



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:09 AM GMT

PDB ID : 2VYC
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

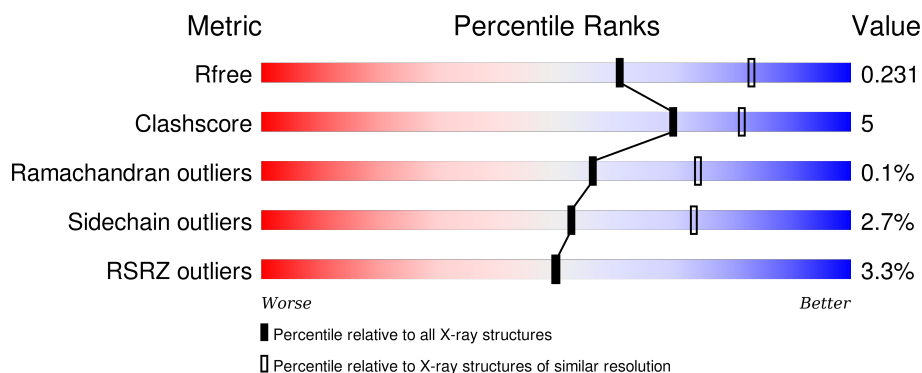
1 Overall quality at a glance

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>3%</div> <div>88%</div> <div>11%</div> </div>
1	B	755	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
1	C	755	<div> <div>4%</div> <div>87%</div> <div>13%</div> </div>
1	D	755	<div> <div>2%</div> <div>90%</div> <div>10%</div> </div>
1	E	755	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	755	
1	G	755	
1	H	755	
1	I	755	
1	J	755	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	A	1386	-	-	-	X
2	PLP	B	1386	-	-	-	X
2	PLP	C	1386	-	-	-	X
2	PLP	D	1386	-	-	-	X
2	PLP	E	1386	-	-	-	X
2	PLP	F	1386	-	-	-	X
2	PLP	G	1386	-	-	-	X
2	PLP	H	1386	-	-	-	X
2	PLP	I	1386	-	-	-	X
2	PLP	J	1386	-	-	-	X

2 Entry composition

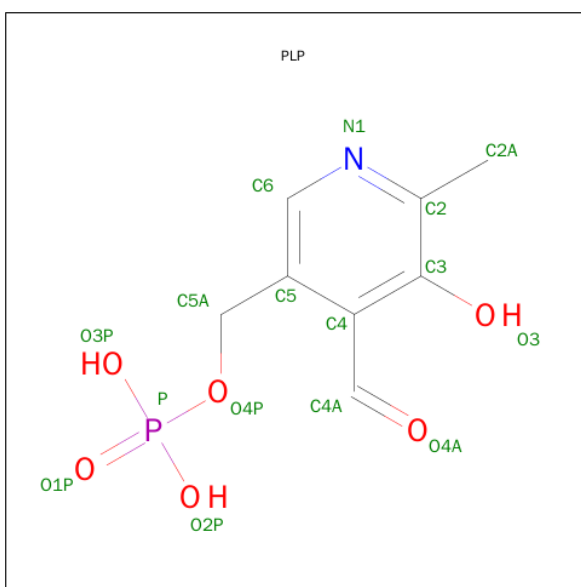
There are 3 unique types of molecules in this entry. The entry contains 62902 atoms, of which 0 are hydrogens and 0 are deuteriums.

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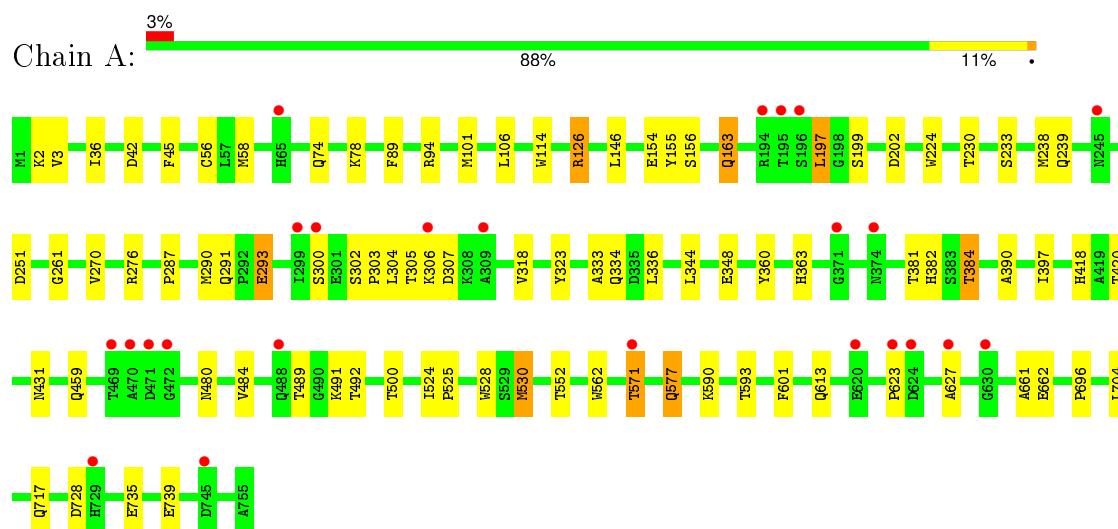
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	219	Total 219	O 219	0	0
3	D	266	Total 266	O 266	0	0
3	E	258	Total 258	O 258	0	0
3	F	268	Total 268	O 268	0	0
3	G	237	Total 237	O 237	0	0
3	H	272	Total 272	O 272	0	0
3	I	262	Total 262	O 262	0	0
3	J	238	Total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

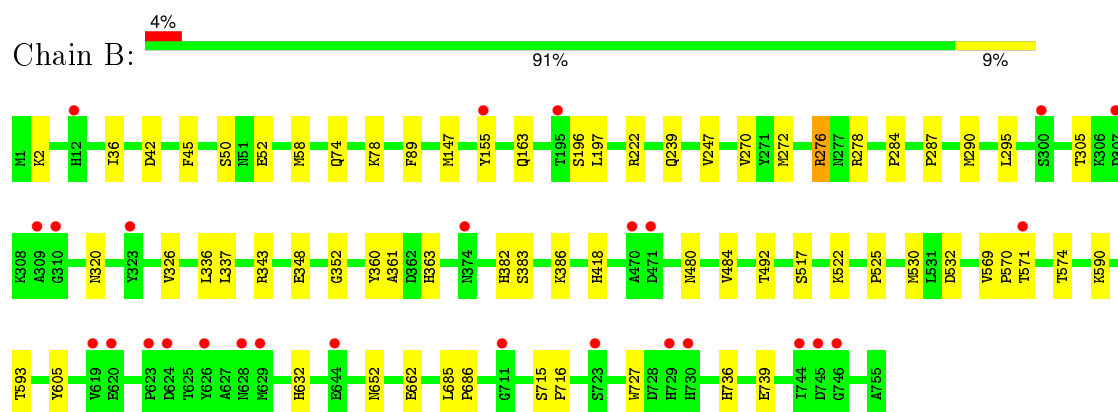
3 Residue-property plots

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

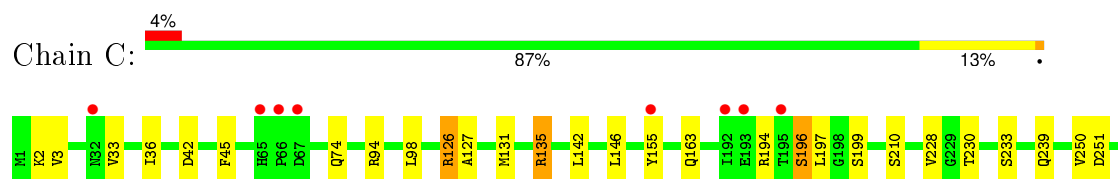
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

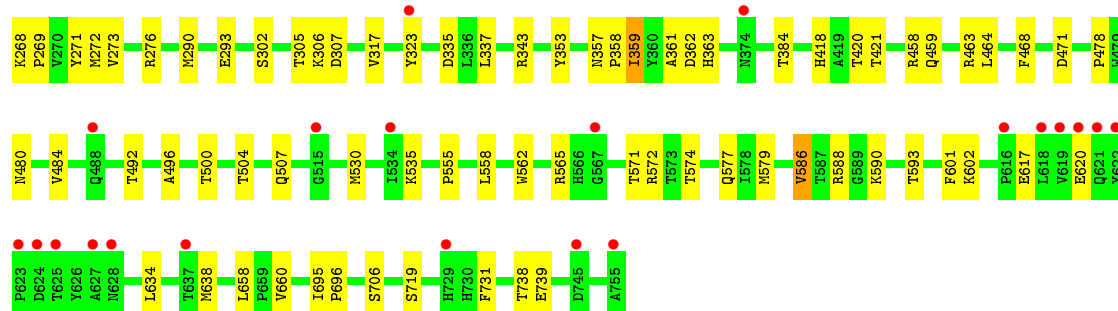


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

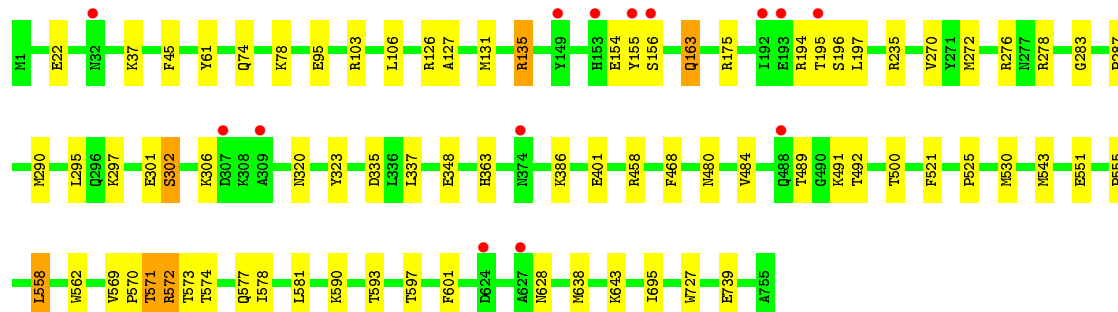
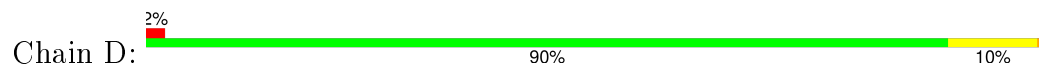


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

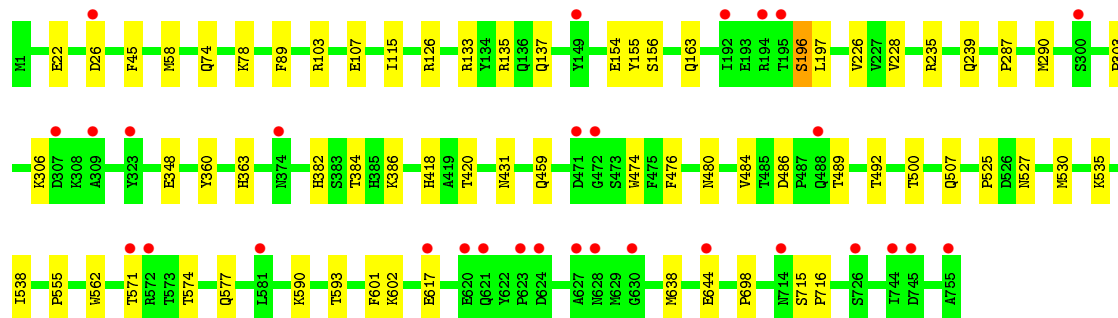
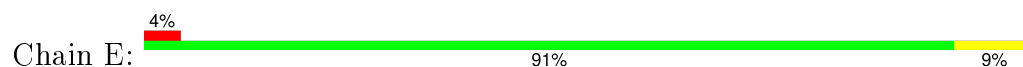




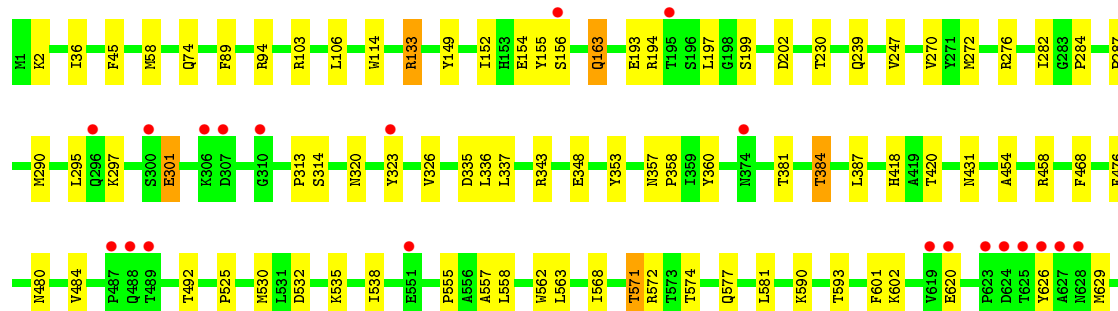
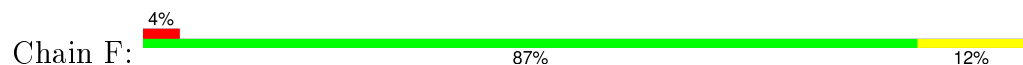
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

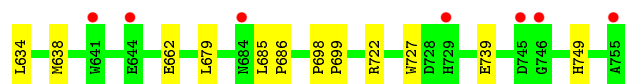


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

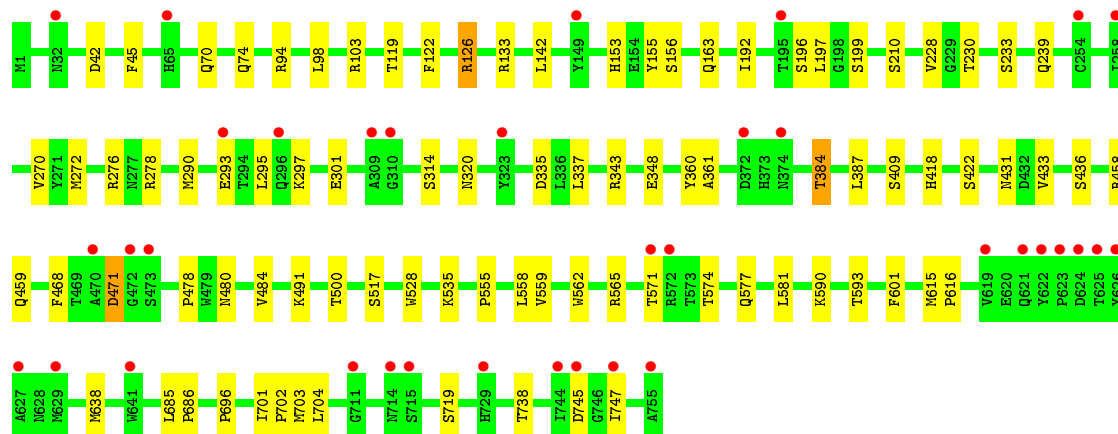
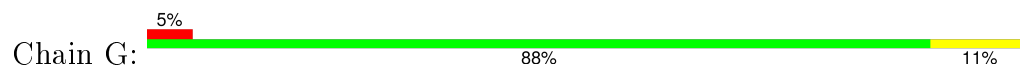


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

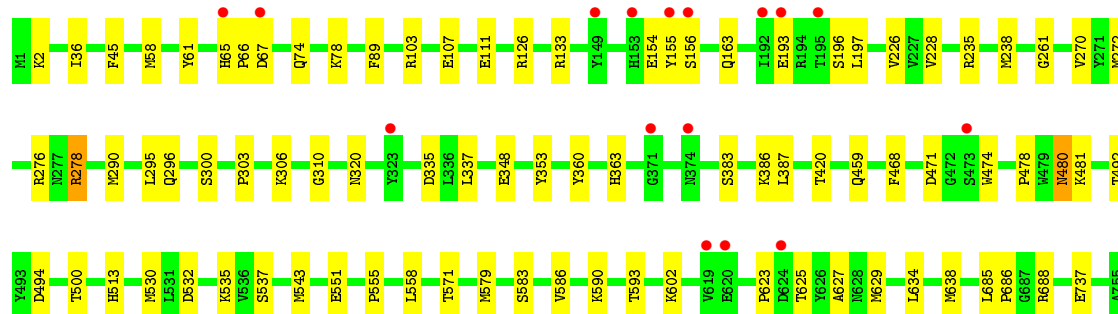
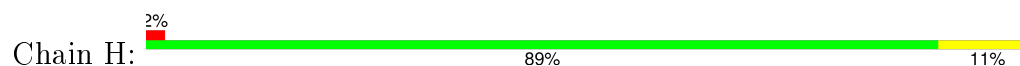




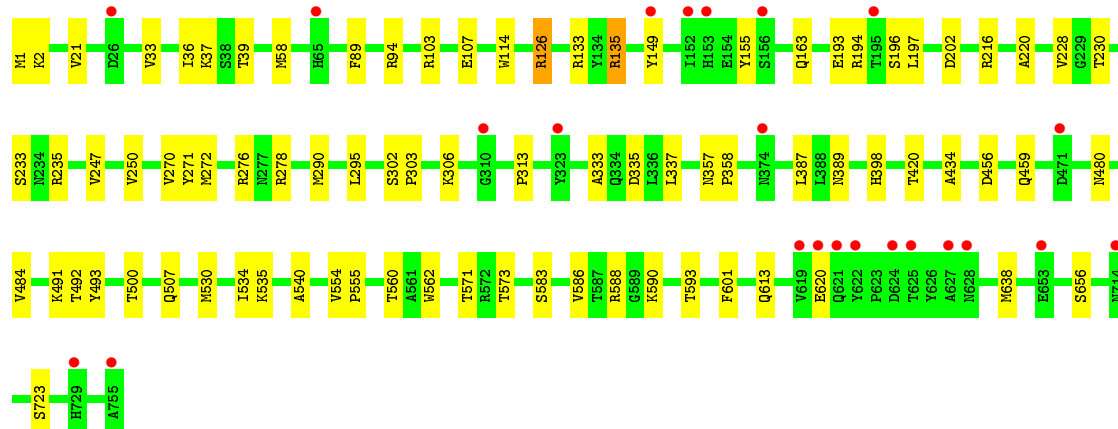
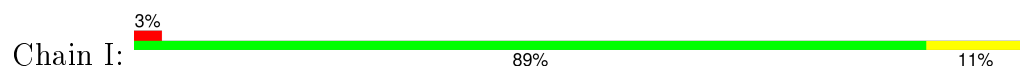
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



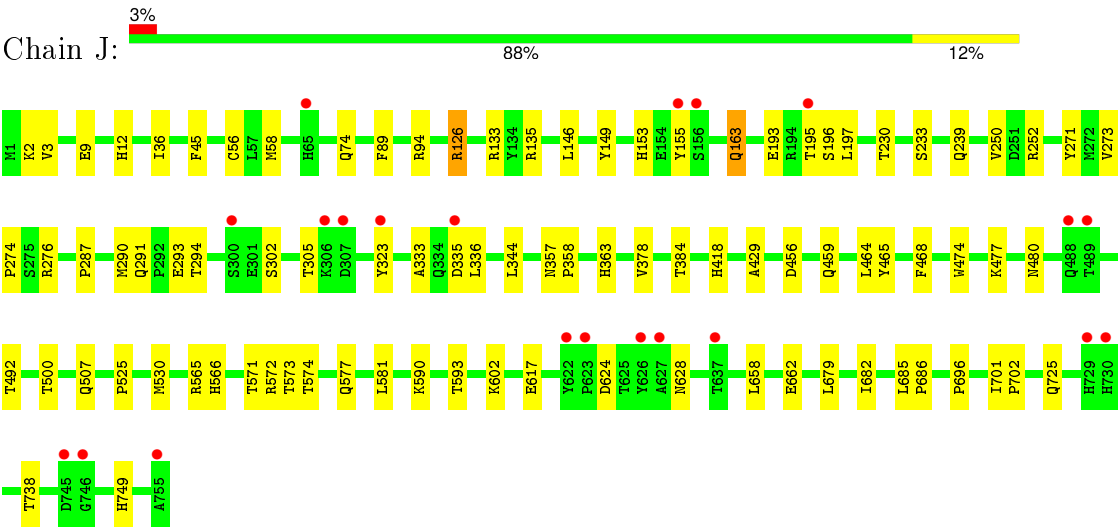
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



• 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 39.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.40) 99.9 (39.82-2.40)	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 (5.30%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 385893 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.61	0/6211	0.67	1/8438 (0.0%)
1	B	0.63	0/6224	0.68	1/8456 (0.0%)
1	C	0.60	0/6211	0.65	3/8438 (0.0%)
1	D	0.65	0/6222	0.69	1/8452 (0.0%)
1	E	0.63	0/6244	0.68	1/8482 (0.0%)
1	F	0.63	0/6224	0.67	0/8456
1	G	0.60	0/6224	0.65	2/8456 (0.0%)
1	H	0.68	0/6257	0.70	3/8499 (0.0%)
1	I	0.65	0/6233	0.70	4/8468 (0.0%)
1	J	0.58	0/6224	0.64	1/8456 (0.0%)
All	All	0.63	0/62274	0.67	17/84601 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	I	235	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	H	235	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	H	688	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	126	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	J	126	ARG	NE-CZ-NH2	-6.62	116.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	278	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	I	278	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	126	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	G	197	LEU	CA-CB-CG	5.50	127.96	115.30
1	E	235	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	532	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	343	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	I	278	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	G	126	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	126	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	I	126	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	52	0
1	B	6016	0	5767	41	0
1	C	6008	0	5762	76	0
1	D	6015	0	5771	52	0
1	E	6028	0	5780	40	0
1	F	6016	0	5767	70	0
1	G	6016	0	5767	61	0
1	H	6036	0	5788	64	0
1	I	6021	0	5771	50	0
1	J	6016	0	5767	57	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
3	C	219	0	0	2	0
3	D	266	0	0	5	0
3	E	258	0	0	3	0
3	F	268	0	0	5	0
3	G	237	0	0	2	0
3	H	272	0	0	1	0
3	I	262	0	0	2	0
3	J	238	0	0	3	0
All	All	62902	0	57762	535	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 (535) 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:HH11	1:C:135[A]:ARG:HG2	1.16	1.11
1:I:135[A]:ARG:HH11	1:I:135[A]:ARG:HG2	1.19	1.05
1:E:384:THR:HG21	1:E:431:ASN:OD1	1.63	0.98
1:J:135[B]:ARG:HH11	1:J:135[B]:ARG:HG2	1.29	0.97
1:H:272:MET:HE1	1:H:337:LEU:HD21	1.45	0.97
1:F:272:MET:HE1	1:F:337:LEU:HD21	1.49	0.92
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:384:THR:HG21	1:F:431:ASN:OD1	1.67	0.91
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:363:HIS:CG	1:D:530:MET:HE3	2.09	0.87
1:C:272:MET:HE1	1:C:290:MET:HG2	1.57	0.86
1:A:155:TYR:O	1:A:163:GLN:NE2	2.09	0.86
1:B:360:TYR:HA	1:B:530:MET:HE1	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:239:GLN:HG3	1:A:418:HIS:NE2	1.93	0.84
1:D:272:MET:HE2	1:D:295:LEU:HD21	1.60	0.83
1:C:45[A]:PHE:CE1	1:C:74[A]:GLN:HG2	2.12	0.83
1:H:155:TYR:C	1:H:163:GLN:HE22	1.82	0.83
1:G:239:GLN:HG3	1:G:418:HIS:NE2	1.93	0.83
1:C:272:MET:HE1	1:C:337:LEU:HD21	1.62	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:J:323[A]:TYR:CE2	1:J:572:ARG:HB2	2.16	0.81
1:I:507:GLN:HG3	1:I:530:MET:HE2	1.63	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:D:155:TYR:O	1:D:163:GLN:NE2	2.15	0.80
1:H:555:PRO:HG2	1:H:638:MET:HE2	1.64	0.80
1:B:590:LYS:HD3	1:C:126:ARG:HD3	1.64	0.79
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: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:C:135[A]:ARG:HG2	1:C:135[A]:ARG:NH1	1.95	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:I:507:GLN:CG	1:I:530:MET:HE2	2.15	0.75
1:I:272:MET:HE1	1:I:337:LEU:HD21	1.69	0.75
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:I:135[A]:ARG:HG2	1:I:135[A]:ARG:NH1	1.94	0.73
1:B:574:THR:HB	3:B:2228:HOH:O	1.88	0.73
1:C:323:TYR:OH	1:C:571:THR:HB	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:SER:HA	1:E:163:GLN:NE2	2.05	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: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:H:363:HIS:CG	1:H:530:MET:HE3	2.26	0.69
1:F:149:TYR:HE2	1:F:193:GLU:HG3	1.55	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:H:272:MET:CE	1:H:337:LEU:HD21	2.23	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:G:468:PHE:CZ	1:H:103:ARG:HD3	2.28	0.68
1:E:363:HIS:CG	1:E:530:MET:HE3	2.29	0.68
1:B:590:LYS:O	1:B:593:THR:HG22	1.94	0.68
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:H:272:MET:HE1	1:H:337:LEU:CD2	2.25	0.66
1:F:323[B]:TYR:HD2	3:F:2154:HOH:O	1.77	0.66
1:F:323[A]:TYR:OH	1:F:571:THR:HB	1.96	0.66
1:E:126:ARG:HD2	3:E:2054:HOH:O	1.95	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:H:2:LYS:HD3	1:H:36:ILE:HD11	1.79	0.64
1:F:58:MET:HG2	1:F:89:PHE:HB2	1.78	0.64
1:I:272:MET:CE	1:I:337:LEU:HD21	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:MET:CE	1:C:337:LEU:HD21	2.28	0.64
1:C:2:LYS:HD3	1:C:36:ILE:CD1	2.26	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: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:A:293:GLU:H	1:A:293:GLU:CD	2.03	0.63
1:F:272:MET:HE1	1:F:337:LEU:CD2	2.27	0.62
1:A:45[A]:PHE:CE1	1:A:74[A]:GLN:HG2	2.34	0.62
1:H:155:TYR:C	1:H:163:GLN:NE2	2.52	0.62
1:C:507:GLN:HE21	1:C:530:MET:HE1	1.63	0.62
1:B:247:VAL:HG22	1:B:305:THR:HG22	1.82	0.61
1:G:590:LYS:CD	1:H:126:ARG:HD3	2.31	0.61
1:B:290:MET:HE3	1:B:337:LEU:HG	1.82	0.61
1:F:287:PRO:HD2	1:F:525:PRO:HG2	1.82	0.61
1:C:507:GLN:NE2	1:C:530:MET:HE1	2.16	0.61
1:I:389:ASN:O	1:I:434:ALA:HB2	2.00	0.60
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:F:679:LEU:HD22	1:F:749:HIS:HB3	1.83	0.59
1:E:303:PRO:HA	1:E:306:LYS:HE3	1.84	0.59
1:J:474:TRP:O	1:J:602:LYS:HE2	2.01	0.59
1:A:290:MET:HE1	1:A:333:ALA:HA	1.84	0.59
1:E:459:GLN:OE1	1:E:500:THR:HG22	2.02	0.59
1:I:149:TYR:HE2	1:I:193:GLU:HG3	1.68	0.59
1:D:638:MET:CE	1:D:727:TRP:HH2	2.15	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:A:360:TYR:HA	1:A:530:MET:HE1	1.84	0.59
1:D:571:THR:HG21	1:D:581:LEU:HB2	1.83	0.59
1:B:287:PRO:HD2	1:B:525:PRO:HG2	1.84	0.58
1:A:363:HIS:CG	1:A:530:MET:HE2	2.39	0.58
1:I:588[A]:ARG:NH2	3:I:2236:HOH:O	2.35	0.58
1:D:290:MET:HE3	1:D:337:LEU:HG	1.86	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:J:290:MET:HE1	1:J:333:ALA:HA	1.86	0.57
1:J:45[A]:PHE:HE1	1:J:74[A]:GLN:HG2	1.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ARG:NH1	1:B:652:ASN:OD1	2.38	0.57
1:F:323[A]:TYR:CE2	1:F:572:ARG:HB2	2.39	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: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:C:45[A]:PHE:HE1	1:C:74[A]:GLN:HG2	1.68	0.56
1:I:507:GLN:CG	1:I:530:MET:CE	2.83	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:E:617:GLU:CD	1:E:617:GLU:H	2.09	0.56
1:J:126:ARG:HD2	3:J:2056:HOH:O	2.05	0.56
1:C:45[A]:PHE:CE1	1:C:74[A]:GLN:CG	2.89	0.55
1:J:574:THR:HB	3:J:2211:HOH:O	2.05	0.55
1:C:588:ARG:HH11	1:C:588:ARG:HG2	1.71	0.55
1:C:272:MET:CE	1:C:290:MET:HG2	2.33	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:D:638:MET:HE3	1:D:727:TRP:CH2	2.42	0.55
1:A:239:GLN:HG2	3:A:2134:HOH:O	2.07	0.55
1:D:555:PRO:HB2	1:D:638:MET:HE1	1.89	0.55
1:A:623:PRO:O	1:A:627:ALA:HB2	2.06	0.55
1:C:478:PRO:HB2	1:C:480:ASN:HD21	1.72	0.55
1:J:323[A]:TYR:HE2	1:J:572:ARG:HB2	1.66	0.55
1:F:468:PHE:CE2	1:F:602:LYS:HE2	2.42	0.55
1:B:272:MET:HE3	1:B:295:LEU:HD21	1.89	0.55
1:H:363:HIS:CE1	1:H:530:MET:HE2	2.42	0.54
1:D:638:MET:HE3	1:D:727:TRP:HH2	1.72	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:D:45[A]:PHE:HE1	1:D:74[A]:GLN:HG2	1.72	0.54
1:C:302:SER:HB3	1:C:305:THR:OG1	2.08	0.54
1:H:555:PRO:HB2	1:H:638:MET:CE	2.38	0.54
1:I:272:MET:HE2	1:I:295:LEU:HD21	1.88	0.54
1:B:363:HIS:CD2	1:B:530:MET:HG2	2.42	0.54
1:C:696:PRO:HA	1:C:738:THR:HG23	1.90	0.54
1:C:230:THR:HA	1:C:233:SER:HB2	1.88	0.54
1:H:634:LEU:O	1:H:638:MET:HG3	2.08	0.54
1:B:290:MET:CE	1:B:337:LEU:HG	2.38	0.54
1:B:278:ARG:NH2	1:B:517:SER:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:590:LYS:O	1:G:593:THR:HG22	2.08	0.53
1:E:226:VAL:HG12	1:E:228:VAL:H	1.73	0.53
1:H:272:MET:HE2	1:H:295:LEU:HD21	1.89	0.53
1:I:507:GLN:CD	1:I:530:MET:HE1	2.29	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:574:THR:HB	3:E:2232:HOH:O	2.09	0.53
1:E:287:PRO:HD2	1:E:525:PRO:HG2	1.89	0.53
1:G:290:MET:HE2	1:G:528:TRP:HH2	1.72	0.53
1:D:468:PHE:CZ	1:E:103:ARG:HD3	2.43	0.53
1:A:224:TRP:HB2	1:A:397:ILE:HB	1.90	0.53
1:A:3:VAL:HG22	1:A:56:CYS:HB3	1.91	0.53
1:B:383:SER:CB	1:B:386:LYS:HD2	2.39	0.53
1:A:146:LEU:HD23	1:A:197:LEU:HD21	1.91	0.53
1:J:468:PHE:CE2	1:J:602:LYS:HE3	2.44	0.53
1:J:363:HIS:CG	1:J:530:MET:HE3	2.44	0.52
1:E:22[A]:GLU:OE2	1:E:26[A]:ASP:OD1	2.28	0.52
1:D:272:MET:HE2	1:D:295:LEU:CD2	2.35	0.52
1:H:65:HIS:CD2	1:H:66:PRO:HD2	2.45	0.52
1:F:722:ARG:NH1	3:F:2266:HOH:O	2.42	0.52
1:H:290:MET:HE3	1:H:337:LEU:HG	1.92	0.52
1:C:468:PHE:CE2	1:C:602:LYS:HE3	2.45	0.52
1:G:272:MET:CE	1:G:337:LEU:HD21	2.39	0.51
1:I:555:PRO:CB	1:I:638:MET:HE2	2.40	0.51
1:A:739:GLU:HG2	3:A:2144:HOH:O	2.10	0.51
1:I:555:PRO:HB2	1:I:638:MET:CE	2.40	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:G:230:THR:HA	1:G:233:SER:HB2	1.93	0.51
1:D:363:HIS:CG	1:D:530:MET:CE	2.89	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:F:272:MET:HE2	1:F:295:LEU:HD21	1.93	0.51
1:G:239:GLN:HG2	3:G:2117:HOH:O	2.10	0.51
1:I:216[A]:ARG:HH11	1:I:216[A]:ARG:HG2	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:GLN:HG3	1:C:418:HIS:NE2	2.26	0.50
1:H:272:MET:CE	1:H:337:LEU:CD2	2.87	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:F:133[B]:ARG:HH21	1:J:566:HIS:HD2	1.59	0.50
1:C:323:TYR:CE2	1:C:572:ARG:HB2	2.47	0.50
1:F:149:TYR:CE2	1:F:193:GLU:HG3	2.43	0.50
1:J:574:THR:HG1	1:J:577:GLN:HB3	1.77	0.50
1:G:272:MET:HE1	1:G:290:MET:HG2	1.93	0.50
1:E:386:LYS:NZ	2:E:1386:PLP:O3	2.45	0.50
1:C:555:PRO:HB2	1:C:638:MET:CE	2.42	0.50
1:A:363:HIS:CG	1:A:530:MET:CE	2.94	0.50
1:F:272:MET:CE	1:F:337:LEU:HD21	2.32	0.50
1:A:384:THR:HG21	1:A:431:ASN:OD1	2.11	0.50
1:A:199:SER:HB3	1:A:202:ASP:HB2	1.92	0.50
1:F:133[B]:ARG:NH2	1:J:566:HIS:HD2	2.10	0.49
1:C:3:VAL:HG23	1:C:33:VAL:HG11	1.92	0.49
1:H:155:TYR:HB3	1:H:163:GLN:HE21	1.77	0.49
1:A:290:MET:HE2	1:A:528:TRP:HH2	1.76	0.49
1:G:192:ILE:HD11	1:G:199:SER:HB2	1.95	0.49
1:G:478:PRO:HB2	1:G:480:ASN:ND2	2.27	0.49
1:I:387:LEU:HD11	1:I:535:LYS:HE3	1.94	0.49
1:E:574:THR:HG22	1:E:698:PRO:HB3	1.94	0.49
1:C:463:ARG:HG3	1:C:496:ALA:HB1	1.94	0.49
1:F:555:PRO:HB2	1:F:638:MET:HE1	1.94	0.49
1:H:45[A]:PHE:CE1	1:H:74[A]:GLN:NE2	2.80	0.49
1:I:250:VAL:O	1:I:271:TYR:HA	2.13	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: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:F:290:MET:HE3	1:F:337:LEU:HG	1.94	0.49
1:G:320:ASN:O	1:G:348:GLU:HA	2.12	0.49
1:J:363:HIS:CD2	1:J:530:MET:HG2	2.48	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:D:320:ASN:O	1:D:348:GLU:HA	2.13	0.48
1:A:94[A]:ARG:HG3	1:A:114:TRP:CE2	2.47	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:I:534:ILE:HG13	1:I:535:LYS:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:507:GLN:NE2	1:E:530:MET:HE1	2.29	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:J:153:HIS:HE1	1:J:193:GLU:OE2	1.97	0.48
1:B:383:SER:HB2	1:B:386:LYS:HD2	1.95	0.47
1:B:352:GLY:HA2	1:B:382:HIS:CD2	2.48	0.47
1:B:58:MET:HG2	1:B:89:PHE:HB2	1.96	0.47
1:C:42:ASP:HA	1:C:45[B]:PHE:CD2	2.49	0.47
1:G:272:MET:HE2	1:G:295:LEU:HD21	1.96	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:J:302:SER:HB3	1:J:305:THR:OG1	2.15	0.47
1:F:685:LEU:N	1:F:686:PRO:CD	2.77	0.47
1:I:194:ARG:NH1	1:I:202:ASP:OD2	2.47	0.47
1:E:555:PRO:HB2	1:E:638:MET:CE	2.45	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:HE3	1:F:290:MET:HB3	1.74	0.47
1:D:290:MET:CE	1:D:337:LEU:HG	2.44	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:I:302:SER:O	1:I:306:LYS:HG3	2.15	0.47
1:H:320:ASN:O	1:H:348:GLU:HA	2.15	0.47
1:H:238:MET:SD	1:H:261:GLY:HA3	2.55	0.47
1:F:272:MET:CE	1:F:337:LEU:CD2	2.93	0.47
1:A:156:SER:HA	1:A:163:GLN:HE22	1.80	0.47
1:J:685:LEU:N	1:J:686:PRO:CD	2.78	0.47
1:C:273:VAL:HG22	1:C:658:LEU:HD21	1.97	0.47
1:F:468:PHE:CE2	1:G:103:ARG:HD3	2.50	0.47
1:B:272:MET:CE	1:B:337:LEU:HD21	2.45	0.46
1:F:574:THR:HB	3:F:2241:HOH:O	2.13	0.46
1:D:574:THR:HB	3:D:2230:HOH:O	2.15	0.46
1:B:363:HIS:CG	1:B:530:MET:HE2	2.50	0.46
1:C:363:HIS:CG	1:C:530:MET:HE3	2.50	0.46
1:I:230:THR:HA	1:I:233:SER:HB2	1.97	0.46
1:H:163:GLN:HE21	1:H:163:GLN:HA	1.80	0.46
1:H:363:HIS:ND1	1:H:530:MET:HE2	2.30	0.46
1:A:363:HIS:ND1	1:A:530:MET:HE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:555:PRO:HB2	1:I:638:MET:HE2	1.97	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:B:727:TRP:CD1	1:B:736:HIS:CD2	3.03	0.46
1:H:290:MET:CE	1:H:337:LEU:HG	2.46	0.46
1:E:476:PHE:HB3	1:E:538:ILE:HG23	1.97	0.46
1:J:565:ARG:NH1	1:J:617:GLU:OE1	2.43	0.46
1:C:574:THR:OG1	1:C:577:GLN:HB3	2.16	0.46
1:J:146:LEU:HD12	1:J:429:ALA:HB2	1.97	0.46
1:B:290:MET:HE3	1:B:290:MET:HB3	1.77	0.46
1:H:353:TYR:OH	1:H:532:ASP:OD2	2.28	0.46
1:A:489:THR:HG21	1:A:491:LYS:HB2	1.98	0.46
1:C:590:LYS:CD	1:D:126:ARG:HD3	2.46	0.46
1:H:45[A]:PHE:CE1	1:H:74[A]:GLN:HG2	2.51	0.46
1:G:228:VAL:O	1:G:228:VAL:HG12	2.16	0.46
1:H:290:MET:HE3	1:H:290:MET:HB3	1.73	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:A:304:LEU:HD11	1:A:661:ALA:HB1	1.98	0.45
1:H:555:PRO:HB2	1:H:638:MET:HE3	1.98	0.45
1:E:363:HIS:CG	1:E:530:MET:CE	2.98	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:A:58:MET:HG2	1:A:89:PHE:HB2	1.99	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:H:154:GLU:OE2	1:H:156:SER:HB2	2.15	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:G:471:ASP:O	1:G:471:ASP:CG	2.55	0.45
1:C:572:ARG:NH1	3:C:2196:HOH:O	2.49	0.45
1:I:126:ARG:HD2	3:I:2060:HOH:O	2.16	0.45
1:D:562:TRP:CD1	1:D:601:PHE:HB2	2.52	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:C:228:VAL:O	1:C:228:VAL:HG12	2.16	0.45
1:J:252:ARG:HB3	1:J:274:PRO:HD3	1.99	0.45
1:G:290:MET:HE3	1:G:290:MET:HB3	1.81	0.45
1:F:297:LYS:HG2	1:F:301:GLU:OE2	2.17	0.45
1:B:50:SER:C	1:B:52:GLU:H	2.20	0.45
1:D:468:PHE:CE2	1:E:103:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:HD11	1:D:106:LEU:HD11	1.99	0.45
1:G:360:TYR:O	1:G:361:ALA:C	2.53	0.45
1:E:562:TRP:CD1	1:E:601:PHE:HB2	2.52	0.45
1:D:558:LEU:HD12	1:D:558:LEU:HA	1.73	0.45
1:A:363:HIS:CE1	1:A:530:MET:HE2	2.52	0.44
1:H:387:LEU:CD1	1:H:535:LYS:HE2	2.47	0.44
1:C:290:MET:HE3	1:C:290:MET:HB3	1.71	0.44
1:A:290:MET:HE2	1:A:336:LEU:HD12	1.99	0.44
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:D:283:GLY:HA3	1:D:521:PHE:CE1	2.52	0.44
1:D:154:GLU:OE2	1:D:156:SER:CB	2.64	0.44
1:B:272:MET:HE2	1:B:337:LEU:HD21	1.98	0.44
1:F:638:MET:HE2	1:F:638:MET:HB3	1.91	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:H:156:SER:HA	1:H:163:GLN:OE1	2.17	0.44
1:F:247:VAL:O	1:F:313:PRO:HA	2.18	0.44
1:J:679:LEU:HD22	1:J:749:HIS:HB3	1.98	0.44
1:A:101:MET:SD	1:A:106:LEU:HD21	2.57	0.44
1:J:291:GLN:HB2	1:J:294:THR:OG1	2.17	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:D:135[A]:ARG:HD2	3:D:2078:HOH:O	2.16	0.44
1:I:290:MET:HE1	1:I:333:ALA:HA	1.99	0.44
1:F:557:ALA:HB3	1:F:638:MET:HE3	2.00	0.44
1:B:284:PRO:HD3	1:B:326:VAL:HG11	2.00	0.44
1:F:284:PRO:HD3	1:F:326:VAL:HG11	2.00	0.44
1:H:228:VAL:O	1:H:228:VAL:HG12	2.18	0.44
1:J:572:ARG:NH1	3:J:2209:HOH:O	2.51	0.44
1:G:615:MET:N	1:G:616:PRO:HD3	2.33	0.44
1:E:115:ILE:O	1:E:115:ILE:HG13	2.17	0.44
1:D:323:TYR:CE2	1:D:572:ARG:HB2	2.53	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:E:486:ASP:O	1:E:489:THR:O	2.36	0.43
1:I:560:THR:OG1	1:I:573:THR:HG21	2.17	0.43
1:H:555:PRO:HG2	1:H:638:MET:CE	2.40	0.43
1:I:58:MET:HG2	1:I:89:PHE:HB2	1.98	0.43
1:E:360:TYR:HA	1:E:530:MET:HE1	2.01	0.43
1:G:272:MET:HE3	1:G:337:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2:LYS:HD3	1:J:36:ILE:HD11	1.99	0.43
1:A:2:LYS:HD3	1:A:36:ILE:HD11	2.00	0.43
1:J:682:ILE:HD13	1:J:725:GLN:NE2	2.34	0.43
1:F:287:PRO:HB3	1:F:336:LEU:HD11	1.98	0.43
1:F:287:PRO:CD	1:F:525:PRO:HG2	2.47	0.43
1:D:290:MET:HE3	1:D:290:MET:HB3	1.79	0.43
1:C:695:ILE:HB	1:C:739:GLU:HB2	2.00	0.43
1:G:555:PRO:HB2	1:G:638:MET:HE3	1.99	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:E:290:MET:HE3	1:E:290:MET:HB3	1.65	0.43
1:C:290:MET:HE3	1:C:337:LEU:HG	1.99	0.43
1:J:574:THR:OG1	1:J:577:GLN:HB3	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:G:745:ASP:O	1:G:747:ILE:HD12	2.18	0.43
1:G:387:LEU:CD1	1:G:535:LYS:HE3	2.49	0.43
1:J:357:ASN:HA	1:J:358:PRO:HD3	1.89	0.43
1:F:638:MET:CE	1:F:727:TRP:HH2	2.32	0.43
1:A:384:THR:OG1	1:A:390:ALA:CB	2.66	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:C:361:ALA:O	1:C:362:ASP:HB2	2.19	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:F:563:LEU:HD22	1:F:568:ILE:HG21	2.01	0.43
1:I:562:TRP:CD1	1:I:601:PHE:HB2	2.54	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:E:535:LYS:HE3	3:E:2140:HOH:O	2.17	0.43
1:C:290:MET:CE	1:C:337:LEU:HG	2.49	0.42
1:C:468:PHE:CE2	1:D:103:ARG:HD3	2.52	0.42
1:B:42:ASP:HA	1:B:45[B]:PHE:CD2	2.54	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: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:F:94[A]:ARG:HG3	1:F:114:TRP:CE2	2.54	0.42
1:H:537:SER:OG	1:H:579:MET:HG3	2.19	0.42
1:F:320:ASN:O	1:F:348:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:459:GLN:OE1	1:J:500:THR:HG22	2.19	0.42
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:565:ARG:NH1	1:C:617:GLU:OE2	2.52	0.42
1:C:251:ASP:HB2	1:C:317:VAL:O	2.18	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:A:577:GLN:HB3	1:A:577:GLN:HE21	1.63	0.42
1:F:679:LEU:HD22	1:F:749:HIS:CB	2.50	0.42
1:D:572:ARG:HG3	1:D:573:THR:N	2.35	0.42
1:G:272:MET:HE1	1:G:337:LEU:HD21	2.02	0.42
1:C:638:MET:HA	1:C:731:PHE:CZ	2.54	0.42
1:C:459:GLN:OE1	1:C:500:THR:CG2	2.59	0.42
1:H:360:TYR:HA	1:H:530:MET:HE1	2.02	0.42
1:J:507:GLN:OE1	1:J:530:MET:HE1	2.19	0.42
1:H:226:VAL:HG12	1:H:228:VAL:H	1.84	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: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:B:287:PRO:CD	1:B:525:PRO:HG2	2.49	0.42
1:C:558:LEU:HD11	1:C:634:LEU:HD23	2.02	0.42
1:B:715:SER:HA	1:B:716:PRO:HD2	1.97	0.42
1:I:357:ASN:HA	1:I:358:PRO:HD3	1.94	0.42
1:G:119:THR:HB	1:G:122:PHE:CD2	2.55	0.42
1:H:296:GLN:HE22	1:H:310:GLY:H	1.68	0.42
1:D:638:MET:HE2	1:D:727:TRP:HH2	1.84	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:H:2:LYS:HB2	1:H:2:LYS:HE3	1.85	0.41
1:G:272:MET:HE3	1:G:337:LEU:CD2	2.50	0.41
1:H:387:LEU:HD11	1:H:535:LYS:HE2	2.02	0.41
1:G:555:PRO:HB2	1:G:638:MET:CE	2.50	0.41
1:C:586:VAL:HG12	3:C:2199:HOH:O	2.19	0.41
1:A:348:GLU:HB2	1:A:382:HIS:CD2	2.55	0.41
1:E:715:SER:HA	1:E:716:PRO:HD3	1.92	0.41
1:B:685:LEU:N	1:B:686:PRO:CD	2.82	0.41
1:H:363:HIS:CB	1:H:530:MET:HE3	2.49	0.41
1:J:291:GLN:HB3	1:J:293:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ARG:NH2	3:B:2142:HOH:O	2.51	0.41
1:H:363:HIS:ND1	1:H:530:MET:CE	2.84	0.41
1:F:558:LEU:HD11	1:F:634:LEU:HD23	2.01	0.41
1:A:459:GLN:OE1	1:A:500:THR:HG22	2.20	0.41
1:B:155:TYR:O	1:B:163:GLN:CG	2.59	0.41
1:J:290:MET:HE2	1:J:336:LEU:HD12	2.03	0.41
1:H:478:PRO:HB2	1:H:480:ASN:OD1	2.21	0.41
1:A:238:MET:SD	1:A:261:GLY:HA3	2.61	0.41
1:D:287:PRO:HD2	1:D:525:PRO:HG2	2.02	0.41
1:D:22[A]:GLU:OE1	1:D:37:LYS:NZ	2.49	0.41
1:C:239:GLN:CG	1:C:418:HIS:NE2	2.84	0.41
1:I:290:MET:HB3	1:I:290:MET:HE3	1.87	0.41
1:G:565:ARG:NH1	1:G:616:PRO:HD2	2.36	0.41
1:D:386:LYS:NZ	2:D:1386:PLP:O3	2.53	0.41
1:H:58:MET:HG2	1:H:89:PHE:HB2	2.02	0.41
1:D:278:ARG:O	1:D:543:MET:HE3	2.19	0.41
1:B:239:GLN:HG3	1:B:418:HIS:CD2	2.55	0.41
1:I:590:LYS:HD3	1:J:126:ARG:HD3	2.03	0.41
1:F:535:LYS:HE2	3:F:2153:HOH:O	2.21	0.41
1:C:194:ARG:O	1:C:196:SER:N	2.53	0.41
1:I:1:MET:HE3	1:I:33:VAL:HG22	2.03	0.41
1:J:344:LEU:O	1:J:378:VAL:HA	2.19	0.41
1:J:468:PHE:CD2	1:J:602:LYS:HE3	2.55	0.41
1:I:303:PRO:HA	1:I:306:LYS:HE2	2.01	0.41
1:F:320:ASN:O	1:F:348:GLU:HA	2.21	0.41
1:G:701:ILE:HB	1:G:702:PRO:HD2	2.02	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:A:728:ASP:OD1	1:A:735:GLU:HA	2.20	0.41
1:G:314:SER:O	1:G:343:ARG:HD3	2.21	0.41
1:C:507:GLN:NE2	1:C:530:MET:CE	2.83	0.41
1:J:617:GLU:OE1	1:J:617:GLU:N	2.53	0.41
1:A:524:ILE:HA	1:A:525:PRO:HD3	1.92	0.41
1:F:353:TYR:OH	1:F:535:LYS:NZ	2.53	0.41
1:E:348:GLU:HB2	1:E:382:HIS:CD2	2.56	0.41
1:A:562:TRP:CD1	1:A:601:PHE:HB2	2.56	0.41
1:F:562:TRP:CD1	1:F:601:PHE:HB2	2.56	0.41
1:C:353:TYR:OH	1:C:535:LYS:NZ	2.53	0.40
1:G:293:GLU:CD	1:G:293:GLU:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:557:ALA:HB3	1:F:638:MET:CE	2.51	0.40
1:H:468:PHE:CE2	1:I:103:ARG:HD3	2.56	0.40
1:D:569:VAL:HG12	1:D:570:PRO:O	2.20	0.40
1:D:175:ARG:NH2	3:D:2095:HOH:O	2.53	0.40
1:H:685:LEU:N	1:H:686:PRO:CD	2.84	0.40
1:C:359:ILE:O	1:C:530:MET:HE1	2.20	0.40
1:F:360:TYR:HA	1:F:530:MET:HE1	2.02	0.40
1:G:558:LEU:HD12	1:G:558:LEU:HA	1.85	0.40
1:C:323:TYR:HE2	1:C:572:ARG:HB2	1.84	0.40
1:C:588:ARG:NH1	1:C:588:ARG:HG2	2.35	0.40
1:B:386:LYS:NZ	2:B:1386:PLP:O3	2.51	0.40
1:A:334:GLN:HG3	1:A:344:LEU:CD1	2.52	0.40
1:F:353:TYR:OH	1:F:532:ASP:OD2	2.37	0.40
1:D:297:LYS:HE2	1:D:301:GLU:OE2	2.22	0.40
1:F:387:LEU:HD11	1:F:581:LEU:HD11	2.03	0.40
1:F:314:SER:O	1:F:343:ARG:HD3	2.22	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:D:272:MET:CE	1:D:295:LEU:HD21	2.42	0.40
1:G:387:LEU:HD11	1:G:581:LEU:HD11	2.03	0.40
1:G:153:HIS:HD2	1:G:155:TYR:CE1	2.40	0.40
1:I:94:ARG:HG3	1:I:114:TRP:CE2	2.55	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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	766/755 (102%)	742 (97%)	22 (3%)	2 (0%)	46	63
1	C	765/755 (101%)	741 (97%)	23 (3%)	1 (0%)	56	74
1	D	766/755 (102%)	747 (98%)	19 (2%)	0	100	100
1	E	768/755 (102%)	745 (97%)	22 (3%)	1 (0%)	56	74
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%)	56	74

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%)	629 (97%)	20 (3%)	47	69
1	B	650/637 (102%)	637 (98%)	13 (2%)	63	81
1	C	649/637 (102%)	629 (97%)	20 (3%)	47	69
1	D	650/637 (102%)	624 (96%)	26 (4%)	38	58
1	E	652/637 (102%)	639 (98%)	13 (2%)	63	81
1	F	650/637 (102%)	631 (97%)	19 (3%)	50	71
1	G	650/637 (102%)	635 (98%)	15 (2%)	58	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	653/637 (102%)	631 (97%)	22 (3%)	44	65
1	I	651/637 (102%)	631 (97%)	20 (3%)	47	69
1	J	650/637 (102%)	634 (98%)	16 (2%)	55	76
All	All	6504/6370 (102%)	6320 (97%)	184 (3%)	52	72

All (184) 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	276	ARG
1	A	293	GLU
1	A	300	SER
1	A	307	ASP
1	A	384	THR
1	A	420	THR
1	A	480	ASN
1	A	484	VAL
1	A	492	THR
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	696	PRO
1	B	78	LYS
1	B	147	MET
1	B	197	LEU
1	B	222	ARG
1	B	270	VAL
1	B	276	ARG
1	B	480	ASN
1	B	484	VAL
1	B	492	THR
1	B	522	LYS
1	B	571	THR
1	B	662	GLU
1	B	739	GLU

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Mol	Chain	Res	Type
1	C	135[A]	ARG
1	C	135[B]	ARG
1	C	196	SER
1	C	199	SER
1	C	276	ARG
1	C	293	GLU
1	C	335	ASP
1	C	359	ILE
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	579	MET
1	C	586	VAL
1	C	620	GLU
1	C	660	VAL
1	C	706	SER
1	C	719	SER
1	D	61	TYR
1	D	78	LYS
1	D	95	GLU
1	D	135[A]	ARG
1	D	135[B]	ARG
1	D	163	GLN
1	D	194	ARG
1	D	195	THR
1	D	196	SER
1	D	197	LEU
1	D	270	VAL
1	D	276	ARG
1	D	302	SER
1	D	335	ASP
1	D	401	GLU
1	D	484	VAL
1	D	492	THR
1	D	500	THR
1	D	551	GLU
1	D	558	LEU
1	D	571	THR
1	D	572	ARG

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Mol	Chain	Res	Type
1	D	593	THR
1	D	597	THR
1	D	628	ASN
1	D	643	LYS
1	E	78	LYS
1	E	107	GLU
1	E	133[A]	ARG
1	E	133[B]	ARG
1	E	137	GLN
1	E	196	SER
1	E	197	LEU
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	133[A]	ARG
1	F	133[B]	ARG
1	F	152	ILE
1	F	163	GLN
1	F	194	ARG
1	F	197	LEU
1	F	270	VAL
1	F	276	ARG
1	F	301	GLU
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	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	196	SER
1	G	270	VAL
1	G	276	ARG

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Mol	Chain	Res	Type
1	G	335	ASP
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	571	THR
1	G	719	SER
1	H	61	TYR
1	H	78	LYS
1	H	107	GLU
1	H	133[A]	ARG
1	H	133[B]	ARG
1	H	196	SER
1	H	197	LEU
1	H	270	VAL
1	H	276	ARG
1	H	300	SER
1	H	335	ASP
1	H	420	THR
1	H	471	ASP
1	H	480	ASN
1	H	492	THR
1	H	494	ASP
1	H	551	GLU
1	H	558	LEU
1	H	571	THR
1	H	625	THR
1	H	629	MET
1	H	737	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	270	VAL
1	I	276	ARG
1	I	335	ASP

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Mol	Chain	Res	Type
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	723	SER
1	J	133[A]	ARG
1	J	133[B]	ARG
1	J	163	GLN
1	J	195	THR
1	J	196	SER
1	J	197	LEU
1	J	276	ARG
1	J	335	ASP
1	J	384	THR
1	J	480	ASN
1	J	492	THR
1	J	573	THR
1	J	581	LEU
1	J	624	ASP
1	J	628	ASN
1	J	662	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	C	480	ASN
1	C	507	GLN
1	C	692	ASN
1	D	31	GLN
1	D	163	GLN
1	D	480	ASN
1	D	507	GLN
1	D	613	GLN
1	E	80	HIS
1	E	163	GLN
1	E	239	GLN
1	E	374	ASN
1	E	389	ASN
1	E	393	GLN
1	E	507	GLN
1	F	19	ASN
1	F	163	GLN
1	F	239	GLN
1	F	374	ASN
1	F	507	GLN
1	F	628	ASN
1	F	632	HIS
1	G	31	GLN
1	G	153	HIS
1	G	163	GLN
1	G	239	GLN
1	G	374	ASN
1	G	389	ASN
1	G	480	ASN
1	G	507	GLN
1	H	65	HIS
1	H	163	GLN
1	H	296	GLN
1	H	389	ASN
1	H	393	GLN
1	H	566	HIS
1	I	389	ASN
1	I	393	GLN
1	I	692	ASN
1	I	749	HIS
1	J	153	HIS
1	J	163	GLN

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Mol	Chain	Res	Type
1	J	239	GLN
1	J	645	ASN
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 carbohydrates 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	A	1386	1	15,15,16	2.06	4 (26%)	21,22,23	1.65	4 (19%)
2	PLP	B	1386	1	15,15,16	1.97	4 (26%)	21,22,23	2.05	5 (23%)
2	PLP	C	1386	1	15,15,16	1.93	4 (26%)	21,22,23	1.89	4 (19%)
2	PLP	D	1386	1	15,15,16	1.90	3 (20%)	21,22,23	1.92	4 (19%)
2	PLP	E	1386	1	15,15,16	1.97	3 (20%)	21,22,23	1.84	3 (14%)
2	PLP	F	1386	1	15,15,16	1.97	4 (26%)	21,22,23	2.17	6 (28%)
2	PLP	G	1386	1	15,15,16	1.97	5 (33%)	21,22,23	2.21	6 (28%)
2	PLP	H	1386	1	15,15,16	2.04	4 (26%)	21,22,23	2.26	4 (19%)
2	PLP	I	1386	1	15,15,16	2.11	5 (33%)	21,22,23	2.15	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	J	1386	1	15,15,16	2.08	5 (33%)	21,22,23	1.85	5 (23%)

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	A	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	C	1386	1	-	0/6/6/8	0/1/1/1
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	F	1386	1	-	0/6/6/8	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	I	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	J	1386	1	-	0/6/6/8	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1386	PLP	O3-C3	-6.15	1.22	1.37
2	I	1386	PLP	O3-C3	-5.98	1.23	1.37
2	E	1386	PLP	O3-C3	-5.96	1.23	1.37
2	J	1386	PLP	O3-C3	-5.96	1.23	1.37
2	H	1386	PLP	O3-C3	-5.94	1.23	1.37
2	G	1386	PLP	O3-C3	-5.84	1.23	1.37
2	D	1386	PLP	O3-C3	-5.75	1.23	1.37
2	B	1386	PLP	O3-C3	-5.65	1.23	1.37
2	F	1386	PLP	O3-C3	-5.63	1.23	1.37
2	C	1386	PLP	O3-C3	-5.61	1.23	1.37
2	J	1386	PLP	C3-C2	-3.17	1.38	1.40
2	H	1386	PLP	C3-C2	-3.16	1.38	1.40
2	F	1386	PLP	P-O2P	-2.72	1.44	1.54
2	B	1386	PLP	C3-C2	-2.71	1.38	1.40
2	A	1386	PLP	P-O2P	-2.63	1.45	1.54
2	I	1386	PLP	C3-C2	-2.59	1.39	1.40
2	H	1386	PLP	P-O2P	-2.53	1.45	1.54
2	B	1386	PLP	P-O2P	-2.52	1.45	1.54
2	J	1386	PLP	P-O2P	-2.49	1.45	1.54
2	C	1386	PLP	P-O2P	-2.46	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1386	PLP	P-O2P	-2.41	1.46	1.54
2	I	1386	PLP	P-O2P	-2.33	1.46	1.54
2	E	1386	PLP	P-O2P	-2.29	1.46	1.54
2	E	1386	PLP	P-O3P	-2.29	1.46	1.54
2	F	1386	PLP	P-O3P	-2.26	1.46	1.54
2	D	1386	PLP	P-O3P	-2.21	1.46	1.54
2	G	1386	PLP	P-O2P	-2.18	1.46	1.54
2	A	1386	PLP	C3-C2	-2.17	1.39	1.40
2	G	1386	PLP	C3-C2	-2.16	1.39	1.40
2	G	1386	PLP	P-O3P	-2.14	1.47	1.54
2	I	1386	PLP	P-O3P	-2.10	1.47	1.54
2	F	1386	PLP	C3-C2	-2.10	1.39	1.40
2	C	1386	PLP	P-O3P	-2.06	1.47	1.54
2	J	1386	PLP	P-O3P	-2.04	1.47	1.54
2	H	1386	PLP	P-O3P	-2.03	1.47	1.54
2	B	1386	PLP	P-O3P	-2.03	1.47	1.54
2	I	1386	PLP	C5-C4	-2.02	1.38	1.40
2	J	1386	PLP	C2-N1	2.09	1.38	1.34
2	G	1386	PLP	C2-N1	2.11	1.38	1.34
2	A	1386	PLP	C2-N1	2.22	1.38	1.34
2	C	1386	PLP	C2-N1	2.47	1.39	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1386	PLP	O4P-P-O1P	-4.88	94.73	107.14
2	G	1386	PLP	O4P-P-O1P	-4.76	95.02	107.14
2	C	1386	PLP	O4P-P-O1P	-4.45	95.81	107.14
2	D	1386	PLP	O4P-P-O1P	-4.38	95.99	107.14
2	F	1386	PLP	O4P-P-O1P	-4.35	96.08	107.14
2	H	1386	PLP	O4P-P-O1P	-4.07	96.79	107.14
2	I	1386	PLP	O4P-P-O1P	-3.59	97.99	107.14
2	J	1386	PLP	O4P-P-O1P	-3.33	98.66	107.14
2	E	1386	PLP	O4P-P-O1P	-3.25	98.88	107.14
2	F	1386	PLP	C4A-C4-C5	-2.89	117.88	120.88
2	B	1386	PLP	C5-C6-N1	-2.77	119.06	123.86
2	A	1386	PLP	O4P-P-O1P	-2.45	100.91	107.14
2	J	1386	PLP	C5-C6-N1	-2.44	119.62	123.86
2	G	1386	PLP	C4A-C4-C5	-2.34	118.45	120.88
2	G	1386	PLP	C5-C6-N1	-2.25	119.96	123.86
2	I	1386	PLP	C5-C6-N1	-2.13	120.16	123.86
2	D	1386	PLP	C5-C6-N1	-2.12	120.18	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1386	PLP	C5-C6-N1	-2.08	120.25	123.86
2	F	1386	PLP	C5-C6-N1	-2.05	120.30	123.86
2	A	1386	PLP	C6-C5-C4	2.08	119.91	118.15
2	G	1386	PLP	C6-C5-C4	2.17	119.99	118.15
2	A	1386	PLP	O3P-P-O2P	2.17	115.64	107.38
2	H	1386	PLP	O2P-P-O1P	2.23	117.77	110.58
2	I	1386	PLP	O2P-P-O1P	2.30	118.00	110.58
2	E	1386	PLP	C6-C5-C4	2.38	120.16	118.15
2	J	1386	PLP	O2P-P-O1P	2.49	118.59	110.58
2	C	1386	PLP	O2P-P-O1P	2.54	118.75	110.58
2	C	1386	PLP	C6-C5-C4	2.55	120.31	118.15
2	D	1386	PLP	C6-C5-C4	2.69	120.43	118.15
2	F	1386	PLP	O2P-P-O1P	2.73	119.36	110.58
2	F	1386	PLP	C6-C5-C4	2.79	120.51	118.15
2	G	1386	PLP	O2P-P-O1P	2.83	119.68	110.58
2	B	1386	PLP	C6-C5-C4	2.83	120.55	118.15
2	I	1386	PLP	C6-C5-C4	2.85	120.56	118.15
2	B	1386	PLP	O2P-P-O1P	2.97	120.13	110.58
2	J	1386	PLP	C6-C5-C4	3.35	120.99	118.15
2	J	1386	PLP	O4P-C5A-C5	4.72	116.79	108.99
2	A	1386	PLP	O4P-C5A-C5	4.98	117.23	108.99
2	C	1386	PLP	O4P-C5A-C5	5.30	117.75	108.99
2	B	1386	PLP	O4P-C5A-C5	5.48	118.04	108.99
2	D	1386	PLP	O4P-C5A-C5	5.81	118.59	108.99
2	F	1386	PLP	O4P-C5A-C5	5.94	118.81	108.99
2	E	1386	PLP	O4P-C5A-C5	6.12	119.11	108.99
2	G	1386	PLP	O4P-C5A-C5	6.94	120.46	108.99
2	I	1386	PLP	O4P-C5A-C5	7.32	121.09	108.99
2	H	1386	PLP	O4P-C5A-C5	7.88	122.03	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1386	PLP	1	0
2	D	1386	PLP	1	0
2	E	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%)	-0.07	24 (3%)	51	51	10, 23, 41, 56	4 (0%)
1	B	755/755 (100%)	0.06	27 (3%)	46	47	11, 22, 40, 55	5 (0%)
1	C	755/755 (100%)	0.06	29 (3%)	44	45	11, 25, 43, 58	4 (0%)
1	D	755/755 (100%)	-0.18	14 (1%)	70	69	8, 18, 34, 57	3 (0%)
1	E	755/755 (100%)	0.04	30 (3%)	42	43	8, 21, 39, 54	4 (0%)
1	F	755/755 (100%)	0.02	28 (3%)	45	46	10, 22, 38, 57	2 (0%)
1	G	755/755 (100%)	0.08	36 (4%)	34	35	9, 25, 42, 60	7 (0%)
1	H	755/755 (100%)	-0.22	16 (2%)	67	66	6, 15, 32, 59	3 (0%)
1	I	755/755 (100%)	-0.06	23 (3%)	54	53	7, 18, 36, 54	1 (0%)
1	J	755/755 (100%)	-0.00	21 (2%)	56	55	8, 26, 42, 55	4 (0%)
All	All	7550/7550 (100%)	-0.03	248 (3%)	50	50	6, 22, 40, 60	37 (0%)

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	323[A]	TYR	8.5
1	J	323[A]	TYR	7.3
1	F	323[A]	TYR	7.2
1	E	323[A]	TYR	6.9
1	I	323[A]	TYR	6.8
1	B	323[A]	TYR	6.4
1	H	323[A]	TYR	4.9
1	H	155	TYR	4.7
1	C	620	GLU	4.7
1	C	195	THR	4.6
1	F	625	THR	4.6
1	C	623	PRO	4.5
1	E	745	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	195	THR	4.1
1	E	374	ASN	4.1
1	J	300	SER	4.0
1	B	195	THR	3.9
1	D	374	ASN	3.9
1	C	619	VAL	3.9
1	C	755	ALA	3.9
1	F	627	ALA	3.8
1	G	623	PRO	3.8
1	C	193	GLU	3.8
1	D	193	GLU	3.7
1	G	627	ALA	3.6
1	G	572	ARG	3.6
1	F	623	PRO	3.6
1	G	744	ILE	3.6
1	J	729	HIS	3.6
1	D	192	ILE	3.5
1	D	307	ASP	3.5
1	C	65	HIS	3.5
1	J	745	ASP	3.4
1	H	156	SER	3.4
1	G	571	THR	3.4
1	A	195	THR	3.4
1	C	374	ASN	3.3
1	F	489	THR	3.3
1	G	715	SER	3.3
1	H	65	HIS	3.2
1	D	627	ALA	3.2
1	J	488	GLN	3.2
1	A	630	GLY	3.2
1	I	620	GLU	3.2
1	C	624	ASP	3.2
1	J	65	HIS	3.2
1	F	488	GLN	3.2
1	F	745	ASP	3.2
1	B	310	GLY	3.2
1	B	746	GLY	3.1
1	F	729	HIS	3.1
1	B	623	PRO	3.1
1	E	630	GLY	3.1
1	F	374	ASN	3.1
1	G	195	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	619	VAL	3.1
1	G	374	ASN	3.1
1	E	195	THR	3.1
1	D	155	TYR	3.0
1	A	729	HIS	3.0
1	H	153	HIS	3.0
1	F	620	GLU	3.0
1	G	729	HIS	3.0
1	G	619	VAL	3.0
1	E	472	GLY	3.0
1	G	747	ILE	3.0
1	I	624	ASP	3.0
1	F	628	ASN	3.0
1	H	374	ASN	3.0
1	I	619	VAL	3.0
1	C	621	GLN	3.0
1	E	627	ALA	3.0
1	E	471	ASP	2.9
1	C	534	ILE	2.9
1	B	624	ASP	2.9
1	G	309	ALA	2.9
1	E	488	GLN	2.9
1	F	487	PRO	2.9
1	D	195	THR	2.9
1	I	65	HIS	2.9
1	E	307	ASP	2.8
1	B	300	SER	2.8
1	C	515	GLY	2.8
1	E	624	ASP	2.8
1	A	470	ALA	2.8
1	F	624	ASP	2.8
1	C	622	TYR	2.8
1	A	194	ARG	2.8
1	I	621	GLN	2.8
1	E	755	ALA	2.8
1	E	620	GLU	2.7
1	A	469	THR	2.7
1	A	374	ASN	2.7
1	B	471	ASP	2.7
1	F	300	SER	2.7
1	E	623	PRO	2.7
1	G	745	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	626	TYR	2.7
1	A	472	GLY	2.7
1	C	729	HIS	2.7
1	J	489	THR	2.7
1	D	309	ALA	2.7
1	H	371	GLY	2.7
1	B	729	HIS	2.7
1	E	744	ILE	2.6
1	F	746	GLY	2.6
1	G	622	TYR	2.6
1	H	192	ILE	2.6
1	J	156	SER	2.6
1	E	617	GLU	2.6
1	J	627	ALA	2.6
1	B	628	ASN	2.6
1	J	155	TYR	2.6
1	E	726	SER	2.6
1	G	714	ASN	2.6
1	C	625	THR	2.6
1	B	155	TYR	2.5
1	C	323	TYR	2.5
1	G	626	TYR	2.5
1	I	625	THR	2.5
1	C	745	ASP	2.5
1	F	296	GLN	2.5
1	D	156	SER	2.5
1	G	296	GLN	2.5
1	G	621	GLN	2.5
1	A	620	GLU	2.5
1	B	374	ASN	2.5
1	J	746	GLY	2.5
1	I	627	ALA	2.5
1	G	65	HIS	2.5
1	B	711	GLY	2.5
1	B	619	VAL	2.4
1	G	470	ALA	2.4
1	F	641	TRP	2.4
1	A	306	LYS	2.4
1	F	156	SER	2.4
1	H	473	SER	2.4
1	B	470	ALA	2.4
1	E	149	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	755	ALA	2.4
1	C	67	ASP	2.4
1	G	755	ALA	2.4
1	B	730	HIS	2.4
1	G	472	GLY	2.4
1	F	307	ASP	2.4
1	I	149	TYR	2.4
1	B	644	GLU	2.4
1	D	488	GLN	2.4
1	G	254	CYS	2.4
1	F	551	GLU	2.4
1	J	623	PRO	2.4
1	I	628	ASN	2.4
1	F	306	LYS	2.4
1	E	621	GLN	2.4
1	A	623	PRO	2.3
1	C	567	GLY	2.3
1	I	622	TYR	2.3
1	I	153	HIS	2.3
1	G	32[A]	ASN	2.3
1	B	620	GLU	2.3
1	H	620	GLU	2.3
1	I	653	GLU	2.3
1	B	571	THR	2.3
1	H	195	THR	2.3
1	E	572	ARG	2.3
1	F	644	GLU	2.3
1	D	149	TYR	2.3
1	F	626	TYR	2.3
1	D	153	HIS	2.3
1	J	195	THR	2.3
1	A	471	ASP	2.3
1	A	745	ASP	2.3
1	D	624	ASP	2.3
1	C	192	ILE	2.3
1	A	488	GLN	2.3
1	G	641	TRP	2.3
1	I	26[A]	ASP	2.3
1	C	618	LEU	2.3
1	E	714	ASN	2.3
1	I	374	ASN	2.3
1	G	625	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	149	TYR	2.3
1	H	619	VAL	2.3
1	J	307	ASP	2.2
1	B	309	ALA	2.2
1	A	300	SER	2.2
1	I	714	ASN	2.2
1	I	471	ASP	2.2
1	A	371	GLY	2.2
1	C	155	TYR	2.2
1	G	624	ASP	2.2
1	I	156	SER	2.2
1	I	755	ALA	2.2
1	J	755	ALA	2.2
1	G	372	ASP	2.2
1	A	196	SER	2.2
1	J	306	LYS	2.2
1	A	245	ASN	2.2
1	B	629	MET	2.2
1	G	258	ILE	2.2
1	I	195	THR	2.2
1	G	473	SER	2.2
1	I	152	ILE	2.2
1	E	194	ARG	2.2
1	J	637	THR	2.2
1	B	745	ASP	2.2
1	I	729	HIS	2.1
1	A	309	ALA	2.1
1	C	627	ALA	2.1
1	G	293	GLU	2.1
1	J	622	TYR	2.1
1	B	744	ILE	2.1
1	E	26[A]	ASP	2.1
1	E	571	THR	2.1
1	G	310	GLY	2.1
1	G	149	TYR	2.1
1	C	628	ASN	2.1
1	G	711	GLY	2.1
1	A	624	ASP	2.1
1	E	628	ASN	2.1
1	C	637	THR	2.1
1	E	300	SER	2.1
1	G	629	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	299	ILE	2.1
1	F	310	GLY	2.1
1	A	627	ALA	2.1
1	C	488	GLN	2.1
1	B	723	SER	2.1
1	E	309	ALA	2.1
1	A	65	HIS	2.1
1	E	644	GLU	2.1
1	I	310	GLY	2.1
1	J	626	TYR	2.1
1	A	571	THR	2.1
1	F	684	ASN	2.0
1	H	193	GLU	2.0
1	B	12	HIS	2.0
1	E	192	ILE	2.0
1	H	67	ASP	2.0
1	C	32[A]	ASN	2.0
1	D	32[A]	ASN	2.0
1	J	730	HIS	2.0
1	B	307	ASP	2.0
1	H	624	ASP	2.0
1	C	66	PRO	2.0
1	C	616	PRO	2.0
1	J	335	ASP	2.0
1	E	581	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	PLP	A	1386	15/16	0.97	0.43	12.06	2,2,2,4	15
2	PLP	D	1386	15/16	0.98	0.49	10.04	2,2,2,2	15
2	PLP	C	1386	15/16	0.98	0.45	9.83	2,2,4,6	15
2	PLP	H	1386	15/16	0.98	0.44	4.16	2,2,2,2	15
2	PLP	E	1386	15/16	0.97	0.53	4.03	2,2,2,4	15
2	PLP	I	1386	15/16	0.96	0.52	3.80	2,2,2,4	15
2	PLP	B	1386	15/16	0.96	0.46	3.30	2,2,3,5	15
2	PLP	J	1386	15/16	0.97	0.49	3.27	2,2,4,6	15
2	PLP	F	1386	15/16	0.98	0.47	2.97	2,2,2,3	15
2	PLP	G	1386	15/16	0.98	0.50	2.85	2,2,5,8	15

6.5 Other polymers [i](#)

There are no such residues in this entry.