



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:44 AM UTC

PDB ID : 1TBL / pdb_00001tbl
Title : H141N mutant of rat liver arginase I
Authors : Cama, E.; Cox, J.D.; Ash, D.E.; Christianson, D.W.
Deposited on : 2004-05-20
Resolution : 3.10 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

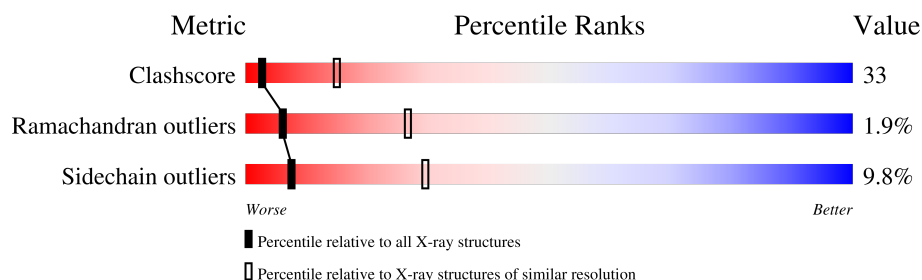
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	C	314	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7217 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 Arginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2394	1526	404	457	7			
1	B	314	Total	C	N	O	S	0	0	0
			2394	1526	404	457	7			
1	C	314	Total	C	N	O	S	0	0	0
			2394	1526	404	457	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ASN	HIS	engineered mutation	UNP P07824
B	141	ASN	HIS	engineered mutation	UNP P07824
C	141	ASN	HIS	engineered mutation	UNP P07824

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	8	Total	O	0	0
			8	8		

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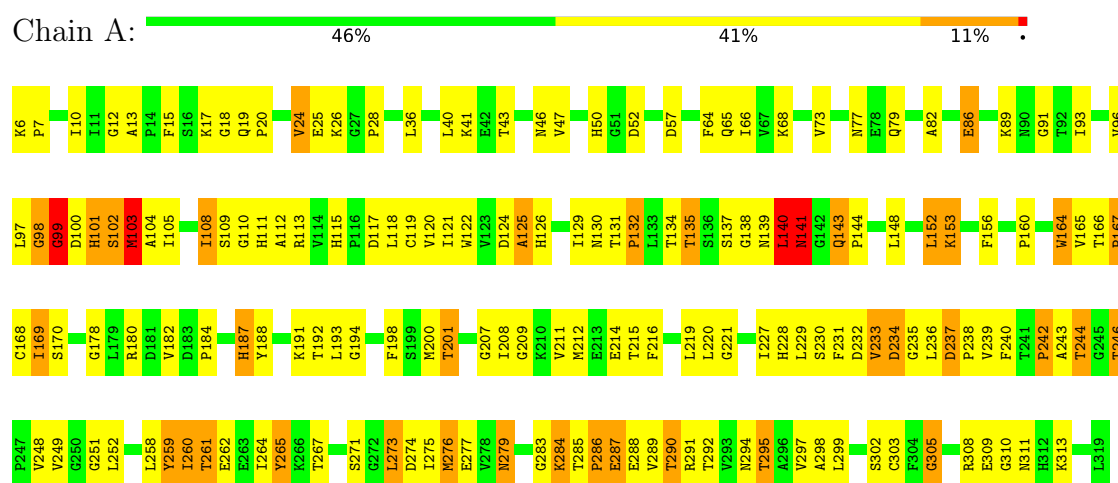
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	12	Total	O	0	0
			12	12		

3 Residue-property plots

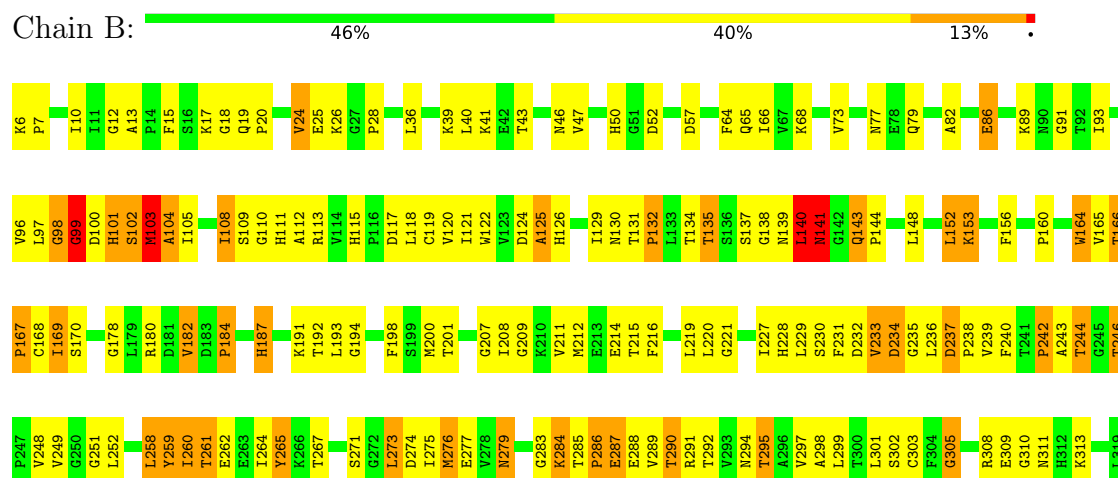
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: Arginase 1

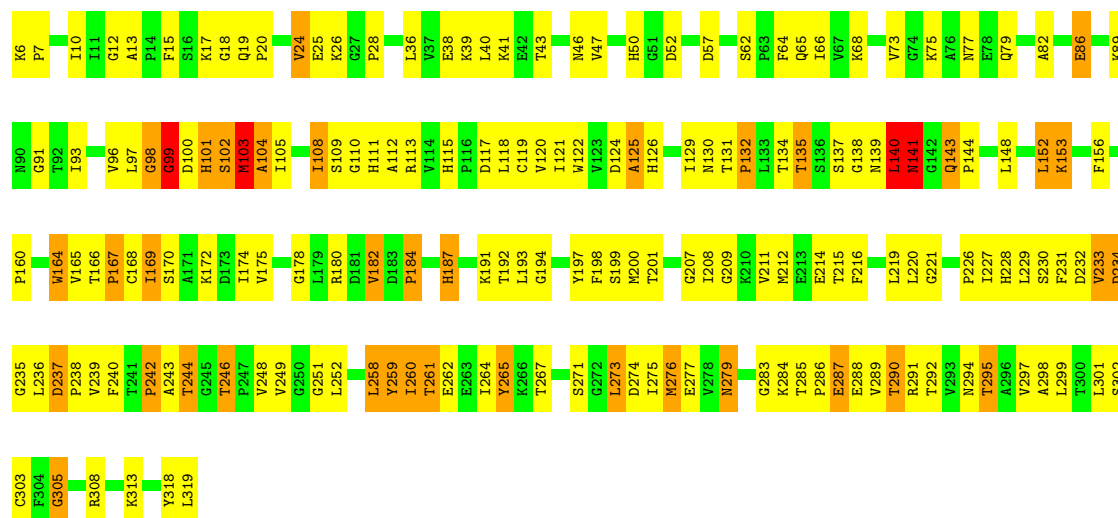


• Molecule 1: Arginase 1



• Molecule 1: Arginase 1





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	88.33Å 88.33Å 113.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.56 – 3.10	Depositor
% Data completeness (in resolution range)	98.8 (45.56-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.298 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7217	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.71	1/2446 (0.0%)	1.18	27/3321 (0.8%)
1	B	0.72	1/2446 (0.0%)	1.18	28/3321 (0.8%)
1	C	0.72	1/2446 (0.0%)	1.18	28/3321 (0.8%)
All	All	0.72	3/7338 (0.0%)	1.18	83/9963 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	LYS	CE-NZ	-7.91	1.25	1.49
1	C	153	LYS	CE-NZ	-7.90	1.25	1.49
1	B	153	LYS	CE-NZ	-7.89	1.25	1.49

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	GLY	N-CA-C	7.62	125.83	115.32
1	B	305	GLY	N-CA-C	7.61	125.82	115.32
1	C	305	GLY	N-CA-C	7.61	125.82	115.32
1	C	125	ALA	N-CA-C	-7.05	104.56	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ALA	N-CA-C	-7.04	104.57	113.72
1	A	125	ALA	N-CA-C	-7.03	104.59	113.72
1	C	265	TYR	N-CA-C	-6.79	103.81	111.14
1	B	265	TYR	N-CA-C	-6.78	103.82	111.14
1	A	265	TYR	N-CA-C	-6.77	103.83	111.14
1	B	96	VAL	N-CA-C	6.68	118.16	107.73
1	A	96	VAL	N-CA-C	6.67	118.14	107.73
1	C	96	VAL	N-CA-C	6.67	118.13	107.73
1	C	99	GLY	N-CA-C	6.30	128.12	113.18
1	C	187	HIS	N-CA-C	-6.29	104.66	112.90
1	B	99	GLY	N-CA-C	6.29	128.08	113.18
1	A	99	GLY	N-CA-C	6.28	128.07	113.18
1	A	187	HIS	N-CA-C	-6.27	104.69	112.90
1	B	187	HIS	N-CA-C	-6.25	104.71	112.90
1	A	234	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	234	ASP	CA-CB-CG	6.20	118.80	112.60
1	B	234	ASP	CA-CB-CG	6.17	118.77	112.60
1	B	249	VAL	N-CA-C	6.08	117.43	109.58
1	C	249	VAL	N-CA-C	6.07	117.41	109.58
1	A	249	VAL	N-CA-C	6.06	117.40	109.58
1	A	108	ILE	N-CA-C	-5.82	105.42	111.58
1	C	108	ILE	N-CA-C	-5.81	105.42	111.58
1	A	86	GLU	N-CA-C	5.81	117.28	111.07
1	B	108	ILE	N-CA-C	-5.81	105.42	111.58
1	B	140	LEU	CA-C-N	-5.78	113.40	122.65
1	B	140	LEU	C-N-CA	-5.78	113.40	122.65
1	C	86	GLU	N-CA-C	5.78	117.25	111.07
1	B	86	GLU	N-CA-C	5.78	117.25	111.07
1	C	182	VAL	N-CA-C	5.77	116.16	107.80
1	A	182	VAL	N-CA-C	5.76	116.15	107.80
1	A	140	LEU	CA-C-N	-5.75	113.44	122.65
1	A	140	LEU	C-N-CA	-5.75	113.44	122.65
1	B	182	VAL	N-CA-C	5.75	116.14	107.80
1	C	140	LEU	CA-C-N	-5.75	113.45	122.65
1	C	140	LEU	C-N-CA	-5.75	113.45	122.65
1	A	141	ASN	CB-CA-C	5.66	120.12	110.56
1	C	141	ASN	CB-CA-C	5.66	120.12	110.56
1	B	141	ASN	CB-CA-C	5.62	120.06	110.56
1	B	259	TYR	N-CA-C	-5.60	104.18	111.02
1	A	164	TRP	N-CA-C	5.60	118.32	111.82
1	A	259	TYR	N-CA-C	-5.59	104.20	111.02
1	C	259	TYR	N-CA-C	-5.58	104.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	TRP	N-CA-C	5.57	118.28	111.82
1	C	164	TRP	N-CA-C	5.57	118.28	111.82
1	C	104	ALA	N-CA-C	-5.54	105.40	111.82
1	A	104	ALA	N-CA-C	-5.53	105.41	111.82
1	B	104	ALA	N-CA-C	-5.51	105.42	111.82
1	C	246	THR	N-CA-C	5.46	118.90	108.97
1	B	246	THR	N-CA-C	5.44	118.86	108.97
1	A	246	THR	N-CA-C	5.43	118.86	108.97
1	C	237	ASP	CA-C-N	5.38	125.03	119.05
1	C	237	ASP	C-N-CA	5.38	125.03	119.05
1	B	237	ASP	CA-C-N	5.38	125.03	119.05
1	B	237	ASP	C-N-CA	5.38	125.03	119.05
1	A	237	ASP	CA-C-N	5.36	124.99	119.05
1	A	237	ASP	C-N-CA	5.36	124.99	119.05
1	C	290	THR	N-CA-C	-5.35	105.36	111.14
1	C	242	PRO	N-CA-C	5.34	120.56	113.57
1	A	290	THR	N-CA-C	-5.34	105.38	111.14
1	A	242	PRO	N-CA-C	5.33	120.55	113.57
1	B	290	THR	N-CA-C	-5.31	105.40	111.14
1	B	242	PRO	N-CA-C	5.30	120.52	113.57
1	C	276	MET	N-CA-C	5.30	118.36	110.14
1	A	276	MET	N-CA-C	5.28	118.33	110.14
1	B	276	MET	N-CA-C	5.28	118.32	110.14
1	C	47	VAL	N-CA-C	5.26	115.47	108.11
1	A	47	VAL	N-CA-C	5.25	115.47	108.11
1	B	47	VAL	N-CA-C	5.23	115.43	108.11
1	C	279	ASN	CA-C-N	5.12	126.24	119.84
1	C	279	ASN	C-N-CA	5.12	126.24	119.84
1	A	279	ASN	CA-C-N	5.12	126.24	119.84
1	A	279	ASN	C-N-CA	5.12	126.24	119.84
1	B	279	ASN	CA-C-N	5.11	126.23	119.84
1	B	279	ASN	C-N-CA	5.11	126.23	119.84
1	B	258	LEU	N-CA-C	-5.05	105.86	111.36
1	B	103	MET	CG-SD-CE	5.03	111.97	100.90
1	C	103	MET	CG-SD-CE	5.03	111.97	100.90
1	A	103	MET	CG-SD-CE	5.03	111.96	100.90
1	C	258	LEU	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	GLY	Peptide
1	B	98	GLY	Peptide
1	C	98	GLY	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	2394	0	2419	163	1
1	B	2394	0	2419	167	1
1	C	2394	0	2419	172	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	9	0	0	1	0
3	B	8	0	0	2	0
3	C	12	0	0	2	0
All	All	7217	0	7257	482	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:SER:HB2	3:C:824:HOH:O	1.59	1.00
1:C:93:ILE:HG23	1:C:271:SER:O	1.71	0.91
1:B:180:ARG:HG3	1:B:248:VAL:HG11	1.53	0.90
1:A:180:ARG:HG3	1:A:248:VAL:HG11	1.53	0.90
1:B:93:ILE:HG23	1:B:271:SER:O	1.71	0.90
1:A:93:ILE:HG23	1:A:271:SER:O	1.71	0.89
1:C:125:ALA:HA	1:C:178:GLY:O	1.73	0.88
1:B:125:ALA:HA	1:B:178:GLY:O	1.73	0.88
1:A:125:ALA:HA	1:A:178:GLY:O	1.73	0.88
1:C:180:ARG:HG3	1:C:248:VAL:HG11	1.54	0.87
1:C:258:LEU:HD23	1:C:299:LEU:HD23	1.58	0.85
1:B:258:LEU:HD23	1:B:299:LEU:HD23	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HD23	1:A:299:LEU:HD23	1.58	0.82
1:A:20:PRO:HA	3:A:820:HOH:O	1.81	0.80
1:C:119:CYS:SG	1:C:227:ILE:HG12	2.23	0.79
1:A:143:GLN:H	1:A:144:PRO:HD3	1.47	0.79
1:C:143:GLN:H	1:C:144:PRO:HD3	1.47	0.79
1:B:119:CYS:SG	1:B:227:ILE:HG12	2.23	0.79
1:B:135:THR:HB	1:B:137:SER:O	1.83	0.78
1:B:143:GLN:H	1:B:144:PRO:HD3	1.47	0.78
1:C:135:THR:HB	1:C:137:SER:O	1.83	0.78
1:A:119:CYS:SG	1:A:227:ILE:HG12	2.23	0.78
1:A:135:THR:HB	1:A:137:SER:O	1.83	0.78
1:C:125:ALA:HB1	1:C:180:ARG:HG2	1.67	0.77
1:B:139:ASN:C	1:B:141:ASN:H	1.92	0.76
1:B:233:VAL:HG12	1:B:244:THR:HG21	1.67	0.76
1:A:125:ALA:HB1	1:A:180:ARG:HG2	1.67	0.76
1:A:233:VAL:HG12	1:A:244:THR:HG21	1.67	0.76
1:B:125:ALA:HB1	1:B:180:ARG:HG2	1.67	0.76
1:C:233:VAL:HG12	1:C:244:THR:HG21	1.67	0.76
1:B:130:ASN:HB3	1:B:135:THR:HG23	1.68	0.76
1:C:130:ASN:HB3	1:C:135:THR:HG23	1.68	0.76
1:C:139:ASN:C	1:C:141:ASN:H	1.92	0.75
1:A:258:LEU:O	1:A:262:GLU:HG3	1.87	0.75
1:C:258:LEU:O	1:C:262:GLU:HG3	1.87	0.75
1:A:130:ASN:HB3	1:A:135:THR:HG23	1.68	0.74
1:A:101:HIS:HA	1:A:276:MET:HE3	1.70	0.74
1:C:101:HIS:HA	1:C:276:MET:HE3	1.70	0.74
1:A:139:ASN:C	1:A:141:ASN:H	1.92	0.74
1:C:18:GLY:O	1:C:141:ASN:HB3	1.88	0.73
1:B:28:PRO:HD3	1:B:98:GLY:O	1.89	0.73
1:B:258:LEU:O	1:B:262:GLU:HG3	1.87	0.73
1:A:219:LEU:O	1:A:220:LEU:HD23	1.89	0.73
1:A:18:GLY:O	1:A:141:ASN:HB3	1.88	0.73
1:B:219:LEU:O	1:B:220:LEU:HD23	1.89	0.72
1:C:219:LEU:O	1:C:220:LEU:HD23	1.89	0.72
1:B:18:GLY:O	1:B:141:ASN:HB3	1.88	0.72
1:A:28:PRO:HD3	1:A:98:GLY:O	1.89	0.72
1:B:101:HIS:HA	1:B:276:MET:HE3	1.70	0.72
1:C:28:PRO:HD3	1:C:98:GLY:O	1.89	0.72
1:B:143:GLN:N	1:B:144:PRO:CD	2.53	0.71
1:A:143:GLN:N	1:A:144:PRO:CD	2.53	0.71
1:C:143:GLN:N	1:C:144:PRO:CD	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ARG:NH2	1:C:251:GLY:CA	2.54	0.71
1:A:180:ARG:NH2	1:A:251:GLY:CA	2.54	0.71
1:B:180:ARG:NH2	1:B:251:GLY:CA	2.53	0.71
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.26	0.70
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.26	0.70
1:A:153:LYS:HD2	1:A:167:PRO:HG2	1.74	0.70
1:B:153:LYS:HD2	1:B:167:PRO:HG2	1.74	0.70
1:C:153:LYS:HD2	1:C:167:PRO:HG2	1.74	0.69
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.26	0.69
1:A:12:GLY:HA3	1:A:52:ASP:OD1	1.93	0.68
1:B:12:GLY:HA3	1:B:52:ASP:OD1	1.93	0.68
1:A:6:LYS:HE2	1:A:91:GLY:O	1.94	0.67
1:C:12:GLY:HA3	1:C:52:ASP:OD1	1.93	0.67
1:B:6:LYS:HE2	1:B:91:GLY:O	1.94	0.66
1:C:25:GLU:HG2	1:C:26:LYS:N	2.09	0.66
1:B:180:ARG:HD2	1:B:248:VAL:HB	1.77	0.66
1:C:6:LYS:HE2	1:C:91:GLY:O	1.94	0.66
1:A:25:GLU:HG2	1:A:26:LYS:N	2.09	0.66
1:B:25:GLU:HG2	1:B:26:LYS:N	2.09	0.66
1:C:139:ASN:C	1:C:141:ASN:N	2.53	0.66
1:A:118:LEU:O	1:A:118:LEU:HD12	1.96	0.66
1:C:258:LEU:CD2	1:C:299:LEU:HD23	2.27	0.65
1:B:118:LEU:HD12	1:B:118:LEU:O	1.96	0.65
1:A:180:ARG:HD2	1:A:248:VAL:HB	1.77	0.65
1:C:118:LEU:HD12	1:C:118:LEU:O	1.96	0.65
1:C:180:ARG:HD2	1:C:248:VAL:HB	1.77	0.65
1:B:168:CYS:SG	1:B:169:ILE:HG23	2.37	0.65
1:C:168:CYS:SG	1:C:169:ILE:HG23	2.37	0.64
1:A:180:ARG:NH2	1:A:251:GLY:HA3	2.13	0.64
1:A:168:CYS:SG	1:A:169:ILE:HG23	2.37	0.64
1:A:198:PHE:CD2	1:A:211:VAL:HG13	2.33	0.64
1:C:198:PHE:CD2	1:C:211:VAL:HG13	2.33	0.64
1:C:180:ARG:NH2	1:C:251:GLY:HA3	2.13	0.63
1:B:110:GLY:O	1:B:113:ARG:HB2	1.99	0.63
1:B:198:PHE:CD2	1:B:211:VAL:HG13	2.33	0.63
1:C:110:GLY:O	1:C:113:ARG:HB2	1.99	0.63
1:A:110:GLY:O	1:A:113:ARG:HB2	1.99	0.63
1:A:188:TYR:CD2	1:C:318:TYR:HB2	2.34	0.63
1:B:139:ASN:C	1:B:141:ASN:N	2.53	0.63
1:A:311:ASN:O	1:B:184:PRO:HA	1.99	0.62
1:A:258:LEU:CD2	1:A:299:LEU:HD23	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:PHE:CB	1:C:103:MET:SD	2.87	0.62
1:A:15:PHE:CB	1:A:103:MET:SD	2.87	0.62
1:B:15:PHE:CB	1:B:103:MET:SD	2.87	0.62
1:B:180:ARG:NH2	1:B:251:GLY:HA3	2.13	0.62
1:B:258:LEU:CD2	1:B:299:LEU:HD23	2.27	0.62
1:B:143:GLN:N	1:B:144:PRO:HD3	2.14	0.62
1:C:211:VAL:O	1:C:215:THR:HG23	2.00	0.62
1:A:211:VAL:O	1:A:215:THR:HG23	2.00	0.62
1:A:40:LEU:O	1:A:43:THR:HG23	2.00	0.61
1:B:180:ARG:NH2	1:B:235:GLY:O	2.29	0.61
1:A:233:VAL:HG12	1:A:244:THR:CG2	2.30	0.61
1:C:40:LEU:O	1:C:43:THR:HG23	2.00	0.61
1:B:233:VAL:HG12	1:B:244:THR:CG2	2.30	0.61
1:A:188:TYR:HE2	1:C:319:LEU:HG	1.64	0.61
1:C:283:GLY:HA3	1:C:289:VAL:CG2	2.31	0.61
1:A:50:HIS:O	1:A:50:HIS:ND1	2.34	0.61
1:B:50:HIS:O	1:B:50:HIS:ND1	2.34	0.61
1:C:50:HIS:O	1:C:50:HIS:ND1	2.34	0.60
1:A:283:GLY:HA3	1:A:289:VAL:CG2	2.31	0.60
1:B:283:GLY:HA3	1:B:289:VAL:CG2	2.31	0.60
1:B:40:LEU:O	1:B:43:THR:HG23	2.00	0.60
1:B:211:VAL:O	1:B:215:THR:HG23	2.00	0.60
1:C:180:ARG:NH2	1:C:251:GLY:HA2	2.17	0.60
1:A:180:ARG:NH2	1:A:235:GLY:O	2.29	0.60
1:A:192:THR:HG22	1:A:193:LEU:HD12	1.84	0.60
1:C:233:VAL:HG12	1:C:244:THR:CG2	2.30	0.60
1:B:311:ASN:O	1:C:184:PRO:HA	2.02	0.59
1:B:12:GLY:HA3	1:B:52:ASP:HA	1.82	0.59
1:C:12:GLY:HA3	1:C:52:ASP:HA	1.83	0.59
1:C:192:THR:HG22	1:C:193:LEU:HD12	1.84	0.59
1:A:12:GLY:HA3	1:A:52:ASP:HA	1.82	0.59
1:B:192:THR:HG22	1:B:193:LEU:HD12	1.84	0.59
1:A:180:ARG:HG3	1:A:248:VAL:CG1	2.31	0.59
1:C:143:GLN:N	1:C:144:PRO:HD3	2.14	0.59
1:A:180:ARG:CZ	1:A:251:GLY:HA3	2.33	0.59
1:A:139:ASN:C	1:A:141:ASN:N	2.53	0.59
1:C:180:ARG:CZ	1:C:251:GLY:HA3	2.33	0.59
1:A:180:ARG:NH2	1:A:251:GLY:HA2	2.17	0.58
1:B:180:ARG:NH2	1:B:251:GLY:HA2	2.17	0.58
1:C:285:THR:OG1	1:C:288:GLU:HG3	2.04	0.58
1:B:285:THR:OG1	1:B:288:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:PRO:HD3	1:C:139:ASN:ND2	2.19	0.57
1:B:20:PRO:HD3	1:B:139:ASN:ND2	2.19	0.57
1:A:285:THR:OG1	1:A:288:GLU:HG3	2.04	0.57
1:C:180:ARG:HG3	1:C:248:VAL:CG1	2.31	0.57
1:B:180:ARG:CZ	1:B:251:GLY:HA3	2.33	0.57
1:C:258:LEU:HD23	1:C:299:LEU:CD2	2.34	0.57
1:A:20:PRO:HD3	1:A:139:ASN:ND2	2.19	0.57
1:B:100:ASP:OD1	1:B:102:SER:OG	2.23	0.57
1:B:143:GLN:H	1:B:144:PRO:CD	2.13	0.57
1:C:180:ARG:NH2	1:C:235:GLY:O	2.29	0.56
1:B:258:LEU:HD23	1:B:299:LEU:CD2	2.34	0.56
1:B:180:ARG:HG3	1:B:248:VAL:CG1	2.31	0.56
1:A:258:LEU:HD23	1:A:299:LEU:CD2	2.34	0.56
1:B:180:ARG:CZ	1:B:251:GLY:CA	2.84	0.55
1:C:198:PHE:CE1	1:C:215:THR:HG22	2.41	0.55
1:A:188:TYR:CD1	1:C:318:TYR:HD2	2.24	0.55
1:A:180:ARG:CZ	1:A:251:GLY:CA	2.84	0.55
1:C:180:ARG:CZ	1:C:251:GLY:CA	2.84	0.55
1:A:201:THR:CG2	1:C:308:ARG:HB2	2.37	0.55
1:A:198:PHE:CE1	1:A:215:THR:HG22	2.41	0.55
1:B:15:PHE:CG	1:B:103:MET:SD	3.00	0.55
1:B:308:ARG:NH1	1:C:200:MET:HB3	2.21	0.55
1:B:198:PHE:CE1	1:B:215:THR:HG22	2.41	0.55
1:A:232:ASP:OD1	1:A:234:ASP:OD2	2.26	0.54
1:A:200:MET:HB3	1:C:308:ARG:NH1	2.22	0.54
1:B:232:ASP:OD1	1:B:234:ASP:OD2	2.26	0.54
1:C:232:ASP:OD1	1:C:234:ASP:OD2	2.26	0.54
1:A:231:PHE:CZ	1:A:299:LEU:HD13	2.42	0.54
1:B:231:PHE:CZ	1:B:299:LEU:HD13	2.42	0.54
1:C:15:PHE:CG	1:C:103:MET:SD	3.00	0.54
1:A:15:PHE:CG	1:A:103:MET:SD	3.00	0.54
1:A:101:HIS:CE1	1:A:122:TRP:CZ2	2.96	0.54
1:C:231:PHE:CZ	1:C:299:LEU:HD13	2.42	0.53
1:B:101:HIS:CE1	1:B:122:TRP:CZ2	2.96	0.53
1:B:244:THR:CG2	1:B:277:GLU:O	2.57	0.53
1:C:101:HIS:CE1	1:C:122:TRP:CZ2	2.96	0.53
1:A:309:GLU:OE2	1:B:187:HIS:NE2	2.38	0.53
1:B:36:LEU:HD13	1:B:297:VAL:HG13	1.90	0.53
1:C:244:THR:CG2	1:C:277:GLU:O	2.57	0.53
1:A:132:PRO:HD2	1:A:156:PHE:CD2	2.44	0.53
1:C:132:PRO:HD2	1:C:156:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LEU:HD12	1:B:229:LEU:C	2.34	0.53
1:C:36:LEU:HD13	1:C:297:VAL:HG13	1.90	0.53
1:A:36:LEU:HD13	1:A:297:VAL:HG13	1.90	0.52
1:A:100:ASP:OD1	1:A:102:SER:OG	2.23	0.52
1:A:244:THR:CG2	1:A:277:GLU:O	2.57	0.52
1:A:283:GLY:HA3	1:A:289:VAL:HG23	1.91	0.52
1:B:273:LEU:HD13	1:B:275:ILE:HD11	1.92	0.52
1:C:229:LEU:C	1:C:229:LEU:HD12	2.34	0.52
1:C:283:GLY:HA3	1:C:289:VAL:HG23	1.91	0.52
1:A:200:MET:HB2	1:C:308:ARG:HD2	1.91	0.52
1:B:131:THR:N	1:B:134:THR:OG1	2.42	0.51
1:B:283:GLY:HA3	1:B:289:VAL:HG23	1.91	0.51
1:C:212:MET:CE	1:C:260:ILE:HG23	2.40	0.51
1:A:228:HIS:NE2	1:A:274:ASP:OD2	2.42	0.51
1:A:229:LEU:O	1:A:273:LEU:HD23	2.10	0.51
1:C:100:ASP:OD1	1:C:102:SER:OG	2.23	0.51
1:A:86:GLU:O	1:A:89:LYS:HB3	2.11	0.51
1:A:229:LEU:C	1:A:229:LEU:HD12	2.34	0.51
1:B:132:PRO:HD2	1:B:156:PHE:CD2	2.44	0.51
1:B:212:MET:CE	1:B:260:ILE:HG23	2.40	0.51
1:B:287:GLU:HG3	1:B:288:GLU:N	2.25	0.51
1:A:273:LEU:HD13	1:A:275:ILE:HD11	1.92	0.51
1:B:73:VAL:HG11	1:B:140:LEU:HD13	1.92	0.51
1:C:15:PHE:CD2	1:C:103:MET:SD	3.04	0.51
1:C:287:GLU:HG3	1:C:288:GLU:N	2.25	0.51
1:B:229:LEU:O	1:B:273:LEU:HD23	2.10	0.51
1:C:73:VAL:HG11	1:C:140:LEU:HD13	1.93	0.51
1:A:212:MET:CE	1:A:260:ILE:HG23	2.40	0.51
1:A:15:PHE:CD2	1:A:103:MET:SD	3.04	0.50
1:A:287:GLU:HG3	1:A:288:GLU:N	2.25	0.50
1:C:229:LEU:O	1:C:273:LEU:HD23	2.10	0.50
1:A:152:LEU:CD1	1:A:193:LEU:HD21	2.42	0.50
1:B:15:PHE:CD2	1:B:103:MET:SD	3.04	0.50
1:B:64:PHE:O	1:B:65:GLN:HB2	2.12	0.50
1:B:86:GLU:O	1:B:89:LYS:HB3	2.11	0.50
1:C:152:LEU:CD1	1:C:193:LEU:HD21	2.42	0.50
1:C:228:HIS:NE2	1:C:274:ASP:OD2	2.41	0.50
1:A:73:VAL:HG11	1:A:140:LEU:HD13	1.92	0.50
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.94	0.50
1:C:64:PHE:O	1:C:65:GLN:HB2	2.12	0.50
1:C:143:GLN:H	1:C:144:PRO:CD	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLU:O	1:C:89:LYS:HB3	2.11	0.50
1:A:310:GLY:HA3	1:B:182:VAL:HB	1.94	0.50
1:C:273:LEU:HD13	1:C:275:ILE:HD11	1.92	0.50
1:B:152:LEU:CD1	1:B:193:LEU:HD21	2.41	0.50
1:A:13:ALA:HB3	1:A:97:LEU:O	2.12	0.50
1:A:64:PHE:O	1:A:65:GLN:HB2	2.12	0.50
1:B:13:ALA:HB3	1:B:97:LEU:O	2.12	0.50
1:C:19:GLN:HB2	1:C:20:PRO:HD2	1.94	0.50
1:C:121:ILE:CD1	1:C:264:ILE:HD11	2.42	0.50
1:A:121:ILE:CD1	1:A:264:ILE:HD11	2.42	0.49
1:A:291:ARG:O	1:A:292:THR:C	2.55	0.49
1:B:291:ARG:O	1:B:292:THR:C	2.55	0.49
1:A:299:LEU:O	1:A:302:SER:HB3	2.13	0.49
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.94	0.49
1:B:124:ASP:HA	1:B:232:ASP:HB3	1.95	0.49
1:B:236:LEU:HB3	1:B:252:LEU:O	2.12	0.49
1:C:240:PHE:C	1:C:242:PRO:HD3	2.38	0.49
1:C:131:THR:N	1:C:134:THR:OG1	2.42	0.49
1:C:299:LEU:O	1:C:302:SER:HB3	2.13	0.49
1:C:236:LEU:HB3	1:C:252:LEU:O	2.12	0.49
1:C:291:ARG:O	1:C:292:THR:C	2.55	0.49
1:A:111:HIS:CE1	1:A:271:SER:HB3	2.48	0.49
1:A:232:ASP:CG	1:A:234:ASP:OD2	2.56	0.49
1:B:299:LEU:O	1:B:302:SER:HB3	2.13	0.49
1:C:13:ALA:HB3	1:C:97:LEU:O	2.12	0.49
1:C:124:ASP:HA	1:C:232:ASP:HB3	1.95	0.49
1:A:236:LEU:HB3	1:A:252:LEU:O	2.12	0.49
1:B:228:HIS:NE2	1:B:274:ASP:OD2	2.41	0.49
1:B:121:ILE:HD13	1:B:264:ILE:HD11	1.95	0.48
1:C:111:HIS:CE1	1:C:271:SER:HB3	2.48	0.48
1:A:121:ILE:HD13	1:A:264:ILE:HD11	1.95	0.48
1:A:124:ASP:HA	1:A:232:ASP:HB3	1.95	0.48
1:A:240:PHE:C	1:A:242:PRO:HD3	2.38	0.48
1:B:111:HIS:CE1	1:B:271:SER:HB3	2.48	0.48
1:A:131:THR:N	1:A:134:THR:OG1	2.42	0.48
1:B:121:ILE:CD1	1:B:264:ILE:HD11	2.42	0.48
1:B:240:PHE:C	1:B:242:PRO:HD3	2.38	0.48
1:B:230:SER:HA	1:B:274:ASP:HB2	1.96	0.48
1:C:232:ASP:CG	1:C:234:ASP:OD2	2.56	0.48
1:B:193:LEU:O	1:B:194:GLY:C	2.57	0.48
1:B:232:ASP:OD1	1:B:234:ASP:CG	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ASP:CG	1:B:234:ASP:OD2	2.56	0.48
1:A:290:THR:HG22	1:A:294:ASN:OD1	2.14	0.48
1:B:6:LYS:HD2	1:B:7:PRO:HD3	1.96	0.48
1:A:232:ASP:OD1	1:A:234:ASP:CG	2.57	0.47
1:C:121:ILE:HD13	1:C:264:ILE:HD11	1.95	0.47
1:C:290:THR:HG22	1:C:294:ASN:OD1	2.14	0.47
1:A:6:LYS:HD2	1:A:7:PRO:HD3	1.96	0.47
1:B:117:ASP:OD1	1:B:117:ASP:N	2.44	0.47
1:B:216:PHE:CZ	1:B:267:THR:HG21	2.49	0.47
1:C:40:LEU:O	1:C:41:LYS:C	2.58	0.47
1:C:232:ASP:OD1	1:C:234:ASP:CG	2.57	0.47
1:A:117:ASP:OD1	1:A:117:ASP:N	2.44	0.47
1:A:193:LEU:O	1:A:194:GLY:C	2.57	0.47
1:A:230:SER:HA	1:A:274:ASP:HB2	1.96	0.47
1:B:290:THR:HG22	1:B:294:ASN:OD1	2.14	0.47
1:C:6:LYS:HD2	1:C:7:PRO:HD3	1.96	0.47
1:C:68:LYS:HG3	1:C:138:GLY:HA3	1.96	0.47
1:C:216:PHE:CZ	1:C:267:THR:HG21	2.49	0.47
1:A:102:SER:HA	1:A:144:PRO:HG3	1.96	0.47
1:A:216:PHE:CZ	1:A:267:THR:HG21	2.49	0.47
1:B:68:LYS:HG3	1:B:138:GLY:HA3	1.96	0.47
1:A:68:LYS:HG3	1:A:138:GLY:HA3	1.96	0.47
1:C:230:SER:HA	1:C:274:ASP:HB2	1.96	0.47
1:C:236:LEU:HD23	1:C:252:LEU:HB2	1.97	0.47
1:A:102:SER:O	1:A:105:ILE:HG13	2.15	0.46
1:B:236:LEU:HD23	1:B:252:LEU:HB2	1.97	0.46
1:B:309:GLU:OE1	1:C:197:TYR:OH	2.24	0.46
1:C:102:SER:HA	1:C:144:PRO:HG3	1.96	0.46
1:C:193:LEU:O	1:C:194:GLY:C	2.57	0.46
1:A:236:LEU:HD23	1:A:252:LEU:HB2	1.97	0.46
1:B:40:LEU:O	1:B:41:LYS:C	2.58	0.46
1:B:102:SER:O	1:B:105:ILE:HG13	2.15	0.46
1:B:126:HIS:CE1	1:B:234:ASP:OD1	2.69	0.46
1:A:40:LEU:O	1:A:41:LYS:C	2.58	0.46
1:A:208:ILE:HG23	1:A:209:GLY:N	2.31	0.46
1:A:258:LEU:O	1:A:259:TYR:C	2.59	0.46
1:A:187:HIS:O	1:A:191:LYS:HG2	2.16	0.46
1:B:187:HIS:O	1:B:191:LYS:HG2	2.16	0.46
1:C:244:THR:HG23	1:C:277:GLU:O	2.16	0.46
1:B:139:ASN:O	1:B:141:ASN:N	2.49	0.46
1:B:102:SER:HA	1:B:144:PRO:HG3	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:HIS:CE1	1:A:234:ASP:OD1	2.69	0.45
1:A:139:ASN:O	1:A:141:ASN:N	2.49	0.45
1:A:15:PHE:O	1:A:99:GLY:HA3	2.16	0.45
1:A:214:GLU:O	1:A:215:THR:C	2.60	0.45
1:A:15:PHE:HB3	1:A:103:MET:SD	2.57	0.45
1:B:308:ARG:NH1	1:C:200:MET:CB	2.79	0.45
1:C:139:ASN:O	1:C:141:ASN:N	2.49	0.45
1:C:236:LEU:HA	1:C:252:LEU:HB2	1.99	0.45
1:B:259:TYR:O	1:B:260:ILE:C	2.59	0.45
1:C:101:HIS:O	1:C:103:MET:N	2.50	0.45
1:C:102:SER:O	1:C:105:ILE:HG13	2.15	0.45
1:C:126:HIS:CE1	1:C:234:ASP:OD1	2.69	0.45
1:B:208:ILE:HG23	1:B:209:GLY:N	2.31	0.45
1:A:244:THR:HG23	1:A:277:GLU:O	2.16	0.45
1:B:101:HIS:O	1:B:103:MET:N	2.50	0.45
1:B:236:LEU:HA	1:B:252:LEU:HB2	1.99	0.45
1:C:15:PHE:HB3	1:C:103:MET:SD	2.57	0.45
1:C:258:LEU:O	1:C:259:TYR:C	2.59	0.45
1:B:15:PHE:O	1:B:99:GLY:HA3	2.16	0.45
1:A:124:ASP:OD1	1:A:234:ASP:OD1	2.35	0.45
1:A:259:TYR:O	1:A:260:ILE:C	2.59	0.45
1:B:214:GLU:O	1:B:215:THR:C	2.60	0.45
1:B:265:TYR:CD1	1:B:305:GLY:N	2.85	0.45
1:B:124:ASP:OD1	1:B:234:ASP:OD1	2.35	0.45
1:C:187:HIS:O	1:C:191:LYS:HG2	2.16	0.45
1:C:208:ILE:HG13	1:C:259:TYR:HD2	1.82	0.45
1:C:265:TYR:CD1	1:C:305:GLY:N	2.85	0.45
1:A:101:HIS:O	1:A:103:MET:N	2.50	0.44
1:B:258:LEU:O	1:B:259:TYR:C	2.59	0.44
1:B:310:GLY:HA3	1:C:182:VAL:HB	1.99	0.44
1:C:208:ILE:HG23	1:C:209:GLY:N	2.31	0.44
1:A:208:ILE:CG2	1:A:209:GLY:N	2.81	0.44
1:A:308:ARG:NH1	1:B:200:MET:HB3	2.32	0.44
1:A:265:TYR:CD1	1:A:305:GLY:N	2.85	0.44
1:C:15:PHE:O	1:C:99:GLY:HA3	2.16	0.44
1:C:180:ARG:CZ	1:C:251:GLY:HA2	2.48	0.44
1:A:208:ILE:HG13	1:A:259:TYR:HD2	1.82	0.44
1:B:207:GLY:O	1:B:208:ILE:C	2.61	0.44
1:C:208:ILE:CG2	1:C:209:GLY:N	2.81	0.44
1:C:214:GLU:O	1:C:215:THR:C	2.60	0.44
1:B:15:PHE:HB3	1:B:103:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:CZ	1:B:251:GLY:HA2	2.48	0.44
1:C:124:ASP:OD1	1:C:234:ASP:OD1	2.35	0.44
1:C:295:THR:O	1:C:298:ALA:HB3	2.18	0.44
1:C:198:PHE:CG	1:C:211:VAL:HG13	2.53	0.44
1:A:207:GLY:O	1:A:208:ILE:C	2.61	0.44
1:A:236:LEU:HA	1:A:252:LEU:HB2	1.99	0.44
1:B:180:ARG:HD2	1:B:248:VAL:CB	2.47	0.44
1:B:198:PHE:CG	1:B:211:VAL:HG13	2.53	0.44
1:B:207:GLY:O	1:B:211:VAL:HG23	2.18	0.44
1:A:231:PHE:CZ	1:A:299:LEU:CD1	3.01	0.43
1:B:231:PHE:CZ	1:B:299:LEU:CD1	3.01	0.43
1:B:295:THR:O	1:B:298:ALA:HB3	2.18	0.43
1:C:209:GLY:HA2	1:C:259:TYR:CE2	2.53	0.43
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.83	0.43
1:A:295:THR:O	1:A:298:ALA:HB3	2.18	0.43
1:B:209:GLY:HA2	1:B:259:TYR:CE2	2.53	0.43
1:B:164:TRP:CZ3	1:B:165:VAL:HG22	2.53	0.43
1:C:207:GLY:O	1:C:211:VAL:HG23	2.18	0.43
1:A:180:ARG:HD2	1:A:248:VAL:CB	2.47	0.43
1:A:200:MET:HB3	1:C:308:ARG:HH11	1.84	0.43
1:B:260:ILE:O	1:B:262:GLU:N	2.52	0.43
1:C:20:PRO:HD3	1:C:139:ASN:CG	2.44	0.43
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.92	0.43
1:A:180:ARG:CZ	1:A:251:GLY:HA2	2.48	0.43
1:A:260:ILE:O	1:A:261:THR:C	2.62	0.43
1:B:166:THR:CG2	3:B:819:HOH:O	2.67	0.43
1:C:164:TRP:CZ3	1:C:165:VAL:HG22	2.53	0.43
1:A:244:THR:HG22	1:A:277:GLU:O	2.18	0.43
1:B:101:HIS:O	1:B:104:ALA:N	2.40	0.43
1:B:244:THR:HG23	1:B:277:GLU:O	2.16	0.43
1:C:15:PHE:HE2	1:C:73:VAL:HG22	1.84	0.43
1:A:15:PHE:HE2	1:A:73:VAL:HG22	1.84	0.43
1:B:10:ILE:N	1:B:10:ILE:HD12	2.34	0.43
1:C:172:LYS:HA	1:C:172:LYS:HD2	1.82	0.43
1:C:231:PHE:CZ	1:C:299:LEU:CD1	3.01	0.43
1:A:10:ILE:HD12	1:A:10:ILE:N	2.34	0.43
1:A:207:GLY:O	1:A:211:VAL:HG23	2.18	0.43
1:A:209:GLY:HA2	1:A:259:TYR:CE2	2.53	0.43
1:B:15:PHE:HE2	1:B:73:VAL:HG22	1.84	0.43
1:B:208:ILE:HG13	1:B:259:TYR:HD2	1.82	0.43
1:B:244:THR:HG22	1:B:277:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PRO:HD3	1:A:139:ASN:CG	2.44	0.43
1:A:260:ILE:O	1:A:262:GLU:N	2.52	0.43
1:B:208:ILE:CG2	1:B:209:GLY:N	2.81	0.43
1:C:260:ILE:O	1:C:262:GLU:N	2.52	0.43
1:B:166:THR:HG21	3:B:819:HOH:O	2.18	0.42
1:A:198:PHE:CG	1:A:211:VAL:HG13	2.53	0.42
1:C:101:HIS:O	1:C:102:SER:C	2.62	0.42
1:C:244:THR:HG22	1:C:277:GLU:O	2.18	0.42
1:C:259:TYR:O	1:C:260:ILE:C	2.59	0.42
1:A:164:TRP:CZ3	1:A:165:VAL:HG22	2.53	0.42
1:A:239:VAL:O	1:A:239:VAL:HG12	2.20	0.42
1:C:120:VAL:HG22	1:C:228:HIS:HB3	2.02	0.42
1:C:220:LEU:O	1:C:221:GLY:C	2.62	0.42
1:A:79:GLN:O	1:A:82:ALA:HB3	2.19	0.42
1:B:79:GLN:O	1:B:82:ALA:HB3	2.19	0.42
1:B:101:HIS:O	1:B:102:SER:C	2.62	0.42
1:A:101:HIS:O	1:A:102:SER:C	2.62	0.42
1:A:220:LEU:O	1:A:221:GLY:C	2.62	0.42
1:B:308:ARG:HH11	1:C:200:MET:CB	2.32	0.42
1:C:243:ALA:HB1	1:C:279:ASN:O	2.20	0.42
1:C:285:THR:C	1:C:287:GLU:N	2.77	0.42
1:B:20:PRO:HD3	1:B:139:ASN:CG	2.44	0.42
1:C:239:VAL:O	1:C:239:VAL:HG12	2.20	0.42
1:C:118:LEU:HD12	1:C:118:LEU:C	2.45	0.42
1:A:129:ILE:HG12	1:A:129:ILE:O	2.20	0.42
1:C:10:ILE:HD12	1:C:10:ILE:N	2.34	0.42
1:C:233:VAL:C	1:C:235:GLY:H	2.28	0.42
1:A:152:LEU:HD13	1:A:193:LEU:HD21	2.02	0.42
1:A:233:VAL:C	1:A:235:GLY:H	2.28	0.42
1:A:243:ALA:HB1	1:A:279:ASN:O	2.20	0.42
1:B:129:ILE:HG12	1:B:129:ILE:O	2.20	0.42
1:C:24:VAL:HB	1:C:99:GLY:HA2	2.02	0.41
1:C:129:ILE:HG12	1:C:129:ILE:O	2.20	0.41
1:A:121:ILE:HD12	1:A:264:ILE:CD1	2.51	0.41
1:B:109:SER:O	1:B:113:ARG:HG3	2.20	0.41
1:B:118:LEU:HD12	1:B:118:LEU:C	2.45	0.41
1:B:237:ASP:OD1	1:B:238:PRO:HD2	2.20	0.41
1:C:79:GLN:O	1:C:82:ALA:HB3	2.19	0.41
1:C:121:ILE:HD12	1:C:264:ILE:CD1	2.51	0.41
1:C:226:PRO:N	3:C:803:HOH:O	2.53	0.41
1:B:121:ILE:HD12	1:B:264:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LEU:O	1:B:221:GLY:C	2.62	0.41
1:A:118:LEU:HD12	1:A:118:LEU:C	2.45	0.41
1:B:152:LEU:HD13	1:B:193:LEU:HD21	2.02	0.41
1:B:243:ALA:HB1	1:B:279:ASN:O	2.20	0.41
1:C:101:HIS:O	1:C:104:ALA:N	2.40	0.41
1:C:237:ASP:OD1	1:C:238:PRO:HD2	2.20	0.41
1:C:261:THR:HB	1:C:303:CYS:SG	2.61	0.41
1:A:109:SER:O	1:A:113:ARG:HG3	2.20	0.41
1:A:237:ASP:OD1	1:A:238:PRO:HD2	2.20	0.41
1:B:112:ALA:HA	1:B:115:HIS:O	2.20	0.41
1:B:233:VAL:C	1:B:235:GLY:H	2.28	0.41
1:B:239:VAL:O	1:B:239:VAL:HG12	2.20	0.41
1:C:152:LEU:HD13	1:C:193:LEU:HD21	2.02	0.41
1:C:219:LEU:C	1:C:220:LEU:HD23	2.45	0.41
1:A:24:VAL:HB	1:A:99:GLY:HA2	2.02	0.41
1:A:120:VAL:HG22	1:A:228:HIS:HB3	2.02	0.41
1:A:188:TYR:CD1	1:C:318:TYR:CD2	3.07	0.41
1:A:212:MET:SD	1:A:260:ILE:HG12	2.61	0.41
1:B:120:VAL:HG22	1:B:228:HIS:HB3	2.02	0.41
1:B:219:LEU:C	1:B:220:LEU:HD23	2.45	0.41
1:B:261:THR:HB	1:B:303:CYS:SG	2.61	0.41
1:B:285:THR:O	1:B:286:PRO:C	2.64	0.41
1:C:109:SER:O	1:C:113:ARG:HG3	2.20	0.41
1:A:108:ILE:HD12	1:A:148:LEU:CD1	2.51	0.41
1:A:219:LEU:C	1:A:220:LEU:HD23	2.45	0.41
1:B:39:LYS:HB3	1:B:301:LEU:HD11	2.03	0.41
1:B:260:ILE:O	1:B:261:THR:C	2.62	0.41
1:B:284:LYS:HB2	1:B:284:LYS:NZ	2.36	0.41
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.85	0.41
1:B:308:ARG:HD2	1:C:200:MET:HB2	2.03	0.41
1:C:108:ILE:HD12	1:C:148:LEU:CD1	2.50	0.41
1:C:112:ALA:HA	1:C:115:HIS:O	2.20	0.41
1:A:112:ALA:HA	1:A:115:HIS:O	2.20	0.41
1:A:261:THR:OG1	1:A:302:SER:HB3	2.21	0.41
1:B:77:ASN:HB3	1:B:164:TRP:CZ2	2.56	0.41
1:B:108:ILE:HD12	1:B:148:LEU:CD1	2.51	0.41
1:B:212:MET:SD	1:B:260:ILE:HG12	2.61	0.41
1:A:284:LYS:NZ	1:A:284:LYS:HB2	2.36	0.40
1:C:212:MET:SD	1:C:260:ILE:HG12	2.61	0.40
1:A:77:ASN:HB3	1:A:164:TRP:CZ2	2.57	0.40
1:A:261:THR:HB	1:A:303:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:THR:OG1	1:B:302:SER:HB3	2.21	0.40
1:C:117:ASP:OD1	1:C:117:ASP:N	2.44	0.40
1:C:174:ILE:HG12	1:C:175:VAL:N	2.36	0.40
1:C:260:ILE:O	1:C:261:THR:C	2.62	0.40
1:A:100:ASP:OD1	1:A:102:SER:CB	2.70	0.40
1:A:285:THR:C	1:A:287:GLU:N	2.77	0.40
1:B:100:ASP:OD1	1:B:102:SER:CB	2.70	0.40
1:B:262:GLU:O	1:B:265:TYR:HB3	2.22	0.40
1:B:24:VAL:HB	1:B:99:GLY:HA2	2.03	0.40
1:B:208:ILE:HG23	1:B:259:TYR:CD2	2.56	0.40
1:C:75:LYS:HA	1:C:75:LYS:HD2	1.93	0.40
1:A:200:MET:CB	1:C:308:ARG:HH11	2.35	0.40
1:A:236:LEU:CD2	1:A:252:LEU:HB2	2.52	0.40
1:C:38:GLU:H	1:C:38:GLU:CD	2.30	0.40
1:C:39:LYS:HB3	1:C:301:LEU:HD11	2.03	0.40
1:C:77:ASN:HB3	1:C:164:TRP:CZ2	2.56	0.40
1:C:126:HIS:ND1	1:C:234:ASP:OD1	2.55	0.40
1:C:199:SER:O	1:C:200:MET:C	2.64	0.40
1:C:208:ILE:HG23	1:C:259:TYR:CD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PRO:CA	1:B:89:LYS:NZ[3_555]	2.00	0.20

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	312/314 (99%)	263 (84%)	43 (14%)	6 (2%)	6 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	312/314 (99%)	264 (85%)	42 (14%)	6 (2%)	6	27
1	C	312/314 (99%)	263 (84%)	43 (14%)	6 (2%)	6	27
All	All	936/942 (99%)	790 (84%)	128 (14%)	18 (2%)	6	27

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLY
1	B	99	GLY
1	C	99	GLY
1	A	260	ILE
1	B	260	ILE
1	C	260	ILE
1	A	140	LEU
1	A	261	THR
1	B	140	LEU
1	B	261	THR
1	C	140	LEU
1	C	261	THR
1	A	102	SER
1	B	102	SER
1	C	102	SER
1	A	143	GLN
1	B	143	GLN
1	C	143	GLN

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	264/264 (100%)	238 (90%)	26 (10%)	7	29
1	B	264/264 (100%)	238 (90%)	26 (10%)	7	29
1	C	264/264 (100%)	238 (90%)	26 (10%)	7	29
All	All	792/792 (100%)	714 (90%)	78 (10%)	7	29

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	46	ASN
1	A	57	ASP
1	A	66	ILE
1	A	101	HIS
1	A	103	MET
1	A	132	PRO
1	A	135	THR
1	A	141	ASN
1	A	152	LEU
1	A	160	PRO
1	A	166	THR
1	A	167	PRO
1	A	169	ILE
1	A	170	SER
1	A	184	PRO
1	A	201	THR
1	A	233	VAL
1	A	244	THR
1	A	246	THR
1	A	273	LEU
1	A	284	LYS
1	A	286	PRO
1	A	287	GLU
1	A	295	THR
1	A	313	LYS
1	B	24	VAL
1	B	46	ASN
1	B	57	ASP
1	B	66	ILE
1	B	101	HIS
1	B	103	MET
1	B	132	PRO
1	B	135	THR
1	B	141	ASN
1	B	152	LEU
1	B	160	PRO
1	B	166	THR
1	B	167	PRO
1	B	169	ILE
1	B	170	SER
1	B	184	PRO

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Mol	Chain	Res	Type
1	B	201	THR
1	B	233	VAL
1	B	244	THR
1	B	246	THR
1	B	273	LEU
1	B	284	LYS
1	B	286	PRO
1	B	287	GLU
1	B	295	THR
1	B	313	LYS
1	C	24	VAL
1	C	46	ASN
1	C	57	ASP
1	C	66	ILE
1	C	101	HIS
1	C	103	MET
1	C	132	PRO
1	C	135	THR
1	C	141	ASN
1	C	152	LEU
1	C	160	PRO
1	C	166	THR
1	C	167	PRO
1	C	169	ILE
1	C	170	SER
1	C	184	PRO
1	C	201	THR
1	C	233	VAL
1	C	244	THR
1	C	246	THR
1	C	273	LEU
1	C	284	LYS
1	C	286	PRO
1	C	287	GLU
1	C	295	THR
1	C	313	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	B	139	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.