



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:13 PM UTC

PDB ID : 2VYC / pdb_00002vyc
Title : Crystal Structure of Acid Induced Arginine Decarboxylase from E. coli
Authors : Andrell, J.; Hicks, M.G.; Palmer, T.; Carpenter, E.P.; Iwata, S.; Maher, M.J.
Deposited on : 2008-07-22
Resolution : 2.40 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

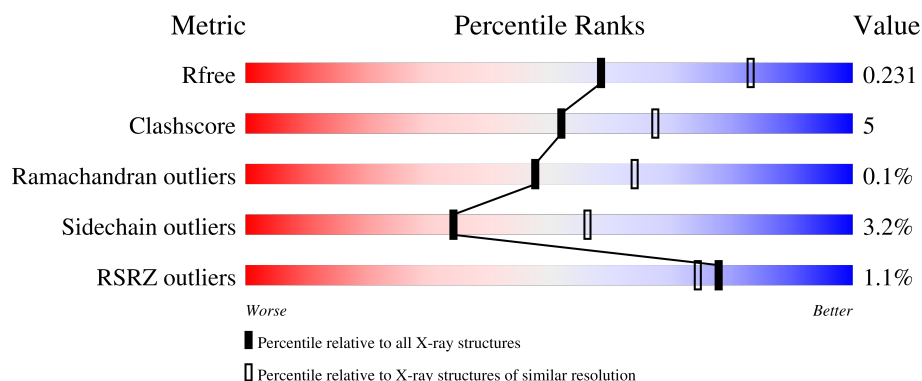
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	755	% 86% 12% .
1	B	755	% 90% 10% .
1	C	755	% 84% 15% .
1	D	755	% 89% 10% .
1	E	755	% 90% 10% .

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Mol	Chain	Length	Quality of chain
1	F	755	% 86%14%•
1	G	755	% 86%13%•
1	H	755	% 87%12%•
1	I	755	% 87%12%
1	J	755	% 87%13%•

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 62902 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 BIODEGRADATIVE ARGININE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	12	0
			6008	3800	1029	1141	38			
1	B	755	Total	C	N	O	S	0	13	0
			6016	3807	1029	1142	38			
1	C	755	Total	C	N	O	S	0	12	0
			6008	3800	1029	1141	38			
1	D	755	Total	C	N	O	S	0	13	0
			6015	3804	1032	1141	38			
1	E	755	Total	C	N	O	S	0	15	0
			6028	3814	1033	1143	38			
1	F	755	Total	C	N	O	S	0	13	0
			6016	3807	1029	1142	38			
1	G	755	Total	C	N	O	S	0	13	0
			6016	3807	1029	1142	38			
1	H	755	Total	C	N	O	S	0	16	0
			6036	3819	1037	1142	38			
1	I	755	Total	C	N	O	S	0	14	0
			6021	3810	1030	1143	38			
1	J	755	Total	C	N	O	S	0	13	0
			6016	3807	1029	1142	38			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	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	299	Total	O	0	0
			299	299		
3	B	253	Total	O	0	0
			253	253		

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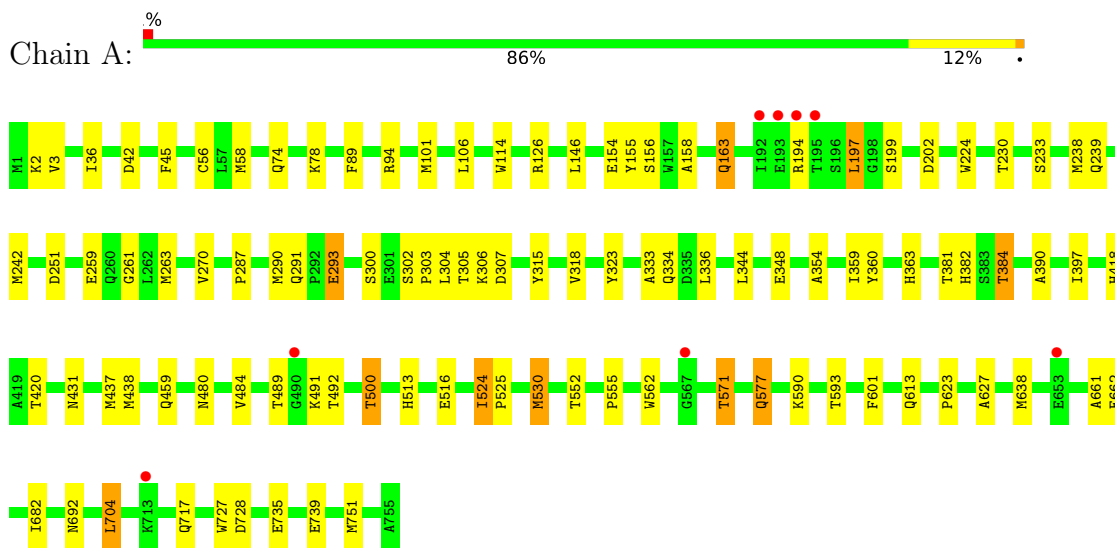
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	219	Total 219	O 219	0	0
3	D	266	Total 266	O 266	0	0
3	E	258	Total 258	O 258	0	0
3	F	268	Total 268	O 268	0	0
3	G	237	Total 237	O 237	0	0
3	H	272	Total 272	O 272	0	0
3	I	262	Total 262	O 262	0	0
3	J	238	Total 238	O 238	0	0

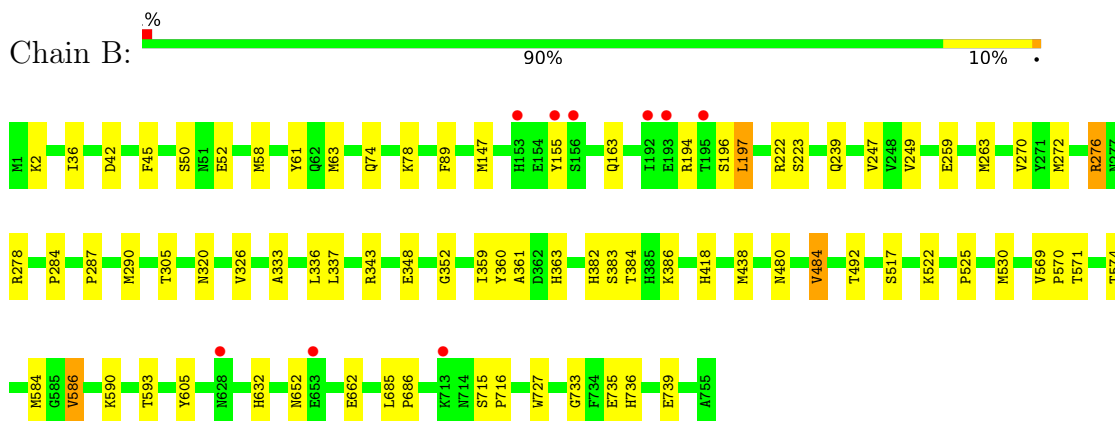
3 Residue-property plots

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

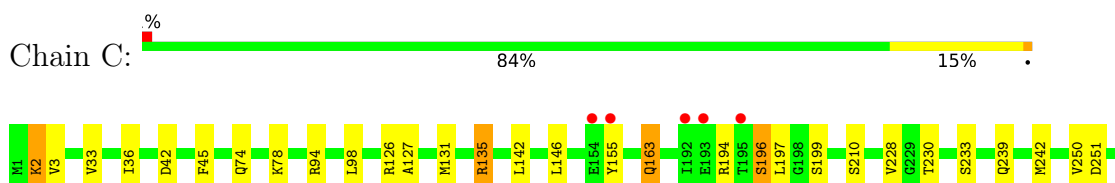
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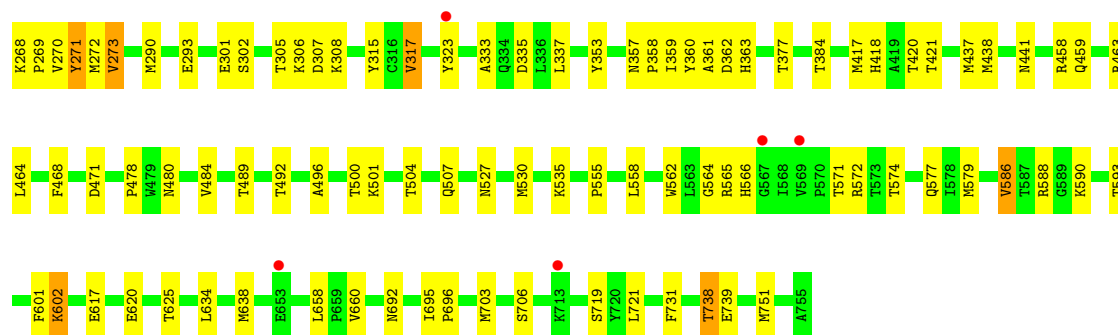


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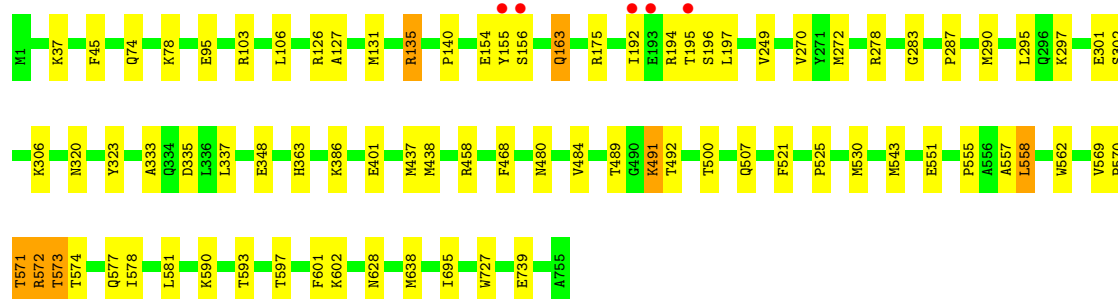
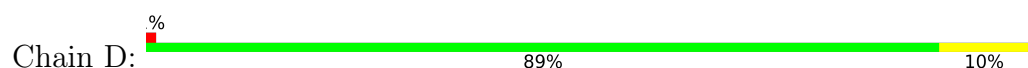


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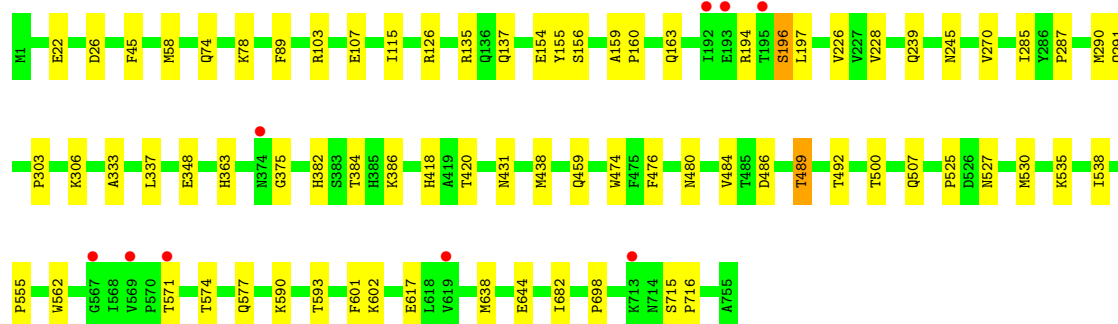
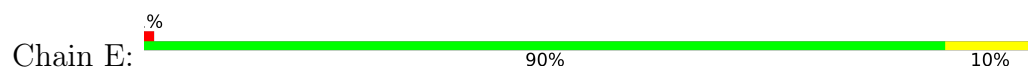




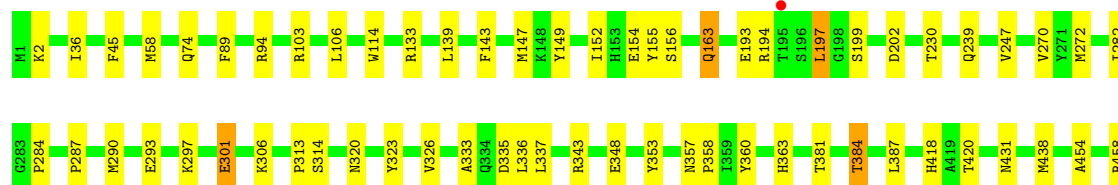
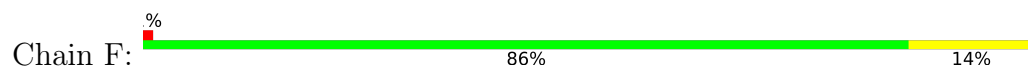
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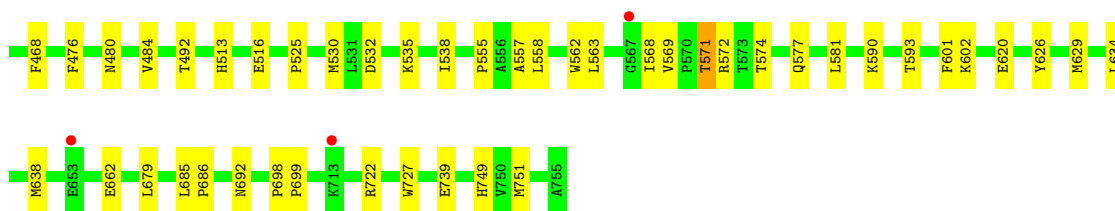


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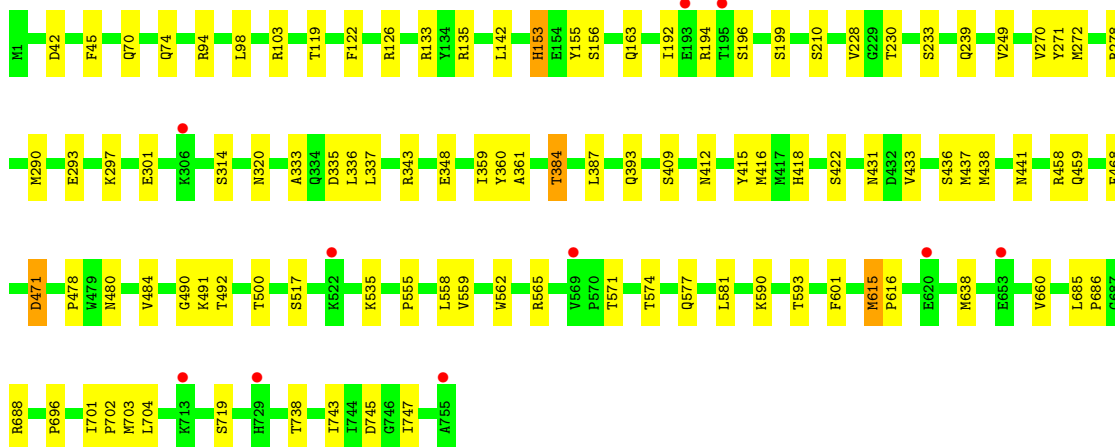
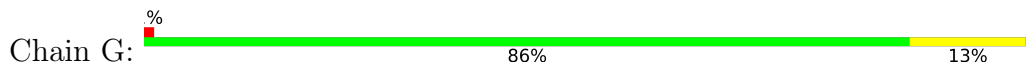


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

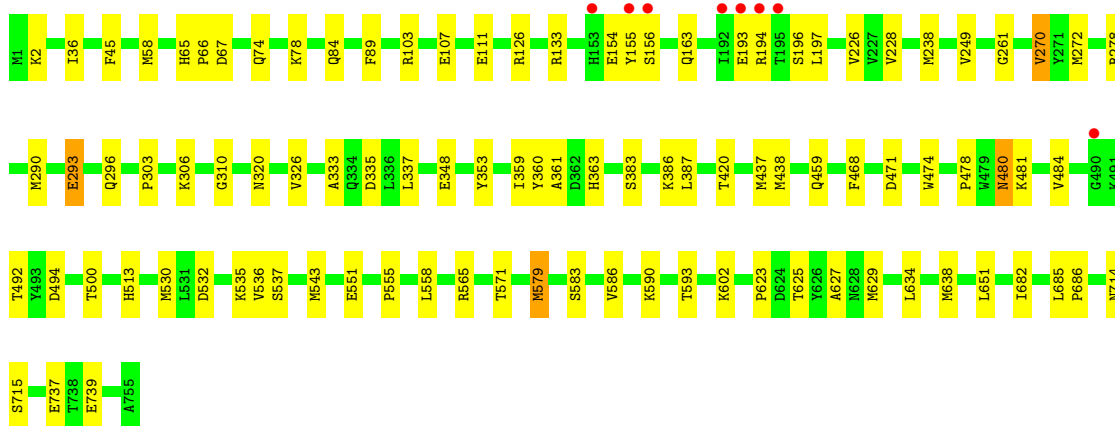
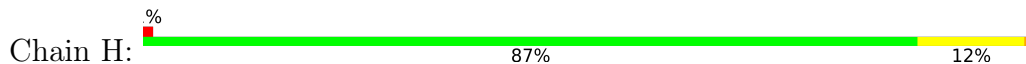




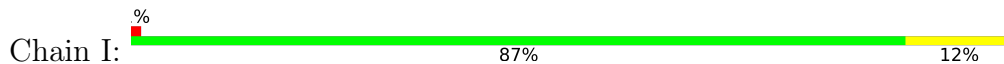
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

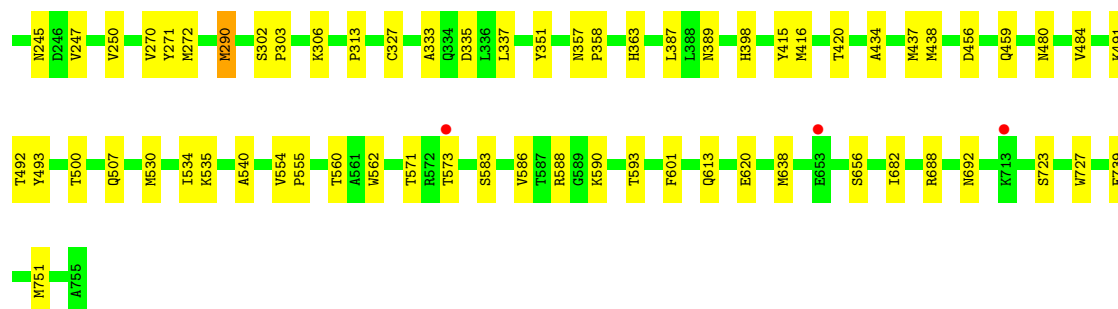


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

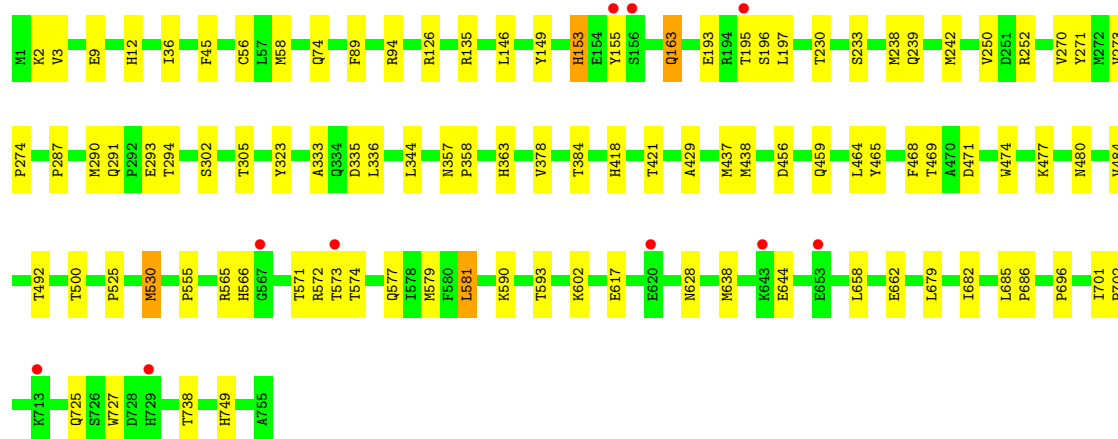
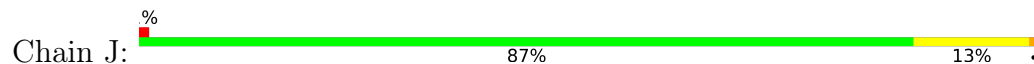


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE





● Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	197.65Å 197.65Å 450.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.40) 99.9 (50.00-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.229 0.180 , 0.231	Depositor DCC
R_{free} test set	19417 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	62902	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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	0.72	0/6211	0.92	3/8438 (0.0%)
1	B	0.76	1/6224 (0.0%)	0.93	3/8456 (0.0%)
1	C	0.72	0/6211	0.93	5/8438 (0.1%)
1	D	0.77	0/6222	0.94	3/8452 (0.0%)
1	E	0.75	0/6244	0.94	8/8482 (0.1%)
1	F	0.75	0/6224	0.92	2/8456 (0.0%)
1	G	0.71	0/6224	0.93	8/8456 (0.1%)
1	H	0.80	1/6257 (0.0%)	0.93	6/8499 (0.1%)
1	I	0.77	0/6233	0.94	4/8468 (0.0%)
1	J	0.69	0/6224	0.91	1/8456 (0.0%)
All	All	0.74	2/62274 (0.0%)	0.93	43/84601 (0.1%)

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	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	VAL	CA-CB	6.08	1.60	1.54
1	H	326	VAL	CA-CB	5.91	1.60	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	N-CA-C	7.86	119.47	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	194	ARG	N-CA-C	7.35	119.08	111.14
1	C	489	THR	N-CA-C	-6.96	101.56	110.19
1	H	536	VAL	N-CA-C	6.87	117.66	107.15
1	E	194	ARG	N-CA-C	6.29	118.13	111.28
1	G	194	ARG	N-CA-C	6.26	118.11	111.28
1	E	489	THR	N-CA-C	-6.12	101.90	110.35
1	I	197	LEU	N-CA-C	5.99	118.77	111.82
1	E	375	GLY	CA-C-N	-5.77	114.81	120.52
1	E	375	GLY	C-N-CA	-5.77	114.81	120.52
1	B	194	ARG	N-CA-C	5.71	117.59	111.36
1	E	682	ILE	N-CA-C	5.70	116.35	110.36
1	H	270	VAL	N-CA-C	-5.64	99.67	108.81
1	C	317	VAL	N-CA-C	5.55	116.11	108.12
1	D	194	ARG	N-CA-C	5.53	117.31	111.28
1	E	291	GLN	CA-C-N	5.52	124.98	119.24
1	E	291	GLN	C-N-CA	5.52	124.98	119.24
1	A	354	ALA	N-CA-C	5.51	118.00	111.33
1	J	153	HIS	N-CA-C	5.47	118.16	109.96
1	I	682	ILE	N-CA-C	5.45	116.08	110.36
1	I	351	TYR	N-CA-CB	-5.45	105.25	111.79
1	G	490	GLY	N-CA-C	-5.41	107.64	115.27
1	B	484	VAL	CB-CA-C	5.40	119.14	110.82
1	F	197	LEU	N-CA-C	5.36	117.87	111.71
1	B	197	LEU	N-CA-C	5.33	117.17	111.36
1	F	194	ARG	N-CA-C	5.32	117.49	111.11
1	G	393	GLN	CB-CA-C	5.25	115.03	109.83
1	C	271	TYR	N-CA-C	5.25	117.46	108.90
1	A	682	ILE	N-CA-C	5.25	115.87	110.36
1	E	285	ILE	N-CA-C	-5.21	102.79	109.30
1	H	84	GLN	CA-C-N	-5.20	114.33	122.65
1	H	84	GLN	C-N-CA	-5.20	114.33	122.65
1	H	682	ILE	N-CA-C	5.20	116.55	110.62
1	G	271	TYR	N-CA-C	5.19	117.42	109.07
1	I	84	GLN	N-CA-C	5.18	117.59	111.33
1	D	140	PRO	CA-C-N	5.13	124.75	119.05
1	D	140	PRO	C-N-CA	5.13	124.75	119.05
1	G	441	ASN	N-CA-C	5.11	116.84	111.28
1	C	441	ASN	N-CA-C	5.08	117.48	111.33
1	C	273	VAL	N-CA-C	5.07	112.88	107.76
1	G	153	HIS	N-CA-C	5.06	117.55	109.96
1	G	615	MET	CA-C-N	5.04	124.83	119.28
1	G	615	MET	C-N-CA	5.04	124.83	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	193	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6008	0	5762	59	0
1	B	6016	0	5767	47	0
1	C	6008	0	5762	87	0
1	D	6015	0	5771	58	0
1	E	6028	0	5780	45	0
1	F	6016	0	5767	76	0
1	G	6016	0	5767	65	0
1	H	6036	0	5788	71	0
1	I	6021	0	5771	60	0
1	J	6016	0	5767	62	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
2	C	15	0	6	0	0
2	D	15	0	6	1	0
2	E	15	0	6	1	0
2	F	15	0	6	0	0
2	G	15	0	6	0	0
2	H	15	0	6	1	0
2	I	15	0	6	0	0
2	J	15	0	6	0	0
3	A	299	0	0	3	0
3	B	253	0	0	3	0
3	C	219	0	0	3	0
3	D	266	0	0	5	0
3	E	258	0	0	4	0
3	F	268	0	0	6	0
3	G	237	0	0	2	0
3	H	272	0	0	1	0
3	I	262	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	238	0	0	3	0
All	All	62902	0	57762	602	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (602) 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:J:155:TYR:O	1:J:163:GLN:NE2	1.78	1.15
1:C:135[A]:ARG:HG2	1:C:135[A]:ARG:HH11	1.16	1.11
1:H:272:MET:HE1	1:H:337:LEU:HD21	1.34	1.09
1:C:272:MET:HE1	1:C:337:LEU:HD21	1.34	1.08
1:I:272:MET:HE1	1:I:337:LEU:HD21	1.33	1.08
1:I:135[A]:ARG:HH11	1:I:135[A]:ARG:HG2	1.19	1.05
1:D:638:MET:HE3	1:D:727:TRP:HH2	1.22	0.99
1:E:384:THR:HG21	1:E:431:ASN:OD1	1.63	0.98
1:G:272:MET:HE1	1:G:337:LEU:HD21	1.46	0.97
1:J:135[B]:ARG:HG2	1:J:135[B]:ARG:HH11	1.29	0.97
1:H:272:MET:HE1	1:H:337:LEU:CD2	1.97	0.94
1:D:638:MET:HE3	1:D:727:TRP:CH2	2.03	0.93
1:F:155:TYR:O	1:F:163:GLN:NE2	2.03	0.92
1:B:239:GLN:HG3	1:B:418:HIS:NE2	1.85	0.92
1:C:458:ARG:HH11	1:C:480:ASN:HD22	1.08	0.91
1:F:272:MET:HE1	1:F:337:LEU:HD21	1.52	0.91
1:F:384:THR:HG21	1:F:431:ASN:OD1	1.67	0.91
1:B:290:MET:HE3	1:B:337:LEU:HG	1.51	0.90
1:G:45[A]:PHE:CE1	1:G:74[A]:GLN:HG2	2.07	0.90
1:J:590:LYS:O	1:J:593:THR:HG22	1.71	0.90
1:J:323[A]:TYR:OH	1:J:571:THR:HB	1.70	0.89
1:D:290:MET:HE3	1:D:337:LEU:HG	1.55	0.89
1:H:155:TYR:C	1:H:163:GLN:HE22	1.82	0.88
1:A:155:TYR:O	1:A:163:GLN:NE2	2.09	0.86
1:H:290:MET:HE3	1:H:337:LEU:HG	1.57	0.85
1:C:290:MET:HE3	1:C:337:LEU:HG	1.56	0.85
1:B:360:TYR:HA	1:B:530:MET:HE1	1.57	0.85
1:G:384:THR:HG21	1:G:431:ASN:OD1	1.76	0.84
1:C:459:GLN:OE1	1:C:500:THR:HG22	1.77	0.84
1:F:272:MET:HE1	1:F:337:LEU:CD2	2.07	0.84
1:A:239:GLN:HG3	1:A:418:HIS:NE2	1.93	0.84
1:C:45[A]:PHE:CE1	1:C:74[A]:GLN:HG2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:239:GLN:HG3	1:G:418:HIS:NE2	1.93	0.83
1:B:272:MET:HE1	1:B:337:LEU:HD21	1.61	0.82
1:B:155:TYR:O	1:B:163:GLN:HG2	1.78	0.82
1:C:2:LYS:HD3	1:C:36:ILE:HD11	1.59	0.82
1:C:590:LYS:O	1:C:593:THR:HG22	1.79	0.81
1:G:458:ARG:HH11	1:G:480:ASN:HD22	1.26	0.81
1:I:507:GLN:CD	1:I:530:MET:HE1	2.05	0.81
1:J:323[A]:TYR:CE2	1:J:572:ARG:HB2	2.16	0.81
1:G:459:GLN:OE1	1:G:500:THR:HG22	1.81	0.81
1:C:135[B]:ARG:HH11	1:C:135[B]:ARG:HG2	1.46	0.80
1:F:638:MET:HE3	1:F:727:TRP:HH2	1.46	0.80
1:D:155:TYR:O	1:D:163:GLN:NE2	2.15	0.80
1:C:272:MET:HE1	1:C:337:LEU:CD2	2.11	0.80
1:F:290:MET:HE3	1:F:337:LEU:HG	1.64	0.80
1:A:638:MET:HE3	1:A:727:TRP:HH2	1.47	0.80
1:B:590:LYS:HD3	1:C:126:ARG:HD3	1.64	0.79
1:I:272:MET:HE1	1:I:337:LEU:CD2	2.12	0.79
1:I:507:GLN:CG	1:I:530:MET:HE1	2.13	0.79
1:A:360:TYR:HA	1:A:530:MET:HE1	1.66	0.78
1:G:278:ARG:NH2	1:G:517:SER:O	2.15	0.78
1:E:156:SER:HA	1:E:163:GLN:HE22	1.47	0.78
1:E:155:TYR:O	1:E:163:GLN:NE2	2.16	0.78
1:F:638:MET:HE3	1:F:727:TRP:CH2	2.18	0.78
1:C:155:TYR:O	1:C:163:GLN:NE2	2.17	0.78
1:F:133[B]:ARG:HD3	3:F:2077:HOH:O	1.84	0.78
1:H:65:HIS:CD2	1:H:67:ASP:H	2.03	0.77
1:D:363:HIS:CG	1:D:530:MET:HE3	2.20	0.77
1:C:135[A]:ARG:HG2	1:C:135[A]:ARG:NH1	1.95	0.77
1:B:259:GLU:HG2	1:B:263:MET:HE2	1.65	0.77
1:F:239:GLN:HG3	1:F:418:HIS:NE2	2.00	0.76
1:H:65:HIS:HD2	1:H:67:ASP:H	1.33	0.76
1:D:45[A]:PHE:CE1	1:D:74[A]:GLN:HG2	2.21	0.76
1:A:290:MET:HE1	1:A:333:ALA:HA	1.68	0.75
1:E:290:MET:HE3	1:E:337:LEU:HG	1.69	0.75
1:G:272:MET:HE1	1:G:337:LEU:CD2	2.17	0.75
1:B:249:VAL:HG11	1:B:272:MET:HE3	1.70	0.74
1:E:45[A]:PHE:CE1	1:E:74[A]:GLN:HG2	2.22	0.74
1:C:458:ARG:NH1	1:C:480:ASN:HD22	1.86	0.73
1:E:239:GLN:HG3	1:E:418:HIS:NE2	2.02	0.73
1:B:574:THR:HB	3:B:2228:HOH:O	1.88	0.73
1:I:135[A]:ARG:HG2	1:I:135[A]:ARG:NH1	1.94	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:TYR:OH	1:C:571:THR:HB	1.88	0.72
1:E:290:MET:HE1	1:E:333:ALA:HA	1.70	0.72
1:J:239:GLN:HG3	1:J:418:HIS:NE2	2.04	0.72
1:D:126:ARG:HD2	3:D:2057:HOH:O	1.90	0.72
1:C:468:PHE:CZ	1:D:103:ARG:HD3	2.25	0.72
1:H:590:LYS:HD2	1:I:126:ARG:HD3	1.71	0.72
1:E:156:SER:HA	1:E:163:GLN:NE2	2.05	0.71
1:I:507:GLN:HG3	1:I:530:MET:HE1	1.72	0.71
1:E:474:TRP:O	1:E:602:LYS:HE2	1.89	0.71
1:C:135[A]:ARG:HH11	1:C:135[A]:ARG:CG	1.99	0.71
1:B:45[A]:PHE:CE1	1:B:74[A]:GLN:HG2	2.26	0.71
1:J:45[A]:PHE:CE1	1:J:74[A]:GLN:HG2	2.24	0.71
1:C:146:LEU:HD23	1:C:197:LEU:HD21	1.72	0.71
1:E:590:LYS:O	1:E:593:THR:HG22	1.91	0.71
1:F:360:TYR:HA	1:F:530:MET:HE1	1.73	0.71
1:B:2:LYS:HD3	1:B:36:ILE:HD11	1.73	0.70
1:H:590:LYS:O	1:H:593:THR:HG22	1.91	0.70
1:H:459:GLN:OE1	1:H:500:THR:HG22	1.90	0.70
1:F:149:TYR:HE2	1:F:193:GLU:HG3	1.55	0.69
1:I:290:MET:HE1	1:I:333:ALA:HA	1.74	0.69
1:A:638:MET:HE3	1:A:727:TRP:CH2	2.27	0.69
1:D:154:GLU:OE2	1:D:156:SER:HB2	1.92	0.69
1:J:682:ILE:HG21	1:J:725:GLN:HE22	1.57	0.69
1:A:323:TYR:OH	1:A:571:THR:HB	1.93	0.68
1:I:590:LYS:O	1:I:593:THR:HG22	1.92	0.68
1:B:239:GLN:CG	1:B:418:HIS:NE2	2.56	0.68
1:I:555:PRO:HB2	1:I:638:MET:HE2	1.75	0.68
1:G:468:PHE:CZ	1:H:103:ARG:HD3	2.28	0.68
1:B:272:MET:HE1	1:B:337:LEU:CD2	2.22	0.68
1:B:590:LYS:O	1:B:593:THR:HG22	1.94	0.68
1:H:555:PRO:HG2	1:H:638:MET:HE2	1.75	0.68
1:H:155:TYR:C	1:H:163:GLN:NE2	2.52	0.67
1:A:293:GLU:CD	1:A:293:GLU:H	2.03	0.67
1:G:45[A]:PHE:CE1	1:G:74[A]:GLN:CG	2.78	0.67
1:D:458:ARG:HH11	1:D:480:ASN:HD22	1.42	0.67
1:A:291:GLN:HB3	1:A:293:GLU:OE2	1.94	0.67
1:D:37:LYS:HE2	3:D:2002:HOH:O	1.94	0.66
1:D:272:MET:HE1	1:D:337:LEU:CD2	2.26	0.66
1:F:323[B]:TYR:HD2	3:F:2154:HOH:O	1.77	0.66
1:E:126:ARG:HD2	3:E:2054:HOH:O	1.95	0.66
1:F:323[A]:TYR:OH	1:F:571:THR:HB	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:437:MET:C	1:G:438:MET:HE2	2.19	0.66
1:G:45[A]:PHE:CD1	1:G:74[A]:GLN:HG2	2.30	0.66
1:G:590:LYS:HD3	1:H:126:ARG:HD3	1.78	0.65
1:J:135[B]:ARG:HG2	1:J:135[B]:ARG:NH1	2.07	0.65
1:G:574:THR:OG1	1:G:577:GLN:HB3	1.96	0.65
1:H:303:PRO:HA	1:H:306:LYS:HE2	1.78	0.65
1:C:302:SER:O	1:C:306:LYS:HG3	1.97	0.64
1:J:230:THR:HA	1:J:233:SER:HB2	1.80	0.64
1:F:557:ALA:HB3	1:F:638:MET:HE1	1.78	0.64
1:H:2:LYS:HD3	1:H:36:ILE:HD11	1.79	0.64
1:H:363:HIS:CG	1:H:530:MET:HE3	2.32	0.64
1:F:58:MET:HG2	1:F:89:PHE:HB2	1.78	0.64
1:H:363:HIS:CG	1:H:530:MET:CE	2.81	0.64
1:C:478:PRO:HB2	1:C:480:ASN:ND2	2.12	0.64
1:E:438:MET:HE3	3:E:2186:HOH:O	1.98	0.64
1:C:2:LYS:HD3	1:C:36:ILE:CD1	2.26	0.63
1:E:507:GLN:NE2	1:E:530:MET:HE1	2.13	0.63
1:G:290:MET:HE3	1:G:337:LEU:HG	1.80	0.63
1:H:126:ARG:HD2	3:H:2053:HOH:O	1.98	0.63
1:J:149:TYR:HE2	1:J:193:GLU:HG3	1.63	0.63
1:I:459:GLN:OE1	1:I:500:THR:HG22	1.99	0.63
1:F:438:MET:HE3	3:F:2177:HOH:O	1.99	0.63
1:I:155:TYR:O	1:I:163:GLN:HG2	1.99	0.63
1:I:387:LEU:CD1	1:I:535:LYS:HE3	2.28	0.63
1:D:272:MET:HE1	1:D:337:LEU:HD21	1.79	0.63
1:A:45[A]:PHE:CE1	1:A:74[A]:GLN:HG2	2.34	0.62
1:G:290:MET:HE1	1:G:333:ALA:HA	1.81	0.62
1:J:363:HIS:CG	1:J:530:MET:HE3	2.33	0.62
1:F:363:HIS:CB	1:F:530:MET:HE2	2.30	0.62
1:D:249:VAL:HG11	1:D:272:MET:HE3	1.82	0.62
1:A:692:ASN:HD22	1:A:751:MET:HE2	1.65	0.61
1:B:247:VAL:HG22	1:B:305:THR:HG22	1.82	0.61
1:A:555:PRO:HB2	1:A:638:MET:HE2	1.82	0.61
1:G:590:LYS:CD	1:H:126:ARG:HD3	2.31	0.61
1:I:555:PRO:CB	1:I:638:MET:HE2	2.30	0.61
1:F:287:PRO:HD2	1:F:525:PRO:HG2	1.82	0.61
1:I:692:ASN:HD22	1:I:751:MET:HE2	1.66	0.61
1:E:617:GLU:H	1:E:617:GLU:CD	2.09	0.60
1:I:438:MET:HE3	3:I:2190:HOH:O	2.01	0.60
1:F:555:PRO:HB2	1:F:638:MET:HE2	1.82	0.60
1:I:389:ASN:O	1:I:434:ALA:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:468:PHE:CZ	1:G:103:ARG:HD3	2.36	0.60
1:A:126:ARG:HD2	3:A:2069:HOH:O	2.02	0.59
1:E:303:PRO:HA	1:E:306:LYS:HE3	1.84	0.59
1:E:459:GLN:OE1	1:E:500:THR:HG22	2.02	0.59
1:F:679:LEU:HD22	1:F:749:HIS:HB3	1.83	0.59
1:J:474:TRP:O	1:J:602:LYS:HE2	2.01	0.59
1:I:149:TYR:HE2	1:I:193:GLU:HG3	1.68	0.59
1:A:290:MET:HE2	1:A:336:LEU:HD12	1.84	0.59
1:D:555:PRO:CB	1:D:638:MET:HE2	2.32	0.59
1:F:574:THR:OG1	1:F:577:GLN:HB3	2.03	0.59
1:D:302:SER:O	1:D:306:LYS:HG3	2.02	0.59
1:D:571:THR:HG21	1:D:581:LEU:HB2	1.83	0.59
1:B:438:MET:HE1	1:B:584:MET:SD	2.43	0.58
1:B:287:PRO:HD2	1:B:525:PRO:HG2	1.84	0.58
1:C:272:MET:CE	1:C:290:MET:HG2	2.33	0.58
1:I:588[A]:ARG:NH2	3:I:2236:HOH:O	2.35	0.58
1:F:590:LYS:CD	1:G:126:ARG:HD3	2.33	0.58
1:C:590:LYS:HD2	1:D:126:ARG:HD3	1.86	0.58
1:F:199:SER:HB3	1:F:202:ASP:HB2	1.86	0.58
1:H:481:LYS:NZ	1:H:513:HIS:CD2	2.72	0.57
1:C:507:GLN:HE21	1:C:530:MET:HE1	1.69	0.57
1:E:363:HIS:CG	1:E:530:MET:HE3	2.40	0.57
1:J:290:MET:HE1	1:J:333:ALA:HA	1.86	0.57
1:F:272:MET:CE	1:F:337:LEU:HD21	2.32	0.57
1:B:276:ARG:NH1	1:B:652:ASN:OD1	2.38	0.57
1:J:45[A]:PHE:HE1	1:J:74[A]:GLN:HG2	1.66	0.57
1:D:572:ARG:HG3	1:D:573:THR:H	1.70	0.57
1:F:154:GLU:OE2	1:F:156:SER:HB2	2.05	0.57
1:F:323[A]:TYR:CE2	1:F:572:ARG:HB2	2.39	0.57
1:A:303:PRO:HA	1:A:306:LYS:HE3	1.87	0.56
1:A:590:LYS:O	1:A:593:THR:HG22	2.05	0.56
1:D:363:HIS:CG	1:D:530:MET:CE	2.89	0.56
1:G:249:VAL:HG11	1:G:272:MET:HE3	1.87	0.56
1:C:45[A]:PHE:HE1	1:C:74[A]:GLN:HG2	1.68	0.56
1:H:363:HIS:CE1	1:H:530:MET:HE2	2.39	0.56
1:G:94[A]:ARG:HH11	1:G:98:LEU:HD12	1.70	0.56
1:I:507:GLN:HG3	1:I:530:MET:CE	2.36	0.56
1:D:574:THR:OG1	1:D:577:GLN:HB3	2.06	0.56
1:J:126:ARG:HD2	3:J:2056:HOH:O	2.05	0.56
1:F:363:HIS:CG	1:F:530:MET:HE2	2.40	0.56
1:C:45[A]:PHE:CE1	1:C:74[A]:GLN:CG	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:MET:HE2	1:C:290:MET:HG2	1.87	0.55
1:C:290:MET:HE1	1:C:333:ALA:HA	1.88	0.55
1:C:588:ARG:HG2	1:C:588:ARG:HH11	1.71	0.55
1:J:574:THR:HB	3:J:2211:HOH:O	2.05	0.55
1:C:272:MET:HE2	1:C:290:MET:HA	1.88	0.55
1:E:574:THR:OG1	1:E:577:GLN:HB3	2.07	0.55
1:G:42:ASP:HA	1:G:45[B]:PHE:CD2	2.41	0.55
1:A:239:GLN:HG2	3:A:2134:HOH:O	2.07	0.55
1:A:623:PRO:O	1:A:627:ALA:HB2	2.06	0.55
1:I:507:GLN:CG	1:I:530:MET:CE	2.83	0.55
1:C:692:ASN:HD22	1:C:751:MET:HE2	1.69	0.55
1:C:478:PRO:HB2	1:C:480:ASN:HD21	1.72	0.55
1:F:468:PHE:CE2	1:F:602:LYS:HE2	2.42	0.55
1:J:323[A]:TYR:HE2	1:J:572:ARG:HB2	1.66	0.55
1:D:272:MET:HE2	1:D:295:LEU:HD21	1.88	0.54
1:F:45[A]:PHE:CE1	1:F:74[A]:GLN:HG2	2.42	0.54
1:C:135[B]:ARG:HG2	1:C:135[B]:ARG:NH1	2.16	0.54
1:C:302:SER:HB3	1:C:305:THR:OG1	2.08	0.54
1:D:45[A]:PHE:HE1	1:D:74[A]:GLN:HG2	1.72	0.54
1:C:437:MET:C	1:C:438:MET:HE2	2.32	0.54
1:H:555:PRO:HB2	1:H:638:MET:CE	2.38	0.54
1:B:363:HIS:CD2	1:B:530:MET:HG2	2.42	0.54
1:C:507:GLN:NE2	1:C:530:MET:HE1	2.23	0.54
1:C:230:THR:HA	1:C:233:SER:HB2	1.88	0.54
1:C:363:HIS:CG	1:C:530:MET:HE3	2.43	0.54
1:C:696:PRO:HA	1:C:738:THR:HG23	1.90	0.54
1:H:634:LEU:O	1:H:638:MET:HG3	2.08	0.54
1:B:278:ARG:NH2	1:B:517:SER:O	2.40	0.54
1:H:583:SER:H	1:H:586:VAL:HG23	1.73	0.54
1:C:458:ARG:HH11	1:C:480:ASN:ND2	1.92	0.53
1:E:226:VAL:HG12	1:E:228:VAL:H	1.73	0.53
1:G:590:LYS:O	1:G:593:THR:HG22	2.08	0.53
1:A:230:THR:HG23	1:A:381:THR:HB	1.90	0.53
1:F:590:LYS:HD2	1:G:126:ARG:HD3	1.89	0.53
1:E:287:PRO:HD2	1:E:525:PRO:HG2	1.89	0.53
1:E:574:THR:HB	3:E:2232:HOH:O	2.09	0.53
1:H:290:MET:HE1	1:H:333:ALA:HA	1.90	0.53
1:A:224:TRP:HB2	1:A:397:ILE:HB	1.90	0.53
1:D:437:MET:C	1:D:438:MET:HE2	2.33	0.53
1:D:468:PHE:CZ	1:E:103:ARG:HD3	2.43	0.53
1:H:272:MET:CE	1:H:337:LEU:HD21	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:VAL:HG22	1:A:56:CYS:HB3	1.91	0.53
1:A:146:LEU:HD23	1:A:197:LEU:HD21	1.91	0.53
1:B:383:SER:CB	1:B:386:LYS:HD2	2.39	0.53
1:J:468:PHE:CE2	1:J:602:LYS:HE3	2.44	0.53
1:A:363:HIS:CG	1:A:530:MET:HE3	2.44	0.53
1:E:22[A]:GLU:OE2	1:E:26[A]:ASP:OD1	2.28	0.52
1:A:242:MET:HE1	1:A:315:TYR:CD2	2.44	0.52
1:F:722:ARG:NH1	3:F:2266:HOH:O	2.42	0.52
1:H:65:HIS:CD2	1:H:66:PRO:HD2	2.45	0.52
1:C:468:PHE:CE2	1:C:602:LYS:HE3	2.45	0.52
1:H:555:PRO:HG2	1:H:638:MET:CE	2.40	0.52
1:B:438:MET:HE3	3:B:2181:HOH:O	2.09	0.51
1:A:739:GLU:HG2	3:A:2144:HOH:O	2.10	0.51
1:F:555:PRO:CB	1:F:638:MET:HE2	2.40	0.51
1:G:412:ASN:ND2	1:G:416:MET:HE3	2.25	0.51
1:I:555:PRO:HB2	1:I:638:MET:CE	2.40	0.51
1:G:230:THR:HA	1:G:233:SER:HB2	1.93	0.51
1:G:685:LEU:N	1:G:686:PRO:HD2	2.25	0.51
1:J:287:PRO:HD2	1:J:525:PRO:HG2	1.92	0.51
1:C:562:TRP:CD1	1:C:601:PHE:HB2	2.46	0.51
1:G:468:PHE:CE2	1:H:103:ARG:HD3	2.45	0.51
1:J:696:PRO:HA	1:J:738:THR:HG23	1.93	0.51
1:B:605:TYR:O	1:B:632:HIS:HB2	2.10	0.51
1:G:239:GLN:HG2	3:G:2117:HOH:O	2.10	0.51
1:I:216[A]:ARG:HG2	1:I:216[A]:ARG:HH11	1.76	0.51
1:I:363:HIS:CE1	1:I:530:MET:HE3	2.45	0.51
1:A:302:SER:HB3	1:A:305:THR:OG1	2.11	0.51
1:H:278:ARG:HG3	1:H:543:MET:HG2	1.93	0.51
1:I:272:MET:HE2	1:I:290:MET:HA	1.92	0.51
1:I:290:MET:HE3	1:I:337:LEU:HG	1.92	0.51
1:C:239:GLN:HG3	1:C:418:HIS:NE2	2.26	0.50
1:E:555:PRO:HG2	1:E:638:MET:HE2	1.92	0.50
1:A:363:HIS:CG	1:A:530:MET:CE	2.94	0.50
1:G:45[A]:PHE:HE1	1:G:74[A]:GLN:HG2	1.69	0.50
1:A:239:GLN:CG	1:A:418:HIS:NE2	2.71	0.50
1:C:323:TYR:CE2	1:C:572:ARG:HB2	2.47	0.50
1:F:133[B]:ARG:HH21	1:J:566:HIS:HD2	1.59	0.50
1:F:149:TYR:CE2	1:F:193:GLU:HG3	2.43	0.50
1:D:507:GLN:NE2	1:D:530:MET:HE1	2.27	0.50
1:E:386:LYS:NZ	2:E:1386:PLP:O3	2.45	0.50
1:B:290:MET:HE3	1:B:337:LEU:CG	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:PRO:HB2	1:C:638:MET:CE	2.42	0.50
1:G:471:ASP:O	1:G:471:ASP:CG	2.55	0.50
1:A:199:SER:HB3	1:A:202:ASP:HB2	1.92	0.50
1:A:384:THR:HG21	1:A:431:ASN:OD1	2.11	0.50
1:C:3:VAL:HG23	1:C:33:VAL:HG11	1.92	0.49
1:F:133[B]:ARG:NH2	1:J:566:HIS:HD2	2.10	0.49
1:B:50:SER:C	1:B:52:GLU:H	2.20	0.49
1:H:155:TYR:HB3	1:H:163:GLN:HE21	1.77	0.49
1:G:360:TYR:O	1:G:361:ALA:C	2.53	0.49
1:J:638:MET:HE3	1:J:727:TRP:CH2	2.48	0.49
1:G:192:ILE:HD11	1:G:199:SER:HB2	1.95	0.49
1:C:463:ARG:HG3	1:C:496:ALA:HB1	1.94	0.49
1:E:574:THR:HG22	1:E:698:PRO:HB3	1.94	0.49
1:G:478:PRO:HB2	1:G:480:ASN:ND2	2.27	0.49
1:H:45[A]:PHE:CE1	1:H:74[A]:GLN:NE2	2.80	0.49
1:I:387:LEU:HD11	1:I:535:LYS:HE3	1.94	0.49
1:H:383:SER:HB2	1:H:386:LYS:HD2	1.94	0.49
1:I:220:ALA:HB2	1:I:398:HIS:HB3	1.94	0.49
1:I:250:VAL:O	1:I:271:TYR:HA	2.13	0.49
1:C:135[A]:ARG:NH1	1:C:135[A]:ARG:CG	2.67	0.49
1:E:135[B]:ARG:HG2	1:E:135[B]:ARG:HH11	1.77	0.49
1:G:320:ASN:O	1:G:348:GLU:HA	2.12	0.49
1:A:94[A]:ARG:HG3	1:A:114:TRP:CE2	2.47	0.48
1:D:272:MET:CE	1:D:295:LEU:HD21	2.42	0.48
1:D:320:ASN:O	1:D:348:GLU:HA	2.13	0.48
1:F:282:ILE:HD11	1:F:699:PRO:HB2	1.95	0.48
1:I:21:VAL:HG12	1:I:37:LYS:HE2	1.95	0.48
1:J:363:HIS:CD2	1:J:530:MET:HG2	2.48	0.48
1:D:590:LYS:HD3	1:E:126:ARG:HD3	1.94	0.48
1:F:230:THR:HG23	1:F:381:THR:HB	1.95	0.48
1:E:507:GLN:HE21	1:E:530:MET:HE1	1.75	0.48
1:D:557:ALA:HB3	1:D:638:MET:HE1	1.96	0.48
1:I:534:ILE:HG13	1:I:535:LYS:HD3	1.95	0.48
1:A:42:ASP:HA	1:A:45[B]:PHE:CD2	2.49	0.48
1:A:251:ASP:HB2	1:A:318:VAL:HA	1.96	0.48
1:D:695:ILE:HD12	1:D:739:GLU:HG2	1.96	0.48
1:H:363:HIS:ND1	1:H:530:MET:HE2	2.28	0.48
1:E:290:MET:HE1	1:E:333:ALA:CA	2.43	0.48
1:I:290:MET:HE1	1:I:333:ALA:CA	2.42	0.48
1:C:555:PRO:HB2	1:C:638:MET:HE2	1.96	0.48
1:J:153:HIS:HE1	1:J:193:GLU:OE2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:MET:HG2	1:B:89:PHE:HB2	1.96	0.47
1:B:352:GLY:HA2	1:B:382:HIS:CD2	2.48	0.47
1:B:383:SER:HB2	1:B:386:LYS:HD2	1.95	0.47
1:A:437:MET:C	1:A:438:MET:HE2	2.40	0.47
1:C:42:ASP:HA	1:C:45[B]:PHE:CD2	2.49	0.47
1:E:58:MET:HG2	1:E:89:PHE:HB2	1.95	0.47
1:G:559:VAL:O	1:G:562:TRP:HB3	2.14	0.47
1:E:555:PRO:HB2	1:E:638:MET:CE	2.45	0.47
1:F:685:LEU:N	1:F:686:PRO:CD	2.77	0.47
1:G:555:PRO:HB2	1:G:638:MET:HE3	1.96	0.47
1:H:278:ARG:O	1:H:543:MET:HE3	2.14	0.47
1:I:194:ARG:NH1	1:I:202:ASP:OD2	2.47	0.47
1:J:302:SER:HB3	1:J:305:THR:OG1	2.15	0.47
1:F:45[A]:PHE:HD2	3:G:2068:HOH:O	1.96	0.47
1:G:562:TRP:CD1	1:G:601:PHE:HB2	2.49	0.47
1:I:456:ASP:OD1	1:J:94[A]:ARG:NH1	2.48	0.47
1:I:583:SER:H	1:I:586:VAL:HG23	1.80	0.47
1:F:290:MET:HE1	1:F:333:ALA:HA	1.97	0.47
1:F:626:TYR:O	1:F:629:MET:HB2	2.14	0.47
1:F:574:THR:HG22	1:F:698:PRO:HB3	1.96	0.47
1:H:238:MET:SD	1:H:261:GLY:HA3	2.55	0.47
1:H:320:ASN:O	1:H:348:GLU:HA	2.15	0.47
1:I:302:SER:O	1:I:306:LYS:HG3	2.15	0.47
1:A:156:SER:HA	1:A:163:GLN:HE22	1.80	0.47
1:C:273:VAL:HG22	1:C:658:LEU:HD21	1.97	0.47
1:C:438:MET:HE3	3:C:2161:HOH:O	2.14	0.47
1:J:685:LEU:N	1:J:686:PRO:CD	2.78	0.47
1:C:417:MET:HE2	1:C:417:MET:HB2	1.89	0.47
1:F:139:LEU:CD1	1:F:147:MET:HE1	2.44	0.47
1:F:468:PHE:CE2	1:G:103:ARG:HD3	2.50	0.47
1:D:574:THR:HB	3:D:2230:HOH:O	2.15	0.46
1:F:574:THR:HB	3:F:2241:HOH:O	2.13	0.46
1:B:363:HIS:CG	1:B:530:MET:HE2	2.50	0.46
1:I:230:THR:HA	1:I:233:SER:HB2	1.97	0.46
1:B:727:TRP:CD1	1:B:736:HIS:CD2	3.03	0.46
1:F:139:LEU:HD13	1:F:147:MET:HE1	1.96	0.46
1:G:156:SER:HA	1:G:163:GLN:NE2	2.30	0.46
1:G:696:PRO:HA	1:G:738:THR:HG23	1.96	0.46
1:H:163:GLN:HE21	1:H:163:GLN:HA	1.80	0.46
1:J:579:MET:HE1	1:J:581:LEU:HD12	1.97	0.46
1:E:476:PHE:HB3	1:E:538:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:THR:OG1	1:C:577:GLN:HB3	2.16	0.46
1:J:565:ARG:NH1	1:J:617:GLU:OE1	2.43	0.46
1:J:146:LEU:HD12	1:J:429:ALA:HB2	1.97	0.46
1:I:437:MET:C	1:I:438:MET:HE2	2.40	0.46
1:A:489:THR:HG21	1:A:491:LYS:HB2	1.98	0.46
1:H:353:TYR:OH	1:H:532:ASP:OD2	2.28	0.46
1:C:590:LYS:CD	1:D:126:ARG:HD3	2.46	0.46
1:E:363:HIS:CG	1:E:530:MET:CE	2.98	0.46
1:G:228:VAL:HG12	1:G:228:VAL:O	2.16	0.46
1:G:293:GLU:CD	1:G:293:GLU:H	2.24	0.46
1:H:45[A]:PHE:CE1	1:H:74[A]:GLN:HG2	2.51	0.46
1:B:363:HIS:ND1	1:B:530:MET:HE2	2.31	0.46
1:F:106:LEU:HD11	1:J:464:LEU:HD11	1.98	0.46
1:J:555:PRO:HB2	1:J:638:MET:HE2	1.97	0.46
1:A:304:LEU:HD11	1:A:661:ALA:HB1	1.98	0.45
1:D:249:VAL:CG1	1:D:272:MET:HE3	2.45	0.45
1:H:363:HIS:CG	1:H:530:MET:HE2	2.51	0.45
1:J:638:MET:HE3	1:J:727:TRP:HH2	1.81	0.45
1:A:58:MET:HG2	1:A:89:PHE:HB2	1.99	0.45
1:A:334:GLN:HG3	1:A:344:LEU:HD12	1.96	0.45
1:I:228:VAL:O	1:I:228:VAL:HG12	2.16	0.45
1:E:507:GLN:NE2	1:E:530:MET:CE	2.80	0.45
1:I:2:LYS:HD3	1:I:36:ILE:HD11	1.97	0.45
1:B:287:PRO:HB3	1:B:336:LEU:HD11	1.98	0.45
1:G:433:VAL:O	1:G:436:SER:HB3	2.16	0.45
1:H:154:GLU:OE2	1:H:156:SER:HB2	2.15	0.45
1:C:572:ARG:NH1	3:C:2196:HOH:O	2.49	0.45
1:D:562:TRP:CD1	1:D:601:PHE:HB2	2.52	0.45
1:I:126:ARG:HD2	3:I:2060:HOH:O	2.16	0.45
1:C:228:VAL:HG12	1:C:228:VAL:O	2.16	0.45
1:G:593:THR:HB	1:H:111:GLU:OE2	2.17	0.45
1:H:474:TRP:CZ2	1:H:602:LYS:HG2	2.51	0.45
1:J:252:ARG:HB3	1:J:274:PRO:HD3	1.99	0.45
1:F:297:LYS:HG2	1:F:301:GLU:OE2	2.17	0.45
1:C:464:LEU:HD11	1:D:106:LEU:HD11	1.99	0.45
1:D:468:PHE:CE2	1:E:103:ARG:HD3	2.52	0.45
1:D:558:LEU:HD12	1:D:558:LEU:HA	1.73	0.45
1:E:562:TRP:CD1	1:E:601:PHE:HB2	2.52	0.45
1:H:387:LEU:CD1	1:H:535:LYS:HE2	2.47	0.44
1:J:437:MET:C	1:J:438:MET:HE2	2.42	0.44
1:D:283:GLY:HA3	1:D:521:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:590:LYS:O	1:F:593:THR:HG22	2.17	0.44
1:H:623:PRO:O	1:H:627:ALA:HB2	2.16	0.44
1:C:703:MET:HE1	1:C:721:LEU:HG	2.00	0.44
1:D:154:GLU:OE2	1:D:156:SER:CB	2.64	0.44
1:F:94[A]:ARG:NH1	1:J:456:ASP:OD1	2.51	0.44
1:G:142:LEU:HB2	1:G:210:SER:HB2	1.98	0.44
1:F:247:VAL:O	1:F:313:PRO:HA	2.18	0.44
1:H:156:SER:HA	1:H:163:GLN:OE1	2.17	0.44
1:A:101:MET:SD	1:A:106:LEU:HD21	2.57	0.44
1:C:360:TYR:O	1:C:361:ALA:C	2.60	0.44
1:H:360:TYR:O	1:H:361:ALA:C	2.61	0.44
1:J:291:GLN:HB2	1:J:294:THR:OG1	2.17	0.44
1:J:679:LEU:HD22	1:J:749:HIS:HB3	1.98	0.44
1:D:135[A]:ARG:HD2	3:D:2078:HOH:O	2.16	0.44
1:D:577:GLN:HG2	1:D:578:ILE:N	2.31	0.44
1:F:476:PHE:HB3	1:F:538:ILE:CG2	2.48	0.44
1:F:513:HIS:HB2	1:F:516:GLU:CD	2.43	0.44
1:B:284:PRO:HD3	1:B:326:VAL:HG11	2.00	0.44
1:C:306:LYS:C	1:C:308:LYS:H	2.25	0.44
1:F:284:PRO:HD3	1:F:326:VAL:HG11	2.00	0.44
1:H:228:VAL:HG12	1:H:228:VAL:O	2.18	0.44
1:H:437:MET:C	1:H:438:MET:HE2	2.43	0.44
1:F:692:ASN:HD22	1:F:751:MET:HE2	1.83	0.44
1:G:290:MET:HE1	1:G:333:ALA:CA	2.47	0.44
1:G:615:MET:N	1:G:616:PRO:HD3	2.33	0.44
1:J:572:ARG:NH1	3:J:2209:HOH:O	2.51	0.44
1:D:290:MET:HE3	1:D:337:LEU:CG	2.39	0.44
1:E:115:ILE:O	1:E:115:ILE:HG13	2.17	0.44
1:F:143:PHE:CZ	1:F:147:MET:HE2	2.53	0.44
1:G:555:PRO:HG2	1:G:638:MET:HE2	1.99	0.44
1:D:323:TYR:CE2	1:D:572:ARG:HB2	2.53	0.43
1:E:486:ASP:O	1:E:489:THR:O	2.36	0.43
1:G:94[A]:ARG:NH1	1:G:98:LEU:HD12	2.33	0.43
1:H:386:LYS:NZ	2:H:1386:PLP:O3	2.49	0.43
1:I:560:THR:OG1	1:I:573:THR:HG21	2.17	0.43
1:I:58:MET:HG2	1:I:89:PHE:HB2	1.98	0.43
1:I:507:GLN:OE1	1:I:530:MET:HE1	2.18	0.43
1:A:2:LYS:HD3	1:A:36:ILE:HD11	2.00	0.43
1:A:156:SER:C	1:A:158:ALA:H	2.26	0.43
1:J:2:LYS:HD3	1:J:36:ILE:HD11	1.99	0.43
1:C:695:ILE:HB	1:C:739:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:PRO:CD	1:F:525:PRO:HG2	2.47	0.43
1:F:287:PRO:HB3	1:F:336:LEU:HD11	1.98	0.43
1:J:682:ILE:HD13	1:J:725:GLN:NE2	2.34	0.43
1:B:320:ASN:O	1:B:348:GLU:HA	2.18	0.43
1:D:127:ALA:O	1:D:131:MET:HG3	2.18	0.43
1:I:201:LEU:HB3	1:I:416:MET:HE3	2.01	0.43
1:G:387:LEU:CD1	1:G:535:LYS:HE3	2.49	0.43
1:G:745:ASP:O	1:G:747:ILE:HD12	2.18	0.43
1:I:491:LYS:HD3	1:I:493:TYR:CZ	2.54	0.43
1:J:3:VAL:HG22	1:J:56:CYS:HB3	1.99	0.43
1:J:58:MET:HG2	1:J:89:PHE:HB2	2.01	0.43
1:J:357:ASN:HA	1:J:358:PRO:HD3	1.89	0.43
1:J:574:THR:OG1	1:J:577:GLN:HB3	2.18	0.43
1:D:507:GLN:HE21	1:D:530:MET:HE1	1.84	0.43
1:G:290:MET:HE2	1:G:336:LEU:HD12	1.99	0.43
1:A:384:THR:OG1	1:A:390:ALA:CB	2.66	0.43
1:C:361:ALA:O	1:C:362:ASP:HB2	2.19	0.43
1:J:9:GLU:HA	1:J:12:HIS:CD2	2.53	0.43
1:J:250:VAL:O	1:J:271:TYR:HA	2.18	0.43
1:H:468:PHE:CZ	1:I:103:ARG:HD3	2.54	0.43
1:C:127:ALA:O	1:C:131:MET:HG3	2.19	0.43
1:E:535:LYS:HE3	3:E:2140:HOH:O	2.17	0.43
1:F:563:LEU:HD22	1:F:568:ILE:HG21	2.01	0.43
1:G:297:LYS:HE3	1:G:301:GLU:OE2	2.17	0.43
1:I:540:ALA:HB1	1:I:554:VAL:O	2.19	0.43
1:I:562:TRP:CD1	1:I:601:PHE:HB2	2.54	0.43
1:B:42:ASP:HA	1:B:45[B]:PHE:CD2	2.54	0.42
1:B:61:TYR:CE2	1:B:63:MET:HE3	2.53	0.42
1:C:468:PHE:CE2	1:D:103:ARG:HD3	2.52	0.42
1:F:558:LEU:HD13	1:F:638:MET:SD	2.58	0.42
1:I:247:VAL:O	1:I:313:PRO:HA	2.19	0.42
1:C:555:PRO:HG2	1:C:638:MET:HE2	2.01	0.42
1:D:363:HIS:CE1	1:D:530:MET:HE2	2.53	0.42
1:A:45[A]:PHE:HE1	1:A:74[A]:GLN:HG2	1.81	0.42
1:A:230:THR:HA	1:A:233:SER:HB2	2.02	0.42
1:D:278:ARG:O	1:D:543:MET:HE3	2.18	0.42
1:F:94[A]:ARG:HG3	1:F:114:TRP:CE2	2.54	0.42
1:F:320:ASN:O	1:F:348:GLU:HG2	2.20	0.42
1:H:537:SER:OG	1:H:579:MET:HG3	2.19	0.42
1:H:651:LEU:HD23	1:H:651:LEU:C	2.44	0.42
1:J:459:GLN:OE1	1:J:500:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:701:ILE:HB	1:J:702:PRO:HD2	2.00	0.42
1:C:94[A]:ARG:NH1	1:C:98:LEU:HD12	2.34	0.42
1:C:251:ASP:HB2	1:C:317:VAL:O	2.18	0.42
1:C:565:ARG:NH1	1:C:617:GLU:OE2	2.52	0.42
1:H:249:VAL:HG11	1:H:272:MET:HE3	2.01	0.42
1:A:577:GLN:HE21	1:A:577:GLN:HB3	1.63	0.42
1:D:290:MET:HE1	1:D:333:ALA:HA	2.02	0.42
1:E:154:GLU:OE2	1:E:156:SER:HB2	2.18	0.42
1:F:103:ARG:HD3	1:J:468:PHE:CZ	2.54	0.42
1:F:454:ALA:O	1:F:458:ARG:HG3	2.20	0.42
1:C:638:MET:HA	1:C:731:PHE:CZ	2.54	0.42
1:D:572:ARG:HG3	1:D:573:THR:N	2.35	0.42
1:F:679:LEU:HD22	1:F:749:HIS:CB	2.50	0.42
1:H:290:MET:HE1	1:H:333:ALA:CA	2.50	0.42
1:I:638:MET:HE3	1:I:727:TRP:HH2	1.85	0.42
1:B:290:MET:HE1	1:B:333:ALA:HA	2.02	0.42
1:C:353:TYR:OH	1:C:535:LYS:NZ	2.53	0.42
1:C:459:GLN:OE1	1:C:500:THR:CG2	2.59	0.42
1:C:564:GLY:C	1:C:566:HIS:H	2.27	0.42
1:A:287:PRO:HG2	1:A:525:PRO:HG2	2.01	0.42
1:A:704:LEU:HD11	1:A:717:GLN:HG2	2.01	0.42
1:C:268:LYS:HA	1:C:269:PRO:HD3	1.88	0.42
1:F:357:ASN:HA	1:F:358:PRO:HD3	1.87	0.42
1:G:703:MET:HG2	1:G:704:LEU:HD12	2.00	0.42
1:H:226:VAL:HG12	1:H:228:VAL:H	1.84	0.42
1:B:287:PRO:CD	1:B:525:PRO:HG2	2.49	0.42
1:B:715:SER:HA	1:B:716:PRO:HD2	1.97	0.42
1:C:558:LEU:HD11	1:C:634:LEU:HD23	2.02	0.42
1:E:159:ALA:HA	1:E:160:PRO:C	2.44	0.42
1:G:119:THR:HB	1:G:122:PHE:CD2	2.55	0.42
1:I:357:ASN:HA	1:I:358:PRO:HD3	1.94	0.42
1:C:242:MET:HE1	1:C:315:TYR:CD2	2.55	0.42
1:H:296:GLN:HE22	1:H:310:GLY:H	1.68	0.42
1:A:259:GLU:HG2	1:A:263:MET:HE2	2.02	0.41
1:C:142:LEU:HB2	1:C:210:SER:HB2	2.01	0.41
1:C:357:ASN:HA	1:C:358:PRO:HD3	1.97	0.41
1:I:159:ALA:HA	1:I:160:PRO:C	2.45	0.41
1:A:348:GLU:HB2	1:A:382:HIS:CD2	2.55	0.41
1:B:685:LEU:N	1:B:686:PRO:CD	2.82	0.41
1:C:586:VAL:HG12	3:C:2199:HOH:O	2.19	0.41
1:E:715:SER:HA	1:E:716:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:555:PRO:HB2	1:G:638:MET:CE	2.50	0.41
1:H:2:LYS:HE3	1:H:2:LYS:HB2	1.85	0.41
1:H:293:GLU:CD	1:H:293:GLU:H	2.28	0.41
1:H:387:LEU:HD11	1:H:535:LYS:HE2	2.02	0.41
1:B:343:ARG:NH2	3:B:2142:HOH:O	2.51	0.41
1:J:291:GLN:HB3	1:J:293:GLU:OE2	2.21	0.41
1:A:459:GLN:OE1	1:A:500:THR:HG22	2.20	0.41
1:F:558:LEU:HD11	1:F:634:LEU:HD23	2.01	0.41
1:H:363:HIS:ND1	1:H:530:MET:CE	2.84	0.41
1:I:363:HIS:NE2	1:I:530:MET:HE3	2.35	0.41
1:A:238:MET:SD	1:A:261:GLY:HA3	2.61	0.41
1:B:155:TYR:O	1:B:163:GLN:CG	2.59	0.41
1:D:287:PRO:HD2	1:D:525:PRO:HG2	2.02	0.41
1:D:555:PRO:HB3	1:D:638:MET:HE2	2.01	0.41
1:H:478:PRO:HB2	1:H:480:ASN:OD1	2.21	0.41
1:H:555:PRO:HB2	1:H:638:MET:HE3	2.02	0.41
1:B:733:GLY:H	1:B:735:GLU:CD	2.29	0.41
1:C:239:GLN:CG	1:C:418:HIS:NE2	2.84	0.41
1:D:386:LYS:NZ	2:D:1386:PLP:O3	2.53	0.41
1:G:415:TYR:CD2	1:G:415:TYR:C	2.99	0.41
1:G:565:ARG:NH1	1:G:616:PRO:HD2	2.36	0.41
1:H:58:MET:HG2	1:H:89:PHE:HB2	2.02	0.41
1:J:469:THR:C	1:J:471:ASP:N	2.76	0.41
1:A:290:MET:HE1	1:A:333:ALA:CA	2.42	0.41
1:B:239:GLN:HG3	1:B:418:HIS:CD2	2.55	0.41
1:C:194:ARG:O	1:C:196:SER:N	2.53	0.41
1:F:535:LYS:HE2	3:F:2153:HOH:O	2.21	0.41
1:G:438:MET:HE2	1:G:438:MET:N	2.35	0.41
1:I:590:LYS:HD3	1:J:126:ARG:HD3	2.03	0.41
1:J:290:MET:HE2	1:J:336:LEU:HD12	2.03	0.41
1:J:344:LEU:O	1:J:378:VAL:HA	2.19	0.41
1:A:728:ASP:OD1	1:A:735:GLU:HA	2.20	0.41
1:D:489:THR:OG1	1:D:491:LYS:HB2	2.20	0.41
1:F:2:LYS:HD3	1:F:36:ILE:HD11	2.02	0.41
1:F:320:ASN:O	1:F:348:GLU:HA	2.21	0.41
1:G:314:SER:O	1:G:343:ARG:HD3	2.21	0.41
1:G:701:ILE:HB	1:G:702:PRO:HD2	2.02	0.41
1:H:363:HIS:CB	1:H:530:MET:HE3	2.50	0.41
1:H:555:PRO:CB	1:H:638:MET:HE3	2.50	0.41
1:H:714:ASN:O	1:H:715:SER:C	2.64	0.41
1:I:303:PRO:HA	1:I:306:LYS:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:468:PHE:CD2	1:J:602:LYS:HE3	2.55	0.41
1:A:524:ILE:HA	1:A:525:PRO:HD3	1.92	0.41
1:A:562:TRP:CD1	1:A:601:PHE:HB2	2.56	0.41
1:C:507:GLN:NE2	1:C:530:MET:CE	2.83	0.41
1:E:348:GLU:HB2	1:E:382:HIS:CD2	2.56	0.41
1:F:353:TYR:OH	1:F:535:LYS:NZ	2.53	0.41
1:F:562:TRP:CD1	1:F:601:PHE:HB2	2.56	0.41
1:H:272:MET:HE2	1:H:290:MET:HA	2.03	0.41
1:J:617:GLU:OE1	1:J:617:GLU:N	2.53	0.41
1:J:238:MET:HA	1:J:242:MET:HE3	2.02	0.40
1:J:273:VAL:HG22	1:J:658:LEU:HD21	2.02	0.40
1:C:500:THR:O	1:C:504:THR:HG23	2.20	0.40
1:D:175:ARG:NH2	3:D:2095:HOH:O	2.53	0.40
1:D:569:VAL:HG12	1:D:570:PRO:O	2.20	0.40
1:H:468:PHE:CE2	1:I:103:ARG:HD3	2.56	0.40
1:H:685:LEU:N	1:H:686:PRO:CD	2.84	0.40
1:G:558:LEU:HD12	1:G:558:LEU:HA	1.85	0.40
1:I:415:TYR:CD2	1:I:415:TYR:C	2.99	0.40
1:A:334:GLN:HG3	1:A:344:LEU:CD1	2.52	0.40
1:A:513:HIS:HB2	1:A:516:GLU:CD	2.46	0.40
1:B:386:LYS:NZ	2:B:1386:PLP:O3	2.51	0.40
1:C:323:TYR:HE2	1:C:572:ARG:HB2	1.84	0.40
1:C:588:ARG:HG2	1:C:588:ARG:NH1	2.35	0.40
1:D:297:LYS:HE2	1:D:301:GLU:OE2	2.22	0.40
1:F:314:SER:O	1:F:343:ARG:HD3	2.22	0.40
1:F:353:TYR:OH	1:F:532:ASP:OD2	2.37	0.40
1:F:387:LEU:HD11	1:F:581:LEU:HD11	2.03	0.40
1:J:465:TYR:CD1	1:J:477:LYS:HB3	2.57	0.40
1:A:154:GLU:OE2	1:A:156:SER:HB2	2.21	0.40
1:B:569:VAL:HA	1:B:570:PRO:HD2	1.97	0.40
1:C:250:VAL:O	1:C:271:TYR:HA	2.21	0.40
1:G:153:HIS:HD2	1:G:155:TYR:CE1	2.40	0.40
1:G:387:LEU:HD11	1:G:581:LEU:HD11	2.03	0.40
1:I:94:ARG:HG3	1:I:114:TRP:CE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	765/755 (101%)	735 (96%)	30 (4%)	0	100	100
1	B	766/755 (102%)	742 (97%)	22 (3%)	2 (0%)	36	50
1	C	765/755 (101%)	741 (97%)	23 (3%)	1 (0%)	48	64
1	D	766/755 (102%)	747 (98%)	19 (2%)	0	100	100
1	E	768/755 (102%)	745 (97%)	22 (3%)	1 (0%)	48	64
1	F	766/755 (102%)	735 (96%)	31 (4%)	0	100	100
1	G	766/755 (102%)	742 (97%)	24 (3%)	0	100	100
1	H	769/755 (102%)	747 (97%)	22 (3%)	0	100	100
1	I	767/755 (102%)	744 (97%)	23 (3%)	0	100	100
1	J	766/755 (102%)	737 (96%)	29 (4%)	0	100	100
All	All	7664/7550 (102%)	7415 (97%)	245 (3%)	4 (0%)	48	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	307	ASP
1	E	196	SER
1	B	196	SER
1	B	361	ALA

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	649/637 (102%)	627 (97%)	22 (3%)	32	54
1	B	650/637 (102%)	633 (97%)	17 (3%)	40	63
1	C	649/637 (102%)	620 (96%)	29 (4%)	24	42
1	D	650/637 (102%)	625 (96%)	25 (4%)	29	49
1	E	652/637 (102%)	639 (98%)	13 (2%)	48	70
1	F	650/637 (102%)	632 (97%)	18 (3%)	38	60
1	G	650/637 (102%)	629 (97%)	21 (3%)	34	56
1	H	653/637 (102%)	628 (96%)	25 (4%)	29	49
1	I	651/637 (102%)	627 (96%)	24 (4%)	30	51
1	J	650/637 (102%)	633 (97%)	17 (3%)	40	63
All	All	6504/6370 (102%)	6293 (97%)	211 (3%)	34	56

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LYS
1	A	163	GLN
1	A	197	LEU
1	A	270	VAL
1	A	293	GLU
1	A	300	SER
1	A	307	ASP
1	A	359	ILE
1	A	384	THR
1	A	420	THR
1	A	480	ASN
1	A	484	VAL
1	A	492	THR
1	A	500	THR
1	A	524	ILE
1	A	530	MET
1	A	552	THR
1	A	571	THR
1	A	577	GLN
1	A	613	GLN
1	A	662	GLU
1	A	704	LEU
1	B	78	LYS
1	B	147	MET

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Mol	Chain	Res	Type
1	B	197	LEU
1	B	222	ARG
1	B	223	SER
1	B	270	VAL
1	B	276	ARG
1	B	359	ILE
1	B	384	THR
1	B	480	ASN
1	B	484	VAL
1	B	492	THR
1	B	522	LYS
1	B	571	THR
1	B	586	VAL
1	B	662	GLU
1	B	739	GLU
1	C	2	LYS
1	C	78	LYS
1	C	135[A]	ARG
1	C	135[B]	ARG
1	C	163	GLN
1	C	196	SER
1	C	199	SER
1	C	270	VAL
1	C	293	GLU
1	C	301	GLU
1	C	335	ASP
1	C	359	ILE
1	C	377	THR
1	C	384	THR
1	C	420	THR
1	C	421	THR
1	C	471	ASP
1	C	484	VAL
1	C	492	THR
1	C	501	LYS
1	C	579	MET
1	C	586	VAL
1	C	602	LYS
1	C	620	GLU
1	C	625	THR
1	C	660	VAL
1	C	706	SER

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Mol	Chain	Res	Type
1	C	719	SER
1	C	738	THR
1	D	78	LYS
1	D	95	GLU
1	D	135[A]	ARG
1	D	135[B]	ARG
1	D	163	GLN
1	D	192	ILE
1	D	195	THR
1	D	196	SER
1	D	197	LEU
1	D	270	VAL
1	D	335	ASP
1	D	401	GLU
1	D	484	VAL
1	D	491	LYS
1	D	492	THR
1	D	500	THR
1	D	551	GLU
1	D	558	LEU
1	D	571	THR
1	D	572	ARG
1	D	573	THR
1	D	593	THR
1	D	597	THR
1	D	602	LYS
1	D	628	ASN
1	E	78	LYS
1	E	107	GLU
1	E	137	GLN
1	E	196	SER
1	E	197	LEU
1	E	245	ASN
1	E	270	VAL
1	E	420	THR
1	E	480	ASN
1	E	484	VAL
1	E	492	THR
1	E	571	THR
1	E	644	GLU
1	F	152	ILE
1	F	163	GLN

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Mol	Chain	Res	Type
1	F	197	LEU
1	F	270	VAL
1	F	293	GLU
1	F	301	GLU
1	F	306	LYS
1	F	335	ASP
1	F	384	THR
1	F	420	THR
1	F	480	ASN
1	F	484	VAL
1	F	492	THR
1	F	569	VAL
1	F	571	THR
1	F	620	GLU
1	F	662	GLU
1	F	739	GLU
1	G	70	GLN
1	G	133[A]	ARG
1	G	133[B]	ARG
1	G	135[A]	ARG
1	G	135[B]	ARG
1	G	196	SER
1	G	270	VAL
1	G	335	ASP
1	G	359	ILE
1	G	384	THR
1	G	409	SER
1	G	422	SER
1	G	471	ASP
1	G	484	VAL
1	G	491	LYS
1	G	492	THR
1	G	571	THR
1	G	660	VAL
1	G	688	ARG
1	G	719	SER
1	G	743	ILE
1	H	78	LYS
1	H	107	GLU
1	H	133[A]	ARG
1	H	133[B]	ARG
1	H	196	SER

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Mol	Chain	Res	Type
1	H	197	LEU
1	H	270	VAL
1	H	293	GLU
1	H	335	ASP
1	H	359	ILE
1	H	420	THR
1	H	471	ASP
1	H	480	ASN
1	H	484	VAL
1	H	492	THR
1	H	494	ASP
1	H	551	GLU
1	H	558	LEU
1	H	565	ARG
1	H	571	THR
1	H	579	MET
1	H	625	THR
1	H	629	MET
1	H	737	GLU
1	H	739	GLU
1	I	39	THR
1	I	107	GLU
1	I	133[A]	ARG
1	I	133[B]	ARG
1	I	135[A]	ARG
1	I	135[B]	ARG
1	I	196	SER
1	I	197	LEU
1	I	245	ASN
1	I	270	VAL
1	I	290	MET
1	I	327	CYS
1	I	335	ASP
1	I	420	THR
1	I	480	ASN
1	I	484	VAL
1	I	492	THR
1	I	571	THR
1	I	613	GLN
1	I	620	GLU
1	I	656	SER
1	I	688	ARG

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Mol	Chain	Res	Type
1	I	723	SER
1	I	739	GLU
1	J	163	GLN
1	J	195	THR
1	J	196	SER
1	J	197	LEU
1	J	270	VAL
1	J	335	ASP
1	J	384	THR
1	J	421	THR
1	J	480	ASN
1	J	484	VAL
1	J	492	THR
1	J	530	MET
1	J	573	THR
1	J	581	LEU
1	J	628	ASN
1	J	644	GLU
1	J	662	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	163	GLN
1	A	239	GLN
1	A	291	GLN
1	A	374	ASN
1	A	389	ASN
1	A	507	GLN
1	A	577	GLN
1	A	632	HIS
1	A	645	ASN
1	A	692	ASN
1	B	19	ASN
1	B	239	GLN
1	B	373	HIS
1	B	393	GLN
1	B	645	ASN
1	C	19	ASN
1	C	31	GLN
1	C	80	HIS

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Mol	Chain	Res	Type
1	C	163	GLN
1	C	480	ASN
1	C	507	GLN
1	C	692	ASN
1	D	30	GLN
1	D	31	GLN
1	D	163	GLN
1	D	389	ASN
1	D	393	GLN
1	D	480	ASN
1	D	507	GLN
1	D	613	GLN
1	D	692	ASN
1	E	137	GLN
1	E	163	GLN
1	E	239	GLN
1	E	389	ASN
1	E	393	GLN
1	E	507	GLN
1	E	613	GLN
1	E	645	ASN
1	E	730	HIS
1	F	19	ASN
1	F	163	GLN
1	F	239	GLN
1	F	389	ASN
1	F	393	GLN
1	F	507	GLN
1	F	628	ASN
1	F	632	HIS
1	F	645	ASN
1	F	692	ASN
1	G	19	ASN
1	G	31	GLN
1	G	163	GLN
1	G	239	GLN
1	G	374	ASN
1	G	389	ASN
1	G	480	ASN
1	G	613	GLN
1	G	645	ASN
1	H	30	GLN

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Mol	Chain	Res	Type
1	H	65	HIS
1	H	163	GLN
1	H	291	GLN
1	H	296	GLN
1	H	374	ASN
1	H	389	ASN
1	H	393	GLN
1	H	566	HIS
1	H	613	GLN
1	H	645	ASN
1	H	692	ASN
1	I	19	ASN
1	I	239	GLN
1	I	393	GLN
1	I	507	GLN
1	I	645	ASN
1	I	692	ASN
1	I	749	HIS
1	J	19	ASN
1	J	30	GLN
1	J	153	HIS
1	J	163	GLN
1	J	239	GLN
1	J	296	GLN
1	J	613	GLN
1	J	645	ASN
1	J	692	ASN
1	J	725	GLN
1	J	749	HIS

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

10 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	D	1386	1	15,15,16	1.94	4 (26%)	21,22,23	1.74	4 (19%)
2	PLP	E	1386	1	15,15,16	2.01	4 (26%)	21,22,23	1.65	3 (14%)
2	PLP	C	1386	1	15,15,16	1.99	4 (26%)	21,22,23	1.72	5 (23%)
2	PLP	F	1386	1	15,15,16	1.98	4 (26%)	21,22,23	2.01	7 (33%)
2	PLP	B	1386	1	15,15,16	1.95	3 (20%)	21,22,23	1.89	5 (23%)
2	PLP	A	1386	1	15,15,16	2.09	3 (20%)	21,22,23	1.53	4 (19%)
2	PLP	I	1386	1	15,15,16	2.12	5 (33%)	21,22,23	1.95	4 (19%)
2	PLP	G	1386	1	15,15,16	1.99	4 (26%)	21,22,23	2.01	6 (28%)
2	PLP	H	1386	1	15,15,16	2.00	4 (26%)	21,22,23	2.04	4 (19%)
2	PLP	J	1386	1	15,15,16	2.05	4 (26%)	21,22,23	1.74	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	D	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	E	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	C	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	F	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	A	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	I	1386	1	-	1/6/6/8	0/1/1/1
2	PLP	G	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	H	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	J	1386	1	-	0/6/6/8	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1386	PLP	O3-C3	-6.24	1.22	1.36
2	I	1386	PLP	O3-C3	-6.07	1.23	1.36
2	E	1386	PLP	O3-C3	-6.05	1.23	1.36
2	J	1386	PLP	O3-C3	-6.04	1.23	1.36
2	H	1386	PLP	O3-C3	-6.02	1.23	1.36
2	G	1386	PLP	O3-C3	-5.92	1.23	1.36
2	D	1386	PLP	O3-C3	-5.84	1.23	1.36
2	B	1386	PLP	O3-C3	-5.73	1.23	1.36
2	F	1386	PLP	O3-C3	-5.71	1.23	1.36
2	C	1386	PLP	O3-C3	-5.69	1.23	1.36
2	C	1386	PLP	C2-N1	3.07	1.39	1.33
2	A	1386	PLP	C2-N1	2.76	1.38	1.33
2	F	1386	PLP	P-O2P	-2.65	1.44	1.54
2	G	1386	PLP	C2-N1	2.63	1.38	1.33
2	J	1386	PLP	C2-N1	2.61	1.38	1.33
2	A	1386	PLP	P-O2P	-2.56	1.45	1.54
2	H	1386	PLP	P-O2P	-2.48	1.45	1.54
2	B	1386	PLP	P-O2P	-2.46	1.45	1.54
2	I	1386	PLP	C2-N1	2.45	1.38	1.33
2	J	1386	PLP	P-O2P	-2.43	1.45	1.54
2	C	1386	PLP	P-O2P	-2.40	1.45	1.54
2	D	1386	PLP	C2-N1	2.39	1.38	1.33
2	D	1386	PLP	P-O2P	-2.36	1.46	1.54
2	F	1386	PLP	C2-N1	2.33	1.38	1.33
2	J	1386	PLP	C3-C2	-2.31	1.38	1.41
2	H	1386	PLP	C3-C2	-2.30	1.38	1.41
2	I	1386	PLP	P-O2P	-2.28	1.46	1.54
2	E	1386	PLP	P-O2P	-2.24	1.46	1.54
2	E	1386	PLP	P-O3P	-2.23	1.46	1.54
2	F	1386	PLP	P-O3P	-2.21	1.46	1.54
2	D	1386	PLP	P-O3P	-2.16	1.46	1.54
2	H	1386	PLP	C2-N1	2.15	1.37	1.33
2	G	1386	PLP	P-O2P	-2.14	1.46	1.54
2	E	1386	PLP	C2-N1	2.13	1.37	1.33
2	B	1386	PLP	C2-N1	2.09	1.37	1.33
2	G	1386	PLP	P-O3P	-2.09	1.47	1.54
2	I	1386	PLP	C5-C4	-2.08	1.38	1.40
2	I	1386	PLP	P-O3P	-2.06	1.47	1.54
2	C	1386	PLP	P-O3P	-2.01	1.47	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1386	PLP	O4P-C5A-C5	6.76	122.03	109.36
2	I	1386	PLP	O4P-C5A-C5	6.26	121.09	109.36
2	G	1386	PLP	O4P-C5A-C5	5.93	120.46	109.36
2	E	1386	PLP	O4P-C5A-C5	5.20	119.11	109.36
2	F	1386	PLP	O4P-C5A-C5	5.04	118.81	109.36
2	D	1386	PLP	O4P-C5A-C5	4.93	118.59	109.36
2	B	1386	PLP	O4P-C5A-C5	4.63	118.04	109.36
2	C	1386	PLP	O4P-C5A-C5	4.48	117.75	109.36
2	B	1386	PLP	O4P-P-O1P	-4.33	94.73	106.44
2	G	1386	PLP	O4P-P-O1P	-4.23	95.02	106.44
2	A	1386	PLP	O4P-C5A-C5	4.20	117.23	109.36
2	J	1386	PLP	O4P-C5A-C5	3.97	116.79	109.36
2	C	1386	PLP	O4P-P-O1P	-3.93	95.81	106.44
2	D	1386	PLP	O4P-P-O1P	-3.87	95.99	106.44
2	F	1386	PLP	O4P-P-O1P	-3.83	96.08	106.44
2	H	1386	PLP	O4P-P-O1P	-3.57	96.79	106.44
2	J	1386	PLP	C6-C5-C4	3.53	120.99	118.10
2	I	1386	PLP	O4P-P-O1P	-3.13	97.99	106.44
2	I	1386	PLP	C6-C5-C4	3.01	120.56	118.10
2	B	1386	PLP	C6-C5-C4	2.99	120.55	118.10
2	F	1386	PLP	C4A-C4-C5	-2.97	117.88	120.94
2	F	1386	PLP	C6-C5-C4	2.94	120.51	118.10
2	B	1386	PLP	C5-C6-N1	-2.93	119.06	123.83
2	J	1386	PLP	O4P-P-O1P	-2.88	98.66	106.44
2	D	1386	PLP	C6-C5-C4	2.85	120.43	118.10
2	E	1386	PLP	O4P-P-O1P	-2.80	98.88	106.44
2	C	1386	PLP	C6-C5-C4	2.70	120.31	118.10
2	J	1386	PLP	C5-C6-N1	-2.59	119.62	123.83
2	E	1386	PLP	C6-C5-C4	2.52	120.16	118.10
2	G	1386	PLP	C4A-C4-C5	-2.42	118.45	120.94
2	B	1386	PLP	O2P-P-O1P	2.39	120.13	110.83
2	G	1386	PLP	C5-C6-N1	-2.38	119.96	123.83
2	G	1386	PLP	C6-C5-C4	2.30	119.99	118.10
2	G	1386	PLP	O2P-P-O1P	2.27	119.68	110.83
2	I	1386	PLP	C5-C6-N1	-2.26	120.16	123.83
2	D	1386	PLP	C5-C6-N1	-2.24	120.18	123.83
2	A	1386	PLP	C6-C5-C4	2.21	119.91	118.10
2	H	1386	PLP	C5-C6-N1	-2.20	120.25	123.83
2	F	1386	PLP	O2P-P-O1P	2.19	119.36	110.83
2	F	1386	PLP	C5-C6-N1	-2.17	120.30	123.83
2	H	1386	PLP	C6-C5-C4	2.12	119.84	118.10
2	A	1386	PLP	O3P-P-O2P	2.09	115.64	107.80
2	F	1386	PLP	O3-C3-C4	2.09	123.55	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1386	PLP	C5-C6-N1	-2.07	120.46	123.83
2	A	1386	PLP	O4P-P-O1P	-2.05	100.91	106.44
2	C	1386	PLP	O2P-P-O1P	2.03	118.75	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1386	PLP	C4-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1386	PLP	1	0
2	E	1386	PLP	1	0
2	B	1386	PLP	1	0
2	H	1386	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	755/755 (100%)	-0.38	8 (1%) 78 74	8, 23, 41, 56	16 (2%)
1	B	755/755 (100%)	-0.23	9 (1%) 76 73	10, 22, 40, 55	18 (2%)
1	C	755/755 (100%)	-0.24	10 (1%) 75 71	11, 25, 43, 58	16 (2%)
1	D	755/755 (100%)	-0.51	5 (0%) 84 81	7, 18, 33, 57	16 (2%)
1	E	755/755 (100%)	-0.35	9 (1%) 76 73	8, 20, 38, 54	19 (2%)
1	F	755/755 (100%)	-0.45	4 (0%) 87 85	10, 21, 38, 57	15 (1%)
1	G	755/755 (100%)	-0.24	10 (1%) 75 71	9, 25, 42, 60	20 (2%)
1	H	755/755 (100%)	-0.62	8 (1%) 78 74	6, 15, 31, 59	19 (2%)
1	I	755/755 (100%)	-0.48	7 (0%) 81 78	7, 18, 36, 54	15 (1%)
1	J	755/755 (100%)	-0.20	10 (1%) 75 71	8, 25, 42, 55	17 (2%)
All	All	7550/7550 (100%)	-0.37	80 (1%) 78 74	6, 22, 40, 60	171 (2%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	729	HIS	10.9
1	D	193	GLU	8.3
1	C	193	GLU	7.9
1	B	628	ASN	7.6
1	G	620	GLU	7.4
1	H	193	GLU	6.9
1	J	643	LYS	6.8
1	A	193	GLU	6.7
1	C	713	LYS	6.5
1	A	713	LYS	6.4
1	J	620	GLU	6.2
1	E	619	VAL	6.2
1	G	193	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	G	522	LYS	5.9
1	J	713	LYS	5.8
1	B	653	GLU	5.8
1	E	193	GLU	5.7
1	F	713	LYS	5.6
1	D	192	ILE	5.6
1	C	192	ILE	5.3
1	H	155	TYR	5.2
1	G	713	LYS	5.1
1	H	192	ILE	4.9
1	B	193	GLU	4.8
1	A	192	ILE	4.8
1	E	192	ILE	4.6
1	F	653	GLU	4.5
1	G	653	GLU	3.9
1	D	155	TYR	3.8
1	B	192	ILE	3.5
1	E	713	LYS	3.5
1	I	713	LYS	3.4
1	B	195	THR	3.3
1	G	306	LYS	3.3
1	B	713	LYS	3.2
1	I	153	HIS	3.1
1	H	156	SER	3.0
1	A	195	THR	3.0
1	B	155	TYR	2.9
1	C	195	THR	2.8
1	I	573	THR	2.8
1	C	567	GLY	2.8
1	G	569	VAL	2.8
1	J	156	SER	2.8
1	H	153	HIS	2.7
1	A	490	GLY	2.7
1	E	567	GLY	2.7
1	E	195	THR	2.6
1	H	490	GLY	2.5
1	G	755	ALA	2.5
1	D	156	SER	2.5
1	I	156	SER	2.5
1	J	155	TYR	2.5
1	C	653	GLU	2.4
1	C	155	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	194	ARG	2.4
1	F	567	GLY	2.4
1	J	653	GLU	2.3
1	F	195	THR	2.3
1	A	567	GLY	2.3
1	B	153	HIS	2.3
1	J	729	HIS	2.3
1	H	195	THR	2.2
1	C	154	GLU	2.2
1	D	195	THR	2.2
1	J	567	GLY	2.2
1	C	323	TYR	2.2
1	J	573	THR	2.2
1	A	653	GLU	2.2
1	J	195	THR	2.1
1	E	569	VAL	2.1
1	I	154	GLU	2.1
1	I	155	TYR	2.1
1	C	569	VAL	2.1
1	I	653	GLU	2.1
1	H	194	ARG	2.1
1	E	374	ASN	2.0
1	G	195	THR	2.0
1	E	571	THR	2.0
1	B	156	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	B	1386	15/16	0.94	0.17	2,2,3,5	15
2	PLP	E	1386	15/16	0.95	0.20	2,2,2,4	15
2	PLP	I	1386	15/16	0.95	0.20	2,2,2,4	15
2	PLP	A	1386	15/16	0.96	0.17	2,2,2,4	15
2	PLP	F	1386	15/16	0.96	0.16	2,2,2,3	15
2	PLP	D	1386	15/16	0.96	0.20	2,2,2,2	15
2	PLP	J	1386	15/16	0.96	0.17	2,2,4,6	15
2	PLP	H	1386	15/16	0.97	0.18	2,2,2,2	15
2	PLP	C	1386	15/16	0.97	0.15	2,2,4,6	15
2	PLP	G	1386	15/16	0.97	0.15	2,2,5,8	15

6.5 Other polymers [i](#)

There are no such residues in this entry.