



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:21 PM UTC

PDB ID : 2ZY5 / pdb_00002zy5
Title : R487A mutant of L-aspartate beta-decarboxylase
Authors : Chen, H.-J.; Ko, T.-P.; Lee, C.-Y.; Wang, N.-C.; Wang, A.H.-J.
Deposited on : 2009-01-13
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

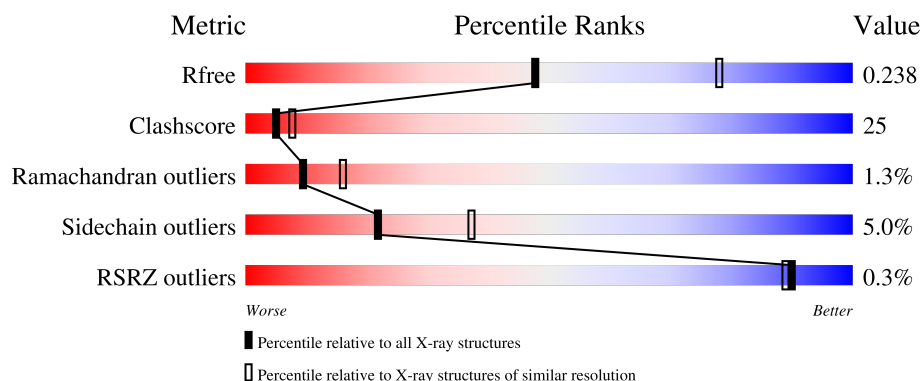
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	546	 49% 39% 6% 7%
1	B	546	 56% 34% • • 6%
1	C	546	 53% 34% 7% • 6%
1	D	546	 54% 34% 6% 6%
1	E	546	 49% 40% 5% 6%

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Mol	Chain	Length	Quality of chain
1	F	546	% 53% 34% 9% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called L-aspartate beta-decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4005	2550	681	757	17			
1	B	515	Total	C	N	O	S	0	0	0
			4048	2576	688	767	17			
1	C	515	Total	C	N	O	S	0	0	0
			4048	2576	688	767	17			
1	D	511	Total	C	N	O	S	0	0	0
			4011	2550	685	759	17			
1	E	511	Total	C	N	O	S	0	0	0
			4018	2558	683	760	17			
1	F	521	Total	C	N	O	S	0	0	0
			4094	2605	696	776	17			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	487	ALA	ARG	engineered mutation	UNP Q93QX0
A	534	LYS	-	expression tag	UNP Q93QX0
A	535	LEU	-	expression tag	UNP Q93QX0
A	536	ALA	-	expression tag	UNP Q93QX0
A	537	ALA	-	expression tag	UNP Q93QX0
A	538	ALA	-	expression tag	UNP Q93QX0
A	539	LEU	-	expression tag	UNP Q93QX0
A	540	GLU	-	expression tag	UNP Q93QX0
A	541	HIS	-	expression tag	UNP Q93QX0
A	542	HIS	-	expression tag	UNP Q93QX0
A	543	HIS	-	expression tag	UNP Q93QX0
A	544	HIS	-	expression tag	UNP Q93QX0
A	545	HIS	-	expression tag	UNP Q93QX0
A	546	HIS	-	expression tag	UNP Q93QX0
B	487	ALA	ARG	engineered mutation	UNP Q93QX0
B	534	LYS	-	expression tag	UNP Q93QX0
B	535	LEU	-	expression tag	UNP Q93QX0

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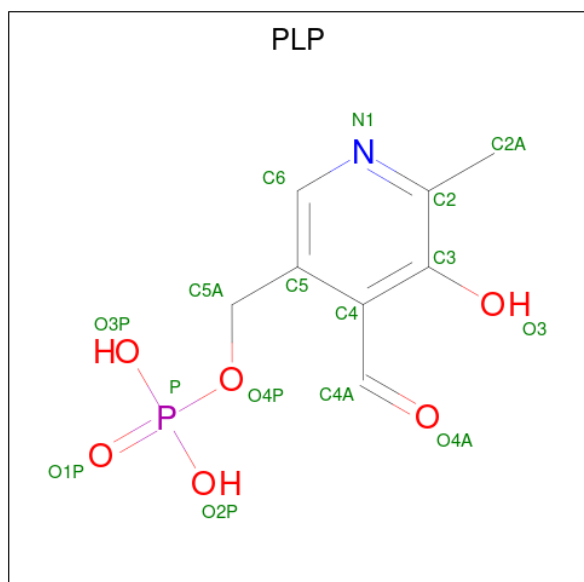
Chain	Residue	Modelled	Actual	Comment	Reference
B	536	ALA	-	expression tag	UNP Q93QX0
B	537	ALA	-	expression tag	UNP Q93QX0
B	538	ALA	-	expression tag	UNP Q93QX0
B	539	LEU	-	expression tag	UNP Q93QX0
B	540	GLU	-	expression tag	UNP Q93QX0
B	541	HIS	-	expression tag	UNP Q93QX0
B	542	HIS	-	expression tag	UNP Q93QX0
B	543	HIS	-	expression tag	UNP Q93QX0
B	544	HIS	-	expression tag	UNP Q93QX0
B	545	HIS	-	expression tag	UNP Q93QX0
B	546	HIS	-	expression tag	UNP Q93QX0
C	487	ALA	ARG	engineered mutation	UNP Q93QX0
C	534	LYS	-	expression tag	UNP Q93QX0
C	535	LEU	-	expression tag	UNP Q93QX0
C	536	ALA	-	expression tag	UNP Q93QX0
C	537	ALA	-	expression tag	UNP Q93QX0
C	538	ALA	-	expression tag	UNP Q93QX0
C	539	LEU	-	expression tag	UNP Q93QX0
C	540	GLU	-	expression tag	UNP Q93QX0
C	541	HIS	-	expression tag	UNP Q93QX0
C	542	HIS	-	expression tag	UNP Q93QX0
C	543	HIS	-	expression tag	UNP Q93QX0
C	544	HIS	-	expression tag	UNP Q93QX0
C	545	HIS	-	expression tag	UNP Q93QX0
C	546	HIS	-	expression tag	UNP Q93QX0
D	487	ALA	ARG	engineered mutation	UNP Q93QX0
D	534	LYS	-	expression tag	UNP Q93QX0
D	535	LEU	-	expression tag	UNP Q93QX0
D	536	ALA	-	expression tag	UNP Q93QX0
D	537	ALA	-	expression tag	UNP Q93QX0
D	538	ALA	-	expression tag	UNP Q93QX0
D	539	LEU	-	expression tag	UNP Q93QX0
D	540	GLU	-	expression tag	UNP Q93QX0
D	541	HIS	-	expression tag	UNP Q93QX0
D	542	HIS	-	expression tag	UNP Q93QX0
D	543	HIS	-	expression tag	UNP Q93QX0
D	544	HIS	-	expression tag	UNP Q93QX0
D	545	HIS	-	expression tag	UNP Q93QX0
D	546	HIS	-	expression tag	UNP Q93QX0
E	487	ALA	ARG	engineered mutation	UNP Q93QX0
E	534	LYS	-	expression tag	UNP Q93QX0
E	535	LEU	-	expression tag	UNP Q93QX0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	536	ALA	-	expression tag	UNP Q93QX0
E	537	ALA	-	expression tag	UNP Q93QX0
E	538	ALA	-	expression tag	UNP Q93QX0
E	539	LEU	-	expression tag	UNP Q93QX0
E	540	GLU	-	expression tag	UNP Q93QX0
E	541	HIS	-	expression tag	UNP Q93QX0
E	542	HIS	-	expression tag	UNP Q93QX0
E	543	HIS	-	expression tag	UNP Q93QX0
E	544	HIS	-	expression tag	UNP Q93QX0
E	545	HIS	-	expression tag	UNP Q93QX0
E	546	HIS	-	expression tag	UNP Q93QX0
F	487	ALA	ARG	engineered mutation	UNP Q93QX0
F	534	LYS	-	expression tag	UNP Q93QX0
F	535	LEU	-	expression tag	UNP Q93QX0
F	536	ALA	-	expression tag	UNP Q93QX0
F	537	ALA	-	expression tag	UNP Q93QX0
F	538	ALA	-	expression tag	UNP Q93QX0
F	539	LEU	-	expression tag	UNP Q93QX0
F	540	GLU	-	expression tag	UNP Q93QX0
F	541	HIS	-	expression tag	UNP Q93QX0
F	542	HIS	-	expression tag	UNP Q93QX0
F	543	HIS	-	expression tag	UNP Q93QX0
F	544	HIS	-	expression tag	UNP Q93QX0
F	545	HIS	-	expression tag	UNP Q93QX0
F	546	HIS	-	expression tag	UNP Q93QX0

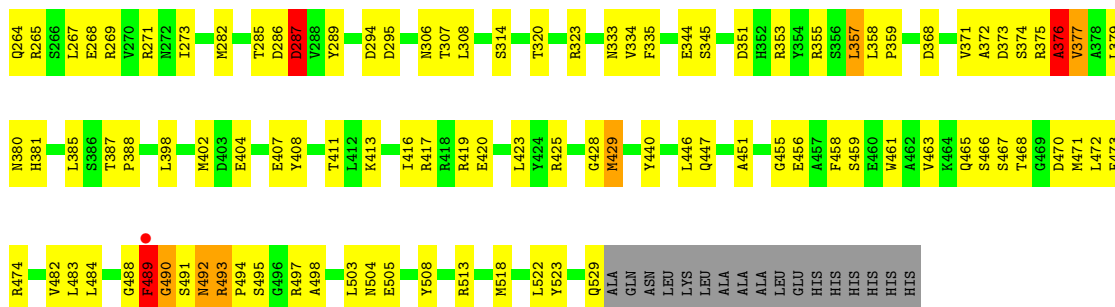
- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

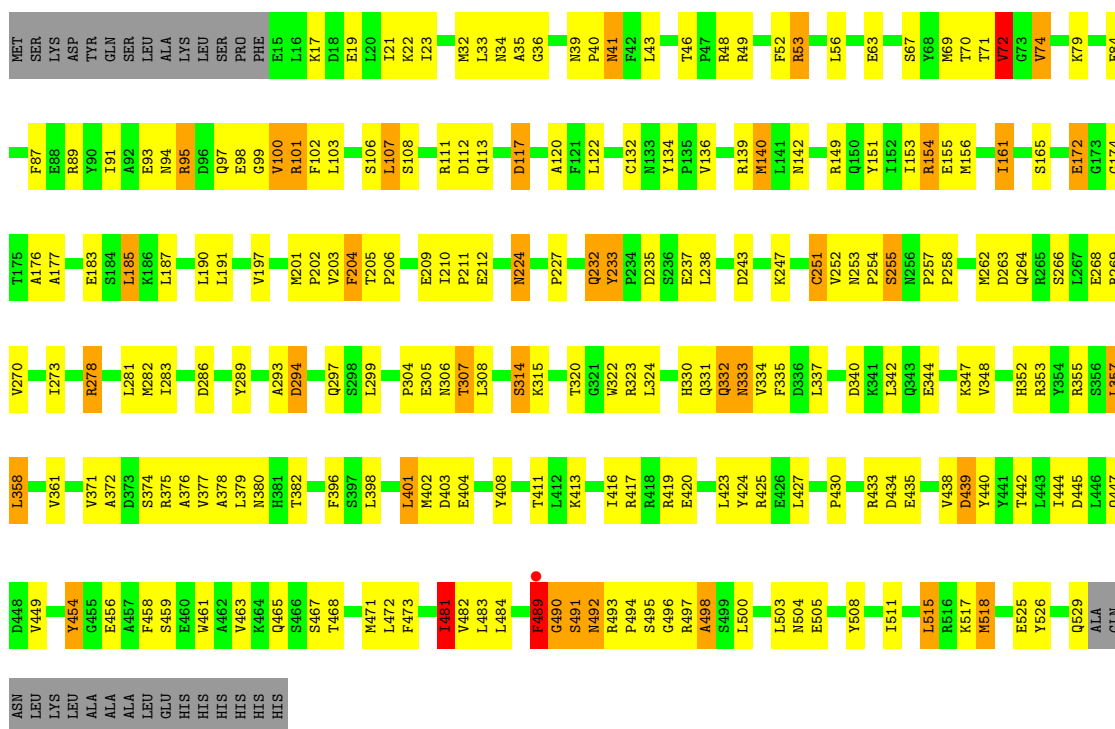
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	318	Total	O	0	0
			318	318		
3	B	355	Total	O	0	0
			355	355		
3	C	337	Total	O	0	0
			337	337		
3	D	342	Total	O	0	0
			342	342		
3	E	282	Total	O	0	0
			282	282		
3	F	265	Total	O	0	0
			265	265		



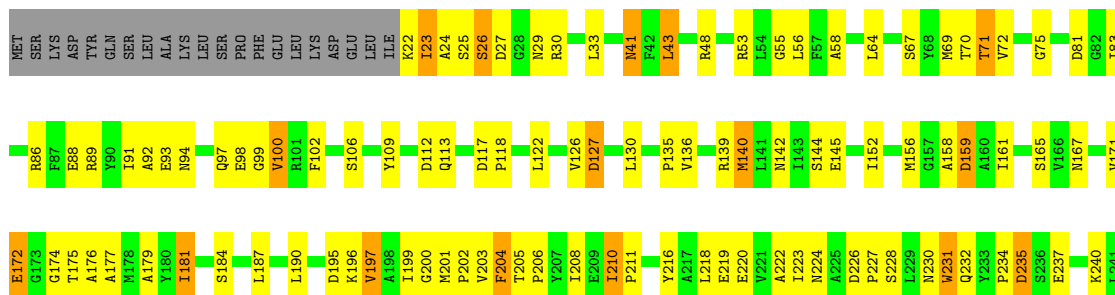
• Molecule 1: L-aspartate beta-decarboxylase

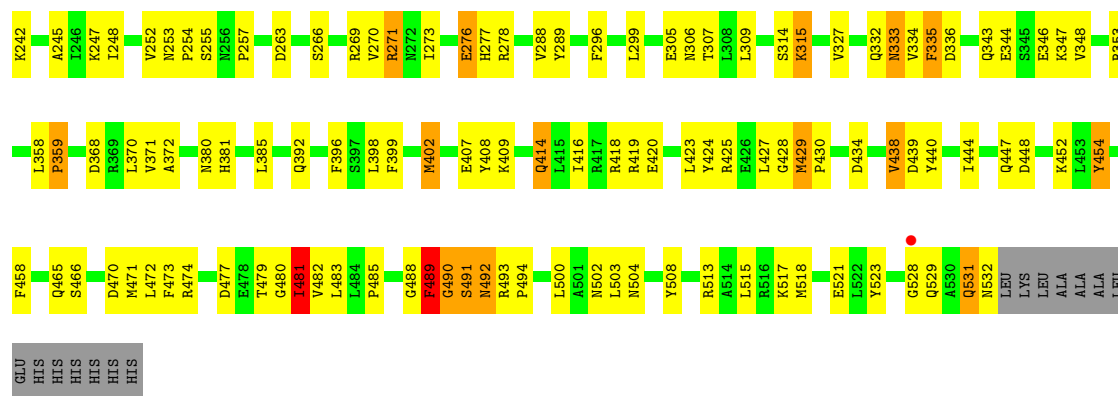
Chain C: 53% 34% 7% 6%



• Molecule 1: L-aspartate beta-decarboxylase

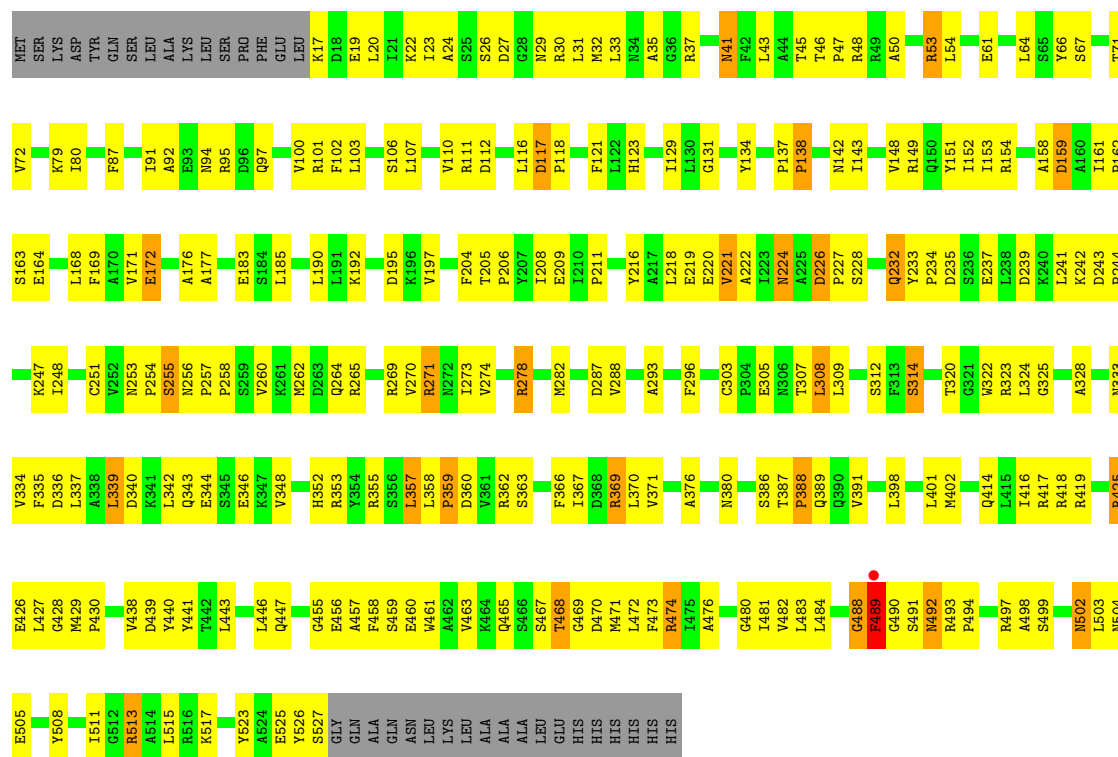
Chain D: 54% 34% 6% 6%





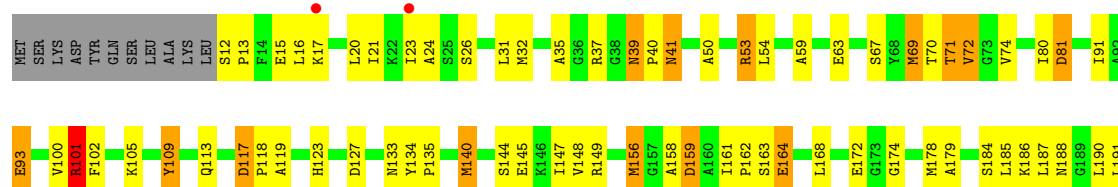
• Molecule 1: L-aspartate beta-decarboxylase

Chain E: 49% 40% 5% 6%



• Molecule 1: L-aspartate beta-decarboxylase

Chain F: 53% 34% 9% 5%



ALA	G455	K192	R271	S345	G456
ALA	E456	A193	V274	E346	E457
LEU	A457	G194	H277	K347	F458
GLU	F458	D195	R278	V348	S459
HIS	S459	K196	P279	R353	E460
HIS	HIS	V197	D280	Y354	W461
HIS	HIS	A198	P279	R355	A462
HIS	HIS	I199	L281	L358	W463
HIS	HIS	G200	M282	P359	K464
HIS	HIS	M201	T285	D360	Q465
		V203	D286	V361	T468
		F204	D287	R362	G469
		T205	Y288	I367	D470
		I208	Y289	R368	M471
		Q215	A293	R369	L472
		E220	F296	L370	F473
		D226	Q297	R375	R474
		P227	Q297	A376	I475
		S228	L299	V377	A476
		L229	F300	A378	D477
		N230	A301	L379	E478
		W231	P304	N380	I481
		P234	E305	T387	V482
		D235	N306	P388	L483
		S236	T307	M402	L484
		E237	L308	D403	A487
		L238	V310	E404	G488
		K240	Y311	R417	F489
		L241	S312	R418	S491
		A245	F313	R419	N492
		I246	S314	E420	R493
		K247	A319	R425	R497
		I248	T320	G428	A501
		N253	W322	M429	Y508
		P254	R323	P430	G512
		S255	L324	R433	R513
		N256	H330	D434	A514
		P257	Q331	E435	L515
		P258	Q332	N436	D520
		S259	N333	N437	Y526
		V260	V334	A437	Q529
		K261	F335	W438	A530
		M262	D336	D439	A531
		D263	L337	Y440	N532
		S266	A338	D445	Q531
		L267	L339	L446	LEU
		E268	D340	Q447	N532
		R269	K341	D448	LEU
		V270	L342	D448	LYS
			Q343		LEU
			E344		ALA

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	149.95Å 216.22Å 208.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 30.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.7 (30.00-2.65) 86.9 (30.00-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.238 0.175 , 0.238	Depositor DCC
R_{free} test set	4320 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26213	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	2/4087 (0.0%)	1.24	35/5536 (0.6%)
1	B	0.84	1/4130 (0.0%)	1.25	34/5593 (0.6%)
1	C	0.84	3/4130 (0.1%)	1.25	42/5593 (0.8%)
1	D	0.84	3/4093 (0.1%)	1.23	39/5544 (0.7%)
1	E	0.79	0/4100	1.20	35/5553 (0.6%)
1	F	0.85	4/4178 (0.1%)	1.27	36/5659 (0.6%)
All	All	0.83	13/24718 (0.1%)	1.24	221/33478 (0.7%)

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	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	MET	SD-CE	8.63	2.01	1.79
1	F	402	MET	SD-CE	-5.89	1.64	1.79
1	D	402	MET	SD-CE	-5.77	1.65	1.79
1	F	282	MET	SD-CE	-5.59	1.65	1.79
1	D	152	ILE	CA-CB	5.55	1.61	1.54
1	C	518	MET	SD-CE	5.50	1.93	1.79
1	F	481	ILE	CA-CB	5.43	1.60	1.54
1	C	416	ILE	CA-CB	5.27	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	VAL	CA-CB	5.17	1.60	1.54
1	F	69	MET	SD-CE	5.14	1.92	1.79
1	A	21	ILE	CA-C	5.14	1.59	1.52
1	C	315	LYS	CE-NZ	-5.10	1.34	1.49
1	A	375	ARG	CA-CB	5.08	1.57	1.53

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	VAL	N-CA-C	-14.34	100.29	111.62
1	F	314	SER	N-CA-C	11.35	123.21	111.07
1	C	440	TYR	N-CA-C	-10.94	99.44	111.36
1	A	142	ASN	N-CA-C	10.89	122.84	110.97
1	B	314	SER	N-CA-C	9.75	122.81	111.11
1	E	440	TYR	N-CA-C	-9.68	100.57	111.71
1	F	435	GLU	N-CA-C	-9.68	101.58	113.97
1	F	440	TYR	N-CA-C	-9.62	100.66	111.82
1	A	314	SER	N-CA-C	9.46	122.46	111.11
1	C	142	ASN	N-CA-C	8.74	120.49	110.97
1	F	67	SER	N-CA-C	8.69	123.94	113.16
1	F	307	THR	N-CA-C	8.65	123.50	109.40
1	C	233	TYR	CA-C-N	-8.42	112.05	120.31
1	C	233	TYR	C-N-CA	-8.42	112.05	120.31
1	B	489	PHE	N-CA-C	8.38	122.04	110.06
1	E	488	GLY	O-C-N	8.25	133.42	122.70
1	E	224	ASN	N-CA-C	8.23	122.30	109.96
1	B	223	ILE	N-CA-C	-8.22	95.17	106.85
1	A	224	ASN	N-CA-C	8.18	121.77	109.25
1	C	224	ASN	N-CA-C	8.06	121.58	109.25
1	A	524	ALA	N-CA-C	-7.85	102.67	111.07
1	B	440	TYR	N-CA-C	-7.84	102.35	112.23
1	D	224	ASN	N-CA-C	7.76	120.99	109.59
1	E	208	ILE	N-CA-C	-7.72	105.65	111.90
1	F	255	SER	N-CA-C	7.68	120.50	110.43
1	B	493	ARG	N-CA-C	7.64	125.39	109.11
1	F	117	ASP	CA-C-N	7.58	126.85	118.97
1	F	117	ASP	C-N-CA	7.58	126.85	118.97
1	D	83	ILE	N-CA-C	7.57	118.37	110.72
1	C	46	THR	CA-C-N	-7.46	112.11	119.87
1	C	46	THR	C-N-CA	-7.46	112.11	119.87
1	A	137	PRO	CA-C-N	7.43	127.45	119.28
1	A	137	PRO	C-N-CA	7.43	127.45	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	440	TYR	N-CA-C	-7.40	103.22	111.28
1	B	505	GLU	N-CA-C	7.38	119.97	111.11
1	B	208	ILE	N-CA-C	-7.34	105.50	111.81
1	F	13	PRO	CA-C-N	-7.29	110.98	122.65
1	F	13	PRO	C-N-CA	-7.29	110.98	122.65
1	D	439	ASP	N-CA-C	7.28	121.55	112.24
1	E	314	SER	N-CA-C	7.27	120.13	111.33
1	A	83	ILE	N-CA-C	7.25	118.02	110.62
1	B	130	LEU	N-CA-C	-7.23	103.12	112.23
1	D	257	PRO	N-CA-C	7.12	130.61	112.10
1	A	430	PRO	CA-C-N	7.09	127.12	119.89
1	A	430	PRO	C-N-CA	7.09	127.12	119.89
1	A	294	ASP	N-CA-C	7.07	118.78	111.14
1	A	307	THR	N-CA-C	7.03	120.64	108.76
1	B	174	GLY	N-CA-C	-7.01	105.67	114.16
1	E	416	ILE	N-CA-C	-6.99	103.85	110.42
1	A	415	LEU	N-CA-C	-6.99	103.74	111.36
1	D	205	THR	N-CA-C	6.97	122.31	113.25
1	E	226	ASP	CA-C-N	6.96	127.25	119.32
1	E	226	ASP	C-N-CA	6.96	127.25	119.32
1	C	205	THR	N-CA-C	6.96	122.29	113.25
1	A	440	TYR	N-CA-C	-6.94	103.77	111.82
1	F	54	LEU	N-CA-C	-6.91	103.81	111.82
1	C	71	THR	N-CA-C	-6.90	104.47	113.17
1	B	294	ASP	N-CA-C	6.89	120.13	111.24
1	D	531	GLN	N-CA-C	-6.89	104.34	112.89
1	D	314	SER	N-CA-C	6.89	119.38	111.11
1	D	438	VAL	N-CA-C	-6.88	105.65	111.56
1	B	287	ASP	N-CA-C	6.88	121.33	112.26
1	F	248	ILE	N-CA-C	6.87	117.68	108.27
1	D	181	ILE	N-CA-C	6.86	117.62	110.62
1	D	190	LEU	N-CA-C	-6.82	105.11	113.50
1	B	112	ASP	N-CA-C	6.82	120.08	111.69
1	D	502	ASN	N-CA-C	6.81	122.54	112.94
1	C	314	SER	N-CA-C	6.81	119.33	111.02
1	C	251	CYS	N-CA-C	6.75	119.12	108.79
1	D	466	SER	N-CA-C	6.74	120.36	110.59
1	E	480	GLY	N-CA-C	-6.74	105.93	115.43
1	C	101	ARG	N-CA-C	-6.71	103.89	111.07
1	B	190	LEU	N-CA-C	-6.68	105.17	113.38
1	B	142	ASN	N-CA-C	6.64	119.12	111.02
1	B	294	ASP	CA-C-N	-6.57	113.01	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	294	ASP	C-N-CA	-6.57	113.01	122.67
1	D	67	SER	N-CA-C	6.55	121.35	113.23
1	A	460	GLU	N-CA-C	6.53	118.40	111.28
1	A	357	LEU	N-CA-C	6.51	118.45	111.36
1	A	358	LEU	N-CA-C	6.49	113.97	108.13
1	A	71	THR	N-CA-C	-6.49	103.64	113.89
1	D	508	TYR	N-CA-C	-6.48	104.22	111.28
1	C	232	GLN	N-CA-C	-6.46	100.96	110.52
1	E	117	ASP	CA-C-N	6.44	126.19	119.05
1	E	117	ASP	C-N-CA	6.44	126.19	119.05
1	A	228	SER	N-CA-C	-6.41	104.72	112.54
1	F	71	THR	N-CA-C	-6.40	103.78	113.89
1	E	255	SER	N-CA-C	6.36	118.23	110.41
1	F	174	GLY	N-CA-C	-6.34	107.69	114.67
1	C	117	ASP	CA-C-N	6.27	126.47	119.32
1	C	117	ASP	C-N-CA	6.27	126.47	119.32
1	E	209	GLU	N-CA-C	6.27	117.91	111.14
1	B	67	SER	N-CA-C	6.27	120.76	113.18
1	B	139	ARG	N-CA-C	6.26	118.91	111.71
1	A	335	PHE	N-CA-C	-6.25	104.55	111.36
1	F	285	THR	N-CA-C	6.24	119.12	109.07
1	D	112	ASP	N-CA-C	6.22	119.35	111.69
1	C	74	VAL	N-CA-C	-6.21	99.20	108.46
1	E	502	ASN	N-CA-C	6.21	120.48	112.41
1	D	210	ILE	CA-C-N	-6.18	113.44	119.87
1	D	210	ILE	C-N-CA	-6.18	113.44	119.87
1	A	76	GLY	N-CA-C	-6.16	103.79	112.60
1	C	278	ARG	CA-C-N	6.15	125.85	119.82
1	C	278	ARG	C-N-CA	6.15	125.85	119.82
1	D	174	GLY	N-CA-C	-6.14	105.19	113.24
1	D	235	ASP	N-CA-C	-6.13	104.51	111.07
1	A	205	THR	N-CA-C	6.11	121.84	113.77
1	F	369	ARG	N-CA-C	-6.06	104.79	111.82
1	E	154	ARG	N-CA-C	6.03	117.53	111.07
1	B	351	ASP	N-CA-C	-6.02	104.72	111.28
1	D	94	ASN	N-CA-C	6.01	118.12	110.61
1	E	142	ASN	N-CA-C	6.00	117.52	110.97
1	F	478	GLU	N-CA-C	6.00	118.61	111.71
1	D	327	VAL	N-CA-C	-6.00	99.10	107.80
1	F	490	GLY	N-CA-C	-5.98	99.00	113.18
1	C	294	ASP	CA-C-N	-5.97	114.96	123.20
1	C	294	ASP	C-N-CA	-5.97	114.96	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	THR	N-CA-C	5.95	119.10	109.40
1	D	307	THR	N-CA-C	5.94	119.50	109.76
1	F	163	SER	N-CA-C	5.90	117.71	111.28
1	B	76	GLY	N-CA-C	-5.86	99.30	113.18
1	F	199	ILE	N-CA-C	5.84	116.41	107.77
1	D	335	PHE	N-CA-C	-5.81	104.54	111.69
1	E	107	LEU	N-CA-C	-5.81	105.02	111.36
1	D	481	ILE	CB-CA-C	-5.80	103.72	110.91
1	D	454	TYR	N-CA-C	5.77	120.15	112.30
1	E	369	ARG	N-CA-C	-5.75	104.62	111.69
1	B	376	ALA	N-CA-C	5.73	123.01	110.80
1	E	260	VAL	N-CA-C	-5.73	99.55	108.44
1	C	297	GLN	N-CA-C	-5.72	98.56	108.69
1	A	208	ILE	N-CA-C	-5.72	104.29	112.35
1	C	489	PHE	N-CA-C	5.71	120.06	109.56
1	E	376	ALA	N-CA-C	5.70	119.54	112.24
1	C	481	ILE	N-CA-C	5.70	116.95	108.23
1	F	438	VAL	N-CA-C	-5.68	107.13	111.62
1	E	342	LEU	N-CA-C	-5.68	103.04	110.53
1	D	416	ILE	N-CA-C	-5.66	104.98	110.42
1	D	208	ILE	N-CA-C	-5.66	105.58	111.58
1	F	358	LEU	N-CA-C	5.64	117.35	108.55
1	E	251	CYS	N-CA-C	5.62	117.95	109.23
1	A	396	PHE	N-CA-C	-5.62	105.24	111.36
1	C	357	LEU	N-CA-C	5.60	120.24	112.45
1	C	161	ILE	CB-CA-C	-5.60	105.73	110.94
1	E	112	ASP	N-CA-C	5.59	118.57	111.69
1	A	130	LEU	N-CA-C	-5.58	106.43	113.18
1	C	255	SER	N-CA-C	5.58	118.74	110.48
1	A	251	CYS	N-CA-C	5.57	118.53	109.24
1	C	107	LEU	N-CA-C	-5.57	104.90	110.97
1	E	308	LEU	N-CA-C	-5.55	98.16	107.99
1	C	396	PHE	N-CA-C	-5.55	105.13	111.07
1	B	37	ARG	CA-C-N	-5.52	117.38	122.29
1	B	37	ARG	C-N-CA	-5.52	117.38	122.29
1	A	502	ASN	N-CA-C	5.51	119.58	112.41
1	D	127	ASP	N-CA-C	-5.50	105.18	111.07
1	F	279	PRO	N-CA-C	-5.50	106.95	114.98
1	E	307	THR	N-CA-C	5.50	118.78	109.76
1	D	305	GLU	N-CA-C	5.48	119.69	112.89
1	F	520	ASP	N-CA-C	-5.46	105.40	111.36
1	C	498	ALA	N-CA-C	-5.44	101.48	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	315	LYS	N-CA-C	5.44	116.89	110.97
1	D	179	ALA	N-CA-C	-5.43	105.26	111.07
1	D	315	LYS	N-CA-C	5.43	118.03	111.40
1	F	119	ALA	N-CA-C	-5.42	105.37	111.28
1	A	96	ASP	N-CA-C	5.42	119.60	113.15
1	E	339	LEU	N-CA-C	-5.42	105.40	112.23
1	F	156	MET	N-CA-C	-5.42	106.68	113.72
1	C	206	PRO	N-CA-C	5.41	120.87	113.84
1	B	257	PRO	N-CA-C	5.40	126.13	112.10
1	D	434	ASP	N-CA-CB	-5.39	103.04	111.56
1	E	303	CYS	CA-C-N	5.39	124.84	119.24
1	E	303	CYS	C-N-CA	5.39	124.84	119.24
1	C	439	ASP	N-CA-C	5.38	122.27	110.80
1	E	271	ARG	N-CA-C	-5.38	105.33	111.14
1	B	71	THR	N-CA-C	-5.36	106.11	113.30
1	C	401	LEU	N-CA-C	5.36	117.12	111.28
1	E	278	ARG	N-CA-C	5.36	119.56	110.02
1	B	495	SER	N-CA-C	5.35	116.66	108.52
1	D	489	PHE	N-CA-C	5.34	117.38	107.60
1	D	299	LEU	N-CA-C	-5.34	105.86	112.38
1	B	295	ASP	N-CA-C	-5.34	99.74	109.56
1	B	416	ILE	N-CA-C	-5.33	105.18	110.62
1	C	100	VAL	N-CA-C	5.31	116.04	110.62
1	E	388	PRO	N-CA-C	-5.31	106.15	113.53
1	B	232	GLN	N-CA-C	-5.29	102.70	110.52
1	B	255	SER	N-CA-C	5.27	117.33	110.43
1	F	232	GLN	N-CA-C	-5.27	102.73	110.52
1	F	159	ASP	N-CA-C	5.26	120.64	113.37
1	B	169	PHE	N-CA-C	-5.26	99.71	108.34
1	C	156	MET	N-CA-C	-5.25	106.65	113.16
1	C	72	VAL	N-CA-C	5.24	117.64	111.09
1	C	185	LEU	N-CA-C	-5.24	105.57	111.28
1	F	101	ARG	N-CA-C	-5.23	104.64	111.02
1	C	307	THR	N-CA-C	5.22	117.58	108.76
1	C	481	ILE	CB-CA-C	-5.21	104.65	110.96
1	A	294	ASP	CA-C-N	-5.18	115.06	122.67
1	A	294	ASP	C-N-CA	-5.18	115.06	122.67
1	E	67	SER	N-CA-C	5.18	119.70	113.17
1	C	454	TYR	N-CA-C	5.16	118.68	111.56
1	A	186	LYS	N-CA-C	-5.16	105.57	111.14
1	D	142	ASN	N-CA-C	5.15	117.31	111.02
1	A	222	ALA	N-CA-C	5.15	117.69	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	39	ASN	CA-C-N	5.13	125.05	119.76
1	F	39	ASN	C-N-CA	5.13	125.05	119.76
1	A	38	GLY	N-CA-C	-5.12	102.05	110.95
1	D	231	TRP	N-CA-C	5.12	121.70	110.80
1	F	226	ASP	N-CA-C	5.10	118.84	109.10
1	F	72	VAL	N-CA-C	5.10	115.82	110.62
1	E	138	PRO	N-CA-C	5.10	120.53	113.65
1	F	109	TYR	N-CA-C	-5.09	105.43	110.97
1	E	221	VAL	N-CA-C	5.08	114.10	106.42
1	C	435	GLU	N-CA-C	5.08	117.55	111.71
1	A	112	ASP	N-CA-C	5.05	119.47	112.45
1	B	377	VAL	CB-CA-C	-5.05	103.01	111.29
1	F	287	ASP	N-CA-C	5.05	118.98	112.41
1	B	420	GLU	N-CA-C	-5.05	105.69	111.14
1	D	276	GLU	N-CA-C	5.03	118.56	112.23
1	F	205	THR	N-CA-C	5.02	120.91	109.81
1	C	35	ALA	N-CA-C	5.02	120.25	113.72
1	A	194	GLY	N-CA-C	-5.01	107.74	114.25
1	D	479	THR	N-CA-C	5.00	120.38	113.97
1	E	233	TYR	N-CA-C	-5.00	103.47	109.72

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	289	TYR	Sidechain
1	D	216	TYR	Sidechain
1	E	134	TYR	Sidechain
1	E	66	TYR	Sidechain
1	F	508	TYR	Sidechain

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	4005	0	3971	230	0
1	B	4048	0	4013	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4048	0	4013	194	2
1	D	4011	0	3970	191	1
1	E	4018	0	3985	217	0
1	F	4094	0	4052	232	1
2	A	15	0	7	0	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	0	0
2	E	15	0	7	0	0
2	F	15	0	6	0	0
3	A	318	0	0	34	0
3	B	355	0	0	22	1
3	C	337	0	0	19	1
3	D	342	0	0	16	0
3	E	282	0	0	19	1
3	F	265	0	0	20	2
All	All	26213	0	24045	1206	5

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 25.

All (1206) 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:425:ARG:HH12	1:D:159:ASP:CA	1.43	1.31
1:A:21:ILE:HD12	3:A:549:HOH:O	1.32	1.23
1:E:17:LYS:HE3	3:E:1349:HOH:O	1.40	1.21
1:B:425:ARG:NH1	1:D:159:ASP:HA	1.58	1.16
1:D:425:ARG:HH22	1:F:159:ASP:HA	1.01	1.14
1:E:446:LEU:HB2	1:E:471:MET:HE1	1.28	1.12
1:A:70:THR:HG22	1:A:72:VAL:H	1.12	1.12
1:D:425:ARG:NH2	1:F:159:ASP:HA	1.66	1.09
1:C:22:LYS:HD2	3:C:747:HOH:O	1.56	1.05
1:F:12:SER:HB3	1:F:15:GLU:HB2	1.39	1.03
1:C:23:ILE:HD11	3:C:747:HOH:O	1.56	1.03
1:E:232:GLN:HE21	1:E:232:GLN:HA	1.20	1.03
1:D:135:PRO:HD2	3:D:1856:HOH:O	1.58	1.01
1:F:333:ASN:HD22	1:F:335:PHE:H	1.02	1.00
1:D:64:LEU:HD23	3:D:791:HOH:O	1.62	1.00
1:F:197:VAL:HG23	1:F:248:ILE:HG23	1.42	0.99
1:B:425:ARG:NH1	1:D:159:ASP:CA	2.18	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:497:ARG:NH1	3:F:1666:HOH:O	1.89	0.96
1:C:333:ASN:HD22	1:C:335:PHE:H	1.04	0.95
1:D:139:ARG:HG3	1:D:371:VAL:HG21	1.49	0.94
1:E:513:ARG:HG3	1:E:513:ARG:HH11	1.31	0.94
1:D:23:ILE:HD12	1:D:23:ILE:H	1.30	0.94
1:C:22:LYS:HD3	1:C:22:LYS:C	1.93	0.93
1:D:333:ASN:HD22	1:D:335:PHE:H	1.16	0.93
1:A:21:ILE:CD1	3:A:549:HOH:O	1.96	0.93
1:E:197:VAL:HG23	1:E:248:ILE:HG23	1.50	0.93
1:A:384:GLY:HA2	3:A:669:HOH:O	1.69	0.93
1:B:26:SER:HB2	3:B:738:HOH:O	1.66	0.93
1:A:362:ARG:HG3	1:A:362:ARG:HH11	1.30	0.92
1:F:448:ASP:HB3	3:F:1711:HOH:O	1.70	0.92
1:F:490:GLY:O	1:F:492:ASN:N	2.03	0.92
1:B:425:ARG:NH1	1:D:159:ASP:C	2.28	0.92
1:B:425:ARG:HH12	1:D:159:ASP:HA	0.75	0.91
1:C:22:LYS:HD2	1:C:23:ILE:CD1	2.01	0.91
1:E:488:GLY:O	1:E:490:GLY:N	2.02	0.90
1:B:159:ASP:HA	1:F:425:ARG:NH2	1.85	0.90
1:B:425:ARG:NH1	1:D:159:ASP:O	2.03	0.90
1:E:257:PRO:HB2	1:E:497:ARG:HD3	1.52	0.90
1:F:257:PRO:HB2	1:F:497:ARG:HD2	1.53	0.90
1:E:226:ASP:OD2	1:E:228:SER:HB3	1.73	0.89
1:C:447:GLN:HG3	1:C:459:SER:OG	1.73	0.88
1:A:20:LEU:HD12	1:A:23:ILE:HG21	1.55	0.88
1:B:254:PRO:HG2	1:B:289:TYR:HB2	1.54	0.88
1:A:172:GLU:HG2	1:A:176:ALA:HB2	1.56	0.87
1:F:159:ASP:OD2	3:F:1268:HOH:O	1.91	0.87
1:A:98:GLU:OE1	3:A:587:HOH:O	1.93	0.87
1:F:491:SER:O	1:F:493:ARG:N	2.06	0.87
1:B:264:GLN:NE2	3:B:859:HOH:O	1.88	0.87
1:F:24:ALA:HB3	1:F:482:VAL:CG2	2.05	0.87
1:F:333:ASN:ND2	1:F:335:PHE:H	1.72	0.86
1:C:232:GLN:HE22	1:C:263:ASP:H	1.23	0.86
1:B:333:ASN:HD22	1:B:335:PHE:H	1.24	0.85
1:E:333:ASN:HD22	1:E:335:PHE:H	1.22	0.85
1:D:490:GLY:O	1:D:492:ASN:ND2	2.09	0.84
1:D:344:GLU:O	1:D:348:VAL:HG23	1.77	0.84
1:E:234:PRO:HG2	1:E:237:GLU:HB2	1.57	0.84
1:F:12:SER:N	3:F:1899:HOH:O	2.10	0.84
1:B:33:LEU:HD11	1:B:482:VAL:HG11	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:PRO:HG2	1:D:237:GLU:HB2	1.57	0.84
1:A:101:ARG:NH2	1:A:105:LYS:HE2	1.92	0.83
1:A:490:GLY:HA3	3:A:1600:HOH:O	1.77	0.83
1:B:15:GLU:HA	3:B:752:HOH:O	1.77	0.83
1:D:227:PRO:HG2	1:D:489:PHE:HB3	1.58	0.82
1:F:353:ARG:HG3	1:F:353:ARG:HH11	1.42	0.82
1:E:20:LEU:HA	1:E:23:ILE:HD12	1.62	0.82
1:A:41:ASN:HD21	1:A:419:ARG:HH22	1.27	0.81
1:E:227:PRO:HG2	1:E:489:PHE:HB3	1.61	0.81
1:B:232:GLN:HE22	1:B:263:ASP:H	1.27	0.81
1:E:443:LEU:HD23	3:E:1492:HOH:O	1.81	0.81
1:B:187:LEU:HD13	1:B:353:ARG:NH2	1.96	0.81
1:C:491:SER:O	1:C:493:ARG:N	2.14	0.80
1:C:22:LYS:HD2	1:C:23:ILE:HD12	1.60	0.80
1:A:172:GLU:HG2	1:A:176:ALA:CB	2.12	0.79
1:C:447:GLN:HG3	1:C:459:SER:HG	1.48	0.79
1:A:447:GLN:HB3	1:A:493:ARG:HH21	1.47	0.79
1:A:72:VAL:HG11	1:B:408:TYR:HA	1.65	0.78
1:D:491:SER:O	1:D:493:ARG:N	2.17	0.78
1:E:255:SER:OG	1:E:258:PRO:HB2	1.84	0.78
1:A:96:ASP:OD2	3:A:1890:HOH:O	2.01	0.78
1:F:101:ARG:HH11	1:F:101:ARG:HG2	1.49	0.78
1:D:41:ASN:HD21	1:D:419:ARG:HH22	1.29	0.78
1:E:195:ASP:OD1	1:E:247:LYS:HG3	1.83	0.78
1:A:513:ARG:HD3	3:A:797:HOH:O	1.84	0.78
1:C:154:ARG:NH2	3:C:951:HOH:O	2.17	0.78
1:A:425:ARG:NH1	3:A:793:HOH:O	2.15	0.78
1:A:64:LEU:HD21	3:D:549:HOH:O	1.83	0.78
1:E:219:GLU:OE2	3:E:1756:HOH:O	2.02	0.78
1:F:489:PHE:O	1:F:491:SER:N	2.17	0.77
1:D:490:GLY:O	1:D:492:ASN:N	2.17	0.77
1:E:232:GLN:HA	1:E:232:GLN:NE2	1.96	0.77
1:E:43:LEU:C	1:E:43:LEU:HD12	2.09	0.77
1:B:159:ASP:HA	1:F:425:ARG:HH22	1.48	0.77
1:C:333:ASN:ND2	1:C:335:PHE:H	1.79	0.77
1:A:234:PRO:HG2	1:A:237:GLU:HB2	1.66	0.77
1:D:232:GLN:HE22	1:D:263:ASP:H	1.29	0.77
1:E:344:GLU:O	1:E:348:VAL:HG23	1.83	0.76
1:F:149:ARG:HB3	1:F:168:LEU:HD11	1.65	0.76
1:D:513:ARG:HG3	1:D:513:ARG:HH11	1.49	0.76
1:E:309:LEU:HB3	1:E:328:ALA:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:GLU:HB3	3:B:759:HOH:O	1.85	0.76
1:C:72:VAL:HG12	1:C:74:VAL:HG23	1.66	0.76
1:D:139:ARG:HG3	1:D:371:VAL:CG2	2.14	0.76
1:A:333:ASN:HD22	1:A:335:PHE:H	1.31	0.76
1:E:488:GLY:C	1:E:490:GLY:H	1.93	0.76
1:D:159:ASP:HB2	3:D:666:HOH:O	1.86	0.75
1:C:41:ASN:HD21	1:C:419:ARG:HH22	1.33	0.75
1:C:471:MET:HE1	1:C:495:SER:HA	1.69	0.75
1:F:24:ALA:HB3	1:F:482:VAL:HG23	1.67	0.75
1:C:89:ARG:NH1	1:C:93:GLU:HG3	2.02	0.74
1:F:355:ARG:NH1	1:F:355:ARG:CB	2.50	0.74
1:A:257:PRO:HB2	1:A:497:ARG:HD2	1.67	0.74
1:C:224:ASN:O	1:C:237:GLU:HG2	1.87	0.74
1:E:131:GLY:HA2	3:E:1428:HOH:O	1.86	0.74
1:E:30:ARG:HG2	1:E:30:ARG:HH11	1.52	0.74
1:E:447:GLN:HE21	1:E:463:VAL:HG21	1.53	0.74
1:E:513:ARG:HD3	3:E:557:HOH:O	1.87	0.74
1:E:387:THR:O	1:E:391:VAL:HG23	1.88	0.73
1:F:201:MET:HE2	1:F:208:ILE:HD11	1.70	0.73
1:B:227:PRO:HG2	1:B:489:PHE:HB3	1.70	0.73
1:F:355:ARG:NH1	1:F:355:ARG:HB2	2.03	0.73
1:A:420:GLU:HG2	1:A:430:PRO:HB3	1.71	0.73
1:E:158:ALA:HB1	1:E:161:ILE:HD12	1.69	0.73
1:E:352:HIS:O	1:E:355:ARG:HG2	1.89	0.73
1:B:490:GLY:O	1:B:492:ASN:N	2.21	0.73
1:B:248:ILE:HG13	1:B:282:MET:O	1.89	0.73
1:D:253:ASN:HA	1:D:254:PRO:C	2.14	0.72
1:E:447:GLN:NE2	1:E:463:VAL:HG21	2.04	0.72
1:C:490:GLY:O	1:C:492:ASN:N	2.22	0.72
1:F:81:ASP:OD2	3:F:1626:HOH:O	2.06	0.72
1:E:106:SER:HB2	1:E:398:LEU:HD13	1.69	0.72
1:C:497:ARG:HD2	3:C:1007:HOH:O	1.89	0.72
1:F:355:ARG:HH11	1:F:355:ARG:HB3	1.55	0.72
1:E:29:ASN:OD1	1:E:482:VAL:HB	1.89	0.72
1:E:205:THR:HB	1:E:206:PRO:HD3	1.72	0.72
1:F:12:SER:CB	1:F:15:GLU:HB2	2.17	0.72
1:E:367:ILE:HA	1:E:370:LEU:HD12	1.71	0.72
1:D:454:TYR:HB2	1:D:458:PHE:CD2	2.24	0.72
1:A:139:ARG:HG3	1:A:371:VAL:HG21	1.72	0.71
1:E:32:MET:O	1:E:484:LEU:HD21	1.90	0.71
1:C:235:ASP:OD1	1:C:269:ARG:HD3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:O	3:A:669:HOH:O	2.09	0.71
1:A:197:VAL:HG23	1:A:248:ILE:HG23	1.72	0.71
1:D:513:ARG:HG3	1:D:513:ARG:NH1	2.05	0.71
1:F:274:VAL:HA	1:F:278:ARG:O	1.89	0.71
1:F:201:MET:CE	1:F:208:ILE:HD11	2.20	0.71
1:E:33:LEU:HD11	1:E:482:VAL:HG11	1.72	0.71
1:B:461:TRP:O	1:B:465:GLN:HG2	1.91	0.70
1:C:111:ARG:HD2	1:C:112:ASP:OD1	1.91	0.70
1:F:281:LEU:HD12	1:F:282:MET:H	1.55	0.70
1:A:408:TYR:HB3	3:A:582:HOH:O	1.90	0.70
1:B:446:LEU:HB2	1:B:471:MET:CE	2.21	0.70
1:C:22:LYS:HD3	1:C:23:ILE:N	2.05	0.70
1:E:353:ARG:HG3	1:E:353:ARG:HH11	1.55	0.70
1:B:451:ALA:HB2	1:B:459:SER:HB2	1.75	0.69
1:B:41:ASN:HD21	1:B:419:ARG:HH22	1.41	0.69
1:D:513:ARG:HD2	3:D:1319:HOH:O	1.91	0.69
1:B:41:ASN:HD21	1:B:419:ARG:HH12	1.41	0.69
1:E:513:ARG:HG3	1:E:513:ARG:NH1	2.03	0.69
1:F:353:ARG:HG3	1:F:353:ARG:NH1	2.08	0.69
1:A:447:GLN:HB2	1:A:463:VAL:HG21	1.74	0.69
1:E:23:ILE:HD13	1:E:473:PHE:CD1	2.28	0.69
1:A:156:MET:HE2	1:A:156:MET:HA	1.74	0.69
1:C:473:PHE:CD1	3:C:720:HOH:O	2.46	0.69
1:E:232:GLN:HE21	1:E:232:GLN:CA	1.99	0.69
1:F:461:TRP:O	1:F:465:GLN:HG2	1.92	0.69
1:A:362:ARG:HG3	1:A:362:ARG:NH1	2.05	0.68
1:D:23:ILE:H	1:D:23:ILE:CD1	2.05	0.68
1:A:253:ASN:HA	1:A:254:PRO:C	2.16	0.68
1:D:232:GLN:NE2	1:D:263:ASP:H	1.92	0.68
1:F:230:ASN:HB3	3:F:1715:HOH:O	1.92	0.68
1:C:70:THR:HG22	1:C:72:VAL:H	1.58	0.68
1:D:97:GLN:O	1:D:100:VAL:HG23	1.93	0.68
1:B:320:THR:O	1:B:323:ARG:HD2	1.91	0.68
1:F:333:ASN:HD22	1:F:335:PHE:N	1.85	0.68
1:A:460:GLU:O	1:A:464:LYS:HG2	1.94	0.68
1:C:95:ARG:NH1	3:C:902:HOH:O	2.24	0.68
1:D:172:GLU:CD	1:D:172:GLU:H	2.02	0.68
1:D:230:ASN:ND2	3:D:1232:HOH:O	2.16	0.68
1:B:139:ARG:HG3	1:B:371:VAL:CG2	2.24	0.68
1:E:481:ILE:HG21	1:E:511:ILE:HD11	1.74	0.68
1:E:197:VAL:HG23	1:E:248:ILE:CG2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:468:THR:O	1:E:472:LEU:HG	1.93	0.67
1:F:434:ASP:O	3:F:1722:HOH:O	2.12	0.67
1:D:407:GLU:OE1	3:D:565:HOH:O	2.12	0.67
1:C:456:GLU:O	1:C:459:SER:HB3	1.94	0.67
1:E:446:LEU:HB2	1:E:471:MET:CE	2.17	0.67
1:A:41:ASN:HD21	1:A:419:ARG:NH2	1.92	0.67
1:A:333:ASN:HD21	1:A:335:PHE:HB2	1.59	0.67
1:C:408:TYR:HA	1:D:72:VAL:HG11	1.77	0.67
1:D:226:ASP:OD2	1:D:228:SER:HB2	1.95	0.67
1:E:401:LEU:O	3:E:1447:HOH:O	2.13	0.67
1:D:201:MET:HE3	1:D:222:ALA:HB2	1.77	0.66
1:A:24:ALA:CB	1:A:482:VAL:HG23	2.25	0.66
1:B:89:ARG:O	1:B:93:GLU:HG2	1.95	0.66
1:A:21:ILE:HG12	3:A:547:HOH:O	1.94	0.66
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.61	0.66
1:B:447:GLN:HB3	1:B:493:ARG:HH21	1.61	0.66
1:F:24:ALA:HB3	1:F:482:VAL:HG21	1.77	0.66
1:A:94:ASN:HB3	1:A:97:GLN:OE1	1.95	0.66
1:A:101:ARG:CZ	1:A:105:LYS:HE2	2.24	0.66
1:B:425:ARG:NH2	1:D:161:ILE:O	2.22	0.66
1:F:69:MET:O	1:F:70:THR:HG23	1.96	0.66
1:D:528:GLY:O	1:D:532:ASN:HB2	1.96	0.66
1:D:26:SER:O	1:D:30:ARG:HG3	1.97	0.65
1:B:84:GLU:O	1:B:88:GLU:HG3	1.95	0.65
1:E:456:GLU:O	1:E:459:SER:HB3	1.96	0.65
1:F:355:ARG:CB	1:F:355:ARG:HH11	2.08	0.65
1:C:333:ASN:HD22	1:C:335:PHE:N	1.87	0.65
1:D:140:MET:HE2	1:D:145:GLU:HA	1.78	0.65
1:A:79:LYS:HB3	3:A:613:HOH:O	1.97	0.65
1:E:366:PHE:HA	1:E:369:ARG:HG3	1.77	0.65
1:E:461:TRP:O	1:E:465:GLN:HG2	1.96	0.65
1:F:433:ARG:HG2	1:F:434:ASP:N	2.12	0.65
1:A:333:ASN:ND2	1:A:335:PHE:H	1.94	0.65
1:B:20:LEU:HA	1:B:23:ILE:HD12	1.79	0.65
1:D:513:ARG:NH2	1:F:164:GLU:HG3	2.12	0.65
1:A:269:ARG:O	1:A:273:ILE:HG13	1.97	0.65
1:D:27:ASP:OD2	1:D:30:ARG:NH1	2.30	0.65
1:C:331:GLN:HB2	1:C:332:GLN:NE2	2.12	0.65
1:C:372:ALA:HA	1:C:380:ASN:HD22	1.60	0.65
1:D:471:MET:HG3	1:D:518:MET:HE1	1.78	0.65
1:A:257:PRO:HG2	1:A:258:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:355:ARG:HB2	1:F:355:ARG:CZ	2.27	0.64
1:D:271:ARG:NH1	1:D:271:ARG:HG2	2.11	0.64
1:C:268:GLU:HB2	3:C:1036:HOH:O	1.96	0.64
1:B:41:ASN:ND2	1:B:419:ARG:HH22	1.95	0.64
1:F:387:THR:OG1	1:F:388:PRO:HD3	1.97	0.64
1:A:70:THR:HG22	1:A:72:VAL:N	1.98	0.64
1:A:159:ASP:HA	1:E:425:ARG:NH2	2.13	0.64
1:A:457:ALA:HB3	3:A:812:HOH:O	1.97	0.64
1:D:333:ASN:ND2	1:D:335:PHE:H	1.92	0.64
1:E:333:ASN:ND2	1:E:335:PHE:HB2	2.12	0.64
1:E:358:LEU:HB2	1:E:359:PRO:HD2	1.78	0.64
1:A:70:THR:HG22	1:A:71:THR:N	2.14	0.63
1:B:111:ARG:HD2	1:B:112:ASP:OD1	1.97	0.63
1:D:201:MET:HE3	1:D:222:ALA:CB	2.28	0.63
1:E:476:ALA:HA	1:E:481:ILE:O	1.98	0.63
1:F:93:GLU:HG3	1:F:93:GLU:O	1.98	0.63
1:D:24:ALA:HB3	1:D:482:VAL:CG2	2.28	0.63
1:E:447:GLN:HB3	1:E:493:ARG:HH21	1.62	0.63
1:E:254:PRO:HD3	1:E:296:PHE:CE1	2.33	0.63
1:F:226:ASP:OD2	1:F:229:LEU:HG	1.98	0.63
1:A:264:GLN:HG3	3:A:752:HOH:O	1.99	0.63
1:A:372:ALA:HA	1:A:380:ASN:HD22	1.63	0.63
1:A:212:GLU:OE1	3:A:732:HOH:O	2.15	0.63
1:B:459:SER:O	1:B:463:VAL:HG23	1.99	0.63
1:D:306:ASN:HA	1:D:334:VAL:HG22	1.80	0.63
1:E:314:SER:HB3	1:E:320:THR:HA	1.79	0.63
1:E:429:MET:HB3	1:E:430:PRO:HD2	1.81	0.63
1:E:446:LEU:CB	1:E:471:MET:HE1	2.19	0.63
1:B:358:LEU:HB2	1:B:359:PRO:HD2	1.80	0.63
1:C:87:PHE:O	1:C:91:ILE:HG12	1.99	0.63
1:E:61:GLU:O	1:E:64:LEU:HB2	1.99	0.63
1:D:23:ILE:HD12	1:D:23:ILE:N	2.10	0.63
1:A:176:ALA:HB1	1:A:180:TYR:CZ	2.34	0.62
1:E:224:ASN:O	1:E:237:GLU:HG2	1.98	0.62
1:F:282:MET:HE3	1:F:335:PHE:CD2	2.34	0.62
1:B:344:GLU:OE1	1:B:344:GLU:HA	1.99	0.62
1:B:425:ARG:HG3	1:D:159:ASP:O	1.98	0.62
1:D:504:ASN:ND2	1:F:113:GLN:HE22	1.96	0.62
1:A:25:SER:HA	1:A:30:ARG:HH12	1.63	0.62
1:F:342:LEU:O	1:F:347:LYS:HE3	1.99	0.62
1:E:398:LEU:O	1:E:402:MET:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:LEU:HB2	1:C:508:TYR:CZ	2.35	0.62
1:D:235:ASP:OD1	1:D:269:ARG:HD3	1.99	0.62
1:D:195:ASP:HB3	1:D:247:LYS:HG3	1.80	0.62
1:C:22:LYS:CD	1:C:23:ILE:HD12	2.29	0.62
1:E:183:GLU:HG2	3:E:1476:HOH:O	1.99	0.62
1:E:426:GLU:O	1:E:427:LEU:HD23	2.00	0.62
1:E:467:SER:O	1:E:470:ASP:N	2.32	0.62
1:A:374:SER:O	1:A:375:ARG:HD3	2.00	0.61
1:B:172:GLU:HG2	1:B:176:ALA:HB2	1.81	0.61
1:D:271:ARG:HG2	1:D:271:ARG:HH11	1.65	0.61
1:E:333:ASN:HD21	1:E:335:PHE:HB2	1.64	0.61
1:A:41:ASN:ND2	1:A:419:ARG:HH22	1.97	0.61
1:B:232:GLN:HE22	1:B:263:ASP:N	1.99	0.61
1:C:22:LYS:CD	3:C:747:HOH:O	2.29	0.61
1:E:53:ARG:HD2	3:E:551:HOH:O	2.00	0.61
1:B:172:GLU:CD	1:B:172:GLU:H	2.08	0.61
1:C:161:ILE:HD11	1:C:304:PRO:HB3	1.82	0.61
1:E:457:ALA:O	3:E:1561:HOH:O	2.16	0.61
1:A:456:GLU:O	1:A:459:SER:HB3	1.99	0.61
1:B:24:ALA:HB3	1:B:482:VAL:HG23	1.82	0.61
1:F:333:ASN:ND2	1:F:335:PHE:N	2.48	0.61
1:C:227:PRO:HG2	1:C:489:PHE:HB3	1.81	0.61
1:C:330:HIS:CE1	1:C:332:GLN:HG2	2.36	0.61
1:C:352:HIS:HB2	3:C:1066:HOH:O	2.00	0.61
1:E:490:GLY:O	1:E:492:ASN:N	2.33	0.61
1:D:41:ASN:HD21	1:D:419:ARG:NH2	1.96	0.61
1:F:17:LYS:NZ	1:F:205:THR:HG21	2.16	0.61
1:F:17:LYS:HZ2	1:F:205:THR:HG21	1.65	0.61
1:D:343:GLN:HB2	1:D:346:GLU:HG3	1.82	0.61
1:F:41:ASN:HD21	1:F:419:ARG:HH12	1.49	0.61
1:A:84:GLU:HG3	3:A:616:HOH:O	2.01	0.60
1:D:187:LEU:HD13	1:D:353:ARG:NH2	2.17	0.60
1:A:70:THR:CG2	1:A:72:VAL:HG23	2.31	0.60
1:C:174:GLY:O	1:C:177:ALA:HB3	2.01	0.60
1:D:488:GLY:O	3:D:1214:HOH:O	2.17	0.60
1:E:523:TYR:O	1:E:527:SER:HB2	2.00	0.60
1:B:235:ASP:OD1	1:B:269:ARG:HD3	2.01	0.60
1:A:72:VAL:HG21	1:B:411:THR:OG1	2.01	0.60
1:C:232:GLN:NE2	1:C:263:ASP:H	1.98	0.60
1:A:205:THR:O	1:A:209:GLU:HG2	2.01	0.60
1:B:158:ALA:HB1	1:B:161:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:GLU:HG3	3:C:831:HOH:O	2.01	0.60
1:C:253:ASN:HA	1:C:254:PRO:C	2.27	0.60
1:E:271:ARG:HG2	1:E:271:ARG:HH11	1.66	0.60
1:F:339:LEU:HD13	1:F:369:ARG:CZ	2.31	0.60
1:A:24:ALA:HB3	1:A:482:VAL:CG2	2.32	0.60
1:D:425:ARG:NH2	1:F:159:ASP:CA	2.56	0.59
1:E:43:LEU:HD12	1:E:43:LEU:O	2.01	0.59
1:F:367:ILE:O	1:F:370:LEU:HB2	2.01	0.59
1:F:489:PHE:N	1:F:489:PHE:CD1	2.70	0.59
1:B:306:ASN:ND2	1:B:334:VAL:HG11	2.17	0.59
1:B:404:GLU:OE1	1:F:418:ARG:HD2	2.02	0.59
1:F:190:LEU:HD22	1:F:338:ALA:HB1	1.83	0.59
1:E:232:GLN:HE22	1:E:262:MET:HA	1.68	0.59
1:B:497:ARG:HD2	3:B:763:HOH:O	2.03	0.59
1:B:513:ARG:HD3	3:B:697:HOH:O	2.02	0.59
1:B:323:ARG:HA	1:B:323:ARG:HH11	1.67	0.59
1:D:24:ALA:HB3	1:D:482:VAL:HG23	1.85	0.59
1:A:31:LEU:HD23	1:A:39:ASN:HB2	1.83	0.58
1:A:70:THR:HB	3:A:600:HOH:O	2.02	0.58
1:F:37:ARG:HG3	1:F:37:ARG:HH11	1.67	0.58
1:B:262:MET:HE2	1:B:267:LEU:HD23	1.85	0.58
1:D:254:PRO:HB3	1:D:438:VAL:HG21	1.86	0.58
1:D:372:ALA:HA	1:D:380:ASN:HD22	1.69	0.58
1:F:80:ILE:HG13	1:F:123:HIS:HB2	1.85	0.58
1:B:248:ILE:HA	1:B:282:MET:O	2.02	0.58
1:F:320:THR:HG23	3:F:1671:HOH:O	2.03	0.58
1:A:490:GLY:O	1:A:492:ASN:N	2.36	0.58
1:E:483:LEU:CD2	1:E:498:ALA:HB2	2.32	0.58
1:A:323:ARG:HH11	1:A:323:ARG:HA	1.68	0.58
1:E:333:ASN:HD22	1:E:335:PHE:N	1.98	0.58
1:B:425:ARG:CZ	1:D:159:ASP:O	2.51	0.58
1:F:489:PHE:C	1:F:491:SER:N	2.61	0.58
1:A:255:SER:OG	1:A:258:PRO:HB2	2.04	0.58
1:A:372:ALA:CA	1:A:380:ASN:HD22	2.17	0.58
1:B:257:PRO:HG2	1:B:258:PRO:HD3	1.86	0.57
1:D:156:MET:HG3	1:D:309:LEU:HD21	1.85	0.57
1:D:358:LEU:N	1:D:358:LEU:HD23	2.19	0.57
1:A:447:GLN:HB2	1:A:463:VAL:CG2	2.33	0.57
1:D:420:GLU:HG2	1:D:430:PRO:HB3	1.85	0.57
1:F:304:PRO:HB2	1:F:330:HIS:HD2	1.68	0.57
1:C:17:LYS:O	1:C:21:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:LYS:HB3	3:E:1400:HOH:O	2.04	0.57
1:E:171:VAL:HG22	1:E:325:GLY:O	2.05	0.57
1:E:227:PRO:CG	1:E:489:PHE:HB3	2.31	0.57
1:A:70:THR:HG22	1:A:71:THR:H	1.70	0.57
1:A:379:LEU:HD23	1:B:206:PRO:HB3	1.87	0.57
1:B:489:PHE:N	1:B:489:PHE:CD2	2.72	0.57
1:C:352:HIS:O	1:C:355:ARG:HG2	2.04	0.57
1:E:41:ASN:C	1:E:41:ASN:HD22	2.13	0.57
1:F:476:ALA:HA	1:F:481:ILE:O	2.05	0.57
1:C:22:LYS:CD	1:C:23:ILE:CD1	2.80	0.57
1:F:41:ASN:HD21	1:F:419:ARG:HH22	1.52	0.57
1:F:281:LEU:HD12	1:F:282:MET:N	2.18	0.57
1:A:24:ALA:HB3	1:A:482:VAL:HG23	1.87	0.57
1:D:237:GLU:OE2	1:D:240:LYS:HE3	2.05	0.57
1:A:158:ALA:HB1	1:A:161:ILE:HD12	1.86	0.57
1:B:446:LEU:HB2	1:B:471:MET:HE3	1.87	0.57
1:D:29:ASN:O	1:D:33:LEU:HG	2.05	0.57
1:E:468:THR:OG1	1:E:494:PRO:HA	2.04	0.57
1:F:304:PRO:HB2	1:F:330:HIS:CD2	2.40	0.57
1:B:41:ASN:HD21	1:B:419:ARG:NH2	2.02	0.57
1:B:456:GLU:H	1:B:456:GLU:CD	2.13	0.57
1:B:446:LEU:HB2	1:B:471:MET:HE1	1.86	0.56
1:E:234:PRO:CG	1:E:237:GLU:HB2	2.30	0.56
1:A:468:THR:OG1	1:A:494:PRO:HA	2.04	0.56
1:B:472:LEU:HD22	1:B:483:LEU:HB2	1.88	0.56
1:E:333:ASN:ND2	1:E:335:PHE:H	1.99	0.56
1:F:459:SER:O	1:F:463:VAL:HG23	2.04	0.56
1:A:226:ASP:OD2	1:A:228:SER:HB2	2.05	0.56
1:C:41:ASN:HD21	1:C:419:ARG:NH2	2.03	0.56
1:D:72:VAL:HG12	1:D:72:VAL:O	2.05	0.56
1:F:23:ILE:HG13	1:F:473:PHE:CZ	2.40	0.56
1:F:254:PRO:HD3	1:F:296:PHE:CZ	2.41	0.56
1:F:322:TRP:HB3	1:F:324:LEU:HG	1.87	0.56
1:E:95:ARG:O	1:E:101:ARG:HD3	2.05	0.56
1:F:232:GLN:HE22	1:F:262:MET:HA	1.70	0.56
1:C:294:ASP:O	3:C:955:HOH:O	2.17	0.56
1:D:106:SER:HB2	1:D:398:LEU:HD13	1.86	0.56
1:D:136:VAL:O	1:D:136:VAL:HG13	2.04	0.56
1:C:41:ASN:ND2	1:C:419:ARG:HH22	2.02	0.56
1:E:270:VAL:O	1:E:274:VAL:HG23	2.05	0.56
1:E:30:ARG:HG2	1:E:30:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ALA:HB1	1:F:161:ILE:HD12	1.87	0.56
1:B:357:LEU:HD11	1:B:372:ALA:HB2	1.88	0.56
1:C:308:LEU:HG	1:C:335:PHE:CZ	2.41	0.56
1:F:195:ASP:OD1	1:F:247:LYS:HD2	2.06	0.56
1:D:531:GLN:NE2	3:D:1333:HOH:O	2.38	0.56
1:F:288:VAL:HG23	1:F:312:SER:HB3	1.87	0.56
1:F:489:PHE:HD1	1:F:489:PHE:H	1.54	0.56
1:B:404:GLU:OE1	1:F:418:ARG:CD	2.55	0.55
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.71	0.55
1:F:156:MET:O	1:F:297:GLN:HA	2.05	0.55
1:F:375:ARG:O	1:F:379:LEU:HB2	2.06	0.55
1:A:357:LEU:HD11	1:A:372:ALA:HB2	1.88	0.55
1:A:362:ARG:HH11	1:A:362:ARG:CG	2.08	0.55
1:D:89:ARG:O	1:D:93:GLU:HB2	2.06	0.55
1:F:320:THR:O	1:F:323:ARG:HD2	2.06	0.55
1:E:456:GLU:H	1:E:456:GLU:CD	2.13	0.55
1:A:111:ARG:HG3	1:A:118:PRO:HB3	1.88	0.55
1:C:113:GLN:OE1	1:C:113:GLN:HA	2.07	0.55
1:D:43:LEU:HB2	1:D:48:ARG:NH1	2.22	0.55
1:F:358:LEU:HB2	1:F:359:PRO:HD2	1.89	0.55
1:C:89:ARG:HH12	1:C:93:GLU:HG3	1.72	0.55
1:C:491:SER:C	1:C:493:ARG:H	2.14	0.55
1:F:305:GLU:HB3	1:F:332:GLN:O	2.07	0.55
1:B:41:ASN:HD21	1:B:419:ARG:NH1	2.03	0.55
1:B:323:ARG:HA	1:B:323:ARG:NH1	2.21	0.55
1:D:200:GLY:HA2	1:D:223:ILE:HB	1.89	0.55
1:E:271:ARG:HG2	1:E:271:ARG:NH1	2.22	0.55
1:F:59:ALA:O	1:F:63:GLU:HG3	2.06	0.55
1:B:225:ALA:HB2	1:B:233:TYR:CE2	2.42	0.55
1:B:232:GLN:NE2	1:B:263:ASP:H	1.99	0.55
1:B:489:PHE:CE1	1:B:493:ARG:HD3	2.42	0.55
1:E:257:PRO:O	1:E:258:PRO:C	2.49	0.55
1:A:46:THR:N	1:A:47:PRO:HD2	2.22	0.54
1:A:87:PHE:O	1:A:91:ILE:HG12	2.06	0.54
1:C:257:PRO:HB2	1:C:497:ARG:HD3	1.89	0.54
1:D:22:LYS:N	1:D:22:LYS:HD2	2.22	0.54
1:D:454:TYR:HB2	1:D:458:PHE:HD2	1.70	0.54
1:E:257:PRO:HB2	1:E:497:ARG:CD	2.31	0.54
1:B:70:THR:HB	1:B:72:VAL:HG12	1.89	0.54
1:B:268:GLU:HB3	1:B:271:ARG:NH2	2.23	0.54
1:D:333:ASN:HD21	1:D:335:PHE:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:THR:HB	1:E:47:PRO:CD	2.36	0.54
1:F:481:ILE:CD1	3:F:1815:HOH:O	2.55	0.54
1:B:72:VAL:N	3:B:782:HOH:O	2.40	0.54
1:C:43:LEU:HB2	1:C:48:ARG:NH1	2.23	0.54
1:C:417:ARG:NH2	1:C:439:ASP:OD2	2.41	0.54
1:E:428:GLY:O	1:E:429:MET:HB2	2.08	0.54
1:F:268:GLU:OE1	1:F:271:ARG:HD3	2.07	0.54
1:A:362:ARG:NH1	1:A:362:ARG:CG	2.69	0.54
1:C:22:LYS:CE	3:C:747:HOH:O	2.51	0.54
1:B:355:ARG:HG2	1:B:355:ARG:NH1	2.22	0.54
1:B:463:VAL:HG13	1:B:494:PRO:HD2	1.89	0.54
1:C:210:ILE:HB	1:C:211:PRO:HD3	1.89	0.54
1:D:72:VAL:O	1:D:72:VAL:CG1	2.55	0.54
1:D:99:GLY:O	1:D:102:PHE:HB3	2.08	0.54
1:E:257:PRO:HG2	1:E:258:PRO:HD3	1.90	0.54
1:A:22:LYS:C	1:A:24:ALA:N	2.64	0.54
1:D:203:VAL:HG22	1:D:204:PHE:N	2.22	0.54
1:E:360:ASP:O	1:E:363:SER:OG	2.26	0.54
1:B:425:ARG:CZ	1:D:159:ASP:C	2.80	0.54
1:C:32:MET:O	1:C:36:GLY:HA2	2.08	0.54
1:C:53:ARG:HG2	1:C:100:VAL:CG2	2.38	0.54
1:A:235:ASP:OD1	1:A:269:ARG:HG3	2.07	0.54
1:B:18:ASP:O	1:B:22:LYS:HG2	2.07	0.54
1:A:169:PHE:CE1	1:A:371:VAL:HG22	2.43	0.54
1:C:374:SER:O	1:C:375:ARG:HD3	2.08	0.54
1:E:234:PRO:HG3	3:E:1497:HOH:O	2.07	0.54
1:B:358:LEU:N	1:B:358:LEU:HD23	2.23	0.53
1:B:372:ALA:HA	1:B:380:ASN:HD22	1.73	0.53
1:C:132:CYS:HB3	1:D:43:LEU:HD22	1.90	0.53
1:D:414:GLN:NE2	3:D:855:HOH:O	2.40	0.53
1:F:257:PRO:HB2	1:F:497:ARG:CD	2.33	0.53
1:B:41:ASN:ND2	1:B:419:ARG:HH12	2.04	0.53
1:B:242:LYS:HD2	3:B:603:HOH:O	2.09	0.53
1:C:165:SER:HA	1:C:331:GLN:HG3	1.89	0.53
1:F:482:VAL:HA	3:F:1742:HOH:O	2.07	0.53
1:D:343:GLN:O	1:D:347:LYS:HG3	2.09	0.53
1:E:461:TRP:CB	3:E:1561:HOH:O	2.55	0.53
1:B:139:ARG:HG3	1:B:371:VAL:HG21	1.90	0.53
1:B:242:LYS:NZ	3:B:603:HOH:O	2.41	0.53
1:C:447:GLN:HE21	1:C:463:VAL:HG21	1.72	0.53
1:E:248:ILE:HG13	1:E:282:MET:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:HD3	3:A:765:HOH:O	2.07	0.53
1:F:192:LYS:O	1:F:195:ASP:HB2	2.09	0.53
1:A:159:ASP:HA	1:E:425:ARG:HH21	1.74	0.53
1:A:212:GLU:HB3	3:A:732:HOH:O	2.07	0.53
1:B:471:MET:HA	1:B:518:MET:HE1	1.91	0.53
1:F:32:MET:HE3	1:F:484:LEU:HG	1.90	0.53
1:C:266:SER:O	1:C:270:VAL:HG23	2.08	0.53
1:B:269:ARG:O	1:B:273:ILE:HG13	2.09	0.53
1:E:26:SER:HB3	1:E:29:ASN:HB2	1.91	0.53
1:E:387:THR:OG1	1:E:388:PRO:HD3	2.08	0.53
1:F:17:LYS:HE3	3:F:1594:HOH:O	2.08	0.53
1:F:474:ARG:NH1	1:F:474:ARG:HG3	2.21	0.53
1:A:398:LEU:O	1:A:402:MET:HG3	2.09	0.53
1:C:22:LYS:HD2	1:C:23:ILE:HD11	1.89	0.53
1:D:58:ALA:CB	1:D:126:VAL:HG13	2.39	0.53
1:E:248:ILE:HA	1:E:282:MET:O	2.07	0.53
1:F:232:GLN:NE2	1:F:263:ASP:H	2.07	0.53
1:C:89:ARG:NH1	1:C:93:GLU:CG	2.70	0.52
1:C:344:GLU:O	1:C:348:VAL:HG23	2.09	0.52
1:D:271:ARG:HH11	1:D:271:ARG:CG	2.21	0.52
1:F:24:ALA:CB	1:F:482:VAL:HG23	2.38	0.52
1:B:53:ARG:HG2	1:B:100:VAL:CG2	2.38	0.52
1:B:379:LEU:HD23	3:B:680:HOH:O	2.08	0.52
1:B:474:ARG:HG2	1:B:518:MET:HE2	1.90	0.52
1:B:373:ASP:HB2	3:B:869:HOH:O	2.09	0.52
1:A:463:VAL:HG13	1:A:494:PRO:CD	2.39	0.52
1:F:187:LEU:HD13	1:F:353:ARG:NH2	2.25	0.52
1:F:188:ASN:HB3	1:F:339:LEU:HD21	1.91	0.52
1:F:433:ARG:CD	3:F:1722:HOH:O	2.56	0.52
1:D:226:ASP:CG	1:D:228:SER:HB2	2.34	0.52
1:F:293:ALA:HB2	1:F:438:VAL:HG22	1.91	0.52
1:B:376:ALA:C	1:B:377:VAL:HG23	2.35	0.52
1:B:458:PHE:CE1	1:B:523:TYR:HA	2.45	0.52
1:B:472:LEU:CD2	1:B:483:LEU:HB2	2.39	0.52
1:A:364:LEU:CD2	1:A:369:ARG:HG2	2.40	0.52
1:F:237:GLU:HA	1:F:240:LYS:HD2	1.92	0.52
1:A:472:LEU:HD11	1:A:485:PRO:HG3	1.90	0.52
1:E:23:ILE:HD13	1:E:473:PHE:HD1	1.72	0.52
1:F:12:SER:O	1:F:16:LEU:HB2	2.10	0.52
1:C:491:SER:C	1:C:493:ARG:N	2.68	0.52
1:D:139:ARG:HD3	1:D:368:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:PRO:HG2	1:E:489:PHE:CB	2.34	0.52
1:F:288:VAL:CG2	1:F:312:SER:HB3	2.40	0.52
1:B:253:ASN:HA	1:B:254:PRO:C	2.34	0.52
1:C:306:ASN:ND2	1:C:334:VAL:HG11	2.25	0.52
1:D:41:ASN:ND2	1:D:419:ARG:HH22	2.04	0.52
1:D:156:MET:HG3	1:D:309:LEU:CD2	2.40	0.52
1:E:243:ASP:C	1:E:243:ASP:OD1	2.52	0.52
1:F:101:ARG:NH2	1:F:105:LYS:NZ	2.58	0.52
1:B:111:ARG:NH2	3:B:1819:HOH:O	2.37	0.51
1:B:151:TYR:CE2	1:B:155:GLU:HG3	2.45	0.51
1:B:255:SER:O	1:B:259:SER:HA	2.09	0.51
1:B:483:LEU:HD22	1:B:498:ALA:HB2	1.93	0.51
1:E:31:LEU:HG	1:E:31:LEU:O	2.08	0.51
1:C:43:LEU:N	1:C:43:LEU:HD23	2.26	0.51
1:C:203:VAL:O	1:C:204:PHE:C	2.52	0.51
1:C:320:THR:O	1:C:323:ARG:HD2	2.10	0.51
1:D:70:THR:HG22	1:D:72:VAL:H	1.75	0.51
1:C:151:TYR:HA	1:C:401:LEU:HD21	1.90	0.51
1:A:111:ARG:NH1	1:A:112:ASP:OD2	2.43	0.51
1:A:196:LYS:HB2	1:A:245:ALA:O	2.11	0.51
1:A:268:GLU:OE2	1:A:271:ARG:NH2	2.41	0.51
1:B:456:GLU:CD	1:B:456:GLU:N	2.69	0.51
1:C:243:ASP:C	1:C:243:ASP:OD1	2.52	0.51
1:D:227:PRO:HG3	1:D:231:TRP:CH2	2.46	0.51
1:E:54:LEU:HB2	1:E:103:LEU:HD21	1.92	0.51
1:E:71:THR:O	1:E:71:THR:HG22	2.10	0.51
1:A:251:CYS:O	1:A:285:THR:HA	2.10	0.51
1:F:202:PRO:HB3	3:F:1598:HOH:O	2.10	0.51
1:F:456:GLU:O	1:F:459:SER:HB3	2.09	0.51
1:A:324:LEU:HD21	1:A:389:GLN:HB3	1.93	0.51
1:C:252:VAL:HG22	1:C:286:ASP:HB3	1.93	0.51
1:F:12:SER:O	1:F:16:LEU:CB	2.59	0.51
1:A:67:SER:HB3	1:D:109:TYR:HA	1.91	0.51
1:A:347:LYS:HD3	1:A:362:ARG:HE	1.76	0.51
1:C:233:TYR:HB2	1:C:238:LEU:HD21	1.93	0.51
1:F:161:ILE:O	1:F:162:PRO:C	2.54	0.51
1:A:294:ASP:O	3:A:768:HOH:O	2.19	0.51
1:E:23:ILE:HD13	1:E:473:PHE:CE1	2.46	0.51
1:E:386:SER:OG	1:E:389:GLN:HB2	2.09	0.51
1:E:523:TYR:O	1:E:527:SER:CB	2.57	0.51
1:B:172:GLU:HG2	1:B:176:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ILE:HD12	1:C:23:ILE:N	2.26	0.51
1:C:305:GLU:O	1:C:334:VAL:HG13	2.11	0.51
1:F:429:MET:HB3	1:F:430:PRO:HD2	1.93	0.51
1:E:472:LEU:HD22	1:E:483:LEU:HB2	1.93	0.51
1:A:156:MET:HG3	1:A:309:LEU:HD11	1.92	0.50
1:A:521:GLU:O	1:A:525:GLU:HG3	2.11	0.50
1:B:53:ARG:HG2	1:B:100:VAL:HG22	1.93	0.50
1:B:333:ASN:ND2	1:B:335:PHE:HB2	2.26	0.50
1:B:398:LEU:O	1:B:402:MET:HG3	2.12	0.50
1:B:489:PHE:H	1:B:489:PHE:HD2	1.58	0.50
1:E:35:ALA:O	1:E:37:ARG:HG3	2.10	0.50
1:F:434:ASP:HB3	1:F:436:ASN:H	1.75	0.50
1:A:404:GLU:OE1	1:E:418:ARG:HD2	2.11	0.50
1:B:80:ILE:HG22	3:B:655:HOH:O	2.10	0.50
1:E:380:ASN:ND2	3:E:1440:HOH:O	2.25	0.50
1:F:253:ASN:HA	1:F:254:PRO:C	2.36	0.50
1:A:525:GLU:O	1:A:528:GLY:N	2.44	0.50
1:B:257:PRO:CD	1:B:258:PRO:HD3	2.42	0.50
1:E:353:ARG:HG3	1:E:353:ARG:NH1	2.23	0.50
1:F:461:TRP:CZ3	1:F:526:TYR:HB2	2.46	0.50
1:E:111:ARG:NH2	3:E:1420:HOH:O	2.33	0.50
1:A:19:GLU:CD	3:A:548:HOH:O	2.54	0.50
1:C:89:ARG:O	1:C:93:GLU:HG2	2.12	0.50
1:D:158:ALA:HB1	1:D:161:ILE:HD12	1.94	0.50
1:E:334:VAL:HA	1:E:337:LEU:HD12	1.93	0.50
1:A:448:ASP:O	1:A:452:LYS:HG3	2.12	0.50
1:C:262:MET:HE3	1:C:266:SER:HB3	1.94	0.50
1:C:139:ARG:HB2	1:C:371:VAL:HG21	1.94	0.50
1:F:40:PRO:HA	1:F:501:ALA:O	2.12	0.50
1:A:437:ALA:HB1	1:A:439:ASP:OD2	2.12	0.50
1:A:458:PHE:CE1	1:A:523:TYR:HA	2.47	0.50
1:B:251:CYS:O	1:B:285:THR:HA	2.12	0.49
1:C:403:ASP:OD1	3:C:1895:HOH:O	2.20	0.49
1:B:243:ASP:OD2	1:B:245:ALA:HB3	2.12	0.49
1:E:264:GLN:O	1:E:265:ARG:C	2.53	0.49
1:E:367:ILE:O	1:E:370:LEU:HB2	2.12	0.49
1:A:491:SER:C	1:A:493:ARG:H	2.19	0.49
1:C:201:MET:HA	1:C:202:PRO:C	2.36	0.49
1:D:196:LYS:HB2	1:D:245:ALA:O	2.11	0.49
1:F:197:VAL:HG23	1:F:248:ILE:CG2	2.30	0.49
1:F:266:SER:O	1:F:270:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:O	1:D:402:MET:HE3	2.12	0.49
1:B:33:LEU:HD23	1:B:484:LEU:HD23	1.95	0.49
1:C:456:GLU:HG2	3:C:1099:HOH:O	2.12	0.49
1:D:172:GLU:HG2	1:D:176:ALA:HB2	1.94	0.49
1:F:41:ASN:C	1:F:41:ASN:HD22	2.19	0.49
1:A:22:LYS:O	1:A:24:ALA:N	2.46	0.49
1:D:71:THR:HG23	1:D:71:THR:O	2.12	0.49
1:E:195:ASP:OD1	1:E:247:LYS:CG	2.58	0.49
1:A:106:SER:HB2	1:A:398:LEU:HD13	1.95	0.49
1:A:248:ILE:HB	1:A:282:MET:HE3	1.94	0.49
1:A:333:ASN:ND2	1:A:335:PHE:HB2	2.25	0.49
1:B:161:ILE:HD12	1:B:161:ILE:N	2.28	0.49
1:F:50:ALA:CB	1:F:102:PHE:HD2	2.26	0.49
1:A:120:ALA:O	3:A:617:HOH:O	2.20	0.49
1:A:304:PRO:HB2	1:A:330:HIS:HD2	1.78	0.49
1:B:357:LEU:O	1:B:358:LEU:HB3	2.11	0.49
1:C:41:ASN:HD22	1:C:41:ASN:H	1.59	0.49
1:C:67:SER:HB3	1:F:109:TYR:HA	1.95	0.49
1:D:472:LEU:HD22	1:D:483:LEU:HB2	1.94	0.49
1:A:150:GLN:NE2	3:A:648:HOH:O	2.46	0.49
1:B:224:ASN:O	1:B:237:GLU:HG2	2.12	0.49
1:B:333:ASN:HD22	1:B:335:PHE:N	2.02	0.49
1:A:221:VAL:HG11	1:A:246:ILE:HD11	1.94	0.49
1:A:248:ILE:HG13	1:A:282:MET:O	2.12	0.49
1:B:171:VAL:C	1:B:385:LEU:HD13	2.38	0.49
1:C:155:GLU:O	3:C:953:HOH:O	2.20	0.49
1:C:314:SER:HB3	1:C:320:THR:HG22	1.94	0.49
1:C:489:PHE:CD1	1:C:489:PHE:N	2.79	0.49
1:D:41:ASN:C	1:D:41:ASN:HD22	2.19	0.49
1:D:140:MET:HE2	1:D:145:GLU:CA	2.41	0.49
1:D:491:SER:C	1:D:493:ARG:H	2.19	0.49
1:C:49:ARG:O	1:C:53:ARG:HB2	2.13	0.49
1:C:72:VAL:HG12	1:C:74:VAL:CG2	2.41	0.49
1:C:252:VAL:O	1:C:255:SER:HA	2.13	0.49
1:C:454:TYR:HB2	1:C:458:PHE:CD2	2.48	0.49
1:C:481:ILE:HG21	1:C:511:ILE:HD11	1.95	0.49
1:D:196:LYS:HE2	1:D:219:GLU:OE1	2.13	0.49
1:E:24:ALA:HB3	1:E:482:VAL:HG23	1.95	0.49
1:F:333:ASN:HD21	1:F:335:PHE:HB2	1.78	0.49
1:A:30:ARG:HG3	1:A:30:ARG:HH11	1.77	0.48
1:C:376:ALA:O	1:C:378:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:LEU:HD23	1:D:358:LEU:H	1.76	0.48
1:F:354:TYR:HB2	1:F:361:VAL:CG1	2.43	0.48
1:A:143:ILE:O	1:A:147:ILE:HG13	2.12	0.48
1:A:196:LYS:HD2	1:A:245:ALA:CB	2.42	0.48
1:A:347:LYS:HB3	1:A:362:ARG:NH2	2.29	0.48
1:C:417:ARG:HA	1:C:417:ARG:HD3	1.55	0.48
1:D:206:PRO:O	1:D:210:ILE:HG13	2.13	0.48
1:E:216:TYR:O	1:E:218:LEU:HD23	2.13	0.48
1:F:144:SER:O	1:F:148:VAL:HG23	2.13	0.48
1:B:257:PRO:CG	1:B:258:PRO:HD3	2.44	0.48
1:C:23:ILE:O	1:C:23:ILE:HG22	2.11	0.48
1:C:106:SER:HB3	1:C:398:LEU:HD13	1.95	0.48
1:C:107:LEU:HD13	1:C:122:LEU:HD21	1.94	0.48
1:D:333:ASN:ND2	1:D:335:PHE:HB2	2.28	0.48
1:E:253:ASN:HA	1:E:254:PRO:C	2.37	0.48
1:E:483:LEU:HD22	1:E:498:ALA:HB2	1.95	0.48
1:F:428:GLY:C	1:F:429:MET:HG2	2.38	0.48
1:A:225:ALA:HB2	1:A:233:TYR:CE2	2.48	0.48
1:D:458:PHE:CE1	1:D:523:TYR:HA	2.48	0.48
1:E:43:LEU:HD11	1:E:45:THR:HG22	1.94	0.48
1:F:298:SER:O	1:F:301:ALA:N	2.41	0.48
1:A:457:ALA:CB	3:A:812:HOH:O	2.58	0.48
1:B:205:THR:O	1:B:209:GLU:HG3	2.13	0.48
1:C:372:ALA:CA	1:C:380:ASN:HD22	2.26	0.48
1:E:499:SER:HB3	1:E:502:ASN:OD1	2.12	0.48
1:F:257:PRO:HD2	1:F:258:PRO:HD3	1.94	0.48
1:F:319:ALA:O	1:F:320:THR:C	2.54	0.48
1:B:522:LEU:HD23	1:B:522:LEU:HA	1.57	0.48
1:C:19:GLU:O	1:C:23:ILE:HD12	2.13	0.48
1:C:473:PHE:HD1	3:C:720:HOH:O	1.88	0.48
1:D:237:GLU:O	1:D:240:LYS:HG3	2.14	0.48
1:F:254:PRO:HB3	1:F:438:VAL:HG21	1.95	0.48
1:F:376:ALA:C	1:F:377:VAL:HG23	2.37	0.48
1:B:358:LEU:N	1:B:358:LEU:CD2	2.76	0.48
1:B:425:ARG:CZ	1:D:159:ASP:HA	2.38	0.48
1:C:41:ASN:HD21	1:C:419:ARG:HH12	1.62	0.48
1:C:358:LEU:HD21	1:C:361:VAL:HA	1.96	0.48
1:D:269:ARG:O	1:D:273:ILE:HG13	2.14	0.48
1:E:95:ARG:O	1:E:101:ARG:CD	2.62	0.48
1:A:23:ILE:HD12	1:A:473:PHE:CE1	2.48	0.48
1:C:423:LEU:HD21	1:C:444:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:PRO:HG2	1:E:220:GLU:OE2	2.14	0.48
1:A:148:VAL:O	1:A:152:ILE:HG12	2.13	0.48
1:A:169:PHE:CD1	1:A:371:VAL:HG22	2.49	0.48
1:A:358:LEU:HD23	1:A:358:LEU:N	2.28	0.48
1:B:387:THR:N	1:B:388:PRO:CD	2.76	0.48
1:B:451:ALA:HB2	1:B:459:SER:CB	2.44	0.48
1:E:43:LEU:C	1:E:43:LEU:CD1	2.85	0.48
1:E:169:PHE:O	1:E:171:VAL:HG13	2.14	0.48
1:E:322:TRP:HB3	1:E:324:LEU:HG	1.95	0.48
1:E:474:ARG:NH1	1:E:474:ARG:HG3	2.28	0.48
1:B:195:ASP:OD1	1:B:247:LYS:NZ	2.42	0.48
1:C:94:ASN:HB3	1:C:97:GLN:OE1	2.13	0.48
1:C:139:ARG:O	1:C:140:MET:HB2	2.14	0.48
1:E:234:PRO:O	1:E:235:ASP:C	2.56	0.48
1:A:204:PHE:HE2	1:A:207:TYR:CD2	2.32	0.47
1:C:43:LEU:HB2	1:C:48:ARG:HH12	1.78	0.47
1:C:53:ARG:HD2	1:D:56:LEU:HD21	1.96	0.47
1:C:379:LEU:HB3	1:D:175:THR:HG23	1.96	0.47
1:D:58:ALA:HB1	1:D:130:LEU:HG	1.95	0.47
1:E:41:ASN:C	1:E:41:ASN:ND2	2.72	0.47
1:E:447:GLN:HG3	1:E:459:SER:OG	2.14	0.47
1:E:467:SER:O	1:E:469:GLY:N	2.47	0.47
1:A:227:PRO:HG2	1:A:489:PHE:HB3	1.96	0.47
1:B:87:PHE:O	1:B:90:TYR:HB3	2.13	0.47
1:B:371:VAL:O	1:B:374:SER:OG	2.32	0.47
1:C:56:LEU:HA	1:C:56:LEU:HD23	1.73	0.47
1:D:127:ASP:OD1	3:D:763:HOH:O	2.20	0.47
1:E:43:LEU:HD13	1:E:48:ARG:NH1	2.28	0.47
1:E:458:PHE:HA	3:E:1561:HOH:O	2.14	0.47
1:F:254:PRO:HD3	1:F:296:PHE:CE1	2.49	0.47
1:A:135:PRO:HG3	1:A:387:THR:HG23	1.97	0.47
1:A:139:ARG:HG3	1:A:371:VAL:CG2	2.44	0.47
1:A:332:GLN:HA	3:A:693:HOH:O	2.15	0.47
1:C:70:THR:HG22	1:C:72:VAL:HB	1.96	0.47
1:C:294:ASP:OD2	1:C:433:ARG:NH2	2.42	0.47
1:D:252:VAL:O	1:D:255:SER:HA	2.14	0.47
1:E:488:GLY:C	1:E:490:GLY:N	2.59	0.47
1:F:491:SER:HB2	3:F:1582:HOH:O	2.13	0.47
1:A:24:ALA:HB1	1:A:29:ASN:ND2	2.30	0.47
1:A:196:LYS:HD2	1:A:245:ALA:HB3	1.97	0.47
1:B:225:ALA:HA	1:B:233:TYR:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:GLN:HA	1:B:529:GLN:NE2	2.28	0.47
1:C:70:THR:CG2	1:C:72:VAL:HB	2.44	0.47
1:D:211:PRO:HG2	1:D:220:GLU:OE1	2.14	0.47
1:E:27:ASP:HA	1:E:30:ARG:HD2	1.96	0.47
1:F:361:VAL:HG12	1:F:361:VAL:O	2.13	0.47
1:A:19:GLU:C	1:A:21:ILE:H	2.22	0.47
1:A:31:LEU:HD21	1:B:134:TYR:CD2	2.50	0.47
1:B:503:LEU:HB2	1:B:508:TYR:CZ	2.50	0.47
1:C:503:LEU:HB2	1:C:508:TYR:CE2	2.50	0.47
1:D:86:ARG:HG2	3:D:572:HOH:O	2.14	0.47
1:A:384:GLY:CA	3:A:669:HOH:O	2.41	0.47
1:A:424:TYR:O	1:A:425:ARG:C	2.58	0.47
1:B:234:PRO:HG2	1:B:237:GLU:HB2	1.97	0.47
1:C:333:ASN:HD21	1:C:335:PHE:HB2	1.79	0.47
1:D:91:ILE:O	1:D:92:ALA:C	2.57	0.47
1:D:425:ARG:CZ	1:F:159:ASP:HA	2.42	0.47
1:E:149:ARG:CA	1:E:168:LEU:HD11	2.45	0.47
1:E:323:ARG:HA	1:E:323:ARG:NH1	2.30	0.47
1:E:503:LEU:HB2	1:E:508:TYR:CZ	2.49	0.47
1:F:282:MET:HE3	1:F:335:PHE:CE2	2.48	0.47
1:F:298:SER:C	1:F:300:PHE:N	2.71	0.47
1:F:354:TYR:HB2	1:F:361:VAL:HG13	1.97	0.47
1:A:254:PRO:HD3	1:A:296:PHE:CE1	2.50	0.47
1:A:482:VAL:O	3:A:576:HOH:O	2.20	0.47
1:B:139:ARG:O	1:B:140:MET:HB2	2.14	0.47
1:C:22:LYS:CD	1:C:23:ILE:HG13	2.45	0.47
1:C:43:LEU:HD23	1:D:75:GLY:O	2.15	0.47
1:F:419:ARG:HB3	1:F:508:TYR:CE2	2.50	0.47
1:A:198:ALA:HB2	1:A:246:ILE:HD13	1.97	0.47
1:C:461:TRP:CH2	1:C:525:GLU:HG2	2.50	0.47
1:E:176:ALA:O	1:E:177:ALA:C	2.57	0.47
1:E:293:ALA:HA	1:E:438:VAL:HG22	1.97	0.47
1:F:199:ILE:O	1:F:201:MET:HG3	2.14	0.47
1:A:30:ARG:O	1:A:34:ASN:HB2	2.15	0.47
1:A:320:THR:O	1:A:323:ARG:HD2	2.14	0.47
1:C:53:ARG:HG2	1:C:100:VAL:HG23	1.97	0.47
1:C:322:TRP:HB3	1:C:324:LEU:HG	1.97	0.47
1:E:91:ILE:HA	1:E:100:VAL:CG1	2.45	0.47
1:F:71:THR:HG22	1:F:71:THR:O	2.14	0.47
1:A:306:ASN:HA	1:A:334:VAL:HG22	1.97	0.46
1:B:333:ASN:HD21	1:B:335:PHE:HB2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ALA:HA	1:C:438:VAL:HG22	1.97	0.46
1:D:358:LEU:HB2	1:D:359:PRO:HD2	1.97	0.46
1:F:17:LYS:O	1:F:21:ILE:HG13	2.15	0.46
1:F:140:MET:HE2	1:F:145:GLU:HA	1.97	0.46
1:F:282:MET:CE	1:F:335:PHE:CE2	2.97	0.46
1:F:355:ARG:CB	1:F:355:ARG:CZ	2.92	0.46
1:F:474:ARG:HG3	1:F:474:ARG:HH11	1.80	0.46
1:D:424:TYR:O	1:D:425:ARG:C	2.57	0.46
1:A:347:LYS:HD3	1:A:362:ARG:NE	2.31	0.46
1:A:357:LEU:HD11	1:A:372:ALA:CB	2.45	0.46
1:B:407:GLU:CG	3:B:659:HOH:O	2.63	0.46
1:B:446:LEU:HD13	1:B:471:MET:HE3	1.97	0.46
1:C:257:PRO:CD	1:C:258:PRO:HD3	2.45	0.46
1:C:423:LEU:HD23	1:C:424:TYR:CE1	2.50	0.46
1:C:461:TRP:CZ3	1:C:526:TYR:HB2	2.50	0.46
1:E:92:ALA:O	1:E:95:ARG:HG3	2.15	0.46
1:F:229:LEU:CD1	1:F:234:PRO:HB3	2.45	0.46
1:F:461:TRP:CE3	1:F:526:TYR:HB2	2.50	0.46
1:A:158:ALA:HB1	1:A:161:ILE:CD1	2.45	0.46
1:A:203:VAL:HA	1:A:256:ASN:O	2.16	0.46
1:B:225:ALA:HB2	1:B:233:TYR:HE2	1.81	0.46
1:C:117:ASP:HB3	1:C:120:ALA:HB3	1.96	0.46
1:F:185:LEU:HD22	1:F:282:MET:HE1	1.97	0.46
1:F:190:LEU:HD22	1:F:338:ALA:CB	2.46	0.46
1:F:344:GLU:O	1:F:348:VAL:HG23	2.15	0.46
1:F:491:SER:C	1:F:493:ARG:H	2.10	0.46
1:A:76:GLY:HA2	1:B:41:ASN:O	2.16	0.46
1:A:257:PRO:CG	1:A:258:PRO:HD3	2.45	0.46
1:A:472:LEU:HD22	1:A:483:LEU:HB2	1.97	0.46
1:B:428:GLY:O	1:B:429:MET:O	2.34	0.46
1:B:447:GLN:HG3	1:B:459:SER:OG	2.15	0.46
1:D:447:GLN:NE2	3:D:1310:HOH:O	2.49	0.46
1:E:456:GLU:CD	1:E:456:GLU:N	2.73	0.46
1:F:468:THR:O	1:F:472:LEU:HG	2.16	0.46
1:A:23:ILE:HD12	1:A:473:PHE:HE1	1.81	0.46
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.73	0.46
1:C:41:ASN:HD22	1:C:41:ASN:N	2.11	0.46
1:E:362:ARG:HG3	1:E:362:ARG:HH11	1.81	0.46
1:E:474:ARG:HG3	1:E:474:ARG:HH11	1.81	0.46
1:F:448:ASP:CB	3:F:1711:HOH:O	2.44	0.46
1:A:463:VAL:HG13	1:A:494:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLU:CD	1:B:172:GLU:N	2.74	0.46
1:C:190:LEU:O	1:C:282:MET:HE1	2.16	0.46
1:D:197:VAL:HG12	1:D:218:LEU:HB3	1.98	0.46
1:D:489:PHE:O	1:D:490:GLY:C	2.59	0.46
1:F:203:VAL:HG23	3:F:1673:HOH:O	2.16	0.46
1:F:310:VAL:O	1:F:310:VAL:HG12	2.15	0.46
1:A:43:LEU:C	1:A:43:LEU:HD12	2.41	0.46
1:A:387:THR:N	1:A:388:PRO:CD	2.79	0.46
1:E:110:VAL:HG11	1:E:121:PHE:CG	2.50	0.46
1:F:53:ARG:HD3	1:F:100:VAL:HG23	1.96	0.46
1:F:190:LEU:CD2	1:F:338:ALA:HB1	2.46	0.46
1:F:234:PRO:O	1:F:235:ASP:C	2.59	0.46
1:A:524:ALA:O	1:A:527:SER:HB2	2.16	0.46
1:D:248:ILE:O	1:D:248:ILE:HG23	2.16	0.46
1:F:201:MET:HE1	1:F:208:ILE:HD11	1.97	0.46
1:A:172:GLU:HG3	1:B:375:ARG:HH21	1.81	0.46
1:A:502:ASN:OD1	1:A:503:LEU:HG	2.16	0.46
1:B:79:LYS:HB2	3:B:778:HOH:O	2.14	0.46
1:B:139:ARG:NH2	3:B:825:HOH:O	2.48	0.46
1:D:474:ARG:NH2	1:D:521:GLU:OE1	2.42	0.46
1:F:257:PRO:CD	1:F:258:PRO:HD3	2.46	0.46
1:A:156:MET:HE2	1:A:156:MET:CA	2.42	0.45
1:C:98:GLU:O	1:C:99:GLY:C	2.57	0.45
1:C:342:LEU:O	1:C:347:LYS:HE3	2.16	0.45
1:F:237:GLU:HA	1:F:240:LYS:CD	2.46	0.45
1:A:433:ARG:HG2	1:A:434:ASP:N	2.31	0.45
1:C:22:LYS:C	1:C:22:LYS:CD	2.66	0.45
1:C:52:PHE:CZ	1:D:55:GLY:HA3	2.51	0.45
1:B:404:GLU:HG2	3:B:653:HOH:O	2.15	0.45
1:C:489:PHE:HD1	1:C:489:PHE:H	1.64	0.45
1:D:418:ARG:HD3	1:F:404:GLU:OE1	2.15	0.45
1:E:102:PHE:CE1	1:E:402:MET:HE3	2.51	0.45
1:F:53:ARG:HD2	3:F:1639:HOH:O	2.15	0.45
1:C:251:CYS:SG	1:C:252:VAL:N	2.89	0.45
1:D:529:GLN:HG2	1:D:529:GLN:O	2.14	0.45
1:E:46:THR:HB	1:E:47:PRO:HD3	1.98	0.45
1:F:101:ARG:NE	1:F:105:LYS:HE3	2.32	0.45
1:F:255:SER:O	1:F:259:SER:HA	2.16	0.45
1:F:330:HIS:ND1	1:F:332:GLN:HG2	2.31	0.45
1:B:32:MET:HE3	1:B:484:LEU:HG	1.99	0.45
1:B:205:THR:HB	1:B:206:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:LYS:O	1:F:261:LYS:HG3	2.17	0.45
1:F:456:GLU:HA	1:F:459:SER:HB3	1.98	0.45
1:F:474:ARG:HH11	1:F:474:ARG:CG	2.29	0.45
1:A:22:LYS:O	1:A:23:ILE:C	2.59	0.45
1:A:253:ASN:O	1:A:287:ASP:HA	2.15	0.45
1:C:33:LEU:HD11	1:C:482:VAL:HG11	1.99	0.45
1:D:470:ASP:CB	3:D:1309:HOH:O	2.64	0.45
1:E:369:ARG:O	1:E:370:LEU:C	2.59	0.45
1:E:461:TRP:HB3	3:E:1561:HOH:O	2.14	0.45
1:A:489:PHE:N	1:A:489:PHE:CD2	2.83	0.45
1:B:32:MET:O	1:B:36:GLY:HA2	2.16	0.45
1:C:172:GLU:HG2	1:C:176:ALA:HB2	1.97	0.45
1:C:185:LEU:HB3	1:C:191:LEU:HB2	1.98	0.45
1:D:201:MET:HA	1:D:202:PRO:C	2.42	0.45
1:E:357:LEU:HB3	1:E:358:LEU:HD23	1.99	0.45
1:E:497:ARG:NE	3:E:1520:HOH:O	2.34	0.45
1:F:101:ARG:HG2	1:F:101:ARG:NH1	2.25	0.45
1:F:270:VAL:O	1:F:274:VAL:HG23	2.17	0.45
1:F:305:GLU:HB2	1:F:333:ASN:HA	1.99	0.45
1:F:474:ARG:O	1:F:478:GLU:HG3	2.17	0.45
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.79	0.45
1:E:287:ASP:N	1:E:287:ASP:OD1	2.47	0.45
1:A:192:LYS:O	1:A:195:ASP:HB2	2.16	0.45
1:C:22:LYS:HE3	1:C:23:ILE:HG13	1.98	0.45
1:C:174:GLY:N	2:C:900:PLP:O3P	2.44	0.45
1:C:281:LEU:O	1:C:306:ASN:HB3	2.17	0.45
1:C:333:ASN:ND2	1:C:333:ASN:C	2.74	0.45
1:C:337:LEU:O	1:C:340:ASP:HB2	2.16	0.45
1:C:408:TYR:CA	1:D:72:VAL:HG11	2.46	0.45
1:E:171:VAL:HA	3:E:1443:HOH:O	2.17	0.45
1:E:456:GLU:HA	1:E:459:SER:HB3	1.98	0.45
1:A:117:ASP:HB3	1:A:120:ALA:HB3	1.99	0.45
1:B:79:LYS:HE3	3:B:654:HOH:O	2.16	0.45
1:C:102:PHE:O	1:C:103:LEU:C	2.60	0.45
1:C:333:ASN:ND2	1:C:335:PHE:N	2.55	0.45
1:E:19:GLU:HA	1:E:22:LYS:HD2	1.99	0.45
1:E:169:PHE:CE1	1:E:371:VAL:HG22	2.51	0.45
1:F:471:MET:HG2	1:F:472:LEU:HD23	1.99	0.45
1:F:490:GLY:O	1:F:492:ASN:ND2	2.50	0.45
1:A:266:SER:O	1:A:267:LEU:C	2.60	0.44
1:B:456:GLU:HA	1:B:459:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:VAL:O	1:E:222:ALA:C	2.59	0.44
1:B:24:ALA:HB3	1:B:482:VAL:CG2	2.45	0.44
1:B:287:ASP:OD1	1:B:287:ASP:N	2.50	0.44
1:B:407:GLU:HG2	3:B:725:HOH:O	2.17	0.44
1:C:201:MET:CB	1:C:202:PRO:HA	2.47	0.44
1:D:491:SER:C	1:D:493:ARG:N	2.74	0.44
1:E:162:PRO:O	1:E:163:SER:C	2.60	0.44
1:A:304:PRO:HB2	1:A:330:HIS:CD2	2.51	0.44
1:A:340:ASP:HB2	3:A:720:HOH:O	2.18	0.44
1:C:447:GLN:HB2	1:C:463:VAL:CG2	2.48	0.44
1:D:140:MET:HE2	1:D:144:SER:C	2.43	0.44
1:D:201:MET:HB3	1:D:202:PRO:HA	1.98	0.44
1:D:396:PHE:O	1:D:399:PHE:HB3	2.16	0.44
1:D:517:LYS:O	1:D:521:GLU:HG3	2.17	0.44
1:A:184:SER:HB2	1:A:370:LEU:HD23	2.00	0.44
1:A:421:THR:O	1:A:425:ARG:HG3	2.17	0.44
1:B:265:ARG:HG2	1:B:265:ARG:HH11	1.81	0.44
1:B:413:LYS:O	1:B:417:ARG:HG2	2.17	0.44
1:B:447:GLN:CG	1:B:459:SER:OG	2.66	0.44
1:C:52:PHE:CE2	1:D:55:GLY:HA3	2.52	0.44
1:C:263:ASP:OD1	1:C:263:ASP:C	2.61	0.44
1:C:468:THR:O	1:C:472:LEU:HG	2.17	0.44
1:D:513:ARG:NH2	1:F:164:GLU:CG	2.80	0.44
1:F:91:ILE:HD13	1:F:100:VAL:HG13	1.99	0.44
1:A:24:ALA:HB3	1:A:482:VAL:HG21	1.99	0.44
1:E:50:ALA:CB	1:E:102:PHE:HD2	2.31	0.44
1:E:87:PHE:CZ	1:E:91:ILE:HD11	2.53	0.44
1:E:425:ARG:HG3	1:E:425:ARG:HH11	1.83	0.44
1:F:343:GLN:O	1:F:344:GLU:C	2.61	0.44
1:A:474:ARG:NH1	3:A:1887:HOH:O	2.44	0.44
1:D:184:SER:CB	1:D:370:LEU:HD23	2.48	0.44
1:E:152:ILE:O	1:E:153:ILE:C	2.60	0.44
1:F:41:ASN:ND2	1:F:419:ARG:HH22	2.14	0.44
1:F:187:LEU:HD13	1:F:353:ARG:HH21	1.81	0.44
1:C:136:VAL:O	1:C:136:VAL:HG13	2.18	0.44
1:D:171:VAL:HG21	1:D:177:ALA:HB2	1.99	0.44
1:E:94:ASN:HB3	1:E:97:GLN:OE1	2.17	0.44
1:A:53:ARG:HG2	1:A:100:VAL:HG23	2.00	0.44
1:A:387:THR:OG1	1:A:388:PRO:HD3	2.18	0.44
1:C:102:PHE:CE1	1:C:402:MET:CE	3.00	0.44
1:D:473:PHE:O	1:D:477:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:TRP:HB2	3:E:1561:HOH:O	2.17	0.44
1:F:127:ASP:OD2	1:F:133:ASN:ND2	2.45	0.44
1:A:19:GLU:C	1:A:21:ILE:N	2.75	0.44
1:A:32:MET:HE3	1:A:484:LEU:HG	2.00	0.44
1:A:232:GLN:HE22	1:A:263:ASP:H	1.64	0.44
1:C:353:ARG:HA	3:C:1878:HOH:O	2.17	0.44
1:D:136:VAL:O	1:D:136:VAL:CG1	2.66	0.44
1:E:117:ASP:HA	1:E:118:PRO:HD2	1.83	0.44
1:A:332:GLN:HG3	3:A:692:HOH:O	2.17	0.43
1:B:463:VAL:HG13	1:B:494:PRO:CD	2.47	0.43
1:C:283:ILE:HG22	1:C:307:THR:HG23	1.99	0.43
1:C:427:LEU:HD22	1:C:449:VAL:HG11	2.00	0.43
1:D:513:ARG:HH11	1:D:513:ARG:CG	2.19	0.43
1:E:32:MET:HE3	1:E:484:LEU:HG	1.99	0.43
1:E:467:SER:C	1:E:469:GLY:N	2.74	0.43
1:F:417:ARG:HD3	1:F:417:ARG:HA	1.68	0.43
1:A:139:ARG:O	1:A:140:MET:HB2	2.17	0.43
1:A:429:MET:HB3	1:A:430:PRO:HD2	1.99	0.43
1:A:525:GLU:O	1:A:526:TYR:C	2.61	0.43
1:C:447:GLN:HB3	1:C:493:ARG:HH21	1.82	0.43
1:E:148:VAL:O	1:E:151:TYR:HB3	2.18	0.43
1:E:314:SER:HB3	1:E:320:THR:HG22	1.99	0.43
1:F:344:GLU:OE2	1:F:362:ARG:NH2	2.41	0.43
1:A:271:ARG:HA	1:A:303:CYS:SG	2.58	0.43
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.73	0.43
1:B:27:ASP:OD1	1:B:30:ARG:NH1	2.51	0.43
1:B:46:THR:N	1:B:47:PRO:HD2	2.33	0.43
1:B:254:PRO:HG2	1:B:289:TYR:CB	2.37	0.43
1:C:517:LYS:O	1:C:518:MET:C	2.61	0.43
1:D:199:ILE:HG22	1:D:201:MET:HG2	2.00	0.43
1:E:192:LYS:HB2	1:E:195:ASP:OD2	2.18	0.43
1:E:288:VAL:HG23	1:E:312:SER:HB3	2.00	0.43
1:F:376:ALA:O	1:F:378:ALA:N	2.49	0.43
1:A:57:PHE:HB2	1:A:90:TYR:CE2	2.54	0.43
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.69	0.43
1:B:108:SER:O	1:B:112:ASP:HB2	2.18	0.43
1:B:242:LYS:CD	3:B:603:HOH:O	2.65	0.43
1:D:242:LYS:HE2	1:D:277:HIS:CD2	2.53	0.43
1:D:254:PRO:HD3	1:D:296:PHE:CE1	2.53	0.43
1:D:481:ILE:HD12	1:D:503:LEU:CD1	2.48	0.43
1:E:172:GLU:CD	1:E:172:GLU:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:482:VAL:O	1:E:482:VAL:HG12	2.18	0.43
1:A:25:SER:HA	1:A:30:ARG:NH1	2.32	0.43
1:B:44:ALA:O	1:B:48:ARG:HG3	2.18	0.43
1:D:271:ARG:NH1	1:D:271:ARG:CG	2.78	0.43
1:E:242:LYS:O	1:E:244:PRO:HD3	2.18	0.43
1:E:471:MET:HE2	1:E:515:LEU:HD11	2.00	0.43
1:F:20:LEU:HD23	1:F:20:LEU:HA	1.89	0.43
1:D:97:GLN:HB2	1:D:100:VAL:HG21	2.01	0.43
1:D:489:PHE:N	1:D:489:PHE:CD1	2.85	0.43
1:F:307:THR:HG22	1:F:308:LEU:N	2.32	0.43
1:F:484:LEU:HB2	1:F:497:ARG:HB2	2.01	0.43
1:A:303:CYS:HB3	3:A:710:HOH:O	2.18	0.43
1:A:426:GLU:O	1:A:427:LEU:HD23	2.18	0.43
1:C:278:ARG:HG3	1:C:278:ARG:NH1	2.32	0.43
1:C:439:ASP:O	1:C:500:LEU:HD12	2.18	0.43
1:D:276:GLU:OE2	1:D:276:GLU:HA	2.18	0.43
1:E:116:LEU:HD13	1:E:143:ILE:HG23	2.01	0.43
1:E:504:ASN:O	1:E:505:GLU:C	2.61	0.43
1:F:337:LEU:O	1:F:340:ASP:HB3	2.17	0.43
1:F:419:ARG:HD3	1:F:508:TYR:HE2	1.83	0.43
1:F:490:GLY:C	1:F:492:ASN:N	2.76	0.43
1:A:210:ILE:N	1:A:211:PRO:HD2	2.34	0.43
1:A:210:ILE:HB	1:A:211:PRO:HD3	2.01	0.43
1:A:351:ASP:OD2	1:A:362:ARG:NH1	2.51	0.43
1:B:257:PRO:HB2	1:B:497:ARG:HD3	2.01	0.43
1:D:254:PRO:HB2	1:D:289:TYR:HB2	2.01	0.43
1:D:408:TYR:O	1:D:409:LYS:C	2.61	0.43
1:D:493:ARG:HA	1:D:494:PRO:HD3	1.78	0.43
1:E:232:GLN:NE2	1:E:232:GLN:CA	2.70	0.43
1:F:529:GLN:O	1:F:532:ASN:HB2	2.19	0.43
1:D:427:LEU:HD13	1:D:515:LEU:HD23	2.00	0.43
1:E:190:LEU:HA	1:E:190:LEU:HD23	1.78	0.43
1:E:461:TRP:CZ3	1:E:526:TYR:HB2	2.54	0.43
1:F:41:ASN:HD21	1:F:419:ARG:NH1	2.16	0.43
1:B:425:ARG:HA	3:B:664:HOH:O	2.19	0.43
1:E:226:ASP:HA	1:E:227:PRO:HD3	1.85	0.43
1:A:23:ILE:CG2	1:A:24:ALA:N	2.82	0.42
1:A:25:SER:CA	1:A:30:ARG:HH12	2.30	0.42
1:A:31:LEU:HD21	1:B:134:TYR:HD2	1.83	0.42
1:A:333:ASN:HD22	1:A:335:PHE:HD1	1.66	0.42
1:B:41:ASN:C	1:B:41:ASN:HD22	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ARG:O	1:B:115:GLY:HA2	2.19	0.42
1:B:140:MET:HG2	1:B:145:GLU:HB2	2.01	0.42
1:B:264:GLN:O	1:B:265:ARG:C	2.62	0.42
1:D:91:ILE:HD12	1:D:100:VAL:HG12	1.99	0.42
1:D:139:ARG:O	1:D:140:MET:HB2	2.17	0.42
1:E:41:ASN:HD21	1:E:419:ARG:HH12	1.66	0.42
1:F:31:LEU:CD2	1:F:39:ASN:HB2	2.49	0.42
1:F:134:TYR:O	1:F:135:PRO:C	2.61	0.42
1:A:28:GLY:HA3	3:A:573:HOH:O	2.19	0.42
1:A:72:VAL:CG1	1:B:408:TYR:HA	2.44	0.42
1:B:17:LYS:O	1:B:21:ILE:HG13	2.19	0.42
1:B:178:MET:HG3	1:B:207:TYR:CE1	2.54	0.42
1:B:262:MET:HE2	1:B:267:LEU:CD2	2.49	0.42
1:C:294:ASP:HA	1:C:413:LYS:NZ	2.34	0.42
1:C:433:ARG:HG2	1:C:433:ARG:HH11	1.83	0.42
1:E:106:SER:HB3	1:E:402:MET:HE1	2.00	0.42
1:E:243:ASP:HA	1:E:244:PRO:HD2	1.90	0.42
1:F:196:LYS:HB2	1:F:245:ALA:O	2.19	0.42
1:F:299:LEU:HD23	1:F:299:LEU:HA	1.89	0.42
1:F:515:LEU:HD12	1:F:515:LEU:HA	1.77	0.42
1:B:404:GLU:CD	1:F:418:ARG:HD2	2.45	0.42
1:B:407:GLU:HG3	3:B:659:HOH:O	2.19	0.42
1:D:333:ASN:HD22	1:D:335:PHE:N	1.98	0.42
1:E:241:LEU:O	1:E:278:ARG:NH1	2.52	0.42
1:F:156:MET:HE2	1:F:156:MET:HA	2.01	0.42
1:F:277:HIS:O	1:F:278:ARG:HD2	2.19	0.42
1:A:252:VAL:O	1:A:255:SER:HA	2.17	0.42
1:B:504:ASN:ND2	1:D:113:GLN:HE22	2.18	0.42
1:D:171:VAL:C	1:D:385:LEU:HD13	2.44	0.42
1:D:235:ASP:HB3	1:D:269:ARG:CZ	2.49	0.42
1:E:110:VAL:HG21	1:E:121:PHE:CZ	2.54	0.42
1:E:221:VAL:O	1:E:221:VAL:HG12	2.20	0.42
1:E:474:ARG:HH21	1:E:517:LYS:HE2	1.83	0.42
1:E:502:ASN:O	1:E:503:LEU:HD23	2.19	0.42
1:E:513:ARG:NH1	1:E:513:ARG:CG	2.73	0.42
1:B:425:ARG:NH1	1:D:159:ASP:CB	2.82	0.42
1:C:467:SER:O	1:C:468:THR:C	2.63	0.42
1:D:122:LEU:O	1:D:126:VAL:HG23	2.19	0.42
1:D:423:LEU:HD21	1:D:444:ILE:HD11	2.01	0.42
1:E:153:ILE:CD1	1:E:163:SER:HA	2.49	0.42
1:E:337:LEU:O	1:E:340:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:GLN:HB2	1:E:463:VAL:CG2	2.49	0.42
1:F:101:ARG:NH2	1:F:105:LYS:HZ2	2.17	0.42
1:F:380:ASN:ND2	3:F:1657:HOH:O	2.30	0.42
1:F:446:LEU:HB2	1:F:471:MET:CE	2.50	0.42
1:A:49:ARG:O	1:A:53:ARG:HB2	2.19	0.42
1:A:430:PRO:HA	1:A:431:PRO:HD3	1.82	0.42
1:C:161:ILE:CD1	1:C:304:PRO:HB3	2.47	0.42
1:C:442:THR:O	1:C:497:ARG:HA	2.19	0.42
1:D:122:LEU:HD23	1:D:122:LEU:HA	1.87	0.42
1:F:330:HIS:CE1	1:F:332:GLN:HG2	2.54	0.42
1:A:70:THR:CG2	1:A:71:THR:N	2.82	0.42
1:A:86:ARG:HD3	1:D:88:GLU:CD	2.45	0.42
1:B:467:SER:O	1:B:468:THR:C	2.61	0.42
1:C:209:GLU:O	1:C:212:GLU:HB3	2.20	0.42
1:C:382:THR:HA	3:C:928:HOH:O	2.20	0.42
1:E:417:ARG:HA	1:E:417:ARG:HD3	1.84	0.42
1:A:53:ARG:HG2	1:A:100:VAL:CG2	2.49	0.42
1:A:139:ARG:HD3	1:A:368:ASP:OD1	2.19	0.42
1:A:351:ASP:HA	1:A:361:VAL:HG11	2.01	0.42
1:A:409:LYS:HG2	1:A:413:LYS:HE3	2.01	0.42
1:A:470:ASP:C	1:A:470:ASP:OD2	2.63	0.42
1:C:299:LEU:HD23	1:C:299:LEU:HA	1.85	0.42
1:E:257:PRO:CB	1:E:497:ARG:HD3	2.37	0.42
1:E:333:ASN:ND2	1:E:335:PHE:N	2.64	0.42
1:E:461:TRP:CE3	1:E:526:TYR:HB2	2.55	0.42
1:F:147:ILE:O	1:F:148:VAL:C	2.60	0.42
1:A:149:ARG:CA	1:A:168:LEU:HD11	2.50	0.42
1:A:420:GLU:HG2	1:A:430:PRO:CB	2.45	0.42
1:C:411:THR:HG21	1:D:70:THR:HG21	2.02	0.42
1:C:420:GLU:HG2	1:C:430:PRO:HB3	2.01	0.42
1:D:358:LEU:N	1:D:358:LEU:CD2	2.82	0.42
1:A:491:SER:C	1:A:493:ARG:N	2.75	0.42
1:D:140:MET:HE2	1:D:145:GLU:N	2.35	0.42
1:D:344:GLU:N	3:D:1267:HOH:O	2.24	0.42
1:D:392:GLN:HG3	1:D:396:PHE:CE2	2.55	0.42
1:D:448:ASP:O	1:D:452:LYS:HG3	2.19	0.42
1:E:30:ARG:NH1	1:E:30:ARG:CG	2.81	0.42
1:F:161:ILE:HD13	1:F:304:PRO:HB3	2.02	0.42
1:F:530:ALA:C	1:F:532:ASN:H	2.28	0.42
1:A:76:GLY:O	1:B:43:LEU:HD21	2.19	0.41
1:B:474:ARG:HG2	1:B:518:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ARG:O	1:C:153:ILE:HG23	2.20	0.41
1:C:247:LYS:HA	1:C:247:LYS:HD3	1.78	0.41
1:C:257:PRO:O	1:C:258:PRO:C	2.61	0.41
1:C:493:ARG:HA	1:C:494:PRO:HD3	1.85	0.41
1:D:22:LYS:N	3:D:1121:HOH:O	2.53	0.41
1:F:195:ASP:OD1	1:F:247:LYS:CD	2.67	0.41
1:A:113:GLN:OE1	1:E:505:GLU:HG3	2.20	0.41
1:A:433:ARG:HG2	1:A:434:ASP:H	1.84	0.41
1:B:102:PHE:CE1	1:B:402:MET:HE2	2.54	0.41
1:B:265:ARG:HG2	1:B:265:ARG:NH1	2.35	0.41
1:D:117:ASP:HA	1:D:118:PRO:HD2	1.94	0.41
1:D:177:ALA:O	1:D:181:ILE:HG13	2.20	0.41
1:D:266:SER:O	1:D:270:VAL:HG23	2.20	0.41
1:D:333:ASN:ND2	1:D:336:ASP:H	2.18	0.41
1:E:352:HIS:CE1	1:E:355:ARG:HH11	2.38	0.41
1:E:481:ILE:HD13	1:E:511:ILE:HD11	2.01	0.41
1:F:35:ALA:HB1	1:F:37:ARG:HH11	1.85	0.41
1:F:194:GLY:HA2	3:F:1700:HOH:O	2.20	0.41
1:F:445:ASP:OD2	1:F:493:ARG:NH2	2.42	0.41
1:F:490:GLY:O	1:F:491:SER:C	2.58	0.41
1:A:229:LEU:O	1:A:230:ASN:CB	2.68	0.41
1:A:261:LYS:O	1:A:262:MET:C	2.63	0.41
1:C:23:ILE:CD1	3:C:747:HOH:O	2.35	0.41
1:C:201:MET:HB3	1:C:202:PRO:HA	2.01	0.41
1:C:269:ARG:O	1:C:273:ILE:HG13	2.20	0.41
1:C:461:TRP:CZ2	1:C:465:GLN:HG3	2.55	0.41
1:C:489:PHE:O	1:C:490:GLY:O	2.38	0.41
1:F:239:ASP:C	1:F:241:LEU:H	2.27	0.41
1:F:333:ASN:ND2	1:F:333:ASN:C	2.79	0.41
1:F:448:ASP:CG	3:F:1711:HOH:O	2.64	0.41
1:B:23:ILE:HD13	1:B:473:PHE:CD1	2.55	0.41
1:B:41:ASN:HD21	1:B:419:ARG:CZ	2.34	0.41
1:B:286:ASP:OD2	2:B:900:PLP:N1	2.53	0.41
1:C:107:LEU:O	1:C:108:SER:C	2.63	0.41
1:D:25:SER:O	1:D:26:SER:HB3	2.20	0.41
1:E:158:ALA:CB	1:E:161:ILE:HD12	2.46	0.41
1:E:461:TRP:CZ2	1:E:465:GLN:OE1	2.73	0.41
1:F:355:ARG:NH1	1:F:355:ARG:HB3	2.20	0.41
1:A:23:ILE:HG23	1:A:24:ALA:N	2.36	0.41
1:E:269:ARG:O	1:E:273:ILE:HG13	2.20	0.41
1:F:344:GLU:O	1:F:345:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:C	1:A:41:ASN:HD22	2.27	0.41
1:A:226:ASP:OD2	1:A:229:LEU:HG	2.21	0.41
1:A:232:GLN:NE2	3:A:740:HOH:O	2.52	0.41
1:A:324:LEU:CD2	1:A:389:GLN:HB3	2.50	0.41
1:B:231:TRP:CZ3	1:B:488:GLY:HA3	2.55	0.41
1:B:255:SER:HB2	1:B:258:PRO:HD2	2.02	0.41
1:D:428:GLY:O	1:D:429:MET:HB2	2.21	0.41
1:E:80:ILE:HG13	1:E:123:HIS:HB2	2.01	0.41
1:F:37:ARG:HH11	1:F:37:ARG:CG	2.32	0.41
1:F:186:LYS:HE3	1:F:215:GLN:O	2.20	0.41
1:F:288:VAL:HG13	1:F:289:TYR:CD1	2.56	0.41
1:A:43:LEU:CD1	1:A:45:THR:HG22	2.50	0.41
1:A:75:GLY:O	1:B:42:PHE:HA	2.21	0.41
1:B:164:GLU:CD	1:B:164:GLU:H	2.28	0.41
1:C:305:GLU:HG2	1:C:332:GLN:O	2.21	0.41
1:D:24:ALA:HB1	1:D:480:GLY:O	2.21	0.41
1:E:185:LEU:HA	1:E:185:LEU:HD23	1.86	0.41
1:F:461:TRP:CE2	1:F:465:GLN:HG3	2.55	0.41
1:F:473:PHE:O	1:F:477:ASP:HB2	2.21	0.41
1:C:483:LEU:HD22	1:C:498:ALA:HB2	2.03	0.41
1:E:336:ASP:HA	1:E:339:LEU:HD12	2.02	0.41
1:F:268:GLU:O	1:F:271:ARG:HB3	2.20	0.41
1:A:43:LEU:HD11	1:A:45:THR:HG22	2.02	0.41
1:A:46:THR:N	1:A:47:PRO:CD	2.83	0.41
1:A:242:LYS:HE2	1:A:277:HIS:CD2	2.56	0.41
1:B:139:ARG:NH1	1:B:368:ASP:OD1	2.46	0.41
1:B:451:ALA:HA	1:B:455:GLY:O	2.21	0.41
1:C:34:ASN:HB3	1:D:381:HIS:CD2	2.55	0.41
1:C:183:GLU:O	1:C:187:LEU:HG	2.21	0.41
1:C:484:LEU:O	1:C:496:GLY:HA2	2.19	0.41
1:C:515:LEU:O	1:C:515:LEU:HD12	2.21	0.41
1:D:278:ARG:HH11	1:D:278:ARG:HG3	1.85	0.41
1:D:288:VAL:HG21	1:D:315:LYS:HG2	2.03	0.41
1:D:500:LEU:HA	1:D:500:LEU:HD23	1.80	0.41
1:E:256:ASN:OD1	1:E:256:ASN:C	2.64	0.41
1:E:343:GLN:O	1:E:346:GLU:N	2.53	0.41
1:F:201:MET:HA	1:F:202:PRO:C	2.45	0.41
1:F:306:ASN:HA	1:F:334:VAL:HG22	2.03	0.41
1:F:512:GLY:O	1:F:513:ARG:C	2.63	0.41
1:A:37:ARG:NH2	3:A:575:HOH:O	2.21	0.41
1:C:172:GLU:CD	1:C:172:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ARG:NH2	1:D:167:ASN:HB3	2.36	0.41
1:E:525:GLU:O	1:E:526:TYR:C	2.64	0.41
1:F:117:ASP:HA	1:F:118:PRO:HD2	1.82	0.41
1:F:178:MET:O	1:F:179:ALA:C	2.63	0.41
1:F:197:VAL:CG2	1:F:248:ILE:HG23	2.31	0.41
1:F:285:THR:OG1	1:F:287:ASP:OD1	2.27	0.41
1:B:139:ARG:HG2	1:B:169:PHE:HA	2.02	0.40
1:B:203:VAL:HG22	1:B:204:PHE:N	2.35	0.40
1:B:271:ARG:HG2	1:B:271:ARG:HH11	1.87	0.40
1:C:39:ASN:HA	1:C:40:PRO:HD3	1.81	0.40
1:F:420:GLU:HG2	1:F:430:PRO:HB3	2.03	0.40
1:F:447:GLN:HE21	1:F:463:VAL:HG21	1.86	0.40
1:A:26:SER:OG	1:A:29:ASN:HB2	2.20	0.40
1:B:199:ILE:O	1:B:201:MET:HG3	2.21	0.40
1:C:403:ASP:O	1:C:404:GLU:C	2.64	0.40
1:C:434:ASP:OD2	1:C:434:ASP:C	2.64	0.40
1:C:504:ASN:O	1:C:505:GLU:C	2.61	0.40
1:D:481:ILE:HD12	1:D:503:LEU:HD13	2.02	0.40
1:E:439:ASP:C	1:E:441:TYR:N	2.74	0.40
1:F:41:ASN:C	1:F:41:ASN:ND2	2.79	0.40
1:A:178:MET:HE3	1:A:250:PHE:HE1	1.85	0.40
1:A:267:LEU:HB3	1:A:302:ILE:HG13	2.04	0.40
1:A:491:SER:O	1:A:493:ARG:N	2.54	0.40
1:C:134:TYR:CD1	1:C:382:THR:HG22	2.56	0.40
1:F:100:VAL:O	1:F:101:ARG:C	2.64	0.40
1:F:197:VAL:O	1:F:220:GLU:HA	2.21	0.40
1:F:454:TYR:HB2	1:F:458:PHE:CD2	2.57	0.40
1:A:461:TRP:O	1:A:465:GLN:HG2	2.22	0.40
1:B:490:GLY:C	1:B:492:ASN:H	2.28	0.40
1:C:283:ILE:CG2	1:C:307:THR:HG23	2.52	0.40
1:E:164:GLU:H	1:E:164:GLU:HG2	1.50	0.40
1:E:226:ASP:CG	1:E:228:SER:HB3	2.44	0.40
1:E:387:THR:N	1:E:388:PRO:CD	2.84	0.40
1:F:360:ASP:C	1:F:362:ARG:N	2.78	0.40
1:A:238:LEU:HD22	1:A:270:VAL:CG2	2.51	0.40
1:A:376:ALA:O	1:A:378:ALA:N	2.49	0.40
1:B:39:ASN:HA	1:B:40:PRO:HD3	1.78	0.40
1:B:86:ARG:NH1	1:B:86:ARG:HG3	2.36	0.40
1:D:418:ARG:HD2	1:F:404:GLU:OE2	2.22	0.40
1:E:137:PRO:HA	1:E:138:PRO:HD3	1.94	0.40
1:F:21:ILE:O	1:F:21:ILE:HG22	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1692:HOH:O	3:F:1692:HOH:O[4_566]	1.88	0.32
1:C:529:GLN:NE2	3:B:600:HOH:O[8_456]	1.97	0.23
1:F:72:VAL:O	3:F:856:HOH:O[4_566]	2.04	0.16
1:D:465:GLN:O	3:C:1068:HOH:O[3_756]	2.12	0.08
1:C:425:ARG:NH2	3:E:1465:HOH:O[4_566]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/546 (93%)	477 (94%)	26 (5%)	5 (1%)	12	20
1	B	513/546 (94%)	488 (95%)	16 (3%)	9 (2%)	6	11
1	C	513/546 (94%)	486 (95%)	22 (4%)	5 (1%)	12	20
1	D	509/546 (93%)	475 (93%)	25 (5%)	9 (2%)	6	11
1	E	509/546 (93%)	451 (89%)	50 (10%)	8 (2%)	7	12
1	F	519/546 (95%)	471 (91%)	43 (8%)	5 (1%)	12	20
All	All	3071/3276 (94%)	2848 (93%)	182 (6%)	41 (1%)	9	16

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	SER
1	B	491	SER
1	C	491	SER
1	C	492	ASN
1	D	491	SER
1	D	492	ASN
1	E	489	PHE
1	E	491	SER

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Mol	Chain	Res	Type
1	F	491	SER
1	F	492	ASN
1	A	490	GLY
1	B	140	MET
1	B	159	ASP
1	B	376	ALA
1	B	490	GLY
1	B	492	ASN
1	C	490	GLY
1	D	159	ASP
1	D	490	GLY
1	E	455	GLY
1	E	468	THR
1	A	492	ASN
1	E	239	ASP
1	A	26	SER
1	B	95	ARG
1	D	140	MET
1	E	159	ASP
1	E	492	ASN
1	B	381	HIS
1	B	429	MET
1	C	140	MET
1	F	140	MET
1	D	26	SER
1	D	98	GLU
1	F	235	ASP
1	D	359	PRO
1	A	23	ILE
1	E	359	PRO
1	D	429	MET
1	F	377	VAL
1	C	377	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/454 (93%)	407 (96%)	16 (4%)	29	49
1	B	428/454 (94%)	405 (95%)	23 (5%)	20	35
1	C	428/454 (94%)	407 (95%)	21 (5%)	22	38
1	D	423/454 (93%)	405 (96%)	18 (4%)	26	44
1	E	425/454 (94%)	408 (96%)	17 (4%)	28	47
1	F	433/454 (95%)	401 (93%)	32 (7%)	13	21
All	All	2560/2724 (94%)	2433 (95%)	127 (5%)	22	37

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	53	ARG
1	A	69	MET
1	A	79	LYS
1	A	172	GLU
1	A	178	MET
1	A	192	LYS
1	A	204	PHE
1	A	205	THR
1	A	218	LEU
1	A	258	PRO
1	A	269	ARG
1	A	272	ASN
1	A	309	LEU
1	A	416	ILE
1	A	489	PHE
1	B	23	ILE
1	B	37	ARG
1	B	41	ASN
1	B	43	LEU
1	B	53	ARG
1	B	71	THR
1	B	81	ASP
1	B	105	LYS
1	B	161	ILE
1	B	172	GLU
1	B	175	THR
1	B	181	ILE
1	B	184	SER
1	B	191	LEU

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Mol	Chain	Res	Type
1	B	204	PHE
1	B	228	SER
1	B	287	ASP
1	B	345	SER
1	B	357	LEU
1	B	423	LEU
1	B	466	SER
1	B	470	ASP
1	B	489	PHE
1	C	41	ASN
1	C	53	ARG
1	C	63	GLU
1	C	69	MET
1	C	72	VAL
1	C	79	LYS
1	C	95	ARG
1	C	101	ARG
1	C	154	ARG
1	C	172	GLU
1	C	197	VAL
1	C	204	PHE
1	C	264	GLN
1	C	332	GLN
1	C	333	ASN
1	C	357	LEU
1	C	358	LEU
1	C	445	ASP
1	C	481	ILE
1	C	489	PHE
1	C	515	LEU
1	D	23	ILE
1	D	41	ASN
1	D	43	LEU
1	D	53	ARG
1	D	71	THR
1	D	81	ASP
1	D	100	VAL
1	D	165	SER
1	D	172	GLU
1	D	197	VAL
1	D	204	PHE
1	D	271	ARG

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Mol	Chain	Res	Type
1	D	332	GLN
1	D	333	ASN
1	D	414	GLN
1	D	481	ILE
1	D	485	PRO
1	D	489	PHE
1	E	41	ASN
1	E	53	ARG
1	E	72	VAL
1	E	129	ILE
1	E	159	ASP
1	E	172	GLU
1	E	204	PHE
1	E	232	GLN
1	E	305	GLU
1	E	308	LEU
1	E	357	LEU
1	E	414	GLN
1	E	425	ARG
1	E	460	GLU
1	E	474	ARG
1	E	489	PHE
1	E	513	ARG
1	F	26	SER
1	F	41	ASN
1	F	53	ARG
1	F	74	VAL
1	F	81	ASP
1	F	93	GLU
1	F	101	ARG
1	F	164	GLU
1	F	172	GLU
1	F	184	SER
1	F	191	LEU
1	F	192	LYS
1	F	195	ASP
1	F	204	PHE
1	F	205	THR
1	F	208	ILE
1	F	227	PRO
1	F	230	ASN
1	F	236	SER

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Mol	Chain	Res	Type
1	F	257	PRO
1	F	258	PRO
1	F	305	GLU
1	F	333	ASN
1	F	346	GLU
1	F	355	ARG
1	F	377	VAL
1	F	434	ASP
1	F	468	THR
1	F	470	ASP
1	F	474	ARG
1	F	489	PHE
1	F	532	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	41	ASN
1	A	224	ASN
1	A	232	GLN
1	A	333	ASN
1	A	380	ASN
1	A	381	HIS
1	A	410	HIS
1	A	447	GLN
1	A	492	ASN
1	B	34	ASN
1	B	39	ASN
1	B	41	ASN
1	B	142	ASN
1	B	215	GLN
1	B	232	GLN
1	B	277	HIS
1	B	306	ASN
1	B	333	ASN
1	B	352	HIS
1	B	380	ASN
1	B	414	GLN
1	B	436	ASN
1	B	447	GLN
1	B	504	ASN

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Mol	Chain	Res	Type
1	B	529	GLN
1	C	34	ASN
1	C	41	ASN
1	C	167	ASN
1	C	188	ASN
1	C	215	GLN
1	C	232	GLN
1	C	264	GLN
1	C	277	HIS
1	C	331	GLN
1	C	333	ASN
1	C	380	ASN
1	C	392	GLN
1	C	436	ASN
1	C	447	GLN
1	C	504	ASN
1	D	34	ASN
1	D	41	ASN
1	D	167	ASN
1	D	215	GLN
1	D	230	ASN
1	D	232	GLN
1	D	331	GLN
1	D	332	GLN
1	D	333	ASN
1	D	380	ASN
1	D	414	GLN
1	D	447	GLN
1	D	504	ASN
1	E	34	ASN
1	E	41	ASN
1	E	150	GLN
1	E	188	ASN
1	E	215	GLN
1	E	232	GLN
1	E	264	GLN
1	E	272	ASN
1	E	277	HIS
1	E	297	GLN
1	E	333	ASN
1	E	414	GLN
1	E	447	GLN

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Mol	Chain	Res	Type
1	E	504	ASN
1	F	34	ASN
1	F	41	ASN
1	F	142	ASN
1	F	215	GLN
1	F	232	GLN
1	F	332	GLN
1	F	333	ASN
1	F	447	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	PLP	B	900	1	15,15,16	2.35	9 (60%)	21,22,23	1.09	1 (4%)
2	PLP	A	900	1	15,15,16	1.85	3 (20%)	21,22,23	2.05	7 (33%)
2	PLP	C	900	1	15,15,16	2.15	3 (20%)	21,22,23	1.79	4 (19%)
2	PLP	E	900	1	15,15,16	1.91	5 (33%)	21,22,23	1.45	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	D	900	1	15,15,16	2.40	7 (46%)	21,22,23	1.97	5 (23%)
2	PLP	F	900	1	15,15,16	2.08	6 (40%)	21,22,23	1.43	4 (19%)

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	PLP	B	900	1	-	2/6/6/8	0/1/1/1
2	PLP	A	900	1	-	3/6/6/8	0/1/1/1
2	PLP	C	900	1	-	0/6/6/8	0/1/1/1
2	PLP	E	900	1	-	1/6/6/8	0/1/1/1
2	PLP	D	900	1	-	1/6/6/8	0/1/1/1
2	PLP	F	900	1	-	0/6/6/8	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	900	PLP	C4A-C4	5.24	1.62	1.51
2	C	900	PLP	C3-C2	-5.13	1.35	1.41
2	D	900	PLP	C2-N1	4.62	1.42	1.33
2	C	900	PLP	C4A-C4	4.45	1.60	1.51
2	B	900	PLP	C3-C2	4.31	1.45	1.41
2	E	900	PLP	C2A-C2	4.25	1.57	1.50
2	D	900	PLP	C6-C5	3.62	1.44	1.37
2	D	900	PLP	C4A-C4	3.61	1.58	1.51
2	D	900	PLP	C5A-C5	3.51	1.60	1.50
2	A	900	PLP	C2-N1	3.50	1.40	1.33
2	A	900	PLP	O3-C3	3.45	1.44	1.36
2	B	900	PLP	C6-N1	3.15	1.40	1.34
2	B	900	PLP	C4A-C4	3.13	1.57	1.51
2	B	900	PLP	C2-N1	3.03	1.39	1.33
2	F	900	PLP	C3-C2	-2.97	1.37	1.41
2	E	900	PLP	C4A-C4	2.90	1.57	1.51
2	F	900	PLP	C2-N1	2.82	1.38	1.33
2	B	900	PLP	P-O4P	-2.76	1.51	1.60
2	B	900	PLP	C3-C4	2.66	1.45	1.40
2	E	900	PLP	C3-C4	2.65	1.45	1.40
2	F	900	PLP	O3-C3	-2.49	1.31	1.36
2	A	900	PLP	P-O3P	-2.40	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	PLP	P-O2P	2.39	1.63	1.54
2	D	900	PLP	C5-C4	2.38	1.43	1.40
2	D	900	PLP	C6-N1	2.37	1.39	1.34
2	D	900	PLP	P-O3P	-2.33	1.46	1.54
2	B	900	PLP	P-O3P	-2.28	1.46	1.54
2	C	900	PLP	C5-C4	2.24	1.43	1.40
2	E	900	PLP	O3-C3	2.21	1.41	1.36
2	E	900	PLP	C5A-C5	2.18	1.56	1.50
2	F	900	PLP	C6-N1	2.18	1.38	1.34
2	F	900	PLP	P-O3P	-2.10	1.47	1.54
2	B	900	PLP	C5A-C5	2.03	1.56	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	PLP	O4P-P-O1P	-5.39	91.86	106.44
2	D	900	PLP	O4P-C5A-C5	4.95	118.64	109.36
2	C	900	PLP	O2P-P-O4P	-4.75	94.30	106.67
2	F	900	PLP	O4P-C5A-C5	-4.38	101.15	109.36
2	D	900	PLP	O2P-P-O4P	-4.22	95.67	106.67
2	E	900	PLP	O3P-P-O1P	3.18	123.21	110.83
2	D	900	PLP	C2A-C2-C3	-3.16	117.10	120.80
2	A	900	PLP	O4P-C5A-C5	3.14	115.25	109.36
2	A	900	PLP	C4A-C4-C5	3.01	124.04	120.94
2	C	900	PLP	C5-C6-N1	-3.00	118.95	123.83
2	A	900	PLP	O3P-P-O4P	3.00	114.49	106.67
2	A	900	PLP	C4A-C4-C3	-2.79	115.88	120.52
2	E	900	PLP	O4P-C5A-C5	-2.70	104.29	109.36
2	D	900	PLP	C4A-C4-C5	2.57	123.58	120.94
2	D	900	PLP	O3P-P-O1P	2.46	120.42	110.83
2	B	900	PLP	O3P-P-O4P	2.30	112.66	106.67
2	A	900	PLP	C5A-C5-C6	-2.17	115.82	119.36
2	C	900	PLP	C6-N1-C2	2.16	123.12	119.20
2	F	900	PLP	O3P-P-O4P	2.15	112.27	106.67
2	F	900	PLP	O3P-P-O1P	2.11	119.06	110.83
2	A	900	PLP	O2P-P-O4P	2.02	111.94	106.67
2	C	900	PLP	O3P-P-O1P	2.02	118.70	110.83
2	F	900	PLP	C5-C6-N1	-2.02	120.55	123.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	PLP	C5A-O4P-P-O2P
2	B	900	PLP	C5A-O4P-P-O2P
2	B	900	PLP	C5A-O4P-P-O3P
2	E	900	PLP	C5A-O4P-P-O1P
2	A	900	PLP	C5A-O4P-P-O1P
2	A	900	PLP	C5A-O4P-P-O3P
2	D	900	PLP	C4-C5-C5A-O4P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	PLP	1	0
2	C	900	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	510/546 (93%)	-0.55	1 (0%) 91 90	19, 38, 77, 117	0
1	B	515/546 (94%)	-0.61	1 (0%) 91 90	18, 34, 67, 101	0
1	C	515/546 (94%)	-0.64	1 (0%) 91 90	14, 35, 65, 115	0
1	D	511/546 (93%)	-0.67	1 (0%) 91 90	17, 34, 54, 115	0
1	E	511/546 (93%)	-0.41	1 (0%) 91 90	20, 42, 74, 117	0
1	F	521/546 (95%)	-0.54	4 (0%) 82 79	18, 36, 64, 117	0
All	All	3083/3276 (94%)	-0.57	9 (0%) 90 89	14, 36, 69, 117	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	489	PHE	2.9
1	D	528	GLY	2.6
1	F	487	ALA	2.6
1	B	489	PHE	2.6
1	F	490	GLY	2.3
1	A	20	LEU	2.3
1	F	17	LYS	2.2
1	C	489	PHE	2.1
1	F	23	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	A	900	15/16	0.98	0.05	26,30,33,33	0
2	PLP	B	900	15/16	0.98	0.04	22,25,28,29	0
2	PLP	C	900	15/16	0.98	0.05	20,22,24,25	0
2	PLP	D	900	15/16	0.98	0.06	26,29,33,34	0
2	PLP	E	900	15/16	0.98	0.05	26,36,39,41	0
2	PLP	F	900	15/16	0.98	0.05	26,29,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.