A:337:GLN:NE2	2.73	0.50
1:E:33:ASN:OD1	1:E:34:GLU:N	2.44	0.50
1:C:253:LEU:HD13	2:C:807:ADP:H2'	1.93	0.50
1:E:134:TYR:OH	1:E:156:GLY:O	2.25	0.50
1:E:158:MET:HG2	1:E:388:MET:HB3	1.92	0.50
1:E:253:LEU:HD13	2:E:807:ADP:H2'	1.93	0.50
1:A:93:ARG:HH21	1:A:194:GLU:HG3	1.75	0.50
1:B:701:GLU:OE2	1:B:735:HIS:NE2	2.42	0.50
1:F:131:PHE:HZ	1:F:184:CYS:H	1.59	0.50
1:D:131:PHE:HA	1:D:135:LEU:HD13	1.93	0.50
1:A:644:TYR:CZ	1:A:646:PRO:HB3	2.46	0.50
1:B:389:LYS:NZ	1:B:446:ALA:HB2	2.26	0.50
1:A:389:LYS:NZ	1:A:446:ALA:HB2	2.26	0.50
1:F:406:HIS:HD2	1:F:410:ASP:HB3	1.77	0.50
1:C:30:GLU:HB3	1:C:96:LEU:HD21	1.93	0.50
1:A:158:MET:HG2	1:A:388:MET:HB3	1.92	0.50
1:B:517:TYR:CZ	1:B:644:TYR:HB2	2.47	0.50
1:B:227:PRO:HB3	1:B:340:HIS:CD2	2.47	0.50
1:C:420:LEU:HD23	1:C:423:ILE:HD12	1.93	0.50
1:D:420:LEU:HD23	1:D:423:ILE:HD12	1.93	0.50
1:F:460:ASN:N	1:F:460:ASN:OD1	2.43	0.50
1:E:406:HIS:HD2	1:E:410:ASP:HB3	1.77	0.50
1:F:158:MET:HG2	1:F:388:MET:HB3	1.92	0.50
1:A:420:LEU:HD23	1:A:423:ILE:HD12	1.93	0.50
1:E:644:TYR:CZ	1:E:646:PRO:HB3	2.46	0.50
1:E:517:TYR:CZ	1:E:644:TYR:HB2	2.46	0.50
1:E:236:LYS:HD2	1:E:237:PRO:HD2	1.92	0.50
1:A:227:PRO:HB3	1:A:340:HIS:CD2	2.47	0.50
1:B:700:ARG:O	1:B:704:GLU:N	2.32	0.50
1:C:700:ARG:O	1:C:704:GLU:N	2.32	0.50
1:F:75:ASP:OD1	1:F:76:THR:N	2.37	0.50
1:E:74:ASP:OD2	1:E:77:CYS:HB3	2.12	0.50
1:B:666:VAL:HA	1:B:731:ILE:HG22	1.94	0.50
1:E:131:PHE:HZ	1:E:184:CYS:H	1.59	0.50
1:C:517:TYR:CZ	1:C:644:TYR:HB2	2.47	0.50
1:B:420:LEU:HD23	1:B:423:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:420:LEU:HD23	1:F:423:ILE:HD12	1.93	0.50
1:C:127:THR:CB	1:C:438:ASP:HA	2.37	0.50
1:F:74:ASP:OD2	1:F:77:CYS:HB3	2.12	0.50
1:A:666:VAL:HA	1:A:731:ILE:HG22	1.94	0.50
1:F:666:VAL:HA	1:F:731:ILE:HG22	1.94	0.50
1:B:131:PHE:HA	1:B:135:LEU:HD13	1.93	0.50
1:F:30:GLU:HB3	1:F:96:LEU:HD21	1.93	0.50
1:B:158:MET:HG2	1:B:388:MET:HB3	1.92	0.50
1:F:33:ASN:OD1	1:F:34:GLU:N	2.43	0.50
1:E:57:VAL:O	1:E:68:VAL:HG13	2.12	0.50
1:B:253:LEU:HD13	2:B:807:ADP:H2'	1.93	0.50
1:E:121:ASP:OD1	1:E:122:THR:N	2.45	0.50
1:F:236:LYS:HD2	1:F:237:PRO:HD2	1.92	0.50
1:E:420:LEU:HD23	1:E:423:ILE:HD12	1.93	0.50
1:C:389:LYS:NZ	1:C:446:ALA:HB2	2.26	0.50
1:A:517:TYR:CZ	1:A:644:TYR:HB2	2.47	0.50
1:D:57:VAL:O	1:D:68:VAL:HG13	2.12	0.50
1:C:227:PRO:HB3	1:C:340:HIS:CD2	2.47	0.50
1:A:294:GLU:CD	1:A:338:ARG:NE	2.61	0.49
1:C:406:HIS:HD2	1:C:410:ASP:HB3	1.77	0.49
1:B:121:ASP:OD1	1:B:122:THR:N	2.45	0.49
1:A:121:ASP:OD1	1:A:122:THR:N	2.45	0.49
1:A:700:ARG:O	1:A:704:GLU:N	2.32	0.49
1:C:57:VAL:O	1:C:68:VAL:HG13	2.12	0.49
1:F:31:ALA:HB2	1:F:84:MET:C	2.33	0.49
1:A:406:HIS:HD2	1:A:410:ASP:HB3	1.77	0.49
1:D:406:HIS:HD2	1:D:410:ASP:HB3	1.77	0.49
1:A:131:PHE:HZ	1:A:184:CYS:H	1.60	0.49
1:F:517:TYR:CZ	1:F:644:TYR:HB2	2.47	0.49
1:F:644:TYR:CZ	1:F:646:PRO:HB3	2.46	0.49
1:D:31:ALA:HB2	1:D:84:MET:C	2.33	0.49
1:A:31:ALA:HB2	1:A:84:MET:C	2.33	0.49
1:E:337:GLN:CA	1:E:337:GLN:NE2	2.73	0.49
1:B:632:ALA:O	1:B:638:ARG:NH1	2.40	0.49
1:F:227:PRO:HB3	1:F:340:HIS:CD2	2.47	0.49
1:E:31:ALA:HB2	1:E:84:MET:C	2.33	0.49
1:F:239:ARG:HH22	1:F:336:LYS:HA	1.78	0.49
1:E:666:VAL:HA	1:E:731:ILE:HG22	1.94	0.49
1:C:666:VAL:HA	1:C:731:ILE:HG22	1.94	0.49
1:E:30:GLU:HB3	1:E:96:LEU:HD21	1.93	0.49
1:D:632:ALA:O	1:D:638:ARG:NH1	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:VAL:O	1:F:68:VAL:HG13	2.12	0.49
1:A:253:LEU:HD13	2:A:807:ADP:H2'	1.93	0.49
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.53	0.49
1:D:74:ASP:OD2	1:D:77:CYS:HB3	2.12	0.49
1:D:169:ASP:O	1:D:171:SER:N	2.46	0.49
1:D:517:TYR:CZ	1:D:644:TYR:HB2	2.47	0.49
1:A:57:VAL:O	1:A:68:VAL:HG13	2.12	0.49
1:D:239:ARG:HH22	1:D:336:LYS:HA	1.78	0.49
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.53	0.49
1:A:169:ASP:O	1:A:171:SER:N	2.46	0.49
1:C:121:ASP:OD1	1:C:122:THR:N	2.45	0.49
1:C:31:ALA:HB2	1:C:84:MET:C	2.33	0.49
1:A:759:ALA:HA	1:A:762:LEU:HD12	1.95	0.49
1:C:74:ASP:OD2	1:C:77:CYS:HB3	2.12	0.49
1:A:74:ASP:OD2	1:A:77:CYS:HB3	2.12	0.49
1:B:406:HIS:HD2	1:B:410:ASP:HB3	1.77	0.49
1:E:169:ASP:O	1:E:171:SER:N	2.46	0.49
1:C:131:PHE:HA	1:C:135:LEU:HD13	1.93	0.49
1:F:253:LEU:HD13	2:F:807:ADP:H2'	1.93	0.49
1:F:121:ASP:OD1	1:F:122:THR:N	2.45	0.49
1:D:227:PRO:HB3	1:D:340:HIS:CD2	2.47	0.49
1:B:239:ARG:HH22	1:B:336:LYS:HA	1.78	0.49
1:F:519:PRO:HG2	1:F:522:CYS:SG	2.53	0.49
1:B:759:ALA:HA	1:B:762:LEU:HD12	1.95	0.49
1:B:294:GLU:CD	1:B:338:ARG:NE	2.61	0.49
1:E:127:THR:CB	1:E:438:ASP:HA	2.37	0.49
1:A:519:PRO:HG2	1:A:522:CYS:SG	2.53	0.49
1:B:169:ASP:O	1:B:171:SER:N	2.46	0.49
1:C:169:ASP:O	1:C:171:SER:N	2.46	0.49
1:B:31:ALA:HB2	1:B:84:MET:C	2.33	0.49
1:E:675:LEU:HA	1:E:678:MET:SD	2.53	0.49
1:B:57:VAL:O	1:B:68:VAL:HG13	2.12	0.49
1:B:675:LEU:HA	1:B:678:MET:SD	2.53	0.49
1:B:74:ASP:OD2	1:B:77:CYS:HB3	2.12	0.48
1:D:131:PHE:HZ	1:D:184:CYS:H	1.60	0.48
1:E:759:ALA:HA	1:E:762:LEU:HD12	1.95	0.48
1:F:759:ALA:HA	1:F:762:LEU:HD12	1.95	0.48
1:E:227:PRO:HB3	1:E:340:HIS:CD2	2.47	0.48
1:D:666:VAL:HA	1:D:731:ILE:HG22	1.94	0.48
1:C:759:ALA:HA	1:C:762:LEU:HD12	1.95	0.48
1:D:681:GLY:HA3	1:D:745:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:675:LEU:HA	1:C:678:MET:SD	2.53	0.48
1:C:681:GLY:HA3	1:C:745:ARG:HH21	1.78	0.48
1:F:675:LEU:HA	1:F:678:MET:SD	2.53	0.48
1:C:60:LYS:HA	1:C:66:GLU:HG2	1.96	0.48
1:B:131:PHE:HZ	1:B:184:CYS:H	1.59	0.48
1:D:121:ASP:OD1	1:D:122:THR:N	2.45	0.48
1:F:364:ASP:N	1:F:364:ASP:OD1	2.35	0.48
1:D:519:PRO:HG2	1:D:522:CYS:SG	2.53	0.48
1:B:60:LYS:HA	1:B:66:GLU:HG2	1.96	0.48
1:C:114:ILE:HD13	1:C:168:THR:HG23	1.96	0.48
1:D:191:ARG:HH21	1:D:195:GLU:HG2	1.79	0.48
1:D:675:LEU:HA	1:D:678:MET:SD	2.53	0.48
1:E:123:VAL:O	1:E:126:ILE:HG12	2.14	0.48
1:C:519:PRO:HG2	1:C:522:CYS:SG	2.53	0.48
1:F:169:ASP:O	1:F:171:SER:N	2.46	0.48
1:D:681:GLY:CA	1:D:745:ARG:HE	2.27	0.48
1:D:759:ALA:HA	1:D:762:LEU:HD12	1.95	0.48
1:F:681:GLY:CA	1:F:745:ARG:HE	2.27	0.48
1:C:681:GLY:CA	1:C:745:ARG:HE	2.27	0.48
1:B:123:VAL:O	1:B:126:ILE:HG12	2.14	0.48
1:D:123:VAL:O	1:D:126:ILE:HG12	2.14	0.48
1:B:284:SER:O	1:B:288:LYS:HG2	2.14	0.48
1:A:675:LEU:HA	1:A:678:MET:SD	2.53	0.48
1:C:627:ASP:N	1:C:627:ASP:OD1	2.46	0.48
1:C:239:ARG:HH22	1:C:336:LYS:HA	1.78	0.48
1:D:127:THR:CB	1:D:438:ASP:HA	2.37	0.48
1:D:60:LYS:HA	1:D:66:GLU:HG2	1.96	0.48
1:B:681:GLY:HA3	1:B:745:ARG:HH21	1.78	0.48
1:C:284:SER:O	1:C:288:LYS:HG2	2.14	0.48
1:E:681:GLY:CA	1:E:745:ARG:HE	2.27	0.48
1:A:284:SER:O	1:A:288:LYS:HG2	2.14	0.48
1:F:123:VAL:O	1:F:126:ILE:HG12	2.14	0.48
1:A:60:LYS:HA	1:A:66:GLU:HG2	1.96	0.48
1:C:131:PHE:HZ	1:C:184:CYS:H	1.59	0.48
1:A:681:GLY:CA	1:A:745:ARG:HE	2.27	0.48
1:E:466:GLU:OE1	1:E:466:GLU:N	2.47	0.48
1:E:336:LYS:O	1:E:337:GLN:C	2.51	0.48
1:E:114:ILE:HD13	1:E:168:THR:HG23	1.96	0.48
1:D:284:SER:O	1:D:288:LYS:HG2	2.14	0.48
1:A:134:TYR:OH	1:A:156:GLY:O	2.25	0.48
1:F:700:ARG:O	1:F:704:GLU:N	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:VAL:HG23	1:E:96:LEU:HA	1.96	0.48
1:E:681:GLY:HA3	1:E:745:ARG:HH21	1.79	0.48
1:A:123:VAL:O	1:A:126:ILE:HG12	2.14	0.48
1:A:239:ARG:HH22	1:A:336:LYS:HA	1.78	0.47
1:A:336:LYS:O	1:A:337:GLN:C	2.51	0.47
1:D:336:LYS:O	1:D:337:GLN:C	2.51	0.47
1:D:337:GLN:NE2	1:D:337:GLN:CA	2.73	0.47
1:B:114:ILE:HD13	1:B:168:THR:HG23	1.96	0.47
1:D:114:ILE:HD13	1:D:168:THR:HG23	1.96	0.47
1:F:466:GLU:N	1:F:466:GLU:OE1	2.47	0.47
1:E:239:ARG:HH22	1:E:336:LYS:HA	1.78	0.47
1:F:681:GLY:HA3	1:F:745:ARG:HH21	1.78	0.47
1:A:681:GLY:HA3	1:A:745:ARG:HH21	1.78	0.47
1:C:191:ARG:HH21	1:C:195:GLU:HG2	1.79	0.47
1:A:389:LYS:HZ2	1:A:446:ALA:HB2	1.77	0.47
1:D:28:VAL:HG23	1:D:96:LEU:HA	1.96	0.47
1:E:191:ARG:HH21	1:E:195:GLU:HG2	1.79	0.47
1:C:123:VAL:O	1:C:126:ILE:HG12	2.14	0.47
1:A:191:ARG:HH21	1:A:195:GLU:HG2	1.79	0.47
1:B:627:ASP:N	1:B:627:ASP:OD1	2.46	0.47
1:E:60:LYS:HA	1:E:66:GLU:HG2	1.96	0.47
1:C:109:LYS:HD3	1:C:173:TYR:CD1	2.50	0.47
1:E:33:ASN:OD1	1:E:35:ASP:N	2.31	0.47
1:F:284:SER:O	1:F:288:LYS:HG2	2.14	0.47
1:C:37:SER:O	1:C:38:VAL:HG23	2.14	0.47
1:A:466:GLU:OE1	1:A:466:GLU:N	2.47	0.47
1:D:37:SER:O	1:D:38:VAL:HG23	2.14	0.47
1:C:337:GLN:NE2	1:C:337:GLN:CA	2.73	0.47
1:F:60:LYS:HA	1:F:66:GLU:HG2	1.96	0.47
1:F:28:VAL:HG23	1:F:96:LEU:HA	1.96	0.47
1:B:681:GLY:CA	1:B:745:ARG:HE	2.27	0.47
1:D:679:THR:HB	1:D:682:PHE:HB2	1.97	0.47
1:F:191:ARG:HH21	1:F:195:GLU:HG2	1.79	0.47
1:C:28:VAL:HG23	1:C:96:LEU:HA	1.96	0.47
1:A:37:SER:O	1:A:38:VAL:HG23	2.14	0.47
1:C:466:GLU:N	1:C:466:GLU:OE1	2.47	0.47
1:A:109:LYS:HD3	1:A:173:TYR:CD1	2.50	0.47
1:F:109:LYS:HD3	1:F:173:TYR:CD1	2.50	0.47
1:E:109:LYS:HD3	1:E:173:TYR:CD1	2.50	0.47
1:D:134:TYR:OH	1:D:156:GLY:O	2.25	0.47
1:C:679:THR:HB	1:C:682:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:SER:O	1:E:288:LYS:HG2	2.14	0.47
1:F:37:SER:O	1:F:38:VAL:HG23	2.14	0.47
1:D:466:GLU:OE1	1:D:466:GLU:N	2.47	0.47
1:A:473:GLN:N	1:A:473:GLN:OE1	2.32	0.47
1:F:134:TYR:OH	1:F:156:GLY:O	2.25	0.47
1:F:337:GLN:CA	1:F:337:GLN:NE2	2.73	0.47
1:F:114:ILE:HD13	1:F:168:THR:HG23	1.96	0.47
1:F:229:LEU:O	1:F:233:ILE:HG22	2.15	0.47
1:F:288:LYS:HA	1:F:291:GLU:OE2	2.15	0.47
1:A:679:THR:HB	1:A:682:PHE:HB2	1.97	0.47
1:D:627:ASP:OD1	1:D:627:ASP:N	2.46	0.47
1:E:644:TYR:CE2	1:E:646:PRO:HB3	2.50	0.47
1:B:58:LEU:HD22	1:B:103:GLN:NE2	2.30	0.47
1:F:679:THR:HB	1:F:682:PHE:HB2	1.97	0.47
1:A:58:LEU:HD22	1:A:103:GLN:NE2	2.30	0.47
1:B:679:THR:HB	1:B:682:PHE:HB2	1.97	0.47
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.50	0.47
1:E:136:LYS:HB2	1:E:137:PRO:HD3	1.97	0.47
1:F:627:ASP:OD1	1:F:627:ASP:N	2.46	0.47
1:B:466:GLU:OE1	1:B:466:GLU:N	2.47	0.47
1:D:700:ARG:O	1:D:704:GLU:N	2.32	0.46
1:D:109:LYS:HD3	1:D:173:TYR:CD1	2.50	0.46
1:A:28:VAL:HG23	1:A:96:LEU:HA	1.96	0.46
1:A:229:LEU:O	1:A:233:ILE:HG22	2.15	0.46
1:B:288:LYS:HA	1:B:291:GLU:OE2	2.15	0.46
1:F:58:LEU:HD22	1:F:103:GLN:NE2	2.30	0.46
1:E:679:THR:HB	1:E:682:PHE:HB2	1.97	0.46
1:B:191:ARG:HH21	1:B:195:GLU:HG2	1.79	0.46
1:F:136:LYS:HB2	1:F:137:PRO:HD3	1.97	0.46
1:E:627:ASP:OD1	1:E:627:ASP:N	2.46	0.46
1:C:58:LEU:HD22	1:C:103:GLN:NE2	2.30	0.46
1:E:22:ARG:NH1	1:E:24:ASN:OD1	2.49	0.46
1:A:114:ILE:HD13	1:A:168:THR:HG23	1.96	0.46
1:B:109:LYS:HD3	1:B:173:TYR:CD1	2.50	0.46
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.96	0.46
1:F:290:PHE:CE2	1:F:331:LEU:HB3	2.51	0.46
1:F:644:TYR:CE2	1:F:646:PRO:HB3	2.50	0.46
1:D:22:ARG:NH1	1:D:24:ASN:OD1	2.49	0.46
1:C:270:ASN:OD1	1:C:272:PRO:HD2	2.16	0.46
1:A:389:LYS:HE3	1:A:443:ASN:O	2.16	0.46
1:D:131:PHE:HZ	1:D:184:CYS:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:644:TYR:CE2	1:D:646:PRO:HB3	2.50	0.46
1:E:288:LYS:HA	1:E:291:GLU:OE2	2.15	0.46
1:E:37:SER:O	1:E:38:VAL:HG23	2.14	0.46
1:C:136:LYS:HB2	1:C:137:PRO:HD3	1.97	0.46
1:B:37:SER:O	1:B:38:VAL:HG23	2.14	0.46
1:E:131:PHE:HZ	1:E:184:CYS:N	2.14	0.46
1:D:288:LYS:HA	1:D:291:GLU:OE2	2.15	0.46
1:B:136:LYS:HB2	1:B:137:PRO:HD3	1.97	0.46
1:F:22:ARG:NH1	1:F:24:ASN:OD1	2.49	0.46
1:D:58:LEU:HD22	1:D:103:GLN:NE2	2.30	0.46
1:F:689:GLU:HA	1:F:692:GLN:HB2	1.97	0.46
1:C:473:GLN:OE1	1:C:473:GLN:N	2.32	0.46
1:B:389:LYS:HE3	1:B:443:ASN:O	2.16	0.46
1:E:229:LEU:O	1:E:233:ILE:HG22	2.15	0.46
1:B:229:LEU:O	1:B:233:ILE:HG22	2.15	0.46
1:B:644:TYR:CE2	1:B:646:PRO:HB3	2.50	0.46
1:A:270:ASN:OD1	1:A:272:PRO:HD2	2.16	0.46
1:F:270:ASN:OD1	1:F:272:PRO:HD2	2.15	0.46
1:A:689:GLU:HA	1:A:692:GLN:HB2	1.97	0.46
1:F:389:LYS:HE3	1:F:443:ASN:O	2.16	0.46
1:A:290:PHE:CE2	1:A:331:LEU:HB3	2.51	0.46
1:C:290:PHE:CE2	1:C:331:LEU:HB3	2.51	0.46
1:C:229:LEU:O	1:C:233:ILE:HG22	2.15	0.46
1:C:33:ASN:OD1	1:C:35:ASP:N	2.31	0.46
1:C:288:LYS:HA	1:C:291:GLU:OE2	2.15	0.46
1:B:270:ASN:OD1	1:B:272:PRO:HD2	2.16	0.46
1:E:58:LEU:HD22	1:E:103:GLN:NE2	2.30	0.46
1:C:22:ARG:NH1	1:C:24:ASN:OD1	2.49	0.46
1:D:270:ASN:OD1	1:D:272:PRO:HD2	2.16	0.46
1:C:336:LYS:O	1:C:337:GLN:C	2.51	0.46
1:B:131:PHE:HZ	1:B:184:CYS:N	2.14	0.46
1:D:229:LEU:O	1:D:233:ILE:HG22	2.15	0.46
1:D:489:LEU:O	1:D:493:VAL:HG22	2.16	0.46
1:A:294:GLU:HG3	1:A:338:ARG:CG	2.46	0.46
1:F:294:GLU:HG3	1:F:338:ARG:CG	2.46	0.46
1:E:290:PHE:CE2	1:E:331:LEU:HB3	2.51	0.46
1:B:689:GLU:HA	1:B:692:GLN:HB2	1.97	0.46
1:A:22:ARG:NH1	1:A:24:ASN:OD1	2.49	0.46
1:A:493:VAL:HG23	1:A:494:GLN:N	2.31	0.46
1:E:364:ASP:N	1:E:364:ASP:OD1	2.35	0.46
1:E:294:GLU:HG3	1:E:338:ARG:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:PHE:HZ	1:F:184:CYS:N	2.14	0.46
1:A:131:PHE:HZ	1:A:184:CYS:N	2.14	0.46
1:D:290:PHE:CE2	1:D:331:LEU:HB3	2.51	0.46
1:A:288:LYS:HA	1:A:291:GLU:OE2	2.15	0.46
1:C:689:GLU:HA	1:C:692:GLN:HB2	1.97	0.46
1:B:22:ARG:NH1	1:B:24:ASN:OD1	2.49	0.46
1:A:627:ASP:OD1	1:A:627:ASP:N	2.46	0.46
1:C:389:LYS:HE3	1:C:443:ASN:O	2.16	0.46
1:C:644:TYR:CE2	1:C:646:PRO:HB3	2.50	0.46
1:E:270:ASN:OD1	1:E:272:PRO:HD2	2.16	0.46
1:F:493:VAL:HG23	1:F:494:GLN:N	2.31	0.46
1:E:389:LYS:HE3	1:E:443:ASN:O	2.16	0.45
1:C:489:LEU:O	1:C:493:VAL:HG22	2.16	0.45
1:A:136:LYS:HB2	1:A:137:PRO:HD3	1.97	0.45
1:E:43:GLN:HB3	1:E:44:PRO:HD3	1.99	0.45
1:C:148:LYS:HE3	1:C:167:GLU:HA	1.98	0.45
1:D:136:LYS:HB2	1:D:137:PRO:HD3	1.97	0.45
1:A:176:VAL:HG13	1:A:180:THR:HG21	1.99	0.45
1:E:176:VAL:HG13	1:E:180:THR:HG21	1.99	0.45
1:C:131:PHE:HZ	1:C:184:CYS:N	2.14	0.45
1:E:661:LEU:O	1:E:664:SER:O	2.35	0.45
1:F:43:GLN:HB3	1:F:44:PRO:HD3	1.99	0.45
1:D:689:GLU:HA	1:D:692:GLN:HB2	1.97	0.45
1:E:489:LEU:O	1:E:493:VAL:HG22	2.16	0.45
1:D:389:LYS:HE3	1:D:443:ASN:O	2.16	0.45
1:F:176:VAL:HG13	1:F:180:THR:HG21	1.99	0.45
1:D:148:LYS:HE3	1:D:167:GLU:HA	1.98	0.45
1:B:290:PHE:CE2	1:B:331:LEU:HB3	2.51	0.45
1:F:661:LEU:O	1:F:664:SER:O	2.35	0.45
1:E:689:GLU:HA	1:E:692:GLN:HB2	1.97	0.45
1:A:112:LYS:O	1:A:181:VAL:HG12	2.17	0.45
1:F:118:PRO:HG3	1:F:130:LEU:HD22	1.99	0.45
1:B:148:LYS:HE3	1:B:167:GLU:HA	1.99	0.45
1:D:323:ARG:NH1	1:E:278:LEU:HD23	2.32	0.45
1:B:323:ARG:NH1	1:C:278:LEU:HD23	2.32	0.45
1:D:294:GLU:HG3	1:D:338:ARG:CG	2.46	0.45
1:B:294:GLU:HG3	1:B:338:ARG:CG	2.46	0.45
1:D:176:VAL:HG13	1:D:180:THR:HG21	1.99	0.45
1:E:474:VAL:HG23	1:E:478:ASP:HB2	1.99	0.45
1:B:459:SER:O	1:B:462:SER:HB2	2.17	0.45
1:B:493:VAL:HG23	1:B:494:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:PRO:HG3	1:E:130:LEU:HD22	1.99	0.45
1:D:118:PRO:HG3	1:D:130:LEU:HD22	1.99	0.45
1:E:140:LEU:HB3	1:E:141:GLU:OE1	2.17	0.45
1:B:140:LEU:HB3	1:B:141:GLU:OE1	2.17	0.45
1:D:140:LEU:HB3	1:D:141:GLU:OE1	2.17	0.45
1:A:278:LEU:HD23	1:F:323:ARG:NH1	2.31	0.45
1:F:474:VAL:HG23	1:F:478:ASP:HB2	1.99	0.45
1:E:148:LYS:HE3	1:E:167:GLU:HA	1.98	0.45
1:B:176:VAL:HG13	1:B:180:THR:HG21	1.99	0.45
1:C:176:VAL:HG13	1:C:180:THR:HG21	1.99	0.45
1:D:112:LYS:O	1:D:181:VAL:HG12	2.17	0.45
1:D:474:VAL:HG23	1:D:478:ASP:HB2	1.99	0.45
1:B:661:LEU:O	1:B:664:SER:O	2.35	0.45
1:B:43:GLN:HB3	1:B:44:PRO:HD3	1.99	0.45
1:C:459:SER:O	1:C:462:SER:HB2	2.17	0.45
1:A:118:PRO:HG3	1:A:130:LEU:HD22	1.99	0.45
1:F:140:LEU:HB3	1:F:141:GLU:OE1	2.17	0.45
1:C:140:LEU:HB3	1:C:141:GLU:OE1	2.17	0.45
1:E:493:VAL:HG23	1:E:494:GLN:N	2.31	0.45
1:B:489:LEU:O	1:B:493:VAL:HG22	2.16	0.45
1:D:364:ASP:OD1	1:D:364:ASP:N	2.35	0.45
1:D:555:SER:O	1:D:555:SER:OG	2.35	0.45
1:F:336:LYS:O	1:F:337:GLN:C	2.51	0.45
1:C:493:VAL:HG23	1:C:494:GLN:N	2.31	0.45
1:A:661:LEU:O	1:A:664:SER:O	2.35	0.45
1:C:112:LYS:O	1:C:181:VAL:HG12	2.17	0.44
1:D:493:VAL:HG23	1:D:494:GLN:N	2.31	0.44
1:C:43:GLN:HB3	1:C:44:PRO:HD3	1.99	0.44
1:E:45:LYS:HG2	1:E:80:GLU:OE2	2.18	0.44
1:C:130:LEU:HD11	1:C:163:PHE:HZ	1.83	0.44
1:D:33:ASN:OD1	1:D:35:ASP:N	2.31	0.44
1:F:489:LEU:O	1:F:493:VAL:HG22	2.16	0.44
1:C:469:VAL:HG22	1:C:540:ILE:HG12	2.00	0.44
1:A:45:LYS:HG2	1:A:80:GLU:OE2	2.18	0.44
1:F:112:LYS:O	1:F:181:VAL:HG12	2.17	0.44
1:C:96:LEU:HD13	1:C:261:GLU:OE2	2.18	0.44
1:D:136:LYS:O	1:D:140:LEU:HD13	2.18	0.44
1:A:474:VAL:HG23	1:A:478:ASP:HB2	1.99	0.44
1:D:459:SER:O	1:D:462:SER:HB2	2.17	0.44
1:D:45:LYS:HG2	1:D:80:GLU:OE2	2.18	0.44
1:B:118:PRO:HG3	1:B:130:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:PRO:HG3	1:C:130:LEU:HD22	1.99	0.44
1:B:33:ASN:OD1	1:B:35:ASP:N	2.31	0.44
1:A:489:LEU:O	1:A:493:VAL:HG22	2.16	0.44
1:B:469:VAL:HG22	1:B:540:ILE:HG12	2.00	0.44
1:D:469:VAL:HG22	1:D:540:ILE:HG12	2.00	0.44
1:C:474:VAL:HG23	1:C:478:ASP:HB2	1.99	0.44
1:C:45:LYS:HG2	1:C:80:GLU:OE2	2.18	0.44
1:E:96:LEU:HD13	1:E:261:GLU:OE2	2.18	0.44
1:A:43:GLN:HB3	1:A:44:PRO:HD3	1.99	0.44
1:F:96:LEU:HD13	1:F:261:GLU:OE2	2.18	0.44
1:C:136:LYS:O	1:C:140:LEU:HD13	2.18	0.44
1:D:43:GLN:HB3	1:D:44:PRO:HD3	1.98	0.44
1:C:294:GLU:HG3	1:C:338:ARG:CG	2.46	0.44
1:F:45:LYS:HG2	1:F:80:GLU:OE2	2.18	0.44
1:B:45:LYS:HG2	1:B:80:GLU:OE2	2.18	0.44
1:B:59:LEU:O	1:B:66:GLU:HA	2.18	0.44
1:D:130:LEU:HD11	1:D:163:PHE:HZ	1.83	0.44
1:A:96:LEU:HD13	1:A:261:GLU:OE2	2.18	0.44
1:C:661:LEU:O	1:C:664:SER:O	2.35	0.44
1:A:323:ARG:NH1	1:B:278:LEU:HD23	2.33	0.44
1:F:148:LYS:HE3	1:F:167:GLU:HA	1.98	0.44
1:D:96:LEU:HD13	1:D:261:GLU:OE2	2.18	0.44
1:F:136:LYS:O	1:F:140:LEU:HD13	2.18	0.44
1:E:469:VAL:HG22	1:E:540:ILE:HG12	2.00	0.44
1:D:661:LEU:O	1:D:664:SER:O	2.35	0.44
1:E:323:ARG:NH1	1:F:278:LEU:HD23	2.32	0.44
1:A:148:LYS:HE3	1:A:167:GLU:HA	1.99	0.44
1:A:459:SER:O	1:A:462:SER:HB2	2.17	0.44
1:D:307:ASP:N	1:D:307:ASP:OD1	2.51	0.44
1:B:336:LYS:O	1:B:337:GLN:C	2.51	0.43
1:C:59:LEU:O	1:C:66:GLU:HA	2.18	0.43
1:B:130:LEU:HD11	1:B:163:PHE:HZ	1.83	0.43
1:E:112:LYS:O	1:E:181:VAL:HG12	2.17	0.43
1:B:112:LYS:O	1:B:181:VAL:HG12	2.17	0.43
1:A:469:VAL:HG22	1:A:540:ILE:HG12	2.00	0.43
1:E:473:GLN:N	1:E:473:GLN:OE1	2.32	0.43
1:F:59:LEU:O	1:F:66:GLU:HA	2.18	0.43
1:D:59:LEU:O	1:D:66:GLU:HA	2.18	0.43
1:C:206:ILE:HG12	1:C:253:LEU:HD23	2.01	0.43
1:B:27:ILE:O	1:B:82:ILE:HG22	2.19	0.43
1:B:136:LYS:O	1:B:140:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LYS:O	1:A:140:LEU:HD13	2.18	0.43
1:A:140:LEU:HB3	1:A:141:GLU:OE1	2.17	0.43
1:F:459:SER:O	1:F:462:SER:HB2	2.17	0.43
1:C:323:ARG:NH1	1:D:278:LEU:HD23	2.33	0.43
1:E:59:LEU:O	1:E:66:GLU:HA	2.18	0.43
1:E:115:HIS:NE2	1:E:185:GLU:HG2	2.34	0.43
1:C:192:GLU:N	1:C:192:GLU:OE1	2.52	0.43
1:B:307:ASP:N	1:B:307:ASP:OD1	2.51	0.43
1:E:441:VAL:O	1:E:444:SER:OG	2.28	0.43
1:E:130:LEU:HD11	1:E:163:PHE:HZ	1.83	0.43
1:B:96:LEU:HD13	1:B:261:GLU:OE2	2.18	0.43
1:F:206:ILE:HG12	1:F:253:LEU:HD23	2.00	0.43
1:F:469:VAL:HG22	1:F:540:ILE:HG12	2.00	0.43
1:B:474:VAL:HG23	1:B:478:ASP:HB2	1.99	0.43
1:B:115:HIS:NE2	1:B:185:GLU:HG2	2.34	0.43
1:B:143:TYR:CE1	1:B:178:PRO:HD3	2.49	0.43
1:C:143:TYR:CE1	1:C:178:PRO:HD3	2.48	0.43
1:E:206:ILE:HG12	1:E:253:LEU:HD23	2.00	0.43
1:B:206:ILE:HG12	1:B:253:LEU:HD23	2.01	0.43
1:D:27:ILE:O	1:D:82:ILE:HG22	2.19	0.43
1:E:459:SER:O	1:E:462:SER:HB2	2.17	0.43
1:E:500:PRO:O	1:E:504:LEU:HD13	2.19	0.43
1:F:473:GLN:OE1	1:F:473:GLN:N	2.32	0.43
1:F:307:ASP:N	1:F:307:ASP:OD1	2.51	0.43
1:F:315:LYS:NZ	1:F:321:GLU:OE2	2.43	0.43
1:A:130:LEU:HD11	1:A:163:PHE:HZ	1.83	0.43
1:F:684:GLY:HA3	2:F:900:ADP:C8	2.54	0.43
1:B:82:ILE:HG12	1:B:84:MET:HG3	2.00	0.43
1:E:136:LYS:O	1:E:140:LEU:HD13	2.18	0.43
1:D:294:GLU:CG	1:D:338:ARG:CG	2.97	0.43
1:A:429:LEU:HD12	1:A:430:ILE:N	2.34	0.43
1:B:130:LEU:HD11	1:B:163:PHE:CZ	2.54	0.43
1:F:130:LEU:HD11	1:F:163:PHE:HZ	1.83	0.43
1:A:684:GLY:HA3	2:A:900:ADP:C8	2.54	0.43
1:A:206:ILE:HG12	1:A:253:LEU:HD23	2.01	0.43
1:B:270:ASN:HA	1:B:304:ASP:HB3	2.00	0.43
1:D:270:ASN:HA	1:D:304:ASP:HB3	2.00	0.43
1:D:758:PHE:O	1:D:761:THR:OG1	2.29	0.43
1:D:500:PRO:O	1:D:504:LEU:HD13	2.19	0.43
1:F:192:GLU:OE1	1:F:192:GLU:N	2.52	0.43
1:C:429:LEU:HD12	1:C:430:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:O	1:A:66:GLU:HA	2.18	0.43
1:E:143:TYR:CE1	1:E:178:PRO:HD3	2.48	0.43
1:D:684:GLY:HA3	2:D:900:ADP:C8	2.54	0.43
1:B:684:GLY:HA3	2:B:900:ADP:C8	2.54	0.43
1:E:270:ASN:HA	1:E:304:ASP:HB3	2.00	0.43
1:F:500:PRO:O	1:F:504:LEU:HD13	2.19	0.43
1:A:115:HIS:NE2	1:A:185:GLU:HG2	2.34	0.43
1:F:216:ILE:O	1:F:220:VAL:HG22	2.19	0.43
1:D:115:HIS:NE2	1:D:185:GLU:HG2	2.34	0.43
1:A:216:ILE:O	1:A:220:VAL:HG22	2.19	0.43
1:C:294:GLU:CG	1:C:338:ARG:CG	2.97	0.43
1:D:206:ILE:HG12	1:D:253:LEU:HD23	2.01	0.43
1:A:192:GLU:N	1:A:192:GLU:OE1	2.52	0.43
1:B:192:GLU:OE1	1:B:192:GLU:N	2.52	0.43
1:B:429:LEU:HD12	1:B:430:ILE:N	2.34	0.43
1:A:130:LEU:HD11	1:A:163:PHE:CZ	2.54	0.43
1:F:130:LEU:HD11	1:F:163:PHE:CZ	2.54	0.43
1:E:684:GLY:HA3	2:E:900:ADP:C8	2.54	0.43
1:F:82:ILE:HG12	1:F:84:MET:HG3	2.01	0.43
1:F:115:HIS:NE2	1:F:185:GLU:HG2	2.34	0.43
1:F:393:ASP:N	1:F:393:ASP:OD1	2.52	0.43
1:B:294:GLU:CG	1:B:338:ARG:CG	2.97	0.42
1:E:429:LEU:HD12	1:E:430:ILE:N	2.34	0.42
1:F:429:LEU:HD12	1:F:430:ILE:N	2.34	0.42
1:D:130:LEU:HD11	1:D:163:PHE:CZ	2.54	0.42
1:A:127:THR:CB	1:A:438:ASP:HA	2.37	0.42
1:E:130:LEU:HD11	1:E:163:PHE:CZ	2.54	0.42
1:D:170:PRO:HB2	1:D:173:TYR:HD2	1.84	0.42
1:D:109:LYS:HE2	1:D:174:CYS:O	2.19	0.42
1:C:27:ILE:O	1:C:82:ILE:HG22	2.19	0.42
1:A:270:ASN:HA	1:A:304:ASP:HB3	2.00	0.42
1:A:27:ILE:O	1:A:82:ILE:HG22	2.19	0.42
1:C:120:ASP:N	1:C:120:ASP:OD1	2.52	0.42
1:D:113:ARG:NH2	1:D:183:HIS:CD2	2.88	0.42
1:C:130:LEU:HD11	1:C:163:PHE:CZ	2.54	0.42
1:F:113:ARG:NH2	1:F:183:HIS:CD2	2.88	0.42
1:E:113:ARG:NH2	1:E:183:HIS:CD2	2.88	0.42
1:E:170:PRO:HB2	1:E:173:TYR:HD2	1.84	0.42
1:F:27:ILE:O	1:F:82:ILE:HG22	2.19	0.42
1:A:307:ASP:N	1:A:307:ASP:OD1	2.51	0.42
1:D:192:GLU:N	1:D:192:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:LEU:HD12	1:D:430:ILE:N	2.34	0.42
1:E:750:ASN:HA	1:E:753:ARG:HG2	2.02	0.42
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.54	0.42
1:E:109:LYS:HE2	1:E:174:CYS:O	2.19	0.42
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.54	0.42
1:D:82:ILE:HG12	1:D:84:MET:HG3	2.00	0.42
1:A:82:ILE:HG12	1:A:84:MET:HG3	2.00	0.42
1:E:82:ILE:HG12	1:E:84:MET:HG3	2.00	0.42
1:E:682:PHE:CZ	1:E:743:ALA:HB1	2.55	0.42
1:A:500:PRO:O	1:A:504:LEU:HD13	2.19	0.42
1:B:216:ILE:O	1:B:220:VAL:HG22	2.19	0.42
1:C:500:PRO:O	1:C:504:LEU:HD13	2.19	0.42
1:E:216:ILE:O	1:E:220:VAL:HG22	2.19	0.42
1:C:307:ASP:OD1	1:C:307:ASP:N	2.51	0.42
1:F:187:GLU:HG2	1:F:187:GLU:O	2.19	0.42
1:F:120:ASP:OD1	1:F:120:ASP:N	2.52	0.42
1:B:109:LYS:HE2	1:B:174:CYS:O	2.19	0.42
1:F:109:LYS:HE2	1:F:174:CYS:O	2.19	0.42
1:D:203:TYR:CE2	1:D:261:GLU:HG2	2.54	0.42
1:F:682:PHE:CZ	1:F:743:ALA:HB1	2.55	0.42
1:C:115:HIS:NE2	1:C:185:GLU:HG2	2.34	0.42
1:E:307:ASP:N	1:E:307:ASP:OD1	2.51	0.42
1:A:294:GLU:CG	1:A:338:ARG:CG	2.97	0.42
1:F:294:GLU:CG	1:F:338:ARG:CG	2.97	0.42
1:C:114:ILE:HG22	1:C:116:VAL:HG13	2.02	0.42
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.54	0.42
1:E:27:ILE:O	1:E:82:ILE:HG22	2.19	0.42
1:D:682:PHE:CZ	1:D:743:ALA:HB1	2.55	0.42
1:B:652:SER:O	1:B:655:ALA:N	2.53	0.42
1:E:192:GLU:OE1	1:E:192:GLU:N	2.52	0.42
1:D:393:ASP:OD1	1:D:393:ASP:N	2.52	0.42
1:A:187:GLU:HG2	1:A:187:GLU:O	2.19	0.42
1:E:120:ASP:OD1	1:E:120:ASP:N	2.52	0.42
1:C:652:SER:O	1:C:655:ALA:N	2.53	0.42
1:E:294:GLU:CG	1:E:338:ARG:CG	2.97	0.42
1:D:750:ASN:HA	1:D:753:ARG:HG2	2.02	0.42
1:F:750:ASN:HA	1:F:753:ARG:HG2	2.02	0.42
1:C:750:ASN:HA	1:C:753:ARG:HG2	2.02	0.42
1:A:109:LYS:HE2	1:A:174:CYS:O	2.19	0.42
1:C:113:ARG:NH2	1:C:183:HIS:CD2	2.88	0.42
1:B:500:PRO:O	1:B:504:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:SER:O	1:A:655:ALA:N	2.53	0.42
1:C:393:ASP:N	1:C:393:ASP:OD1	2.52	0.42
1:E:393:ASP:OD1	1:E:393:ASP:N	2.52	0.42
1:A:143:TYR:CE1	1:A:178:PRO:HD3	2.49	0.42
1:F:114:ILE:HG22	1:F:116:VAL:HG13	2.02	0.42
1:B:114:ILE:HG22	1:B:116:VAL:HG13	2.02	0.42
1:A:114:ILE:HG22	1:A:116:VAL:HG13	2.02	0.42
1:C:109:LYS:HE2	1:C:174:CYS:O	2.19	0.42
1:C:170:PRO:HB2	1:C:173:TYR:HD2	1.84	0.42
1:C:684:GLY:HA3	2:C:900:ADP:C8	2.54	0.42
1:C:82:ILE:HG12	1:C:84:MET:HG3	2.00	0.42
1:D:652:SER:O	1:D:655:ALA:N	2.53	0.42
1:C:216:ILE:O	1:C:220:VAL:HG22	2.19	0.42
1:F:652:SER:O	1:F:655:ALA:N	2.53	0.42
1:B:120:ASP:OD1	1:B:120:ASP:N	2.52	0.42
1:B:750:ASN:HA	1:B:753:ARG:HG2	2.02	0.42
1:B:170:PRO:HB2	1:B:173:TYR:HD2	1.84	0.42
1:C:270:ASN:HA	1:C:304:ASP:HB3	2.00	0.42
1:F:270:ASN:HA	1:F:304:ASP:HB3	2.00	0.42
1:D:216:ILE:O	1:D:220:VAL:HG22	2.19	0.42
1:D:187:GLU:HG2	1:D:187:GLU:O	2.19	0.42
1:B:187:GLU:HG2	1:B:187:GLU:O	2.19	0.42
1:E:42:SER:HB2	1:E:45:LYS:HZ3	1.85	0.41
1:D:114:ILE:HG22	1:D:116:VAL:HG13	2.02	0.41
1:A:113:ARG:NH2	1:A:183:HIS:CD2	2.88	0.41
1:A:170:PRO:HB2	1:A:173:TYR:HD2	1.84	0.41
1:B:393:ASP:OD1	1:B:393:ASP:N	2.52	0.41
1:A:393:ASP:OD1	1:A:393:ASP:N	2.52	0.41
1:F:476:TRP:CZ3	1:F:486:LYS:HG2	2.55	0.41
1:C:682:PHE:CZ	1:C:743:ALA:HB1	2.55	0.41
1:F:397:GLU:O	1:F:401:ASN:N	2.39	0.41
1:A:120:ASP:OD1	1:A:120:ASP:N	2.52	0.41
1:F:203:TYR:CE2	1:F:261:GLU:HG2	2.54	0.41
1:B:517:TYR:HA	1:B:623:THR:O	2.20	0.41
1:A:682:PHE:CZ	1:A:743:ALA:HB1	2.55	0.41
1:D:155:ARG:HE	1:D:386:LYS:HZ2	1.69	0.41
1:E:652:SER:O	1:E:655:ALA:N	2.53	0.41
1:A:519:PRO:HD2	1:A:645:ILE:O	2.21	0.41
1:A:750:ASN:HA	1:A:753:ARG:HG2	2.02	0.41
1:F:170:PRO:HB2	1:F:173:TYR:HD2	1.84	0.41
1:B:113:ARG:NH2	1:B:183:HIS:CD2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:ASP:HB2	1:D:397:GLU:OE1	2.21	0.41
1:D:580:ASP:HB3	1:D:629:ILE:HD11	2.02	0.41
1:E:114:ILE:HG22	1:E:116:VAL:HG13	2.02	0.41
1:B:682:PHE:CZ	1:B:743:ALA:HB1	2.55	0.41
1:C:580:ASP:HB3	1:C:629:ILE:HD11	2.02	0.41
1:D:120:ASP:OD1	1:D:120:ASP:N	2.52	0.41
1:E:476:TRP:CZ3	1:E:486:LYS:HG2	2.55	0.41
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.54	0.41
1:D:517:TYR:HA	1:D:623:THR:O	2.20	0.41
1:E:517:TYR:HA	1:E:623:THR:O	2.20	0.41
1:C:395:ASP:HB2	1:C:397:GLU:OE1	2.21	0.41
1:D:55:ASP:OD1	1:D:71:VAL:HG22	2.21	0.41
1:B:395:ASP:HB2	1:B:397:GLU:OE1	2.21	0.41
1:E:187:GLU:O	1:E:187:GLU:HG2	2.19	0.41
1:D:669:ASP:OD1	1:D:669:ASP:N	2.54	0.41
1:E:669:ASP:N	1:E:669:ASP:OD1	2.54	0.41
1:C:517:TYR:HA	1:C:623:THR:O	2.20	0.41
1:F:38:VAL:HA	1:F:70:ILE:O	2.21	0.41
1:C:55:ASP:OD1	1:C:71:VAL:HG22	2.21	0.41
1:F:127:THR:CB	1:F:438:ASP:HA	2.37	0.41
1:E:519:PRO:HD2	1:E:645:ILE:O	2.21	0.41
1:A:476:TRP:CZ3	1:A:486:LYS:HG2	2.55	0.41
1:F:517:TYR:HA	1:F:623:THR:O	2.20	0.41
1:A:38:VAL:HA	1:A:70:ILE:O	2.21	0.41
1:B:38:VAL:HA	1:B:70:ILE:O	2.21	0.41
1:D:657:LEU:HD23	1:D:657:LEU:HA	1.92	0.41
1:C:187:GLU:HG2	1:C:187:GLU:O	2.19	0.41
1:F:519:PRO:HD2	1:F:645:ILE:O	2.21	0.41
1:B:482:LEU:O	1:B:486:LYS:HG3	2.21	0.41
1:D:476:TRP:CZ3	1:D:486:LYS:HG2	2.55	0.41
1:D:143:TYR:CE1	1:D:178:PRO:HD3	2.49	0.41
1:D:377:ARG:NE	1:D:403:THR:O	2.54	0.41
1:A:290:PHE:CD2	1:A:331:LEU:HB3	2.56	0.41
1:A:517:TYR:HA	1:A:623:THR:O	2.20	0.41
1:E:55:ASP:OD1	1:E:71:VAL:HG22	2.21	0.41
1:A:395:ASP:HB2	1:A:397:GLU:OE1	2.21	0.41
1:C:669:ASP:OD1	1:C:669:ASP:N	2.54	0.41
1:B:55:ASP:OD1	1:B:71:VAL:HG22	2.21	0.41
1:B:127:THR:CB	1:B:438:ASP:HA	2.37	0.41
1:B:441:VAL:O	1:B:444:SER:OG	2.28	0.41
1:A:109:LYS:O	1:A:175:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:PHE:CD2	1:B:331:LEU:HB3	2.56	0.41
1:A:688:THR:O	1:A:692:GLN:HG3	2.21	0.41
1:D:688:THR:O	1:D:692:GLN:HG3	2.21	0.41
1:C:519:PRO:HD2	1:C:645:ILE:O	2.21	0.40
1:C:476:TRP:CZ3	1:C:486:LYS:HG2	2.55	0.40
1:D:482:LEU:O	1:D:486:LYS:HG3	2.21	0.40
1:B:377:ARG:NE	1:B:403:THR:O	2.54	0.40
1:E:377:ARG:NE	1:E:403:THR:O	2.54	0.40
1:E:395:ASP:HB2	1:E:397:GLU:OE1	2.21	0.40
1:F:310:ALA:HA	1:F:325:VAL:HG22	2.03	0.40
1:B:580:ASP:HB3	1:B:629:ILE:HD11	2.02	0.40
1:F:669:ASP:OD1	1:F:669:ASP:N	2.54	0.40
1:B:519:PRO:HD2	1:B:645:ILE:O	2.21	0.40
1:C:290:PHE:CD2	1:C:331:LEU:HB3	2.56	0.40
1:F:688:THR:O	1:F:692:GLN:HG3	2.21	0.40
1:A:580:ASP:HB3	1:A:629:ILE:HD11	2.02	0.40
1:E:580:ASP:HB3	1:E:629:ILE:HD11	2.02	0.40
1:C:426:LYS:HD2	1:C:426:LYS:HA	1.88	0.40
1:A:482:LEU:O	1:A:486:LYS:HG3	2.21	0.40
1:B:476:TRP:CZ3	1:B:486:LYS:HG2	2.55	0.40
1:E:349:ARG:HA	1:E:350:PRO:HD3	1.97	0.40
1:B:109:LYS:O	1:B:175:ILE:HB	2.22	0.40
1:B:688:THR:O	1:B:692:GLN:HG3	2.21	0.40
1:F:580:ASP:HB3	1:F:629:ILE:HD11	2.02	0.40
1:F:55:ASP:OD1	1:F:71:VAL:HG22	2.21	0.40
1:D:519:PRO:HD2	1:D:645:ILE:O	2.21	0.40
1:A:377:ARG:NE	1:A:403:THR:O	2.54	0.40
1:A:426:LYS:HA	1:A:426:LYS:HD2	1.88	0.40
1:B:315:LYS:NZ	1:B:321:GLU:OE2	2.42	0.40
1:F:143:TYR:CE1	1:F:178:PRO:HD3	2.48	0.40
1:E:482:LEU:O	1:E:486:LYS:HG3	2.21	0.40
1:F:377:ARG:NE	1:F:403:THR:O	2.54	0.40
1:F:395:ASP:HB2	1:F:397:GLU:OE1	2.21	0.40
1:A:55:ASP:OD1	1:A:71:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	26	66
1	B	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	26	66
1	C	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	26	66
1	D	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	26	66
1	E	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	26	66
1	F	719/806 (89%)	670 (93%)	44 (6%)	5 (1%)	26	66
All	All	4314/4836 (89%)	4020 (93%)	264 (6%)	30 (1%)	31	66

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	ASP
1	B	169	ASP
1	C	169	ASP
1	D	169	ASP
1	E	169	ASP
1	F	169	ASP
1	A	339	ALA
1	B	339	ALA
1	C	339	ALA
1	D	339	ALA
1	E	339	ALA
1	F	339	ALA
1	A	170	PRO
1	B	170	PRO
1	C	170	PRO
1	D	170	PRO
1	E	170	PRO
1	F	170	PRO
1	A	315	LYS
1	B	315	LYS

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Mol	Chain	Res	Type
1	C	315	LYS
1	D	315	LYS
1	E	315	LYS
1	F	315	LYS
1	A	172	PRO
1	B	172	PRO
1	C	172	PRO
1	D	172	PRO
1	E	172	PRO
1	F	172	PRO

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	615/678 (91%)	615 (100%)	0	100	100
1	B	615/678 (91%)	615 (100%)	0	100	100
1	C	615/678 (91%)	615 (100%)	0	100	100
1	D	615/678 (91%)	615 (100%)	0	100	100
1	E	615/678 (91%)	615 (100%)	0	100	100
1	F	615/678 (91%)	615 (100%)	0	100	100
All	All	3690/4068 (91%)	3690 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	285	ASN
1	A	337	GLN
1	A	340	HIS
1	A	421	GLN
1	A	533	ASN

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Mol	Chain	Res	Type
1	A	538	ASN
1	B	36	ASN
1	B	285	ASN
1	B	337	GLN
1	B	340	HIS
1	B	421	GLN
1	B	533	ASN
1	B	538	ASN
1	C	36	ASN
1	C	285	ASN
1	C	337	GLN
1	C	340	HIS
1	C	421	GLN
1	C	533	ASN
1	C	538	ASN
1	D	36	ASN
1	D	285	ASN
1	D	337	GLN
1	D	340	HIS
1	D	421	GLN
1	D	533	ASN
1	D	538	ASN
1	E	36	ASN
1	E	337	GLN
1	E	340	HIS
1	E	421	GLN
1	E	533	ASN
1	E	538	ASN
1	F	36	ASN
1	F	285	ASN
1	F	337	GLN
1	F	340	HIS
1	F	421	GLN
1	F	533	ASN
1	F	538	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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	ADP	A	807	-	24,29,29	1.02	1 (4%)	23,45,45	1.72	2 (8%)
2	ADP	A	900	-	24,29,29	0.94	1 (4%)	23,45,45	1.80	1 (4%)
2	ADP	B	807	-	24,29,29	1.02	1 (4%)	23,45,45	1.72	2 (8%)
2	ADP	B	900	-	24,29,29	0.93	1 (4%)	23,45,45	1.81	2 (8%)
2	ADP	C	807	-	24,29,29	1.03	1 (4%)	23,45,45	1.72	2 (8%)
2	ADP	C	900	-	24,29,29	0.94	1 (4%)	23,45,45	1.80	1 (4%)
2	ADP	D	807	-	24,29,29	1.02	1 (4%)	23,45,45	1.72	2 (8%)
2	ADP	D	900	-	24,29,29	0.94	1 (4%)	23,45,45	1.81	1 (4%)
2	ADP	E	807	-	24,29,29	1.02	1 (4%)	23,45,45	1.72	2 (8%)
2	ADP	E	900	-	24,29,29	0.93	1 (4%)	23,45,45	1.80	1 (4%)
2	ADP	F	807	-	24,29,29	1.03	1 (4%)	23,45,45	1.73	2 (8%)
2	ADP	F	900	-	24,29,29	0.93	1 (4%)	23,45,45	1.81	1 (4%)

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	ADP	A	807	-	-	0/12/32/32	0/3/3/3
2	ADP	A	900	-	-	0/12/32/32	0/3/3/3
2	ADP	B	807	-	-	0/12/32/32	0/3/3/3
2	ADP	B	900	-	-	0/12/32/32	0/3/3/3
2	ADP	C	807	-	-	0/12/32/32	0/3/3/3
2	ADP	C	900	-	-	0/12/32/32	0/3/3/3
2	ADP	D	807	-	-	0/12/32/32	0/3/3/3
2	ADP	D	900	-	-	0/12/32/32	0/3/3/3
2	ADP	E	807	-	-	0/12/32/32	0/3/3/3
2	ADP	E	900	-	-	0/12/32/32	0/3/3/3
2	ADP	F	807	-	-	0/12/32/32	0/3/3/3
2	ADP	F	900	-	-	0/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	807	ADP	C5-C4	2.27	1.45	1.40
2	F	807	ADP	C5-C4	2.27	1.45	1.40
2	A	807	ADP	C5-C4	2.27	1.45	1.40
2	D	807	ADP	C5-C4	2.27	1.45	1.40
2	E	807	ADP	C5-C4	2.28	1.45	1.40
2	B	807	ADP	C5-C4	2.29	1.45	1.40
2	B	900	ADP	C5-C4	2.44	1.46	1.40
2	E	900	ADP	C5-C4	2.44	1.46	1.40
2	A	900	ADP	C5-C4	2.45	1.46	1.40
2	D	900	ADP	C5-C4	2.45	1.46	1.40
2	C	900	ADP	C5-C4	2.45	1.46	1.40
2	F	900	ADP	C5-C4	2.45	1.46	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	ADP	N3-C2-N1	-6.73	123.58	128.87
2	F	900	ADP	N3-C2-N1	-6.72	123.59	128.87
2	D	900	ADP	N3-C2-N1	-6.72	123.59	128.87
2	A	900	ADP	N3-C2-N1	-6.68	123.62	128.87
2	C	900	ADP	N3-C2-N1	-6.67	123.63	128.87
2	E	900	ADP	N3-C2-N1	-6.67	123.64	128.87
2	F	807	ADP	N3-C2-N1	-5.88	124.25	128.87
2	C	807	ADP	N3-C2-N1	-5.86	124.27	128.87
2	A	807	ADP	N3-C2-N1	-5.86	124.27	128.87
2	D	807	ADP	N3-C2-N1	-5.86	124.27	128.87
2	E	807	ADP	N3-C2-N1	-5.82	124.30	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	807	ADP	N3-C2-N1	-5.80	124.31	128.87
2	A	807	ADP	C2'-C1'-N9	-2.37	107.13	113.47
2	E	807	ADP	C2'-C1'-N9	-2.37	107.13	113.47
2	B	807	ADP	C2'-C1'-N9	-2.36	107.14	113.47
2	D	807	ADP	C2'-C1'-N9	-2.36	107.15	113.47
2	F	807	ADP	C2'-C1'-N9	-2.36	107.15	113.47
2	C	807	ADP	C2'-C1'-N9	-2.35	107.17	113.47
2	B	900	ADP	N6-C6-N1	2.01	121.89	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	807	ADP	1	0
2	A	900	ADP	2	0
2	B	807	ADP	1	0
2	B	900	ADP	2	0
2	C	807	ADP	1	0
2	C	900	ADP	2	0
2	D	807	ADP	1	0
2	D	900	ADP	2	0
2	E	807	ADP	1	0
2	E	900	ADP	2	0
2	F	807	ADP	1	0
2	F	900	ADP	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.