



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:57 AM UTC

PDB ID : 2ZY3 / pdb_00002zy3
Title : dodecameric 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 : 2.50 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

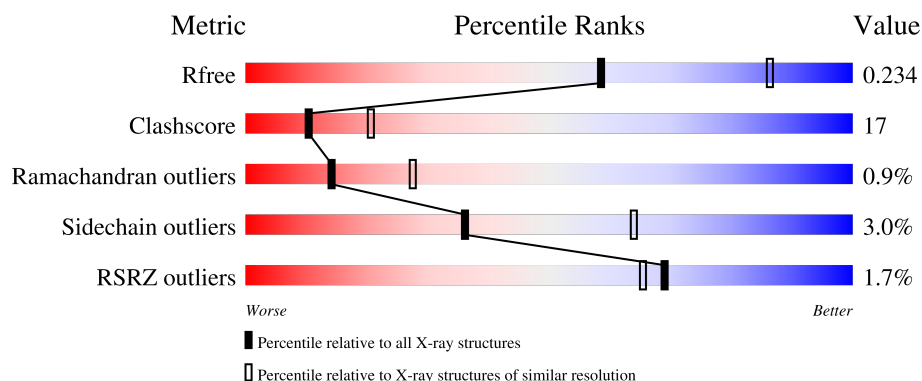
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	 2% 64% 27% • 7%
1	B	546	 1% 64% 28% • 6%
1	C	546	 1% 66% 24% • 5%
1	D	546	 1% 66% 25% • 6%
1	E	546	 2% 60% 30% • 6%

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Mol	Chain	Length	Quality of chain
1	F	546	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26599 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
			4011	2553	684	757	17			
1	B	515	Total	C	N	O	S	0	0	0
			4054	2579	691	767	17			
1	C	516	Total	C	N	O	S	0	0	0
			4065	2588	692	768	17			
1	D	514	Total	C	N	O	S	0	0	0
			4042	2571	692	762	17			
1	E	512	Total	C	N	O	S	0	0	0
			4028	2563	687	761	17			
1	F	523	Total	C	N	O	S	0	0	0
			4116	2620	701	778	17			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	534	LYS	-	expression tag	UNP Q93QX0
B	535	LEU	-	expression tag	UNP Q93QX0
B	536	ALA	-	expression tag	UNP Q93QX0
B	537	ALA	-	expression tag	UNP Q93QX0

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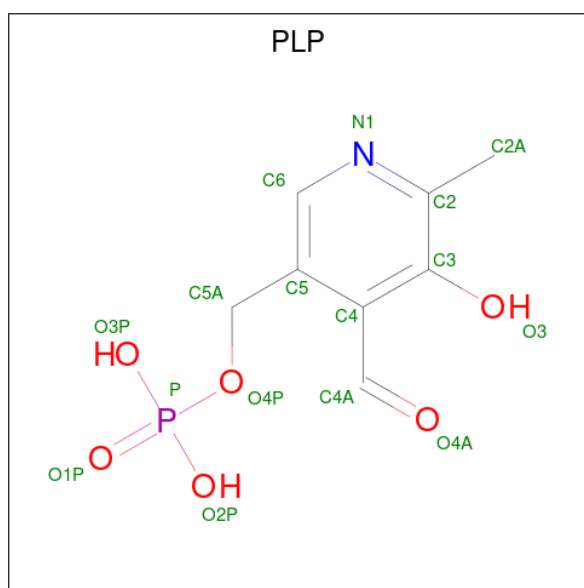
Chain	Residue	Modelled	Actual	Comment	Reference
B	538	ALA	-	expression tag	UNP Q93QX0
B	539	LEU	-	expression tag	UNP Q93QX0
B	540	GLU	-	expression tag	UNP Q93QX0
B	541	HIS	-	expression tag	UNP Q93QX0
B	542	HIS	-	expression tag	UNP Q93QX0
B	543	HIS	-	expression tag	UNP Q93QX0
B	544	HIS	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

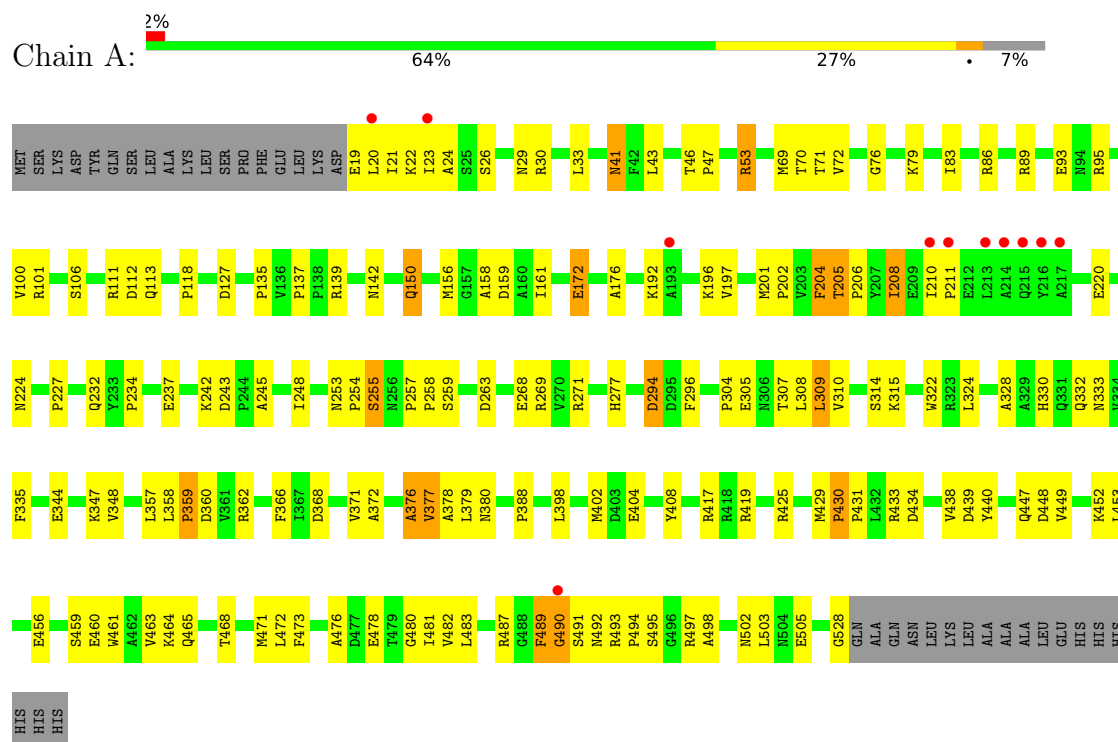
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	369	Total	O	0	0
			369	369		
3	B	431	Total	O	0	0
			431	431		
3	C	403	Total	O	0	0
			403	403		
3	D	353	Total	O	0	0
			353	353		
3	E	329	Total	O	0	0
			329	329		
3	F	308	Total	O	0	0
			308	308		

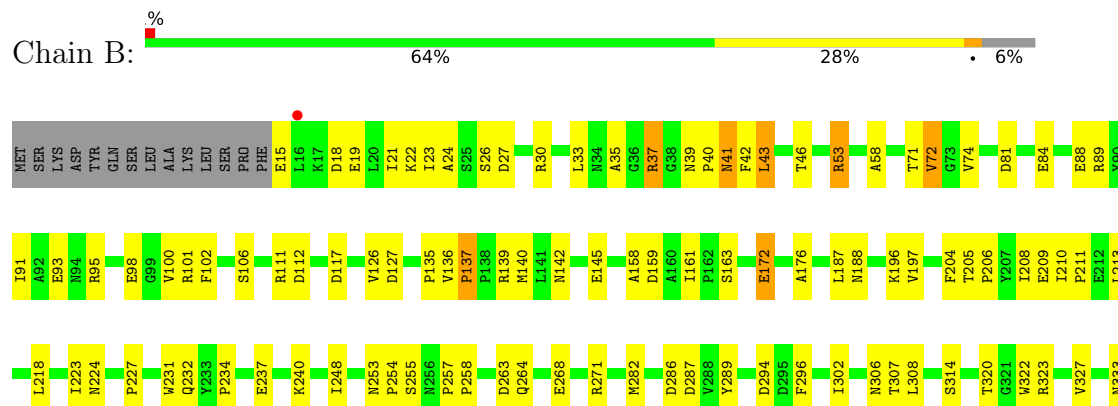
3 Residue-property plots

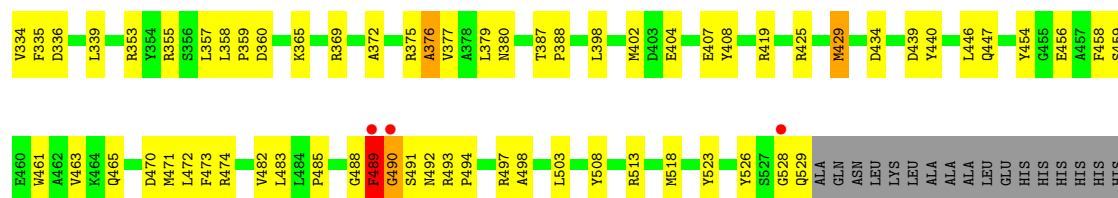
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: L-aspartate beta-decarboxylase

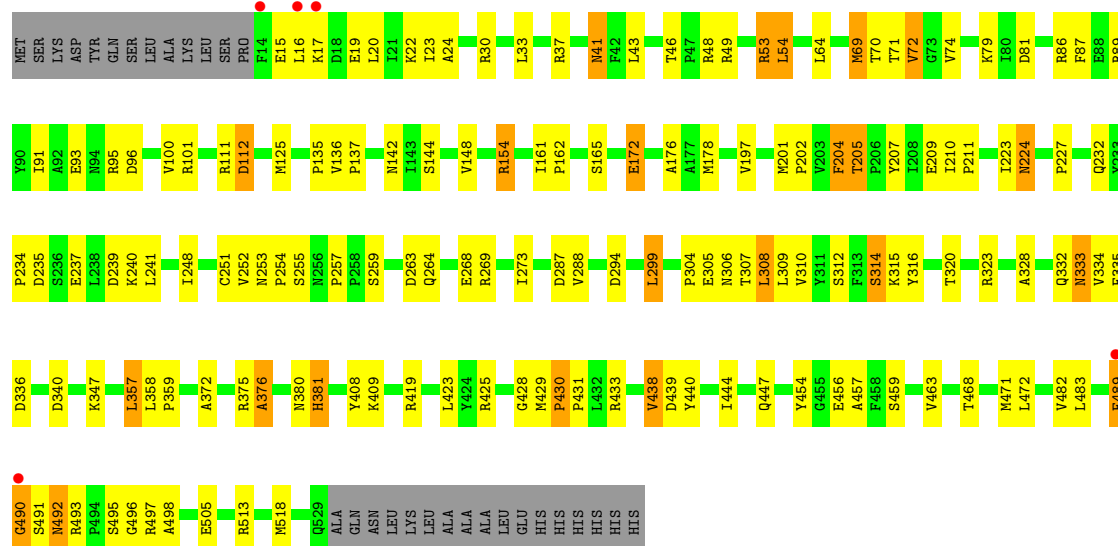


• Molecule 1: L-aspartate beta-decarboxylase

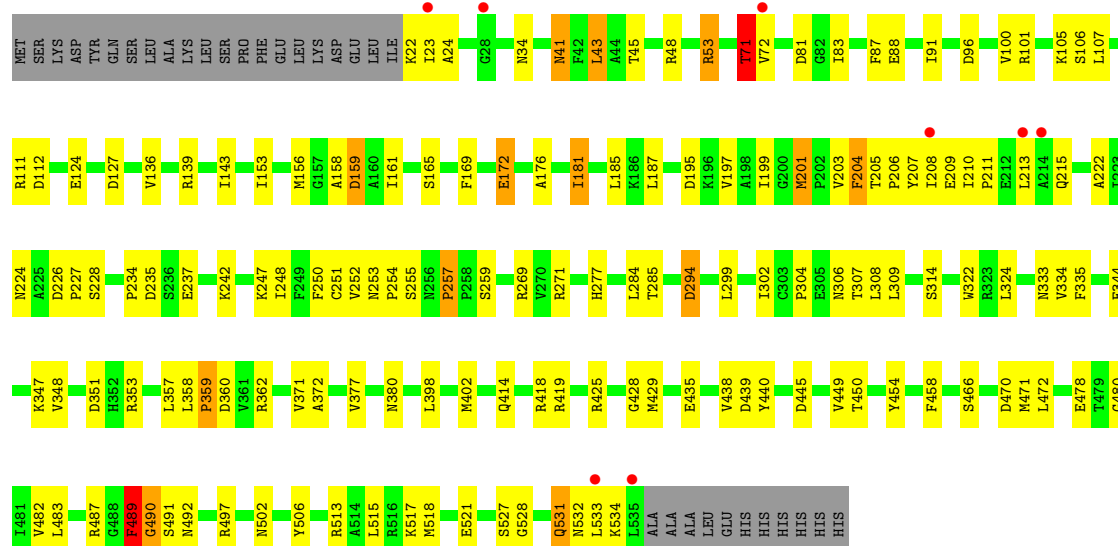




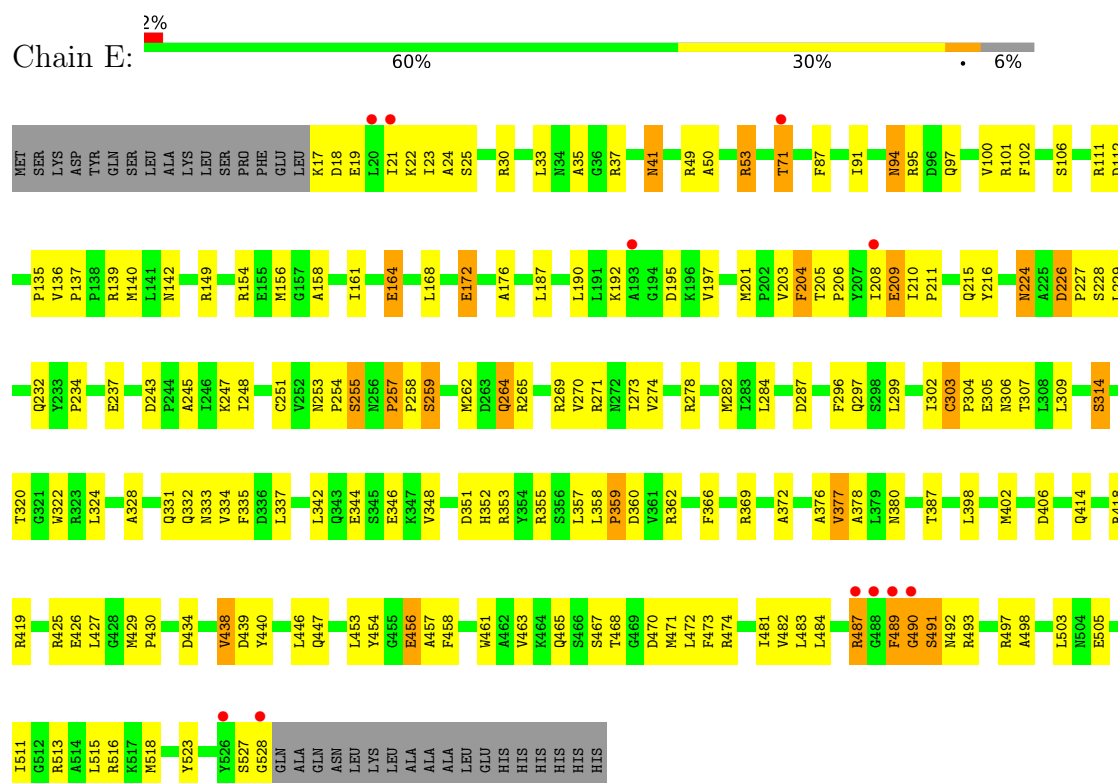
• Molecule 1: L-aspartate beta-decarboxylase



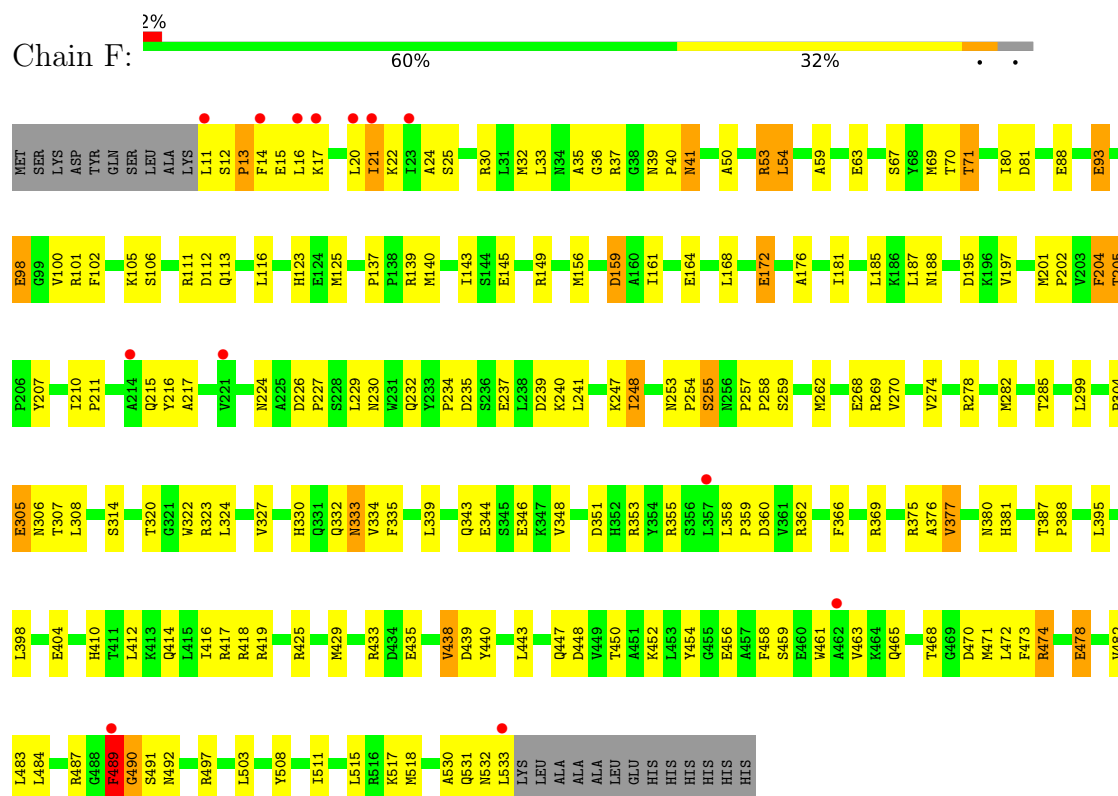
• Molecule 1: L-aspartate beta-decarboxylase



• Molecule 1: L-aspartate beta-decarboxylase



• Molecule 1: L-aspartate beta-decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	149.73Å 216.14Å 208.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.8 (50.00-2.50) 92.7 (50.00-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.234 0.175 , 0.234	Depositor DCC
R_{free} test set	5444 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26599	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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	0.66	0/4093	1.07	27/5543 (0.5%)
1	B	0.68	0/4136	1.06	24/5600 (0.4%)
1	C	0.67	0/4148	1.04	28/5616 (0.5%)
1	D	0.65	0/4124	1.02	21/5584 (0.4%)
1	E	0.65	0/4110	1.03	20/5565 (0.4%)
1	F	0.67	0/4200	1.04	25/5688 (0.4%)
All	All	0.66	0/24811	1.04	145/33596 (0.4%)

There are no bond length outliers.

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	440	TYR	N-CA-C	-9.86	100.61	111.36
1	F	440	TYR	N-CA-C	-8.90	101.50	111.82
1	C	440	TYR	N-CA-C	-8.89	101.59	111.28
1	B	314	SER	N-CA-C	8.84	121.72	111.11
1	A	438	VAL	N-CA-C	-8.71	104.74	111.62
1	A	307	THR	N-CA-C	8.69	123.45	108.76
1	A	440	TYR	N-CA-C	-8.38	102.07	111.71
1	A	142	ASN	N-CA-C	8.06	120.78	111.11
1	E	307	THR	N-CA-C	8.01	121.95	108.90
1	C	142	ASN	N-CA-C	7.83	120.57	111.02
1	B	72	VAL	N-CA-C	7.67	118.46	110.72
1	F	307	THR	N-CA-C	7.35	121.51	109.24
1	A	314	SER	N-CA-C	7.26	119.83	111.11
1	F	67	SER	N-CA-C	7.19	121.90	113.20
1	A	294	ASP	N-CA-C	7.08	118.89	111.03
1	D	314	SER	N-CA-C	7.00	119.51	111.11
1	B	294	ASP	CA-C-N	-7.00	113.66	123.03
1	B	294	ASP	C-N-CA	-7.00	113.66	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	440	TYR	N-CA-C	-6.95	103.71	111.71
1	E	440	TYR	N-CA-C	-6.92	103.80	111.82
1	F	314	SER	N-CA-C	6.90	119.44	111.02
1	C	294	ASP	CA-C-N	-6.86	113.83	123.03
1	C	294	ASP	C-N-CA	-6.86	113.83	123.03
1	B	307	THR	N-CA-C	6.83	120.53	109.40
1	E	142	ASN	N-CA-C	6.68	119.12	111.11
1	B	142	ASN	N-CA-C	6.68	119.17	111.02
1	E	255	SER	N-CA-C	6.57	119.42	110.55
1	F	435	GLU	N-CA-C	-6.48	105.37	113.28
1	C	314	SER	N-CA-C	6.45	118.89	111.02
1	C	299	LEU	N-CA-C	-6.36	104.62	112.38
1	E	251	CYS	N-CA-C	6.36	119.86	109.24
1	A	505	GLU	N-CA-C	6.32	118.69	111.11
1	C	439	ASP	N-CA-C	6.24	120.23	112.24
1	B	117	ASP	CA-C-N	6.24	125.46	118.97
1	B	117	ASP	C-N-CA	6.24	125.46	118.97
1	D	478	GLU	N-CA-C	6.23	118.15	111.36
1	D	307	THR	N-CA-C	6.23	119.61	109.59
1	D	257	PRO	N-CA-C	6.18	128.18	112.10
1	E	71	THR	N-CA-C	-6.17	105.03	113.30
1	F	439	ASP	N-CA-C	6.16	120.13	112.24
1	F	248	ILE	N-CA-C	6.16	116.48	108.35
1	A	294	ASP	CA-C-N	-6.10	114.08	122.87
1	A	294	ASP	C-N-CA	-6.10	114.08	122.87
1	F	369	ARG	N-CA-C	-6.09	104.76	111.82
1	E	299	LEU	N-CA-C	-6.08	105.12	112.54
1	D	224	ASN	N-CA-C	6.05	119.04	109.96
1	E	314	SER	N-CA-C	6.00	118.32	111.11
1	F	255	SER	N-CA-C	6.00	118.45	110.53
1	B	429	MET	CA-C-N	5.97	124.02	119.66
1	B	429	MET	C-N-CA	5.97	124.02	119.66
1	C	505	GLU	N-CA-C	5.92	118.21	111.11
1	F	71	THR	N-CA-C	-5.83	104.87	113.61
1	A	502	ASN	N-CA-C	5.78	120.34	112.88
1	C	257	PRO	N-CA-C	5.78	127.12	112.10
1	D	502	ASN	N-CA-C	5.76	121.20	113.72
1	C	224	ASN	N-CA-C	5.75	118.91	109.76
1	C	307	THR	N-CA-C	5.75	118.28	108.90
1	F	224	ASN	N-CA-C	5.75	118.59	109.96
1	C	54	LEU	N-CA-C	-5.74	105.16	111.82
1	B	224	ASN	N-CA-C	5.73	118.56	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	THR	CA-C-N	-5.73	113.86	119.64
1	B	46	THR	C-N-CA	-5.73	113.86	119.64
1	F	205	THR	N-CA-C	5.69	120.65	113.25
1	B	137	PRO	CA-C-N	5.68	125.80	119.32
1	B	137	PRO	C-N-CA	5.68	125.80	119.32
1	E	438	VAL	N-CA-C	-5.67	106.15	111.48
1	D	83	ILE	N-CA-C	5.67	118.14	111.05
1	C	205	THR	N-CA-C	5.66	120.61	113.25
1	C	315	LYS	N-CA-C	5.66	118.31	111.40
1	D	181	ILE	N-CA-C	5.66	115.85	110.42
1	D	45	THR	N-CA-C	5.65	118.64	111.69
1	B	327	VAL	N-CA-C	-5.61	99.67	107.80
1	E	454	TYR	N-CA-C	5.60	118.05	110.88
1	A	224	ASN	N-CA-C	5.60	118.66	109.76
1	B	377	VAL	N-CA-C	5.60	120.98	109.34
1	A	150	GLN	N-CA-C	-5.55	105.31	111.36
1	A	430	PRO	CA-C-N	5.54	125.85	119.92
1	A	430	PRO	C-N-CA	5.54	125.85	119.92
1	C	430	PRO	CA-C-N	5.54	125.49	119.78
1	C	430	PRO	C-N-CA	5.54	125.49	119.78
1	F	438	VAL	N-CA-C	-5.53	106.80	111.56
1	F	98	GLU	N-CA-C	5.53	117.77	111.02
1	A	127	ASP	N-CA-C	-5.52	105.17	111.07
1	A	478	GLU	N-CA-C	5.50	120.05	113.23
1	F	299	LEU	N-CA-C	-5.50	105.67	112.38
1	C	454	TYR	N-CA-C	5.47	119.12	111.56
1	F	285	THR	N-CA-C	5.47	117.82	108.90
1	B	376	ALA	N-CA-C	5.45	122.40	110.80
1	E	209	GLU	N-CA-C	5.43	119.07	112.23
1	A	296	PHE	N-CA-C	5.43	118.18	110.10
1	F	54	LEU	N-CA-C	-5.41	105.49	111.71
1	D	377	VAL	N-CA-C	5.40	120.58	109.34
1	E	224	ASN	N-CA-C	5.39	118.13	110.10
1	A	315	LYS	N-CA-C	5.38	118.31	111.69
1	B	489	PHE	N-CA-C	5.38	119.42	109.24
1	D	531	GLN	N-CA-C	-5.38	105.98	112.54
1	C	376	ALA	N-CA-C	5.36	122.23	110.80
1	B	439	ASP	N-CA-C	5.33	118.93	111.74
1	D	439	ASP	N-CA-C	5.30	119.33	112.86
1	D	209	GLU	N-CA-C	5.30	118.21	111.69
1	A	439	ASP	N-CA-C	5.30	119.02	112.24
1	D	71	THR	N-CA-C	-5.29	105.48	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	GLU	N-CA-C	5.29	117.96	111.82
1	A	83	ILE	N-CA-C	5.29	116.06	110.72
1	A	255	SER	N-CA-C	5.28	117.50	110.53
1	A	430	PRO	N-CA-C	5.28	115.54	110.47
1	D	299	LEU	N-CA-C	-5.26	105.96	112.38
1	F	517	LYS	N-CA-C	-5.26	105.44	111.07
1	F	377	VAL	N-CA-C	5.26	120.28	109.34
1	D	489	PHE	N-CA-C	5.25	119.17	109.24
1	B	454	TYR	N-CA-C	5.25	119.44	112.30
1	D	466	SER	N-CA-C	5.25	118.22	110.46
1	F	489	PHE	N-CA-C	5.24	119.14	109.24
1	F	376	ALA	N-CA-C	5.22	118.79	111.90
1	E	94	ASN	N-CA-C	5.20	117.54	110.88
1	A	243	ASP	CA-C-N	5.20	124.91	119.82
1	A	243	ASP	C-N-CA	5.20	124.91	119.82
1	D	294	ASP	CA-C-N	-5.18	115.84	122.79
1	D	294	ASP	C-N-CA	-5.18	115.84	122.79
1	C	438	VAL	N-CA-C	-5.17	107.11	111.56
1	F	381	HIS	N-CA-C	5.15	119.43	113.20
1	E	303	CYS	CA-C-N	5.15	125.19	119.32
1	E	303	CYS	C-N-CA	5.15	125.19	119.32
1	C	71	THR	N-CA-C	-5.15	106.40	113.30
1	C	112	ASP	N-CA-C	5.14	117.67	111.40
1	B	223	ILE	N-CA-C	-5.13	99.29	106.53
1	E	257	PRO	N-CA-C	5.13	125.45	112.10
1	E	439	ASP	N-CA-C	5.13	118.84	112.58
1	A	377	VAL	N-CA-C	5.11	119.97	109.34
1	F	511	ILE	N-CA-C	-5.10	105.73	110.53
1	E	226	ASP	CA-C-N	5.09	125.12	119.32
1	E	226	ASP	C-N-CA	5.09	125.12	119.32
1	C	251	CYS	N-CA-C	5.08	117.45	108.75
1	F	327	VAL	N-CA-C	-5.08	101.06	108.17
1	F	478	GLU	N-CA-C	5.08	118.74	112.54
1	C	308	LEU	N-CA-C	-5.06	100.48	108.73
1	D	127	ASP	N-CA-C	-5.05	105.77	111.28
1	C	46	THR	CA-C-N	-5.04	114.47	119.56
1	C	46	THR	C-N-CA	-5.04	114.47	119.56
1	B	127	ASP	N-CA-C	-5.04	105.78	111.28
1	C	223	ILE	N-CA-C	-5.03	99.70	106.85
1	C	381	HIS	N-CA-C	5.02	119.12	113.15
1	E	377	VAL	N-CA-C	5.01	119.76	109.34
1	A	137	PRO	CA-C-N	5.00	124.60	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	PRO	C-N-CA	5.00	124.60	119.05

There are no chirality outliers.

There are no planarity outliers.

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	4011	0	3978	134	0
1	B	4054	0	4021	148	0
1	C	4065	0	4029	114	1
1	D	4042	0	4013	132	0
1	E	4028	0	3996	157	0
1	F	4116	0	4082	173	0
2	A	15	0	7	0	0
2	B	15	0	7	1	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
2	E	15	0	7	0	0
2	F	15	0	6	0	0
3	A	369	0	0	12	0
3	B	431	0	0	15	0
3	C	403	0	0	11	0
3	D	353	0	0	14	0
3	E	329	0	0	16	1
3	F	308	0	0	18	0
All	All	26599	0	24160	824	1

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 (824) 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:D:105:LYS:HE3	3:D:1343:HOH:O	1.46	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:GLN:HE21	1:E:463:VAL:HG21	1.14	1.10
1:B:425:ARG:HH12	1:D:159:ASP:HA	1.21	1.02
1:F:530:ALA:O	1:F:533:LEU:HG	1.65	0.97
1:E:446:LEU:HB2	1:E:471:MET:HE1	1.50	0.94
1:B:333:ASN:HD22	1:B:335:PHE:H	1.17	0.93
1:A:333:ASN:HD22	1:A:335:PHE:H	1.10	0.93
1:B:227:PRO:HG2	1:B:489:PHE:HB3	1.49	0.91
1:F:333:ASN:HD22	1:F:335:PHE:H	1.07	0.90
1:E:201:MET:HE3	1:E:208:ILE:HD11	1.53	0.89
1:F:197:VAL:HG23	1:F:248:ILE:HG23	1.54	0.89
1:A:41:ASN:HD21	1:A:419:ARG:HH22	1.19	0.89
1:E:264:GLN:H	1:E:264:GLN:HE21	1.21	0.88
1:B:254:PRO:HG2	1:B:289:TYR:HB2	1.57	0.87
1:F:11:LEU:HG	3:F:1852:HOH:O	1.74	0.87
1:F:227:PRO:HG2	1:F:489:PHE:HB3	1.56	0.86
1:B:358:LEU:HB2	1:B:359:PRO:HD2	1.59	0.85
1:D:425:ARG:HH22	1:F:159:ASP:HA	1.42	0.84
1:D:333:ASN:HD22	1:D:335:PHE:H	1.22	0.84
1:A:333:ASN:HD21	1:A:335:PHE:HB2	1.43	0.83
1:A:333:ASN:ND2	1:A:335:PHE:H	1.77	0.83
1:B:158:ALA:HB1	1:B:161:ILE:HD13	1.59	0.83
1:E:41:ASN:HD21	1:E:419:ARG:HH22	1.26	0.83
1:D:227:PRO:HG2	1:D:489:PHE:HB3	1.60	0.83
1:E:447:GLN:HB3	1:E:493:ARG:HH21	1.44	0.82
1:C:89:ARG:NH1	1:C:93:GLU:HG3	1.95	0.82
1:D:139:ARG:HG3	1:D:371:VAL:HG21	1.61	0.81
1:D:471:MET:HG3	1:D:518:MET:HE1	1.63	0.81
1:C:471:MET:HG3	1:C:518:MET:HE1	1.64	0.79
1:E:447:GLN:NE2	1:E:463:VAL:HG21	1.96	0.79
1:F:333:ASN:ND2	1:F:335:PHE:H	1.81	0.79
1:A:72:VAL:HG11	1:B:408:TYR:HA	1.66	0.78
1:F:139:ARG:NH2	3:F:1966:HOH:O	2.16	0.78
1:D:425:ARG:NH2	1:F:159:ASP:HA	1.98	0.78
1:E:106:SER:HB2	1:E:398:LEU:HD13	1.66	0.78
1:B:471:MET:HA	1:B:518:MET:HE1	1.66	0.77
1:A:358:LEU:HB2	1:A:359:PRO:HD2	1.67	0.77
1:A:205:THR:HB	1:A:206:PRO:HD3	1.66	0.77
1:D:197:VAL:HG23	1:D:248:ILE:HG23	1.66	0.77
1:E:227:PRO:HG2	1:E:489:PHE:HB3	1.67	0.77
1:C:64:LEU:HD22	3:F:953:HOH:O	1.84	0.77
1:E:257:PRO:HB2	1:E:497:ARG:HD3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:PRO:HG2	1:E:237:GLU:HB2	1.67	0.76
1:C:268:GLU:HB2	3:C:1218:HOH:O	1.85	0.76
1:A:70:THR:HG22	1:A:72:VAL:H	1.50	0.76
1:E:456:GLU:H	1:E:456:GLU:CD	1.93	0.75
1:A:242:LYS:HE2	1:A:277:HIS:CD2	2.21	0.75
1:B:425:ARG:NH1	1:D:159:ASP:HA	2.01	0.75
1:C:227:PRO:HG2	1:C:489:PHE:HB3	1.67	0.75
1:E:17:LYS:HG3	3:E:1573:HOH:O	1.87	0.75
1:E:297:GLN:NE2	1:E:302:ILE:HD11	2.02	0.74
1:B:205:THR:HB	1:B:206:PRO:HD3	1.68	0.74
1:F:306:ASN:ND2	1:F:334:VAL:HG11	2.02	0.73
1:A:172:GLU:HG2	1:A:176:ALA:HB2	1.71	0.73
1:B:33:LEU:HD11	1:B:482:VAL:HG11	1.70	0.73
1:B:257:PRO:HB2	1:B:497:ARG:HD3	1.69	0.73
1:E:358:LEU:HB2	1:E:359:PRO:HD2	1.71	0.73
1:F:226:ASP:OD2	1:F:229:LEU:HG	1.89	0.73
1:D:344:GLU:O	1:D:348:VAL:HG23	1.89	0.72
1:D:96:ASP:HB3	3:D:1342:HOH:O	1.90	0.72
1:E:197:VAL:HG23	1:E:248:ILE:HG23	1.72	0.72
1:F:333:ASN:HD22	1:F:335:PHE:N	1.86	0.72
1:D:358:LEU:HB2	1:D:359:PRO:HD2	1.72	0.71
1:C:53:ARG:HG2	1:C:100:VAL:HG23	1.71	0.71
1:B:26:SER:O	1:B:30:ARG:HG3	1.91	0.71
1:C:408:TYR:HA	1:D:72:VAL:HG11	1.71	0.71
1:B:15:GLU:HB3	3:B:894:HOH:O	1.90	0.70
1:F:93:GLU:HG3	1:F:93:GLU:O	1.90	0.70
1:F:471:MET:HE3	1:F:515:LEU:HD11	1.73	0.70
1:E:333:ASN:ND2	1:E:335:PHE:HB2	2.05	0.70
1:F:101:ARG:HH11	1:F:101:ARG:HG2	1.56	0.70
1:F:358:LEU:HB2	1:F:359:PRO:HD2	1.71	0.70
1:A:372:ALA:HA	1:A:380:ASN:HD22	1.57	0.70
1:C:19:GLU:O	1:C:23:ILE:HD12	1.92	0.70
1:D:234:PRO:HG2	1:D:237:GLU:HB2	1.74	0.70
1:A:333:ASN:ND2	1:A:335:PHE:HB2	2.05	0.70
1:C:33:LEU:HD11	1:C:482:VAL:HG11	1.72	0.70
1:F:187:LEU:HD13	1:F:353:ARG:NH2	2.07	0.70
1:E:528:GLY:C	3:E:1841:HOH:O	2.34	0.70
1:A:471:MET:HE1	1:A:495:SER:HA	1.72	0.69
1:B:333:ASN:HD22	1:B:335:PHE:N	1.88	0.69
1:E:461:TRP:HB2	3:E:1826:HOH:O	1.92	0.69
1:A:227:PRO:HG2	1:A:489:PHE:HB3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLU:O	1:B:88:GLU:HG3	1.93	0.69
1:C:372:ALA:HA	1:C:380:ASN:HD22	1.56	0.69
1:D:172:GLU:HG2	1:D:176:ALA:HB2	1.73	0.69
1:D:372:ALA:HA	1:D:380:ASN:HD22	1.58	0.69
1:E:513:ARG:HD3	3:E:560:HOH:O	1.92	0.69
1:A:139:ARG:HG3	1:A:371:VAL:HG21	1.75	0.69
1:F:282:MET:HE3	1:F:335:PHE:CD2	2.28	0.68
1:E:158:ALA:HB1	1:E:161:ILE:HD12	1.75	0.68
1:F:490:GLY:O	1:F:492:ASN:N	2.25	0.68
1:A:448:ASP:O	1:A:452:LYS:HG3	1.93	0.68
1:E:474:ARG:HG3	1:E:518:MET:HE3	1.75	0.68
1:D:306:ASN:HA	1:D:334:VAL:HG22	1.73	0.68
1:C:70:THR:HG22	1:C:72:VAL:H	1.59	0.67
1:D:23:ILE:HD12	1:D:23:ILE:H	1.59	0.67
1:C:234:PRO:HG2	1:C:237:GLU:HB2	1.77	0.67
1:A:41:ASN:HD21	1:A:419:ARG:NH2	1.92	0.67
1:B:461:TRP:O	1:B:465:GLN:HG2	1.94	0.67
1:A:257:PRO:HB2	1:A:497:ARG:HD2	1.77	0.67
1:D:139:ARG:HG3	1:D:371:VAL:CG2	2.24	0.67
1:D:418:ARG:HD3	1:F:404:GLU:OE1	1.94	0.67
1:F:156:MET:HE2	1:F:156:MET:HA	1.75	0.66
1:C:15:GLU:C	1:C:17:LYS:H	2.02	0.66
1:C:41:ASN:HD21	1:C:419:ARG:HH12	1.43	0.66
1:E:471:MET:HE2	1:E:515:LEU:HD11	1.77	0.66
1:F:353:ARG:HG3	1:F:353:ARG:HH11	1.61	0.66
1:F:41:ASN:HD21	1:F:419:ARG:HH22	1.42	0.66
1:A:490:GLY:O	1:A:492:ASN:N	2.28	0.66
1:C:19:GLU:O	1:C:22:LYS:HB3	1.96	0.66
1:D:294:ASP:O	3:D:1372:HOH:O	2.13	0.66
1:E:353:ARG:HG3	1:E:353:ARG:HH11	1.60	0.66
1:A:41:ASN:ND2	1:A:419:ARG:HH22	1.93	0.65
1:A:294:ASP:O	3:A:795:HOH:O	2.14	0.65
1:A:24:ALA:HB3	1:A:482:VAL:HG23	1.76	0.65
1:F:24:ALA:HB3	1:F:482:VAL:HG23	1.78	0.65
1:F:111:ARG:HD2	1:F:112:ASP:OD1	1.97	0.65
1:A:21:ILE:HG23	1:A:22:LYS:N	2.12	0.64
1:B:490:GLY:O	1:B:492:ASN:N	2.31	0.64
1:B:24:ALA:HB3	1:B:482:VAL:HG23	1.80	0.64
1:B:172:GLU:CD	1:B:172:GLU:H	2.05	0.63
1:E:33:LEU:HD11	1:E:482:VAL:HG11	1.79	0.63
1:C:333:ASN:HD22	1:C:335:PHE:H	1.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PRO:HD2	3:A:671:HOH:O	1.97	0.63
1:C:210:ILE:HB	1:C:211:PRO:HD3	1.81	0.63
1:A:53:ARG:HG2	1:A:100:VAL:CG2	2.29	0.63
1:A:234:PRO:HG2	1:A:237:GLU:HB2	1.80	0.63
1:A:197:VAL:HG23	1:A:248:ILE:HG23	1.81	0.63
1:C:253:ASN:HA	1:C:254:PRO:C	2.24	0.63
1:D:515:LEU:HD12	1:D:518:MET:HE2	1.81	0.63
1:E:333:ASN:HD22	1:E:335:PHE:H	1.46	0.63
1:B:197:VAL:HG21	1:B:218:LEU:HD13	1.81	0.62
1:C:89:ARG:HH12	1:C:93:GLU:HG3	1.63	0.62
1:C:489:PHE:CE2	1:C:493:ARG:HD3	2.34	0.62
1:A:29:ASN:O	1:A:33:LEU:HG	1.98	0.62
1:F:195:ASP:OD1	1:F:247:LYS:HD2	2.00	0.62
1:B:15:GLU:HA	3:B:886:HOH:O	1.98	0.62
1:E:362:ARG:HG3	1:E:362:ARG:HH11	1.64	0.62
1:E:232:GLN:HE21	1:E:232:GLN:HA	1.65	0.62
1:A:232:GLN:HE22	1:A:263:ASP:H	1.48	0.62
1:A:53:ARG:HG2	1:A:100:VAL:HG23	1.80	0.62
1:B:446:LEU:HD13	1:B:471:MET:HE3	1.81	0.62
1:C:456:GLU:O	1:C:459:SER:HB3	2.00	0.62
1:E:30:ARG:HG2	1:E:30:ARG:HH11	1.64	0.62
1:E:201:MET:HE3	1:E:208:ILE:CD1	2.29	0.62
1:C:87:PHE:O	1:C:91:ILE:HG12	2.00	0.61
1:B:23:ILE:HD13	1:B:473:PHE:CD1	2.35	0.61
1:C:333:ASN:ND2	1:C:336:ASP:H	1.98	0.61
1:C:333:ASN:HD22	1:C:335:PHE:N	1.97	0.61
1:B:106:SER:HB2	1:B:398:LEU:HD13	1.82	0.61
1:C:172:GLU:HG2	1:C:176:ALA:HB2	1.81	0.61
1:C:490:GLY:O	1:C:492:ASN:N	2.33	0.61
1:D:172:GLU:CD	1:D:172:GLU:H	2.08	0.61
1:A:24:ALA:HB3	1:A:482:VAL:CG2	2.31	0.61
1:B:483:LEU:HD22	1:B:498:ALA:HB2	1.82	0.61
1:A:333:ASN:ND2	1:A:335:PHE:N	2.49	0.61
1:C:447:GLN:HB3	1:C:493:ARG:HH21	1.66	0.61
1:D:210:ILE:N	1:D:211:PRO:HD2	2.16	0.61
1:E:17:LYS:HD2	3:E:1572:HOH:O	2.00	0.61
1:E:172:GLU:HG2	1:E:176:ALA:HB2	1.82	0.60
1:E:271:ARG:HG2	1:E:271:ARG:HH11	1.66	0.60
1:B:333:ASN:ND2	1:B:335:PHE:H	1.94	0.60
1:D:210:ILE:O	1:D:213:LEU:HB2	2.01	0.60
1:D:213:LEU:HD13	1:D:215:GLN:OE1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ASP:HB2	3:D:1523:HOH:O	2.02	0.60
1:F:387:THR:OG1	1:F:388:PRO:HD3	2.01	0.60
1:D:490:GLY:O	1:D:492:ASN:N	2.34	0.60
1:E:232:GLN:HA	1:E:232:GLN:NE2	2.17	0.60
1:A:447:GLN:HB2	1:A:463:VAL:CG2	2.32	0.60
1:C:224:ASN:O	1:C:237:GLU:HG2	2.02	0.60
1:E:41:ASN:HD21	1:E:419:ARG:NH2	1.99	0.60
1:E:481:ILE:HD13	1:E:503:LEU:HD13	1.84	0.60
1:B:135:PRO:HD2	3:B:779:HOH:O	2.01	0.60
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.66	0.60
1:F:24:ALA:HB3	1:F:482:VAL:CG2	2.31	0.59
1:B:21:ILE:HG12	1:B:33:LEU:HD12	1.84	0.59
1:B:404:GLU:OE1	1:F:418:ARG:HD2	2.02	0.59
1:F:412:LEU:O	1:F:416:ILE:HG12	2.03	0.59
1:C:471:MET:HE1	1:C:495:SER:HA	1.85	0.59
1:D:333:ASN:HD22	1:D:335:PHE:N	1.99	0.59
1:D:358:LEU:HD23	1:D:358:LEU:H	1.68	0.59
1:E:461:TRP:O	1:E:465:GLN:HG2	2.03	0.59
1:A:156:MET:HG3	1:A:309:LEU:HD11	1.84	0.59
1:D:513:ARG:HD2	3:D:1534:HOH:O	2.03	0.59
1:F:41:ASN:HD21	1:F:419:ARG:HH12	1.49	0.59
1:F:172:GLU:H	1:F:172:GLU:CD	2.10	0.59
1:F:492:ASN:ND2	3:F:2011:HOH:O	2.32	0.59
1:E:352:HIS:O	1:E:355:ARG:HG2	2.02	0.59
1:B:187:LEU:HD13	1:B:353:ARG:NH2	2.18	0.58
1:C:255:SER:O	1:C:259:SER:HA	2.01	0.58
1:A:253:ASN:HA	1:A:254:PRO:C	2.26	0.58
1:C:154:ARG:NH2	3:C:1108:HOH:O	2.35	0.58
1:C:381:HIS:ND1	1:D:34:ASN:HB3	2.18	0.58
1:E:446:LEU:HB2	1:E:471:MET:CE	2.28	0.58
1:E:94:ASN:HB3	1:E:97:GLN:OE1	2.02	0.58
1:E:461:TRP:CB	3:E:1826:HOH:O	2.48	0.58
1:A:472:LEU:HD22	1:A:483:LEU:HB2	1.85	0.58
1:B:41:ASN:HD21	1:B:419:ARG:HH12	1.50	0.58
1:B:353:ARG:NH1	3:B:881:HOH:O	2.36	0.58
1:B:490:GLY:C	1:B:492:ASN:H	2.12	0.58
1:C:204:PHE:HE2	1:C:207:TYR:CG	2.22	0.58
1:F:35:ALA:HB1	1:F:37:ARG:HH11	1.68	0.58
1:C:513:ARG:HD3	3:C:1283:HOH:O	2.02	0.58
1:D:199:ILE:O	1:D:201:MET:HG2	2.04	0.58
1:D:271:ARG:NH1	1:D:302:ILE:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:THR:HB	1:D:206:PRO:CD	2.33	0.58
1:F:172:GLU:HG2	1:F:176:ALA:HB2	1.85	0.57
1:F:257:PRO:HB2	1:F:497:ARG:HD2	1.84	0.57
1:B:306:ASN:ND2	1:B:334:VAL:HG11	2.19	0.57
1:A:106:SER:HB2	1:A:398:LEU:HD13	1.86	0.57
1:B:41:ASN:HD21	1:B:419:ARG:HH22	1.53	0.57
3:B:789:HOH:O	1:D:159:ASP:HA	2.05	0.57
1:F:333:ASN:ND2	1:F:335:PHE:N	2.50	0.57
1:F:489:PHE:N	1:F:489:PHE:HD1	2.03	0.57
1:F:461:TRP:O	1:F:465:GLN:HG2	2.04	0.57
1:F:473:PHE:HE2	3:F:1875:HOH:O	1.86	0.57
1:F:489:PHE:N	1:F:489:PHE:CD1	2.72	0.57
1:E:487:ARG:HG3	1:E:487:ARG:HH11	1.70	0.57
1:A:196:LYS:HD2	1:A:245:ALA:HB3	1.85	0.57
1:A:447:GLN:HB2	1:A:463:VAL:HG21	1.85	0.57
1:B:425:ARG:NH2	1:D:153:ILE:CG2	2.68	0.57
1:D:106:SER:HB2	1:D:398:LEU:HD13	1.85	0.57
1:D:195:ASP:HB3	1:D:247:LYS:HG3	1.86	0.57
1:E:111:ARG:HD2	1:E:112:ASP:OD1	2.04	0.57
1:F:472:LEU:HD22	1:F:483:LEU:HB2	1.87	0.57
1:C:232:GLN:HE22	1:C:263:ASP:H	1.53	0.57
1:D:41:ASN:HD21	1:D:419:ARG:HH12	1.51	0.57
1:D:253:ASN:HA	1:D:254:PRO:C	2.30	0.57
1:B:210:ILE:N	1:B:211:PRO:HD2	2.20	0.57
1:A:172:GLU:HG2	1:A:176:ALA:CB	2.34	0.57
1:D:235:ASP:OD1	1:D:269:ARG:HD3	2.05	0.57
1:F:490:GLY:C	1:F:492:ASN:H	2.13	0.57
1:F:59:ALA:O	1:F:63:GLU:HG3	2.05	0.56
1:A:21:ILE:HG23	1:A:22:LYS:HG3	1.87	0.56
1:C:23:ILE:HD13	3:C:853:HOH:O	2.04	0.56
1:D:101:ARG:HD3	3:D:557:HOH:O	2.04	0.56
1:E:172:GLU:CD	1:E:172:GLU:H	2.13	0.56
1:F:253:ASN:HA	1:F:254:PRO:C	2.30	0.56
1:E:334:VAL:HA	1:E:337:LEU:HD12	1.88	0.56
1:F:270:VAL:O	1:F:274:VAL:HG23	2.05	0.56
1:A:20:LEU:HD12	1:A:23:ILE:HG21	1.88	0.56
1:B:98:GLU:HB2	3:B:834:HOH:O	2.05	0.56
1:C:235:ASP:OD1	1:C:269:ARG:HD3	2.06	0.56
1:C:197:VAL:HG23	1:C:248:ILE:HG23	1.88	0.56
1:F:452:LYS:HE2	3:F:2002:HOH:O	2.04	0.56
1:A:86:ARG:HD3	1:D:88:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:GLU:H	1:B:456:GLU:CD	2.14	0.55
1:A:21:ILE:HG23	1:A:22:LYS:H	1.69	0.55
1:D:24:ALA:HB3	1:D:482:VAL:CG2	2.36	0.55
1:E:226:ASP:OD2	1:E:229:LEU:HG	2.07	0.55
1:A:79:LYS:NZ	3:A:626:HOH:O	2.18	0.55
1:C:178:MET:HE2	1:C:310:VAL:HG11	1.88	0.55
1:C:306:ASN:ND2	1:C:334:VAL:HG11	2.22	0.55
1:D:333:ASN:HD21	1:D:335:PHE:HB2	1.72	0.55
1:D:347:LYS:HD2	1:D:362:ARG:NH1	2.22	0.55
1:E:41:ASN:ND2	1:E:419:ARG:HH22	1.99	0.55
1:E:248:ILE:HD11	1:E:284:LEU:HB2	1.88	0.55
1:E:490:GLY:O	1:E:492:ASN:N	2.40	0.55
1:F:474:ARG:O	1:F:478:GLU:HG3	2.07	0.55
1:C:86:ARG:HD3	1:F:88:GLU:OE1	2.07	0.55
1:D:172:GLU:HG2	1:D:176:ALA:CB	2.37	0.55
1:D:414:GLN:NE2	3:D:1004:HOH:O	2.38	0.55
1:E:309:LEU:HB3	1:E:328:ALA:HB3	1.89	0.55
1:E:483:LEU:HD22	1:E:498:ALA:HB2	1.88	0.55
1:B:253:ASN:HA	1:B:254:PRO:C	2.29	0.55
1:D:187:LEU:HD13	1:D:353:ARG:NH2	2.22	0.55
1:A:332:GLN:HG3	3:A:703:HOH:O	2.06	0.54
1:B:139:ARG:NH2	3:B:589:HOH:O	2.39	0.54
1:C:111:ARG:HD2	1:C:112:ASP:OD1	2.07	0.54
1:F:375:ARG:NE	3:F:2197:HOH:O	2.38	0.54
1:B:53:ARG:HG2	1:B:100:VAL:CG2	2.36	0.54
1:D:306:ASN:HA	1:D:334:VAL:CG2	2.38	0.54
1:F:330:HIS:CE1	1:F:332:GLN:HG2	2.42	0.54
1:B:18:ASP:O	1:B:22:LYS:HG2	2.08	0.54
1:A:101:ARG:NH2	3:A:653:HOH:O	2.38	0.54
1:F:20:LEU:HB3	1:F:482:VAL:HG11	1.89	0.54
1:B:53:ARG:HG2	1:B:100:VAL:HG23	1.89	0.54
1:D:322:TRP:HB3	1:D:324:LEU:HG	1.90	0.54
1:D:358:LEU:HD23	1:D:358:LEU:N	2.22	0.54
1:E:19:GLU:HA	1:E:22:LYS:HD2	1.90	0.54
1:E:468:THR:O	1:E:472:LEU:HG	2.07	0.54
1:A:489:PHE:N	1:A:489:PHE:CD2	2.73	0.54
1:A:490:GLY:C	1:A:492:ASN:H	2.15	0.54
1:B:232:GLN:HE22	1:B:263:ASP:H	1.55	0.54
1:B:513:ARG:HD3	3:B:826:HOH:O	2.06	0.54
1:F:239:ASP:OD2	1:F:269:ARG:NH2	2.37	0.54
1:B:425:ARG:HH12	1:D:159:ASP:CA	2.09	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:PHE:CE1	1:D:371:VAL:HG22	2.42	0.54
1:E:513:ARG:HG3	1:E:513:ARG:HH11	1.73	0.54
1:F:254:PRO:HB3	1:F:438:VAL:HG21	1.88	0.54
1:E:53:ARG:HD3	1:E:100:VAL:HG23	1.89	0.53
1:E:232:GLN:HE21	1:E:232:GLN:CA	2.20	0.53
1:E:255:SER:O	1:E:259:SER:HA	2.08	0.53
1:F:210:ILE:N	1:F:211:PRO:HD2	2.23	0.53
1:B:237:GLU:OE2	1:B:240:LYS:HE3	2.08	0.53
1:D:205:THR:HB	1:D:206:PRO:HD3	1.90	0.53
1:F:232:GLN:HE22	1:F:262:MET:HA	1.71	0.53
1:A:19:GLU:O	1:A:23:ILE:HB	2.09	0.53
1:C:20:LEU:HD13	1:C:482:VAL:HG13	1.89	0.53
1:A:417:ARG:HD2	1:A:433:ARG:NH2	2.22	0.53
1:E:398:LEU:HB3	1:E:402:MET:HE2	1.91	0.53
1:A:23:ILE:CD1	1:A:473:PHE:CE1	2.91	0.53
1:A:158:ALA:HB1	1:A:161:ILE:HD12	1.91	0.53
1:B:320:THR:O	1:B:323:ARG:HD2	2.09	0.53
1:C:447:GLN:HE21	1:C:463:VAL:HG21	1.74	0.53
1:E:226:ASP:OD2	1:E:228:SER:HB3	2.09	0.53
1:F:234:PRO:HG2	1:F:237:GLU:HB2	1.90	0.53
1:A:347:LYS:HD3	1:A:362:ARG:HE	1.73	0.53
1:F:333:ASN:HD21	1:F:335:PHE:HB2	1.73	0.53
1:B:35:ALA:HB1	1:B:37:ARG:HH11	1.73	0.53
1:F:35:ALA:HB1	1:F:37:ARG:NH1	2.24	0.53
1:F:344:GLU:O	1:F:348:VAL:HG23	2.08	0.53
1:A:456:GLU:O	1:A:459:SER:HB3	2.09	0.52
1:F:17:LYS:O	1:F:21:ILE:HG13	2.09	0.52
1:B:355:ARG:HG2	1:B:355:ARG:NH1	2.23	0.52
1:B:398:LEU:O	1:B:402:MET:HG3	2.08	0.52
1:D:254:PRO:HB3	1:D:438:VAL:HG21	1.91	0.52
1:A:255:SER:O	1:A:259:SER:HA	2.08	0.52
1:B:447:GLN:HB3	1:B:493:ARG:HH21	1.74	0.52
1:E:314:SER:HB3	1:E:320:THR:HG22	1.92	0.52
1:D:158:ALA:HB1	1:D:161:ILE:HD12	1.91	0.52
1:F:13:PRO:HG2	1:F:14:PHE:H	1.74	0.52
1:F:106:SER:HB2	1:F:398:LEU:HD13	1.91	0.52
1:A:429:MET:HB3	1:A:430:PRO:HD2	1.92	0.52
1:B:159:ASP:HB2	1:F:429:MET:HE1	1.91	0.52
1:E:205:THR:HB	1:E:206:PRO:HD3	1.91	0.52
1:F:98:GLU:HB2	3:F:548:HOH:O	2.09	0.52
1:B:196:LYS:NZ	3:B:659:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:VAL:O	1:D:136:VAL:HG13	2.08	0.52
1:C:43:LEU:HB2	1:C:48:ARG:NH1	2.23	0.52
1:D:333:ASN:ND2	1:D:335:PHE:H	2.00	0.52
1:B:89:ARG:O	1:B:93:GLU:HG2	2.10	0.52
1:D:257:PRO:HB2	1:D:497:ARG:HD2	1.91	0.52
1:E:333:ASN:HD21	1:E:335:PHE:HB2	1.74	0.52
1:A:196:LYS:HD2	1:A:245:ALA:CB	2.40	0.52
1:E:210:ILE:N	1:E:211:PRO:HD2	2.25	0.52
1:F:308:LEU:HD11	1:F:366:PHE:HE2	1.75	0.52
1:F:448:ASP:HB3	3:F:2002:HOH:O	2.09	0.52
1:F:474:ARG:HG3	1:F:518:MET:HE3	1.92	0.52
1:A:447:GLN:HB3	1:A:493:ARG:HH21	1.76	0.51
1:C:232:GLN:NE2	1:C:263:ASP:H	2.08	0.51
1:B:254:PRO:HG2	1:B:289:TYR:CB	2.37	0.51
1:D:111:ARG:HD2	1:D:112:ASP:OD1	2.10	0.51
1:A:483:LEU:HD22	1:A:498:ALA:HB2	1.91	0.51
1:B:357:LEU:HD11	1:B:372:ALA:HB2	1.93	0.51
1:E:23:ILE:HD13	1:E:473:PHE:CD1	2.45	0.51
1:F:380:ASN:ND2	3:F:1935:HOH:O	2.42	0.51
1:A:172:GLU:HG3	1:B:375:ARG:NH2	2.25	0.51
1:B:459:SER:O	1:B:463:VAL:HG23	2.10	0.51
1:B:529:GLN:HA	1:B:529:GLN:NE2	2.25	0.51
1:D:22:LYS:N	1:D:22:LYS:HD2	2.26	0.51
1:D:333:ASN:ND2	1:D:335:PHE:HB2	2.25	0.51
1:E:87:PHE:O	1:E:91:ILE:HG12	2.10	0.51
1:F:37:ARG:HH11	1:F:37:ARG:HG3	1.75	0.51
1:F:454:TYR:HB2	1:F:458:PHE:CD2	2.45	0.51
1:A:425:ARG:NH1	3:A:830:HOH:O	2.44	0.51
1:B:24:ALA:HB3	1:B:482:VAL:CG2	2.41	0.51
1:B:323:ARG:NH1	1:B:323:ARG:HA	2.26	0.51
1:C:41:ASN:HD21	1:C:419:ARG:HH22	1.57	0.51
1:D:203:VAL:HG22	1:D:204:PHE:N	2.26	0.51
1:A:344:GLU:O	1:A:348:VAL:HG23	2.11	0.51
1:D:226:ASP:OD2	1:D:228:SER:HB2	2.10	0.51
1:F:197:VAL:O	1:F:197:VAL:HG13	2.10	0.51
1:A:111:ARG:HD2	1:A:112:ASP:OD1	2.10	0.51
1:C:41:ASN:HD22	1:C:41:ASN:H	1.57	0.51
1:D:359:PRO:HG2	1:D:360:ASP:H	1.74	0.51
1:E:426:GLU:O	1:E:516:ARG:HD3	2.09	0.51
1:C:358:LEU:HB2	1:C:359:PRO:HD2	1.92	0.51
1:E:215:GLN:HG3	1:E:216:TYR:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:ARG:HG2	1:E:271:ARG:NH1	2.25	0.51
1:C:41:ASN:HD21	1:C:419:ARG:NH1	2.08	0.51
1:F:257:PRO:HB2	1:F:497:ARG:CD	2.41	0.51
1:D:513:ARG:HG3	1:D:513:ARG:HH11	1.75	0.50
1:F:417:ARG:HD2	1:F:433:ARG:NH2	2.26	0.50
1:B:197:VAL:HG22	1:B:248:ILE:CG2	2.41	0.50
1:A:208:ILE:HG22	1:A:220:GLU:OE2	2.11	0.50
1:B:425:ARG:NH2	1:D:158:ALA:O	2.32	0.50
1:D:490:GLY:C	1:D:492:ASN:H	2.20	0.50
1:A:23:ILE:HD12	1:A:473:PHE:CE1	2.45	0.50
1:C:15:GLU:C	1:C:17:LYS:N	2.70	0.50
1:C:72:VAL:HG12	1:C:74:VAL:HG23	1.92	0.50
1:A:379:LEU:HD23	1:B:206:PRO:HB3	1.94	0.50
1:F:50:ALA:CB	1:F:102:PHE:HD2	2.24	0.50
1:A:359:PRO:HG2	1:A:360:ASP:H	1.76	0.50
1:B:358:LEU:HB2	1:B:359:PRO:CD	2.37	0.50
1:B:372:ALA:HA	1:B:380:ASN:HD22	1.76	0.50
1:D:517:LYS:O	1:D:521:GLU:HG3	2.12	0.50
1:F:343:GLN:HB2	1:F:346:GLU:HG3	1.94	0.50
1:A:139:ARG:HG3	1:A:371:VAL:CG2	2.40	0.50
1:A:172:GLU:HG3	1:B:375:ARG:HH21	1.76	0.50
1:E:95:ARG:O	1:E:101:ARG:HD3	2.12	0.50
1:E:523:TYR:O	1:E:527:SER:HB2	2.11	0.50
1:A:72:VAL:CG1	1:B:408:TYR:HA	2.41	0.50
1:A:308:LEU:HD11	1:A:366:PHE:HE2	1.75	0.50
1:B:248:ILE:HA	1:B:282:MET:O	2.12	0.50
1:C:101:ARG:HD3	3:C:939:HOH:O	2.11	0.50
1:D:472:LEU:HD22	1:D:483:LEU:HB2	1.93	0.49
1:D:515:LEU:CD1	1:D:518:MET:HE2	2.42	0.49
1:E:25:SER:OG	1:E:30:ARG:NH2	2.45	0.49
1:E:331:GLN:HE21	1:E:332:GLN:HE21	1.59	0.49
1:A:79:LYS:HB3	3:A:617:HOH:O	2.11	0.49
1:A:476:ALA:HA	1:A:481:ILE:O	2.13	0.49
1:D:450:THR:HB	1:D:458:PHE:CE2	2.47	0.49
1:E:161:ILE:HD11	1:E:304:PRO:HG3	1.94	0.49
1:E:446:LEU:CB	1:E:471:MET:HE1	2.33	0.49
1:F:181:ILE:O	1:F:185:LEU:HG	2.12	0.49
1:F:443:LEU:HD13	1:F:497:ARG:CZ	2.41	0.49
1:D:513:ARG:HG3	1:D:513:ARG:NH1	2.28	0.49
1:E:53:ARG:HD2	3:E:551:HOH:O	2.11	0.49
1:F:188:ASN:HB3	1:F:339:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:TRP:HB3	1:F:324:LEU:HG	1.93	0.49
1:F:359:PRO:HG2	1:F:360:ASP:H	1.76	0.49
1:A:113:GLN:OE1	1:E:505:GLU:HG3	2.13	0.49
1:A:205:THR:O	1:A:208:ILE:HG13	2.12	0.49
1:B:111:ARG:HD2	1:B:112:ASP:OD1	2.12	0.49
1:E:136:VAL:HA	1:E:137:PRO:C	2.37	0.49
1:E:487:ARG:HA	3:E:1758:HOH:O	2.12	0.49
1:F:235:ASP:OD1	1:F:269:ARG:HD3	2.12	0.49
1:A:111:ARG:HG3	1:A:118:PRO:HB3	1.94	0.49
1:B:172:GLU:HG2	1:B:176:ALA:HB2	1.95	0.49
1:B:429:MET:HE1	1:D:159:ASP:HB2	1.94	0.49
1:E:215:GLN:HB3	3:E:1723:HOH:O	2.11	0.49
1:E:270:VAL:O	1:E:274:VAL:HG23	2.12	0.49
1:F:41:ASN:C	1:F:41:ASN:HD22	2.19	0.49
1:A:205:THR:HB	1:A:206:PRO:CD	2.41	0.49
1:A:210:ILE:N	1:A:211:PRO:HD2	2.27	0.49
1:C:269:ARG:O	1:C:273:ILE:HG13	2.13	0.49
1:D:513:ARG:NH1	3:D:1535:HOH:O	2.45	0.49
1:E:353:ARG:HG3	1:E:353:ARG:NH1	2.27	0.49
1:F:450:THR:HB	1:F:458:PHE:CE2	2.48	0.49
1:A:24:ALA:HB1	1:A:480:GLY:O	2.12	0.49
1:D:41:ASN:HD21	1:D:419:ARG:HH22	1.61	0.49
1:F:33:LEU:HD11	1:F:482:VAL:HG11	1.95	0.49
1:F:101:ARG:HG2	1:F:101:ARG:NH1	2.27	0.49
1:A:95:ARG:NH1	3:A:645:HOH:O	2.44	0.49
1:A:201:MET:HB3	1:A:202:PRO:HA	1.94	0.49
1:A:232:GLN:NE2	3:A:759:HOH:O	2.45	0.49
1:E:18:ASP:O	1:E:22:LYS:HG3	2.13	0.49
1:E:257:PRO:HG2	1:E:258:PRO:HD3	1.95	0.49
1:E:306:ASN:ND2	1:E:334:VAL:HG11	2.27	0.49
1:E:457:ALA:O	3:E:1826:HOH:O	2.20	0.49
1:E:481:ILE:HD13	1:E:503:LEU:CD1	2.42	0.49
1:D:24:ALA:HB1	1:D:480:GLY:O	2.13	0.49
1:E:344:GLU:O	1:E:348:VAL:HG23	2.13	0.49
1:A:357:LEU:HD11	1:A:372:ALA:HB2	1.94	0.48
1:B:232:GLN:NE2	1:B:263:ASP:H	2.11	0.48
1:E:472:LEU:HD22	1:E:483:LEU:HB2	1.94	0.48
1:F:25:SER:HB2	1:F:30:ARG:HH22	1.76	0.48
1:C:15:GLU:O	1:C:15:GLU:HG2	2.14	0.48
1:F:425:ARG:NH2	3:F:617:HOH:O	2.29	0.48
1:A:333:ASN:ND2	1:A:335:PHE:CB	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLN:HE21	1:A:463:VAL:HG21	1.78	0.48
1:E:264:GLN:H	1:E:264:GLN:NE2	2.00	0.48
1:D:204:PHE:HE2	1:D:207:TYR:CG	2.32	0.48
1:D:357:LEU:HD11	1:D:372:ALA:HB2	1.96	0.48
1:E:135:PRO:HG3	1:E:387:THR:HG23	1.96	0.48
1:F:282:MET:HE3	1:F:335:PHE:CE2	2.48	0.48
1:A:23:ILE:HD12	1:A:473:PHE:HE1	1.79	0.48
1:A:76:GLY:O	1:B:43:LEU:HD21	2.13	0.48
1:E:491:SER:HB2	3:E:1578:HOH:O	2.13	0.48
1:F:156:MET:HE2	1:F:156:MET:CA	2.44	0.48
1:F:461:TRP:CZ2	1:F:465:GLN:HG3	2.48	0.48
1:B:472:LEU:CD1	1:B:485:PRO:HG3	2.44	0.48
1:C:64:LEU:CD2	3:F:953:HOH:O	2.53	0.48
1:E:322:TRP:HB3	1:E:324:LEU:HG	1.95	0.48
1:E:447:GLN:HB3	1:E:493:ARG:NH2	2.22	0.48
1:F:41:ASN:HD21	1:F:419:ARG:NH2	2.08	0.48
1:A:461:TRP:CE3	1:A:465:GLN:HG3	2.48	0.48
1:B:493:ARG:HD2	3:B:692:HOH:O	2.12	0.48
1:D:487:ARG:NH2	3:D:1265:HOH:O	2.46	0.48
1:E:481:ILE:HG21	1:E:511:ILE:HD11	1.95	0.48
1:F:21:ILE:HG22	1:F:21:ILE:O	2.14	0.48
1:F:25:SER:HB2	1:F:30:ARG:NH2	2.29	0.48
1:F:353:ARG:HG3	1:F:353:ARG:NH1	2.28	0.48
1:B:209:GLU:O	1:B:213:LEU:HG	2.14	0.47
1:D:71:THR:HG23	1:D:71:THR:O	2.14	0.47
1:D:506:TYR:HB3	1:F:113:GLN:O	2.14	0.47
1:E:253:ASN:HA	1:E:254:PRO:C	2.38	0.47
1:F:204:PHE:HE2	1:F:207:TYR:CG	2.32	0.47
1:B:463:VAL:HG13	1:B:494:PRO:HD2	1.96	0.47
1:C:69:MET:O	3:C:1002:HOH:O	2.20	0.47
1:D:372:ALA:CA	1:D:380:ASN:HD22	2.26	0.47
1:E:190:LEU:O	1:E:282:MET:HE1	2.13	0.47
1:F:487:ARG:HG2	3:F:1867:HOH:O	2.14	0.47
1:A:72:VAL:HG22	1:B:407:GLU:HB3	1.97	0.47
1:A:150:GLN:NE2	3:A:657:HOH:O	2.47	0.47
1:F:20:LEU:C	1:F:22:LYS:H	2.22	0.47
1:F:41:ASN:ND2	1:F:419:ARG:HH22	2.09	0.47
1:B:489:PHE:CE1	1:B:493:ARG:HD3	2.50	0.47
1:E:224:ASN:O	1:E:237:GLU:HG2	2.14	0.47
1:F:474:ARG:CG	1:F:518:MET:HE3	2.44	0.47
1:C:41:ASN:ND2	1:C:419:ARG:HH12	2.09	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:THR:O	1:C:323:ARG:HD2	2.14	0.47
1:C:468:THR:O	1:C:472:LEU:HG	2.14	0.47
1:A:24:ALA:CB	1:A:482:VAL:HG23	2.43	0.47
1:C:172:GLU:CD	1:C:172:GLU:H	2.21	0.47
1:C:252:VAL:O	1:C:255:SER:HA	2.15	0.47
1:F:237:GLU:HA	1:F:240:LYS:HD2	1.97	0.47
1:F:305:GLU:CD	1:F:305:GLU:H	2.23	0.47
1:B:208:ILE:O	1:B:211:PRO:HG2	2.14	0.47
1:C:433:ARG:HG2	1:C:433:ARG:HH11	1.80	0.47
1:D:306:ASN:ND2	1:D:334:VAL:HG11	2.29	0.47
1:D:489:PHE:O	1:D:490:GLY:O	2.33	0.47
1:E:197:VAL:HG13	1:E:197:VAL:O	2.14	0.47
1:E:254:PRO:HD3	1:E:296:PHE:CE1	2.50	0.47
1:A:46:THR:N	1:A:47:PRO:HD2	2.30	0.47
1:A:481:ILE:HD13	1:A:503:LEU:HD13	1.97	0.47
1:B:434:ASP:C	1:B:434:ASP:OD1	2.58	0.47
1:A:309:LEU:HD23	1:A:310:VAL:N	2.30	0.47
1:B:425:ARG:NH2	1:D:153:ILE:HG21	2.30	0.47
1:C:305:GLU:O	1:C:334:VAL:HG13	2.15	0.47
1:E:139:ARG:O	1:E:140:MET:HB2	2.14	0.47
1:E:205:THR:CG2	1:E:209:GLU:OE2	2.63	0.47
1:F:230:ASN:HB3	3:F:2006:HOH:O	2.14	0.47
1:B:458:PHE:CE1	1:B:523:TYR:HA	2.51	0.46
1:D:41:ASN:HD21	1:D:419:ARG:NH1	2.13	0.46
1:B:89:ARG:NH1	1:B:93:GLU:HG3	2.31	0.46
1:D:472:LEU:CD2	1:D:483:LEU:HB2	2.45	0.46
1:F:12:SER:O	1:F:16:LEU:HB2	2.15	0.46
1:F:185:LEU:HD22	1:F:282:MET:HE1	1.97	0.46
1:B:95:ARG:NH2	3:B:944:HOH:O	2.49	0.46
1:B:102:PHE:CE1	1:B:402:MET:CE	2.99	0.46
1:B:404:GLU:OE1	1:F:418:ARG:CD	2.63	0.46
1:C:471:MET:HE1	1:C:496:GLY:N	2.30	0.46
1:D:105:LYS:CB	1:D:402:MET:HE1	2.45	0.46
1:F:16:LEU:O	1:F:20:LEU:HG	2.14	0.46
1:F:71:THR:HG22	1:F:71:THR:O	2.16	0.46
1:F:531:GLN:C	1:F:532:ASN:HD22	2.24	0.46
1:A:41:ASN:C	1:A:41:ASN:HD22	2.23	0.46
1:A:159:ASP:CB	1:E:429:MET:HE1	2.45	0.46
1:B:41:ASN:C	1:B:41:ASN:HD22	2.23	0.46
1:E:232:GLN:HE22	1:E:262:MET:HA	1.80	0.46
1:F:471:MET:HA	1:F:518:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:GLY:HA3	3:F:2011:HOH:O	2.15	0.46
1:A:433:ARG:HG2	1:A:434:ASP:N	2.31	0.46
1:C:162:PRO:HG2	1:C:165:SER:OG	2.15	0.46
1:D:107:LEU:HD21	3:D:2093:HOH:O	2.14	0.46
1:D:203:VAL:HG22	1:D:204:PHE:H	1.81	0.46
1:D:533:LEU:HD13	3:D:2205:HOH:O	2.14	0.46
1:E:24:ALA:HB3	1:E:482:VAL:HG23	1.98	0.46
1:E:248:ILE:HA	1:E:282:MET:O	2.15	0.46
1:F:195:ASP:CG	1:F:247:LYS:HD2	2.40	0.46
1:F:474:ARG:CG	1:F:474:ARG:HH11	2.29	0.46
1:B:257:PRO:CD	1:B:258:PRO:HD3	2.46	0.46
1:B:528:GLY:O	1:B:529:GLN:HB3	2.16	0.46
1:F:140:MET:HE2	1:F:145:GLU:HA	1.98	0.46
1:F:282:MET:CE	1:F:335:PHE:CE2	2.98	0.46
1:E:172:GLU:HG2	1:E:176:ALA:CB	2.46	0.46
1:E:376:ALA:O	1:E:378:ALA:N	2.47	0.46
1:F:187:LEU:HD13	1:F:353:ARG:HH21	1.80	0.46
1:A:528:GLY:O	3:A:865:HOH:O	2.20	0.46
1:B:210:ILE:HA	1:B:213:LEU:HG	1.97	0.46
1:B:456:GLU:CD	1:B:456:GLU:N	2.74	0.46
1:C:375:ARG:NH2	1:D:172:GLU:HG3	2.31	0.46
1:C:489:PHE:CD1	1:C:489:PHE:N	2.83	0.46
1:C:490:GLY:C	1:C:492:ASN:H	2.24	0.46
1:B:197:VAL:CG2	1:B:218:LEU:HD13	2.45	0.46
1:F:358:LEU:HD23	1:F:358:LEU:H	1.81	0.46
1:A:159:ASP:HB2	1:E:429:MET:HE1	1.98	0.45
3:B:550:HOH:O	1:F:418:ARG:HD3	2.14	0.45
1:E:30:ARG:HG2	1:E:30:ARG:NH1	2.29	0.45
1:E:264:GLN:HE21	1:E:264:GLN:N	1.99	0.45
1:A:43:LEU:C	1:A:43:LEU:HD12	2.41	0.45
1:E:23:ILE:HD13	1:E:473:PHE:CE1	2.52	0.45
1:F:20:LEU:C	1:F:22:LYS:N	2.74	0.45
1:F:116:LEU:HD13	1:F:143:ILE:HG23	1.98	0.45
1:C:323:ARG:NH1	1:C:323:ARG:HA	2.32	0.45
1:C:471:MET:HG3	1:C:518:MET:CE	2.41	0.45
1:D:348:VAL:O	1:D:351:ASP:HB2	2.16	0.45
1:E:489:PHE:CD2	1:E:489:PHE:N	2.83	0.45
1:F:41:ASN:HD21	1:F:419:ARG:NH1	2.13	0.45
1:F:333:ASN:ND2	1:F:333:ASN:C	2.75	0.45
1:A:489:PHE:N	1:A:489:PHE:HD2	2.13	0.45
1:A:490:GLY:C	1:A:492:ASN:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:THR:OG1	1:B:388:PRO:HD3	2.17	0.45
1:B:489:PHE:N	1:B:489:PHE:CD2	2.85	0.45
1:D:24:ALA:HB3	1:D:482:VAL:HG23	1.97	0.45
1:E:164:GLU:H	1:E:164:GLU:HG2	1.52	0.45
1:F:53:ARG:HD2	3:F:1915:HOH:O	2.16	0.45
1:F:257:PRO:CD	1:F:258:PRO:HD3	2.47	0.45
1:F:447:GLN:HG3	1:F:459:SER:OG	2.17	0.45
1:B:257:PRO:HB2	1:B:497:ARG:CD	2.42	0.45
1:C:340:ASP:O	1:C:347:LYS:NZ	2.44	0.45
1:F:17:LYS:HE3	1:F:487:ARG:NH2	2.32	0.45
1:F:239:ASP:CG	1:F:269:ARG:HH21	2.23	0.45
1:A:30:ARG:HG3	1:A:30:ARG:HH11	1.82	0.45
1:C:72:VAL:CG1	1:C:74:VAL:HG23	2.46	0.45
1:E:195:ASP:CG	1:E:247:LYS:HG3	2.41	0.45
1:F:355:ARG:HB2	1:F:355:ARG:CZ	2.46	0.45
1:B:136:VAL:HA	1:B:137:PRO:C	2.41	0.45
1:E:265:ARG:HG2	1:E:265:ARG:HH11	1.82	0.45
1:A:139:ARG:HD3	1:A:368:ASP:OD1	2.17	0.45
1:B:27:ASP:OD1	1:B:30:ARG:NH1	2.49	0.45
1:C:49:ARG:O	1:C:53:ARG:HB2	2.16	0.45
1:D:527:SER:O	1:D:531:GLN:HG3	2.17	0.45
1:E:453:LEU:HD22	1:E:516:ARG:NH1	2.32	0.45
1:C:136:VAL:HA	1:C:137:PRO:C	2.41	0.45
1:C:314:SER:HB3	1:C:320:THR:HG22	1.99	0.45
1:E:362:ARG:HG3	1:E:362:ARG:NH1	2.30	0.45
1:F:239:ASP:C	1:F:241:LEU:H	2.25	0.45
1:D:105:LYS:HB3	1:D:402:MET:CE	2.47	0.44
1:D:255:SER:O	1:D:259:SER:HA	2.17	0.44
1:E:49:ARG:O	1:E:53:ARG:HG3	2.18	0.44
1:F:355:ARG:HB2	1:F:355:ARG:NH1	2.32	0.44
1:C:24:ALA:HB3	1:C:482:VAL:HG23	2.00	0.44
1:E:192:LYS:O	1:E:195:ASP:HB2	2.17	0.44
1:F:20:LEU:HB3	1:F:482:VAL:CG1	2.46	0.44
1:B:23:ILE:HD13	1:B:473:PHE:CE1	2.53	0.44
1:E:359:PRO:HG2	1:E:360:ASP:H	1.82	0.44
1:A:408:TYR:HA	1:B:72:VAL:HG21	1.99	0.44
1:B:101:ARG:CZ	3:B:860:HOH:O	2.65	0.44
1:C:205:THR:HB	3:C:852:HOH:O	2.17	0.44
1:F:255:SER:O	1:F:259:SER:HA	2.17	0.44
1:B:264:GLN:O	1:B:268:GLU:HG2	2.18	0.44
1:C:54:LEU:HD21	1:C:125:MET:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:GLY:C	1:C:429:MET:HG2	2.43	0.44
1:E:245:ALA:O	3:E:1734:HOH:O	2.21	0.44
1:E:467:SER:O	1:E:470:ASP:HB2	2.17	0.44
1:A:21:ILE:CG2	1:A:22:LYS:N	2.80	0.44
1:A:204:PHE:C	1:A:204:PHE:CD2	2.95	0.44
1:A:309:LEU:HB3	1:A:328:ALA:HB3	1.99	0.44
1:B:23:ILE:HD13	1:B:473:PHE:HD1	1.79	0.44
1:B:333:ASN:ND2	1:B:335:PHE:HB2	2.33	0.44
1:B:456:GLU:O	1:B:459:SER:HB3	2.17	0.44
1:D:181:ILE:O	1:D:185:LEU:HG	2.18	0.44
1:A:71:THR:HG22	1:A:71:THR:O	2.17	0.44
1:B:140:MET:HE2	1:B:145:GLU:HA	1.99	0.44
1:B:287:ASP:OD1	1:B:287:ASP:N	2.50	0.44
1:C:489:PHE:N	1:C:489:PHE:HD1	2.16	0.44
1:D:101:ARG:CD	3:D:557:HOH:O	2.66	0.44
1:D:156:MET:HG3	1:D:309:LEU:HD21	2.00	0.44
1:E:50:ALA:CB	1:E:102:PHE:HD2	2.31	0.44
1:E:269:ARG:O	1:E:273:ILE:HG13	2.16	0.44
1:E:483:LEU:CD2	1:E:498:ALA:HB2	2.48	0.44
1:A:376:ALA:O	1:A:378:ALA:N	2.50	0.43
1:C:41:ASN:HD22	1:C:41:ASN:N	2.13	0.43
1:C:309:LEU:HB3	1:C:328:ALA:HB3	2.00	0.43
1:D:251:CYS:O	1:D:285:THR:HA	2.18	0.43
1:E:528:GLY:O	3:E:1841:HOH:O	2.21	0.43
1:A:430:PRO:HA	1:A:431:PRO:HD3	1.79	0.43
1:B:72:VAL:HG13	1:B:74:VAL:HG23	2.00	0.43
1:C:81:ASP:CG	3:C:1025:HOH:O	2.61	0.43
1:F:69:MET:O	1:F:70:THR:HG23	2.17	0.43
1:A:304:PRO:HB2	1:A:330:HIS:HD2	1.83	0.43
1:A:468:THR:OG1	1:A:494:PRO:HA	2.18	0.43
1:B:234:PRO:HG2	1:B:237:GLU:HB2	1.99	0.43
1:D:136:VAL:O	1:D:136:VAL:CG1	2.67	0.43
1:E:429:MET:HB3	1:E:430:PRO:HD2	2.00	0.43
1:F:39:ASN:HA	1:F:40:PRO:HD3	1.86	0.43
1:F:355:ARG:NH1	1:F:355:ARG:CB	2.81	0.43
1:A:89:ARG:O	1:A:93:GLU:HB2	2.17	0.43
1:A:255:SER:OG	1:A:258:PRO:HB2	2.18	0.43
1:F:54:LEU:HD21	1:F:125:MET:HB3	2.00	0.43
1:A:232:GLN:NE2	1:A:263:ASP:H	2.15	0.43
1:A:487:ARG:HD2	1:A:487:ARG:HA	1.81	0.43
1:B:461:TRP:CZ3	1:B:526:TYR:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASP:OD1	1:C:96:ASP:N	2.50	0.43
1:D:308:LEU:HD23	1:D:308:LEU:HA	1.89	0.43
1:E:287:ASP:N	1:E:287:ASP:OD1	2.51	0.43
1:F:489:PHE:HD1	1:F:489:PHE:H	1.65	0.43
1:C:254:PRO:HB3	1:C:438:VAL:HG21	2.01	0.43
1:D:210:ILE:N	1:D:211:PRO:CD	2.81	0.43
1:F:80:ILE:HG13	1:F:123:HIS:HB2	2.00	0.43
1:A:388:PRO:HG2	1:B:322:TRP:CD2	2.54	0.43
1:B:41:ASN:HD21	1:B:419:ARG:NH1	2.17	0.43
1:B:41:ASN:ND2	1:B:419:ARG:HH12	2.16	0.43
1:B:255:SER:OG	1:B:258:PRO:HB2	2.19	0.43
1:B:359:PRO:HG2	1:B:360:ASP:H	1.84	0.43
1:D:242:LYS:HE2	1:D:277:HIS:CD2	2.54	0.43
1:D:528:GLY:O	1:D:532:ASN:HB2	2.19	0.43
1:E:434:ASP:HB2	3:E:1778:HOH:O	2.19	0.43
1:F:215:GLN:NE2	3:F:1976:HOH:O	2.51	0.43
1:B:497:ARG:HD2	3:B:901:HOH:O	2.18	0.43
1:C:483:LEU:HD22	1:C:498:ALA:HB2	2.01	0.43
1:E:446:LEU:HD13	1:E:471:MET:CE	2.49	0.43
1:F:41:ASN:ND2	1:F:419:ARG:HH12	2.12	0.43
1:C:37:ARG:HG3	1:C:37:ARG:HH11	1.84	0.43
1:C:489:PHE:O	1:C:490:GLY:O	2.37	0.43
1:E:278:ARG:HG3	1:E:278:ARG:HH11	1.84	0.43
1:E:351:ASP:OD2	1:E:362:ARG:NH1	2.48	0.43
1:E:366:PHE:HA	1:E:369:ARG:HG3	2.00	0.43
1:F:53:ARG:HD3	1:F:100:VAL:HG23	2.01	0.43
1:F:149:ARG:HB3	1:F:168:LEU:HD11	2.01	0.43
1:B:333:ASN:ND2	1:B:336:ASP:H	2.16	0.43
1:C:308:LEU:HD23	1:C:308:LEU:HA	1.92	0.43
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.65	0.42
1:B:210:ILE:N	1:B:211:PRO:CD	2.81	0.42
1:C:172:GLU:HG2	1:C:176:ALA:CB	2.48	0.42
1:F:41:ASN:C	1:F:41:ASN:ND2	2.77	0.42
1:A:433:ARG:HD3	3:A:792:HOH:O	2.18	0.42
1:D:87:PHE:O	1:D:91:ILE:HG12	2.20	0.42
1:E:426:GLU:O	1:E:427:LEU:HD23	2.19	0.42
1:E:484:LEU:O	1:E:497:ARG:N	2.48	0.42
1:D:201:MET:CE	1:D:222:ALA:HB2	2.48	0.42
1:F:140:MET:CE	1:F:145:GLU:HA	2.49	0.42
1:F:330:HIS:ND1	1:F:332:GLN:HG2	2.34	0.42
1:F:358:LEU:HD23	1:F:358:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:459:SER:O	1:F:463:VAL:HG23	2.20	0.42
1:F:468:THR:O	1:F:472:LEU:HG	2.19	0.42
1:A:210:ILE:HD11	1:B:379:LEU:HD11	2.02	0.42
1:B:111:ARG:NH2	3:B:2145:HOH:O	2.48	0.42
1:F:137:PRO:HD2	1:F:140:MET:O	2.19	0.42
1:F:282:MET:HE3	1:F:335:PHE:HD2	1.83	0.42
1:B:286:ASP:OD2	2:B:900:PLP:N1	2.52	0.42
1:B:503:LEU:HB2	1:B:508:TYR:CZ	2.55	0.42
1:C:497:ARG:HD2	3:C:1174:HOH:O	2.18	0.42
1:E:187:LEU:HD13	1:E:353:ARG:NH2	2.34	0.42
1:E:406:ASP:HA	3:E:1698:HOH:O	2.19	0.42
1:A:404:GLU:OE1	1:E:418:ARG:HD2	2.18	0.42
1:B:489:PHE:O	1:B:490:GLY:O	2.38	0.42
1:E:21:ILE:HG12	1:E:33:LEU:HD12	2.02	0.42
1:B:365:LYS:O	1:B:369:ARG:HG3	2.20	0.42
1:B:490:GLY:C	1:B:492:ASN:N	2.75	0.42
1:C:237:GLU:OE2	1:C:240:LYS:NZ	2.45	0.42
1:C:239:ASP:C	1:C:241:LEU:N	2.77	0.42
1:C:288:VAL:HG23	1:C:312:SER:HB3	2.02	0.42
1:E:149:ARG:HB3	1:E:168:LEU:HD11	2.01	0.42
1:A:322:TRP:HB3	1:A:324:LEU:HG	2.01	0.42
1:B:271:ARG:HB2	1:B:302:ILE:CG2	2.50	0.42
1:B:333:ASN:HD21	1:B:335:PHE:HB2	1.83	0.42
1:C:423:LEU:HD21	1:C:444:ILE:HD11	2.01	0.42
1:D:257:PRO:HB2	1:D:497:ARG:CD	2.50	0.42
1:E:254:PRO:HB3	1:E:438:VAL:HG21	2.02	0.42
1:F:362:ARG:HD3	3:F:2034:HOH:O	2.20	0.42
1:A:398:LEU:HB3	1:A:402:MET:HE2	2.01	0.42
1:D:208:ILE:O	1:D:211:PRO:HG2	2.20	0.42
1:D:271:ARG:HH11	1:D:302:ILE:HG23	1.84	0.42
1:D:454:TYR:HB2	1:D:458:PHE:CD2	2.55	0.42
1:D:490:GLY:C	1:D:492:ASN:N	2.78	0.42
1:E:226:ASP:CG	1:E:228:SER:HB3	2.44	0.42
1:F:32:MET:O	1:F:484:LEU:HD21	2.19	0.42
1:F:201:MET:HA	1:F:202:PRO:C	2.45	0.42
1:F:216:TYR:O	1:F:217:ALA:HB3	2.20	0.42
1:F:239:ASP:C	1:F:241:LEU:N	2.78	0.42
1:F:344:GLU:CD	1:F:362:ARG:HH22	2.27	0.42
1:A:460:GLU:O	1:A:464:LYS:HG2	2.20	0.41
1:B:41:ASN:ND2	1:B:419:ARG:HH22	2.16	0.41
1:B:254:PRO:HD3	1:B:296:PHE:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ASP:N	1:C:287:ASP:OD1	2.53	0.41
1:C:299:LEU:HD23	1:C:299:LEU:HA	1.94	0.41
1:D:513:ARG:NH1	3:D:1536:HOH:O	2.53	0.41
1:E:156:MET:HA	1:E:156:MET:HE2	2.02	0.41
1:F:139:ARG:O	1:F:140:MET:HB2	2.20	0.41
1:E:154:ARG:NH1	3:E:1690:HOH:O	2.48	0.41
1:E:243:ASP:C	1:E:243:ASP:OD1	2.63	0.41
1:F:101:ARG:NH2	1:F:105:LYS:NZ	2.69	0.41
1:B:529:GLN:HA	1:B:529:GLN:HE21	1.83	0.41
1:C:316:TYR:OH	1:C:409:LYS:HB2	2.19	0.41
1:C:357:LEU:HA	1:C:357:LEU:HD22	1.85	0.41
1:C:457:ALA:HB3	3:C:1294:HOH:O	2.21	0.41
1:D:53:ARG:HD3	1:D:100:VAL:HG23	2.02	0.41
1:D:302:ILE:C	1:D:304:PRO:HD3	2.45	0.41
1:D:489:PHE:CD1	1:D:489:PHE:N	2.88	0.41
1:E:71:THR:O	1:E:71:THR:HG22	2.18	0.41
1:E:302:ILE:C	1:E:304:PRO:HD3	2.46	0.41
1:B:268:GLU:HB3	1:B:271:ARG:NH2	2.35	0.41
1:B:474:ARG:HG2	1:B:518:MET:HE3	2.02	0.41
1:C:459:SER:O	1:C:463:VAL:HG23	2.20	0.41
1:D:445:ASP:O	1:D:449:VAL:HG23	2.20	0.41
1:E:487:ARG:HH11	1:E:487:ARG:CG	2.33	0.41
1:E:490:GLY:C	1:E:492:ASN:H	2.28	0.41
1:F:320:THR:O	1:F:323:ARG:HD2	2.19	0.41
1:F:410:HIS:O	1:F:414:GLN:HB2	2.21	0.41
1:B:231:TRP:CZ3	1:B:488:GLY:HA3	2.55	0.41
1:C:41:ASN:HD21	1:C:419:ARG:NH2	2.17	0.41
1:C:227:PRO:HG2	1:C:489:PHE:CB	2.45	0.41
1:D:333:ASN:ND2	1:D:335:PHE:N	2.66	0.41
1:A:26:SER:O	1:A:30:ARG:HG3	2.21	0.41
1:B:308:LEU:HG	1:B:335:PHE:CE1	2.55	0.41
1:B:323:ARG:HA	1:B:323:ARG:HH11	1.85	0.41
1:C:490:GLY:C	1:C:492:ASN:N	2.79	0.41
1:D:156:MET:HG3	1:D:309:LEU:CD2	2.51	0.41
1:D:435:GLU:HG2	3:D:1447:HOH:O	2.20	0.41
1:F:161:ILE:CD1	1:F:304:PRO:HB3	2.50	0.41
1:F:333:ASN:ND2	1:F:335:PHE:HB2	2.35	0.41
1:B:39:ASN:HA	1:B:40:PRO:HD3	1.90	0.41
1:C:144:SER:O	1:C:148:VAL:HG23	2.21	0.41
1:C:161:ILE:HD11	1:C:304:PRO:HB3	2.02	0.41
1:D:124:GLU:OE2	1:D:143:ILE:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:PHE:CD1	1:D:284:LEU:HD23	2.56	0.41
1:E:297:GLN:HE21	1:E:302:ILE:HD11	1.82	0.41
1:E:372:ALA:HA	1:E:380:ASN:HD22	1.86	0.41
1:A:268:GLU:OE2	1:A:271:ARG:NH2	2.51	0.41
1:B:19:GLU:HA	1:B:22:LYS:CG	2.49	0.41
1:B:41:ASN:C	1:B:41:ASN:ND2	2.78	0.41
1:B:188:ASN:HB3	1:B:339:LEU:HD21	2.02	0.41
1:D:201:MET:HE2	1:D:222:ALA:HB2	2.03	0.41
1:E:303:CYS:N	1:E:304:PRO:HD3	2.36	0.41
1:E:342:LEU:HD22	1:E:346:GLU:OE1	2.21	0.41
1:F:274:VAL:HA	1:F:278:ARG:O	2.20	0.41
1:F:348:VAL:O	1:F:351:ASP:HB2	2.20	0.41
1:A:41:ASN:ND2	1:A:41:ASN:C	2.79	0.41
1:A:172:GLU:CD	1:A:172:GLU:H	2.28	0.41
1:B:58:ALA:CB	1:B:126:VAL:HG13	2.51	0.41
1:C:135:PRO:HD2	3:C:1083:HOH:O	2.21	0.41
1:E:41:ASN:C	1:E:41:ASN:HD22	2.28	0.41
1:F:32:MET:O	1:F:36:GLY:HA2	2.21	0.41
1:F:395:LEU:HD23	1:F:395:LEU:HA	1.88	0.41
1:F:530:ALA:C	1:F:532:ASN:H	2.28	0.41
1:A:449:VAL:O	1:A:453:LEU:HG	2.21	0.41
1:A:489:PHE:HD2	1:A:489:PHE:H	1.68	0.41
1:C:201:MET:HA	1:C:202:PRO:C	2.46	0.41
1:C:430:PRO:HA	1:C:431:PRO:HD3	1.86	0.41
1:C:471:MET:CG	1:C:518:MET:HE1	2.45	0.41
1:D:428:GLY:C	1:D:429:MET:HG2	2.45	0.41
1:E:203:VAL:HG22	1:E:204:PHE:N	2.35	0.41
1:F:448:ASP:O	1:F:452:LYS:HG3	2.21	0.41
1:B:172:GLU:CD	1:B:172:GLU:N	2.76	0.40
1:A:481:ILE:HD13	1:A:503:LEU:CD1	2.51	0.40
1:B:40:PRO:HB3	1:B:42:PHE:CZ	2.57	0.40
1:C:89:ARG:O	1:C:93:GLU:HG2	2.21	0.40
1:D:43:LEU:HB2	1:D:48:ARG:NH1	2.37	0.40
1:E:458:PHE:CE1	1:E:523:TYR:HA	2.57	0.40
1:F:12:SER:HB3	1:F:15:GLU:HB2	2.03	0.40
1:A:22:LYS:C	1:A:24:ALA:N	2.75	0.40
1:C:333:ASN:HD22	1:C:333:ASN:C	2.30	0.40
1:C:372:ALA:CA	1:C:380:ASN:HD22	2.31	0.40
1:D:418:ARG:CD	1:F:404:GLU:OE1	2.64	0.40
1:F:308:LEU:HG	1:F:335:PHE:CE1	2.56	0.40
1:F:503:LEU:HB2	1:F:508:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ILE:HD13	1:B:91:ILE:HA	1.90	0.40
1:D:252:VAL:O	1:D:255:SER:HA	2.21	0.40
1:E:35:ALA:O	1:E:37:ARG:HG3	2.21	0.40

All (1) 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)
1:C:425:ARG:NH2	3:E:1708:HOH:O[4_566]	2.17	0.03

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%)	484 (95%)	19 (4%)	5 (1%)	12	24
1	B	513/546 (94%)	485 (94%)	25 (5%)	3 (1%)	21	38
1	C	514/546 (94%)	491 (96%)	18 (4%)	5 (1%)	12	24
1	D	512/546 (94%)	484 (94%)	24 (5%)	4 (1%)	16	31
1	E	510/546 (93%)	479 (94%)	27 (5%)	4 (1%)	16	31
1	F	521/546 (95%)	487 (94%)	28 (5%)	6 (1%)	10	20
All	All	3078/3276 (94%)	2910 (94%)	141 (5%)	27 (1%)	14	27

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	SER
1	B	491	SER
1	C	491	SER
1	D	491	SER
1	D	534	LYS

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Mol	Chain	Res	Type
1	E	491	SER
1	F	491	SER
1	A	490	GLY
1	B	376	ALA
1	B	490	GLY
1	C	490	GLY
1	D	490	GLY
1	E	490	GLY
1	F	490	GLY
1	A	376	ALA
1	C	492	ASN
1	C	16	LEU
1	C	376	ALA
1	F	13	PRO
1	F	159	ASP
1	A	377	VAL
1	D	359	PRO
1	E	377	VAL
1	A	359	PRO
1	E	359	PRO
1	F	21	ILE
1	F	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	424/455 (93%)	412 (97%)	12 (3%)	38	66
1	B	429/455 (94%)	418 (97%)	11 (3%)	40	68
1	C	430/455 (94%)	415 (96%)	15 (4%)	32	58
1	D	427/455 (94%)	416 (97%)	11 (3%)	40	68
1	E	426/455 (94%)	412 (97%)	14 (3%)	33	61
1	F	436/455 (96%)	421 (97%)	15 (3%)	32	60
All	All	2572/2730 (94%)	2494 (97%)	78 (3%)	36	64

All (78) 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	172	GLU
1	A	192	LYS
1	A	204	PHE
1	A	205	THR
1	A	208	ILE
1	A	269	ARG
1	A	305	GLU
1	A	309	LEU
1	A	489	PHE
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	163	SER
1	B	172	GLU
1	B	204	PHE
1	B	470	ASP
1	B	489	PHE
1	C	30	ARG
1	C	41	ASN
1	C	53	ARG
1	C	69	MET
1	C	72	VAL
1	C	79	LYS
1	C	95	ARG
1	C	154	ARG
1	C	172	GLU
1	C	204	PHE
1	C	264	GLN
1	C	332	GLN
1	C	333	ASN
1	C	357	LEU
1	C	489	PHE
1	D	41	ASN
1	D	43	LEU
1	D	53	ARG
1	D	71	THR

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Mol	Chain	Res	Type
1	D	81	ASP
1	D	159	ASP
1	D	165	SER
1	D	172	GLU
1	D	201	MET
1	D	204	PHE
1	D	489	PHE
1	E	41	ASN
1	E	53	ARG
1	E	164	GLU
1	E	172	GLU
1	E	204	PHE
1	E	259	SER
1	E	264	GLN
1	E	305	GLU
1	E	357	LEU
1	E	414	GLN
1	E	425	ARG
1	E	456	GLU
1	E	487	ARG
1	E	489	PHE
1	F	41	ASN
1	F	53	ARG
1	F	81	ASP
1	F	93	GLU
1	F	164	GLU
1	F	172	GLU
1	F	204	PHE
1	F	205	THR
1	F	268	GLU
1	F	305	GLU
1	F	333	ASN
1	F	456	GLU
1	F	470	ASP
1	F	474	ARG
1	F	489	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	41	ASN

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Mol	Chain	Res	Type
1	A	150	GLN
1	A	232	GLN
1	A	277	HIS
1	A	333	ASN
1	A	352	HIS
1	A	380	ASN
1	A	389	GLN
1	A	392	GLN
1	A	447	GLN
1	A	492	ASN
1	B	34	ASN
1	B	41	ASN
1	B	97	GLN
1	B	224	ASN
1	B	232	GLN
1	B	306	ASN
1	B	333	ASN
1	B	352	HIS
1	B	380	ASN
1	B	414	GLN
1	B	447	GLN
1	B	504	ASN
1	B	529	GLN
1	C	34	ASN
1	C	41	ASN
1	C	142	ASN
1	C	167	ASN
1	C	215	GLN
1	C	224	ASN
1	C	232	GLN
1	C	264	GLN
1	C	272	ASN
1	C	277	HIS
1	C	306	ASN
1	C	333	ASN
1	C	380	ASN
1	C	436	ASN
1	C	447	GLN
1	C	504	ASN
1	D	34	ASN
1	D	39	ASN
1	D	41	ASN

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Mol	Chain	Res	Type
1	D	133	ASN
1	D	142	ASN
1	D	224	ASN
1	D	230	ASN
1	D	232	GLN
1	D	277	HIS
1	D	332	GLN
1	D	333	ASN
1	D	380	ASN
1	D	504	ASN
1	E	34	ASN
1	E	41	ASN
1	E	142	ASN
1	E	150	GLN
1	E	232	GLN
1	E	264	GLN
1	E	297	GLN
1	E	306	ASN
1	E	332	GLN
1	E	333	ASN
1	E	381	HIS
1	E	447	GLN
1	E	504	ASN
1	F	34	ASN
1	F	41	ASN
1	F	142	ASN
1	F	224	ASN
1	F	232	GLN
1	F	297	GLN
1	F	306	ASN
1	F	332	GLN
1	F	333	ASN
1	F	380	ASN
1	F	410	HIS
1	F	447	GLN
1	F	504	ASN
1	F	532	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	900	1	15,15,16	2.25	6 (40%)	21,22,23	1.38	2 (9%)
2	PLP	A	900	1	15,15,16	2.44	5 (33%)	21,22,23	1.70	3 (14%)
2	PLP	C	900	1	15,15,16	2.21	5 (33%)	21,22,23	1.81	5 (23%)
2	PLP	B	900	1	15,15,16	1.80	4 (26%)	21,22,23	1.60	2 (9%)
2	PLP	D	900	1	15,15,16	2.39	7 (46%)	21,22,23	1.63	2 (9%)
2	PLP	F	900	1	15,15,16	1.53	3 (20%)	21,22,23	1.20	2 (9%)

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

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	PLP	C2A-C2	6.14	1.60	1.50
2	A	900	PLP	C2A-C2	5.51	1.59	1.50
2	C	900	PLP	C2A-C2	5.20	1.58	1.50
2	D	900	PLP	C2-N1	4.33	1.41	1.33
2	A	900	PLP	C5A-C5	4.10	1.61	1.50
2	A	900	PLP	C3-C2	-3.78	1.37	1.41
2	D	900	PLP	C5-C4	3.60	1.44	1.40
2	C	900	PLP	O4P-C5A	3.54	1.57	1.44
2	D	900	PLP	O4P-C5A	3.42	1.57	1.44
2	D	900	PLP	C5A-C5	3.36	1.59	1.50
2	B	900	PLP	C4A-C4	3.07	1.57	1.51
2	C	900	PLP	C5A-C5	3.04	1.58	1.50
2	B	900	PLP	O4P-C5A	3.03	1.56	1.44
2	A	900	PLP	O4P-C5A	2.99	1.55	1.44
2	C	900	PLP	C3-C2	-2.95	1.37	1.41
2	F	900	PLP	C4A-C4	2.93	1.57	1.51
2	B	900	PLP	P-O3P	-2.86	1.44	1.54
2	F	900	PLP	O4P-C5A	2.75	1.55	1.44
2	E	900	PLP	C4A-C4	2.74	1.57	1.51
2	D	900	PLP	C6-N1	2.73	1.40	1.34
2	E	900	PLP	O4P-C5A	2.72	1.54	1.44
2	E	900	PLP	C5A-C5	2.67	1.57	1.50
2	D	900	PLP	P-O3P	-2.49	1.45	1.54
2	D	900	PLP	C4A-C4	2.47	1.56	1.51
2	B	900	PLP	C6-N1	2.45	1.39	1.34
2	E	900	PLP	C2-N1	2.21	1.37	1.33
2	C	900	PLP	P-O3P	-2.21	1.46	1.54
2	A	900	PLP	C4A-C4	2.11	1.55	1.51
2	F	900	PLP	C3-C2	-2.08	1.38	1.41
2	E	900	PLP	C5-C4	2.06	1.42	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	PLP	O4P-C5A-C5	6.12	120.83	109.36
2	D	900	PLP	O4P-C5A-C5	5.73	120.09	109.36
2	A	900	PLP	O4P-C5A-C5	5.66	119.96	109.36
2	C	900	PLP	O4P-C5A-C5	5.22	119.14	109.36
2	E	900	PLP	O4P-C5A-C5	3.81	116.50	109.36
2	F	900	PLP	O4P-C5A-C5	3.71	116.30	109.36
2	C	900	PLP	C2A-C2-C3	2.92	124.22	120.80
2	C	900	PLP	C5A-C5-C6	-2.60	115.13	119.36
2	E	900	PLP	O3P-P-O1P	2.51	120.61	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	PLP	O3P-P-O1P	2.43	120.31	110.83
2	B	900	PLP	C5A-C5-C6	-2.17	115.83	119.36
2	A	900	PLP	C5A-C5-C6	-2.13	115.89	119.36
2	D	900	PLP	C5A-C5-C6	-2.12	115.91	119.36
2	C	900	PLP	C6-N1-C2	2.11	123.03	119.20
2	F	900	PLP	O3P-P-O1P	2.05	118.81	110.83
2	C	900	PLP	C5-C6-N1	-2.01	120.56	123.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	PLP	C6-C5-C5A-O4P
2	E	900	PLP	C6-C5-C5A-O4P
2	F	900	PLP	C6-C5-C5A-O4P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.28	11 (2%) 62 58	14, 34, 77, 110	0
1	B	515/546 (94%)	-0.45	4 (0%) 82 80	10, 31, 70, 105	0
1	C	516/546 (94%)	-0.43	5 (0%) 79 76	13, 33, 65, 120	0
1	D	514/546 (94%)	-0.36	8 (1%) 70 67	14, 34, 71, 115	0
1	E	512/546 (93%)	-0.08	11 (2%) 63 59	16, 41, 76, 110	0
1	F	523/546 (95%)	-0.24	13 (2%) 58 54	16, 35, 70, 118	0
All	All	3090/3276 (94%)	-0.31	52 (1%) 69 65	10, 34, 74, 120	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	PHE	4.4
1	A	214	ALA	4.2
1	E	490	GLY	4.2
1	F	23	ILE	4.1
1	D	535	LEU	4.0
1	A	213	LEU	4.0
1	A	490	GLY	3.9
1	A	20	LEU	3.6
1	B	16	LEU	3.4
1	E	489	PHE	3.2
1	F	462	ALA	3.2
1	C	489	PHE	3.1
1	C	16	LEU	3.0
1	E	71	THR	3.0
1	C	14	PHE	2.9
1	A	23	ILE	2.9
1	A	217	ALA	2.8
1	F	11	LEU	2.8
1	D	23	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	20	LEU	2.8
1	F	533	LEU	2.8
1	B	528	GLY	2.7
1	F	20	LEU	2.7
1	E	528	GLY	2.6
1	C	17	LYS	2.6
1	F	21	ILE	2.6
1	A	193	ALA	2.6
1	C	490	GLY	2.6
1	D	28	GLY	2.6
1	D	533	LEU	2.6
1	F	17	LYS	2.6
1	E	487	ARG	2.5
1	F	16	LEU	2.5
1	D	213	LEU	2.5
1	D	214	ALA	2.5
1	A	210	ILE	2.5
1	A	211	PRO	2.4
1	B	490	GLY	2.4
1	E	21	ILE	2.3
1	A	216	TYR	2.3
1	F	489	PHE	2.3
1	E	208	ILE	2.3
1	E	193	ALA	2.2
1	F	14	PHE	2.2
1	F	357	LEU	2.2
1	D	208	ILE	2.2
1	E	488	GLY	2.2
1	E	526	TYR	2.2
1	A	215	GLN	2.1
1	D	72	VAL	2.1
1	F	221	VAL	2.0
1	F	214	ALA	2.0

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(Å ²)	Q<0.9
2	PLP	A	900	15/16	0.97	0.07	24,32,35,35	0
2	PLP	B	900	15/16	0.97	0.07	26,28,30,31	0
2	PLP	E	900	15/16	0.97	0.07	25,37,39,39	0
2	PLP	F	900	15/16	0.97	0.06	26,30,32,32	0
2	PLP	C	900	15/16	0.98	0.06	23,25,29,31	0
2	PLP	D	900	15/16	0.98	0.05	25,28,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.