



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:53 AM UTC

PDB ID : 1HQH / pdb_00001hqh
Title : CRYSTAL STRUCTURE OF THE BINUCLEAR MANGANESE METALLOENZYME ARGINASE COMPLEXED WITH NOR-N-HYDROXY-L-ARGININE
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Deposited on : 2000-12-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

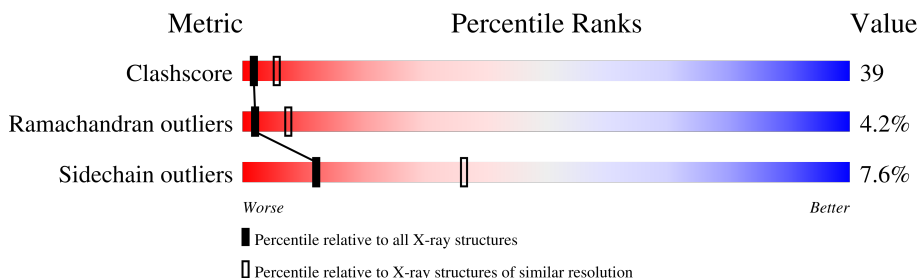
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	323	36% 51% 10% .
1	B	323	35% 52% 10% .
1	C	323	33% 54% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7248 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.

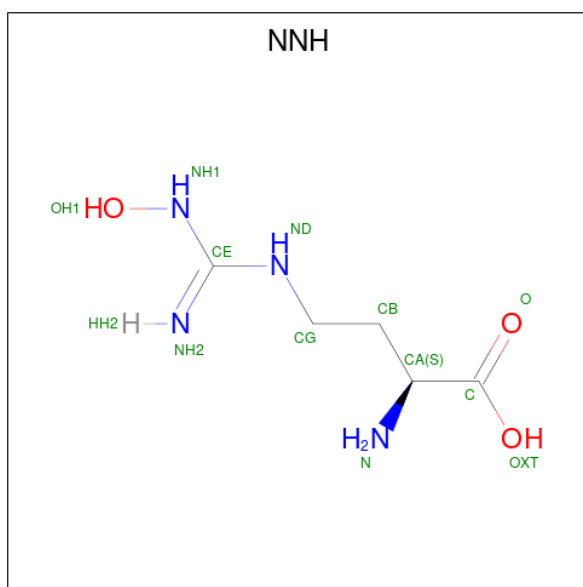
- Molecule 1 is a protein called ARGINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			
1	B	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			
1	C	314	Total	C	N	O	S	0	0	0
			2395	1528	405	455	7			

- 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 NOR-N-OMEGA-HYDROXY-L-ARGININE (CCD ID: NNH) (formula: C₅H₁₂N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	5	4	3		
3	B	1	Total	C	N	O	0	0
			12	5	4	3		
3	C	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 4 is water.

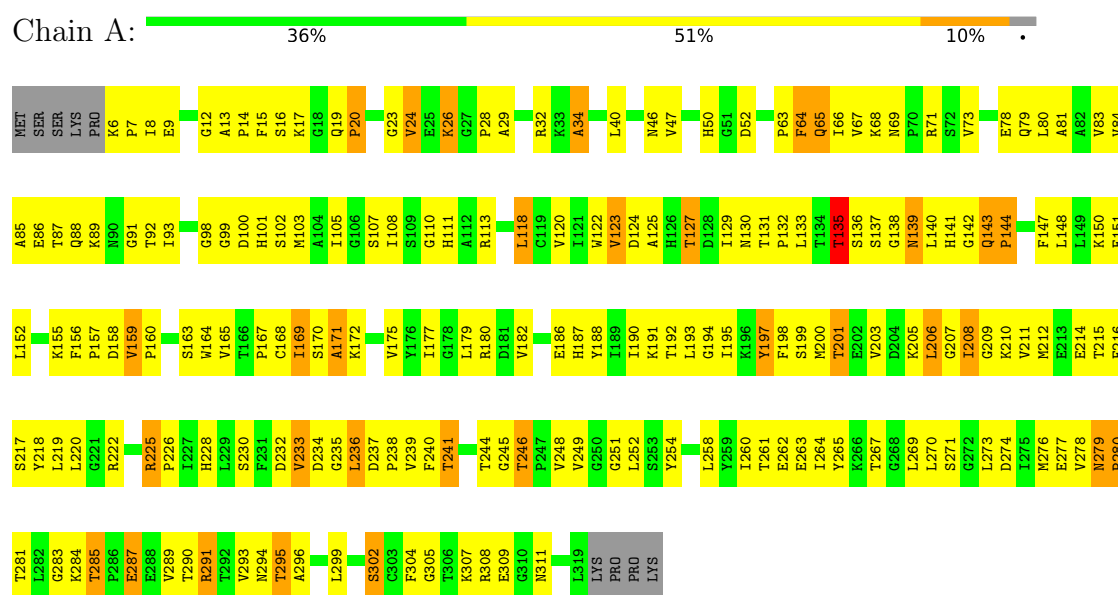
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	8	Total	O	0	0
			8	8		
4	C	8	Total	O	0	0
			8	8		

3 Residue-property plots

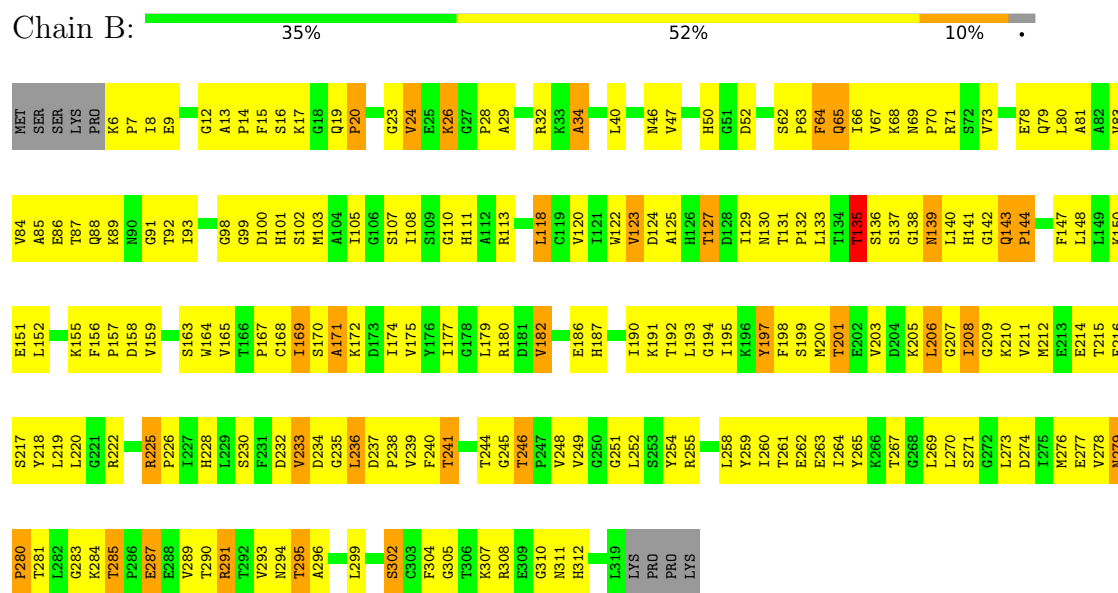
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

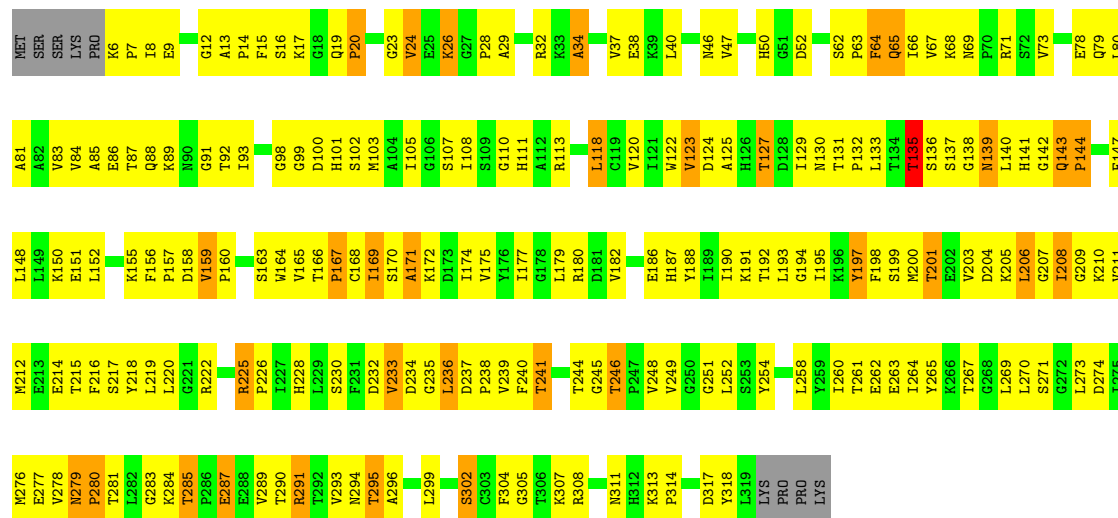
• Molecule 1: ARGINASE 1



• Molecule 1: ARGINASE 1



Chain C: 33% 54% 10% .



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	88.00Å 88.00Å 112.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.80)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.286 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7248	wwPDB-VP
Average B, all atoms (Å ²)	86.0	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: NNH, 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	0.49	0/2448	1.08	21/3325 (0.6%)
1	B	0.50	0/2448	1.08	21/3325 (0.6%)
1	C	0.49	0/2448	1.08	21/3325 (0.6%)
All	All	0.49	0/7344	1.08	63/9975 (0.6%)

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	VAL	N-CA-C	7.94	122.32	109.78
1	C	249	VAL	N-CA-C	7.93	122.31	109.78
1	B	249	VAL	N-CA-C	7.93	122.31	109.78
1	B	236	LEU	N-CA-C	-7.63	100.68	110.53
1	C	236	LEU	N-CA-C	-7.61	100.71	110.53
1	A	236	LEU	N-CA-C	-7.60	100.72	110.53
1	B	241	THR	CA-C-N	6.75	126.71	119.28
1	B	241	THR	C-N-CA	6.75	126.71	119.28
1	A	241	THR	CA-C-N	6.72	126.67	119.28
1	A	241	THR	C-N-CA	6.72	126.67	119.28
1	C	241	THR	CA-C-N	6.71	126.67	119.28
1	C	241	THR	C-N-CA	6.71	126.67	119.28
1	C	20	PRO	N-CA-C	6.46	121.96	114.20
1	A	20	PRO	N-CA-C	6.45	121.94	114.20
1	C	168	CYS	N-CA-C	6.42	121.11	113.28
1	A	136	SER	N-CA-C	-6.42	104.70	113.30
1	C	136	SER	N-CA-C	-6.42	104.70	113.30
1	B	20	PRO	N-CA-C	6.42	121.90	114.20
1	B	136	SER	N-CA-C	-6.41	104.71	113.30
1	B	168	CYS	N-CA-C	6.39	121.07	113.28
1	A	168	CYS	N-CA-C	6.37	121.05	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	VAL	N-CA-C	-6.08	104.59	110.42
1	C	203	VAL	N-CA-C	-6.06	104.60	110.42
1	B	203	VAL	N-CA-C	-6.02	104.64	110.42
1	B	240	PHE	N-CA-C	5.98	119.77	112.23
1	A	240	PHE	N-CA-C	5.96	119.75	112.23
1	A	277	GLU	N-CA-C	5.96	122.79	113.72
1	C	277	GLU	N-CA-C	5.96	122.78	113.72
1	B	277	GLU	N-CA-C	5.96	122.77	113.72
1	C	240	PHE	N-CA-C	5.93	119.71	112.23
1	A	291	ARG	N-CA-C	-5.87	104.57	110.97
1	C	291	ARG	N-CA-C	-5.84	104.60	110.97
1	B	291	ARG	N-CA-C	-5.83	104.62	110.97
1	C	246	THR	CA-C-N	-5.82	113.79	119.78
1	C	246	THR	C-N-CA	-5.82	113.79	119.78
1	B	246	THR	CA-C-N	-5.78	113.83	119.78
1	B	246	THR	C-N-CA	-5.78	113.83	119.78
1	A	246	THR	CA-C-N	-5.77	113.83	119.78
1	A	246	THR	C-N-CA	-5.77	113.83	119.78
1	B	182	VAL	N-CA-C	5.53	116.27	108.36
1	C	182	VAL	N-CA-C	5.52	116.26	108.36
1	A	182	VAL	N-CA-C	5.50	116.23	108.36
1	A	206	LEU	N-CA-C	5.42	117.27	111.36
1	C	206	LEU	N-CA-C	5.42	117.27	111.36
1	B	206	LEU	N-CA-C	5.41	117.25	111.36
1	C	302	SER	N-CA-C	-5.37	105.12	110.97
1	A	302	SER	N-CA-C	-5.35	105.14	110.97
1	C	159	VAL	N-CA-C	5.34	113.71	107.89
1	B	159	VAL	N-CA-C	5.33	113.70	107.89
1	A	159	VAL	N-CA-C	5.32	113.69	107.89
1	B	302	SER	N-CA-C	-5.32	105.17	110.97
1	B	279	ASN	CA-C-N	5.30	126.46	119.84
1	B	279	ASN	C-N-CA	5.30	126.46	119.84
1	C	279	ASN	CA-C-N	5.27	126.42	119.84
1	C	279	ASN	C-N-CA	5.27	126.42	119.84
1	A	279	ASN	CA-C-N	5.26	126.41	119.84
1	A	279	ASN	C-N-CA	5.26	126.41	119.84
1	C	34	ALA	N-CA-C	-5.21	106.94	113.72
1	B	34	ALA	N-CA-C	-5.21	106.95	113.72
1	A	34	ALA	N-CA-C	-5.20	106.96	113.72
1	A	26	LYS	N-CA-C	-5.18	107.03	113.19
1	B	26	LYS	N-CA-C	-5.16	107.05	113.19
1	C	26	LYS	N-CA-C	-5.14	107.07	113.19

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2395	0	2420	191	0
1	B	2395	0	2420	196	0
1	C	2395	0	2420	209	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	12	0	10	0	0
3	B	12	0	10	0	0
3	C	12	0	10	0	0
4	A	5	0	0	0	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
All	All	7248	0	7290	572	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 39.

All (572) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:VAL:HG11	1:B:215:THR:HG22	1.45	0.98
1:C:175:VAL:HG11	1:C:215:THR:HG22	1.45	0.97
1:A:175:VAL:HG11	1:A:215:THR:HG22	1.45	0.96
1:B:143:GLN:H	1:B:144:PRO:CD	1.88	0.86
1:A:140:LEU:O	1:A:144:PRO:HD3	1.75	0.86
1:B:140:LEU:O	1:B:144:PRO:HD3	1.75	0.86
1:A:143:GLN:H	1:A:144:PRO:CD	1.88	0.86
1:C:143:GLN:H	1:C:144:PRO:CD	1.88	0.85
1:A:143:GLN:H	1:A:144:PRO:HD3	1.42	0.85
1:C:244:THR:HG22	1:C:245:GLY:H	1.41	0.85
1:B:143:GLN:H	1:B:144:PRO:HD3	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:O	1:C:144:PRO:HD3	1.75	0.85
1:A:244:THR:HG22	1:A:245:GLY:H	1.41	0.85
1:B:244:THR:HG22	1:B:245:GLY:H	1.41	0.84
1:C:143:GLN:H	1:C:144:PRO:HD3	1.42	0.83
1:B:259:TYR:CE1	1:C:205:LYS:HB2	2.14	0.82
1:C:102:SER:HB3	1:C:141:HIS:HA	1.62	0.81
1:A:102:SER:HB3	1:A:141:HIS:HA	1.62	0.80
1:B:102:SER:HB3	1:B:141:HIS:HA	1.62	0.79
1:A:210:LYS:HE3	1:A:214:GLU:OE2	1.83	0.79
1:B:210:LYS:HE3	1:B:214:GLU:OE2	1.83	0.78
1:C:210:LYS:HE3	1:C:214:GLU:OE2	1.83	0.76
1:A:40:LEU:HD21	1:A:304:PHE:HD2	1.52	0.74
1:C:230:SER:HA	1:C:274:ASP:HB2	1.69	0.73
1:A:230:SER:HA	1:A:274:ASP:HB2	1.69	0.73
1:B:230:SER:HA	1:B:274:ASP:HB2	1.69	0.72
1:C:40:LEU:HD21	1:C:304:PHE:HD2	1.52	0.72
1:B:40:LEU:HD21	1:B:304:PHE:HD2	1.52	0.72
1:A:12:GLY:HA3	1:A:52:ASP:OD1	1.91	0.71
1:B:12:GLY:HA3	1:B:52:ASP:OD1	1.91	0.71
1:A:201:THR:HG22	1:C:308:ARG:HB2	1.73	0.71
1:B:262:GLU:OE1	1:C:201:THR:HB	1.90	0.71
1:B:308:ARG:HB2	1:C:201:THR:HG22	1.73	0.70
1:C:12:GLY:HA3	1:C:52:ASP:OD1	1.91	0.70
1:A:208:ILE:HD11	1:A:260:ILE:HD11	1.73	0.70
1:C:208:ILE:HD11	1:C:260:ILE:HD11	1.73	0.70
1:C:143:GLN:N	1:C:144:PRO:CD	2.55	0.69
1:B:143:GLN:N	1:B:144:PRO:CD	2.55	0.69
1:B:208:ILE:HD11	1:B:260:ILE:HD11	1.73	0.69
1:A:180:ARG:NH1	1:A:248:VAL:O	2.27	0.68
1:B:180:ARG:NH1	1:B:248:VAL:O	2.27	0.68
1:A:143:GLN:N	1:A:144:PRO:CD	2.55	0.67
1:C:118:LEU:HD12	1:C:118:LEU:O	1.94	0.67
1:B:118:LEU:HD12	1:B:118:LEU:O	1.94	0.67
1:C:258:LEU:HD23	1:C:299:LEU:HD23	1.76	0.67
1:C:180:ARG:NH1	1:C:248:VAL:O	2.27	0.67
1:A:258:LEU:HD23	1:A:299:LEU:HD23	1.76	0.67
1:A:118:LEU:O	1:A:118:LEU:HD12	1.94	0.67
1:B:258:LEU:HD23	1:B:299:LEU:HD23	1.76	0.67
1:A:258:LEU:CD2	1:A:299:LEU:HD23	2.25	0.66
1:B:258:LEU:CD2	1:B:299:LEU:HD23	2.25	0.66
1:B:101:HIS:CE1	1:B:122:TRP:CZ2	2.84	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:HIS:CE1	1:A:122:TRP:CZ2	2.84	0.66
1:C:258:LEU:CD2	1:C:299:LEU:HD23	2.25	0.66
1:C:258:LEU:O	1:C:262:GLU:HB2	1.96	0.66
1:C:8:ILE:HD13	1:C:93:ILE:HB	1.78	0.66
1:A:258:LEU:O	1:A:262:GLU:HB2	1.96	0.66
1:B:127:THR:HG23	1:B:179:LEU:HD22	1.78	0.65
1:C:101:HIS:CE1	1:C:122:TRP:CZ2	2.84	0.65
1:A:68:LYS:HG3	1:A:138:GLY:HA3	1.78	0.65
1:B:258:LEU:O	1:B:262:GLU:HB2	1.96	0.65
1:B:8:ILE:HD13	1:B:93:ILE:HB	1.77	0.65
1:C:244:THR:HG22	1:C:245:GLY:N	2.11	0.65
1:A:19:GLN:NE2	1:A:24:VAL:HG21	2.12	0.65
1:A:8:ILE:HD13	1:A:93:ILE:HB	1.77	0.64
1:B:19:GLN:NE2	1:B:24:VAL:HG21	2.12	0.64
1:B:244:THR:HG22	1:B:245:GLY:N	2.11	0.64
1:C:19:GLN:NE2	1:C:24:VAL:HG21	2.12	0.64
1:C:68:LYS:HG3	1:C:138:GLY:HA3	1.78	0.64
1:A:127:THR:HG23	1:A:179:LEU:HD22	1.78	0.64
1:C:6:LYS:HD2	1:C:7:PRO:HD3	1.80	0.64
1:C:127:THR:HG23	1:C:179:LEU:HD22	1.78	0.64
1:A:6:LYS:HD2	1:A:7:PRO:HD3	1.80	0.64
1:B:15:PHE:CE1	1:B:17:LYS:HD3	2.33	0.64
1:A:15:PHE:CE1	1:A:17:LYS:HD3	2.33	0.64
1:B:68:LYS:HG3	1:B:138:GLY:HA3	1.78	0.63
1:C:15:PHE:CE1	1:C:17:LYS:HD3	2.33	0.63
1:A:169:ILE:HD13	1:A:169:ILE:H	1.64	0.63
1:B:98:GLY:HA3	1:B:99:GLY:O	1.99	0.63
1:B:6:LYS:HD2	1:B:7:PRO:HD3	1.80	0.62
1:C:169:ILE:HD13	1:C:169:ILE:H	1.63	0.62
1:A:244:THR:HG22	1:A:245:GLY:N	2.11	0.62
1:B:169:ILE:HD13	1:B:169:ILE:H	1.64	0.62
1:A:98:GLY:HA3	1:A:99:GLY:O	1.99	0.62
1:C:98:GLY:HA3	1:C:99:GLY:O	1.99	0.61
1:A:307:LYS:H	1:A:311:ASN:HD21	1.49	0.60
1:B:169:ILE:HD13	1:B:169:ILE:N	2.16	0.60
1:A:212:MET:CE	1:A:260:ILE:HG23	2.32	0.60
1:C:169:ILE:HD13	1:C:169:ILE:N	2.16	0.60
1:C:212:MET:CE	1:C:260:ILE:HG23	2.31	0.60
1:C:23:GLY:HA3	1:C:279:ASN:OD1	2.02	0.60
1:A:93:ILE:HG23	1:A:271:SER:C	2.27	0.60
1:C:129:ILE:CG2	1:C:186:GLU:HG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:CG2	1:A:186:GLU:HG2	2.32	0.59
1:B:212:MET:CE	1:B:260:ILE:HG23	2.31	0.59
1:B:291:ARG:O	1:B:295:THR:HG23	2.03	0.59
1:A:23:GLY:HA3	1:A:279:ASN:OD1	2.02	0.59
1:A:169:ILE:HD13	1:A:169:ILE:N	2.16	0.59
1:B:225:ARG:HB2	1:B:226:PRO:CD	2.32	0.59
1:C:307:LYS:H	1:C:311:ASN:HD21	1.49	0.59
1:A:118:LEU:HD12	1:A:118:LEU:C	2.28	0.59
1:B:23:GLY:HA3	1:B:279:ASN:OD1	2.02	0.58
1:B:118:LEU:HD12	1:B:118:LEU:C	2.28	0.58
1:B:129:ILE:CG2	1:B:186:GLU:HG2	2.32	0.58
1:B:93:ILE:HG23	1:B:271:SER:C	2.27	0.58
1:B:307:LYS:H	1:B:311:ASN:HD21	1.50	0.58
1:C:93:ILE:HG23	1:C:271:SER:C	2.27	0.58
1:A:205:LYS:HG2	1:A:206:LEU:HD23	1.86	0.58
1:A:225:ARG:HB2	1:A:226:PRO:CD	2.32	0.58
1:A:291:ARG:O	1:A:295:THR:HG23	2.03	0.58
1:C:118:LEU:HD12	1:C:118:LEU:C	2.28	0.58
1:C:225:ARG:HB2	1:C:226:PRO:CD	2.32	0.58
1:C:291:ARG:O	1:C:295:THR:HG23	2.03	0.58
1:B:102:SER:HB3	1:B:141:HIS:CA	2.33	0.58
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.39	0.58
1:A:180:ARG:CZ	1:A:251:GLY:HA3	2.34	0.57
1:A:65:GLN:HE22	1:A:157:PRO:HG3	1.69	0.57
1:B:180:ARG:CZ	1:B:251:GLY:HA3	2.34	0.57
1:C:180:ARG:CZ	1:C:251:GLY:HA3	2.34	0.57
1:A:8:ILE:N	1:A:46:ASN:O	2.38	0.57
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.39	0.57
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.39	0.57
1:C:65:GLN:HE22	1:C:157:PRO:HG3	1.69	0.57
1:C:130:ASN:OD1	1:C:186:GLU:HG3	2.05	0.57
1:C:199:SER:OG	1:C:201:THR:HG23	2.05	0.57
1:B:28:PRO:HD3	1:B:98:GLY:O	2.06	0.56
1:C:28:PRO:HD3	1:C:98:GLY:O	2.05	0.56
1:C:205:LYS:HG2	1:C:206:LEU:HD23	1.86	0.56
1:B:65:GLN:HE22	1:B:157:PRO:HG3	1.69	0.56
1:B:102:SER:HA	1:B:144:PRO:HG3	1.87	0.56
1:B:233:VAL:HG13	1:B:241:THR:HB	1.88	0.56
1:B:130:ASN:OD1	1:B:186:GLU:HG3	2.05	0.56
1:A:130:ASN:OD1	1:A:186:GLU:HG3	2.05	0.56
1:B:50:HIS:O	1:B:50:HIS:ND1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:SER:OG	1:B:201:THR:HG23	2.05	0.56
1:C:233:VAL:HG13	1:C:241:THR:HB	1.87	0.56
1:A:102:SER:HA	1:A:144:PRO:HG3	1.87	0.56
1:A:50:HIS:O	1:A:50:HIS:ND1	2.39	0.56
1:C:50:HIS:O	1:C:50:HIS:ND1	2.39	0.56
1:B:40:LEU:CD2	1:B:304:PHE:HD2	2.18	0.56
1:C:254:TYR:CE1	1:C:295:THR:HB	2.41	0.56
1:B:205:LYS:HG2	1:B:206:LEU:HD23	1.86	0.56
1:A:309:GLU:O	1:B:182:VAL:HB	2.06	0.55
1:B:8:ILE:N	1:B:46:ASN:O	2.38	0.55
1:C:102:SER:HB3	1:C:141:HIS:CA	2.33	0.55
1:C:102:SER:HA	1:C:144:PRO:HG3	1.87	0.55
1:C:219:LEU:O	1:C:220:LEU:HD23	2.07	0.55
1:A:40:LEU:CD2	1:A:304:PHE:HD2	2.18	0.55
1:C:254:TYR:CD1	1:C:295:THR:HB	2.42	0.55
1:A:199:SER:OG	1:A:201:THR:HG23	2.05	0.55
1:A:102:SER:HB3	1:A:141:HIS:CA	2.33	0.55
1:A:219:LEU:O	1:A:220:LEU:HD23	2.07	0.55
1:B:254:TYR:CE1	1:B:295:THR:HB	2.41	0.55
1:C:8:ILE:N	1:C:46:ASN:O	2.38	0.55
1:A:188:TYR:CD2	1:C:318:TYR:HB2	2.42	0.55
1:B:234:ASP:HB3	1:B:244:THR:HG21	1.89	0.55
1:C:40:LEU:CD2	1:C:304:PHE:HD2	2.18	0.55
1:A:28:PRO:HD3	1:A:98:GLY:O	2.05	0.55
1:A:135:THR:HB	1:A:137:SER:O	2.07	0.55
1:A:175:VAL:HG11	1:A:215:THR:CG2	2.30	0.55
1:A:233:VAL:HG13	1:A:241:THR:HB	1.87	0.55
1:B:175:VAL:HG11	1:B:215:THR:CG2	2.30	0.55
1:A:140:LEU:C	1:A:142:GLY:H	2.15	0.54
1:A:254:TYR:CD1	1:A:295:THR:HB	2.42	0.54
1:A:254:TYR:CE1	1:A:295:THR:HB	2.41	0.54
1:B:120:VAL:HG22	1:B:228:HIS:HB3	1.89	0.54
1:C:135:THR:HB	1:C:137:SER:O	2.07	0.54
1:C:140:LEU:C	1:C:142:GLY:H	2.15	0.54
1:A:120:VAL:HG22	1:A:228:HIS:HB3	1.89	0.54
1:B:135:THR:HB	1:B:137:SER:O	2.07	0.54
1:B:219:LEU:O	1:B:220:LEU:HD23	2.07	0.54
1:A:129:ILE:HG22	1:A:186:GLU:HG2	1.90	0.54
1:B:254:TYR:CD1	1:B:295:THR:HB	2.42	0.54
1:B:308:ARG:HB2	1:C:201:THR:CG2	2.36	0.54
1:A:108:ILE:HG12	1:A:228:HIS:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:VAL:HG22	1:C:228:HIS:HB3	1.89	0.54
1:C:129:ILE:HG22	1:C:186:GLU:HG2	1.90	0.54
1:A:234:ASP:HB3	1:A:244:THR:HG21	1.89	0.54
1:C:108:ILE:HG12	1:C:228:HIS:CD2	2.42	0.54
1:C:234:ASP:HB3	1:C:244:THR:HG21	1.89	0.54
1:B:108:ILE:HG12	1:B:228:HIS:CD2	2.42	0.53
1:A:67:VAL:HG21	1:A:132:PRO:HB3	1.90	0.53
1:A:102:SER:HA	1:A:144:PRO:CG	2.38	0.53
1:B:102:SER:HA	1:B:144:PRO:CG	2.38	0.53
1:B:140:LEU:C	1:B:142:GLY:H	2.15	0.53
1:B:259:TYR:CZ	1:C:205:LYS:HB2	2.43	0.53
1:B:287:GLU:OE2	1:B:291:ARG:NH2	2.40	0.53
1:A:188:TYR:CZ	1:C:317:ASP:HA	2.44	0.53
1:A:198:PHE:CE1	1:A:215:THR:HG23	2.44	0.53
1:B:16:SER:HB3	1:B:24:VAL:HG23	1.91	0.53
1:B:198:PHE:CE1	1:B:215:THR:HG23	2.44	0.53
1:A:108:ILE:HG12	1:A:228:HIS:NE2	2.24	0.53
1:A:198:PHE:CD2	1:A:211:VAL:HG13	2.44	0.53
1:B:67:VAL:HG21	1:B:132:PRO:HB3	1.91	0.53
1:C:287:GLU:OE2	1:C:291:ARG:NH2	2.40	0.53
1:A:16:SER:HB3	1:A:24:VAL:HG23	1.91	0.53
1:C:198:PHE:CE1	1:C:215:THR:HG23	2.44	0.53
1:B:129:ILE:HG22	1:B:186:GLU:HG2	1.90	0.52
1:C:108:ILE:HG12	1:C:228:HIS:NE2	2.24	0.52
1:C:220:LEU:HD13	1:C:269:LEU:HD12	1.91	0.52
1:B:198:PHE:CD2	1:B:211:VAL:HG13	2.44	0.52
1:C:102:SER:HA	1:C:144:PRO:CG	2.38	0.52
1:C:278:VAL:O	1:C:280:PRO:HD3	2.10	0.52
1:C:127:THR:HG23	1:C:179:LEU:CD2	2.39	0.52
1:A:278:VAL:O	1:A:280:PRO:HD3	2.10	0.52
1:C:198:PHE:CD2	1:C:211:VAL:HG13	2.44	0.52
1:C:67:VAL:HG21	1:C:132:PRO:HB3	1.90	0.52
1:A:64:PHE:HZ	1:A:157:PRO:HB2	1.74	0.52
1:A:188:TYR:CG	1:C:318:TYR:HD2	2.28	0.52
1:B:135:THR:HG21	1:B:143:GLN:NE2	2.25	0.52
1:A:88:GLN:HG3	1:A:111:HIS:HA	1.92	0.52
1:A:135:THR:HG21	1:A:143:GLN:NE2	2.25	0.52
1:B:127:THR:HG23	1:B:179:LEU:CD2	2.39	0.52
1:C:135:THR:HG21	1:C:143:GLN:NE2	2.25	0.52
1:A:220:LEU:HD13	1:A:269:LEU:HD12	1.91	0.52
1:A:127:THR:HG23	1:A:179:LEU:CD2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ASN:O	1:C:281:THR:N	2.43	0.51
1:B:279:ASN:O	1:B:281:THR:N	2.43	0.51
1:C:7:PRO:HG2	1:C:92:THR:HG22	1.92	0.51
1:A:140:LEU:C	1:A:142:GLY:N	2.68	0.51
1:B:278:VAL:O	1:B:280:PRO:HD3	2.10	0.51
1:C:88:GLN:HG3	1:C:111:HIS:HA	1.92	0.51
1:B:108:ILE:HG12	1:B:228:HIS:NE2	2.24	0.51
1:B:220:LEU:HD13	1:B:269:LEU:HD12	1.91	0.51
1:B:6:LYS:HD2	1:B:7:PRO:CD	2.41	0.51
1:C:64:PHE:HZ	1:C:157:PRO:HB2	1.74	0.51
1:C:180:ARG:NH2	1:C:235:GLY:O	2.44	0.51
1:A:7:PRO:HG2	1:A:92:THR:HG22	1.92	0.51
1:A:279:ASN:O	1:A:281:THR:N	2.43	0.51
1:B:7:PRO:HG2	1:B:92:THR:HG22	1.92	0.51
1:B:64:PHE:HZ	1:B:157:PRO:HB2	1.74	0.51
1:B:132:PRO:HD2	1:B:156:PHE:CD2	2.46	0.51
1:A:180:ARG:NH2	1:A:235:GLY:O	2.44	0.51
1:A:287:GLU:OE2	1:A:291:ARG:NH2	2.40	0.51
1:C:16:SER:HB3	1:C:24:VAL:HG23	1.91	0.51
1:B:88:GLN:HG3	1:B:111:HIS:HA	1.92	0.51
1:C:132:PRO:HD2	1:C:156:PHE:CD2	2.46	0.51
1:A:132:PRO:HD2	1:A:156:PHE:CD2	2.46	0.51
1:A:13:ALA:O	1:A:15:PHE:N	2.45	0.50
1:B:13:ALA:O	1:B:15:PHE:N	2.45	0.50
1:A:308:ARG:O	1:B:180:ARG:HA	2.11	0.50
1:B:218:TYR:HD2	1:B:219:LEU:HG	1.76	0.50
1:C:218:TYR:HD2	1:C:219:LEU:HG	1.77	0.50
1:C:299:LEU:O	1:C:302:SER:HB3	2.12	0.50
1:A:283:GLY:HA3	1:A:289:VAL:HG23	1.93	0.50
1:C:6:LYS:HD2	1:C:7:PRO:CD	2.41	0.50
1:B:283:GLY:HA3	1:B:289:VAL:HG23	1.93	0.50
1:C:13:ALA:O	1:C:15:PHE:N	2.44	0.50
1:B:310:GLY:C	1:C:187:HIS:CD2	2.90	0.50
1:A:299:LEU:O	1:A:302:SER:HB3	2.12	0.50
1:B:180:ARG:NH2	1:B:235:GLY:O	2.44	0.50
1:C:32:ARG:C	1:C:34:ALA:H	2.20	0.50
1:C:140:LEU:C	1:C:142:GLY:N	2.68	0.50
1:C:283:GLY:HA3	1:C:289:VAL:HG23	1.93	0.50
1:A:218:TYR:HD2	1:A:219:LEU:HG	1.77	0.50
1:A:73:VAL:HG12	1:A:73:VAL:O	2.12	0.49
1:B:187:HIS:CE1	1:B:191:LYS:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:HIS:CE1	1:C:191:LYS:HG3	2.47	0.49
1:B:73:VAL:HG12	1:B:73:VAL:O	2.12	0.49
1:B:105:ILE:HA	1:B:148:LEU:HD21	1.94	0.49
1:B:299:LEU:O	1:B:302:SER:HB3	2.12	0.49
1:A:86:GLU:O	1:A:89:LYS:HB3	2.12	0.49
1:B:186:GLU:O	1:B:190:ILE:HG12	2.13	0.49
1:A:32:ARG:C	1:A:34:ALA:H	2.20	0.49
1:A:67:VAL:HA	1:A:138:GLY:HA2	1.95	0.49
1:A:186:GLU:O	1:A:190:ILE:HG12	2.13	0.49
1:C:186:GLU:O	1:C:190:ILE:HG12	2.13	0.49
1:A:187:HIS:CE1	1:A:191:LYS:HG3	2.47	0.49
1:B:140:LEU:C	1:B:142:GLY:N	2.68	0.49
1:C:86:GLU:O	1:C:89:LYS:HB3	2.12	0.49
1:C:258:LEU:HD23	1:C:299:LEU:CD2	2.43	0.49
1:C:192:THR:HG22	1:C:193:LEU:HD12	1.95	0.49
1:C:287:GLU:OE2	1:C:291:ARG:NE	2.45	0.49
1:A:188:TYR:HB2	1:C:318:TYR:CD2	2.48	0.49
1:C:73:VAL:HG12	1:C:73:VAL:O	2.12	0.49
1:C:105:ILE:HA	1:C:148:LEU:HD21	1.94	0.49
1:C:244:THR:CG2	1:C:245:GLY:H	2.21	0.49
1:A:6:LYS:HD2	1:A:7:PRO:CD	2.41	0.49
1:C:6:LYS:HE3	1:C:91:GLY:O	2.14	0.48
1:A:129:ILE:HG12	1:A:129:ILE:O	2.14	0.48
1:A:216:PHE:O	1:A:217:SER:C	2.56	0.48
1:A:279:ASN:C	1:A:281:THR:H	2.22	0.48
1:B:8:ILE:CD1	1:B:93:ILE:HB	2.43	0.48
1:B:32:ARG:C	1:B:34:ALA:H	2.20	0.48
1:C:141:HIS:C	1:C:141:HIS:CD2	2.91	0.48
1:A:6:LYS:HE3	1:A:91:GLY:O	2.14	0.48
1:A:212:MET:HE2	1:A:260:ILE:HG23	1.96	0.48
1:B:67:VAL:HA	1:B:138:GLY:HA2	1.95	0.48
1:A:141:HIS:CD2	1:A:141:HIS:C	2.91	0.48
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.96	0.48
1:A:63:PRO:O	1:A:65:GLN:N	2.47	0.48
1:A:105:ILE:HA	1:A:148:LEU:HD21	1.94	0.48
1:B:258:LEU:HD23	1:B:299:LEU:CD2	2.43	0.48
1:B:312:HIS:CD2	1:C:188:TYR:HD1	2.30	0.48
1:C:67:VAL:HA	1:C:138:GLY:HA2	1.95	0.48
1:C:175:VAL:HG11	1:C:215:THR:CG2	2.30	0.48
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.96	0.48
1:A:188:TYR:CD1	1:C:318:TYR:HD2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:TYR:CE1	1:B:305:GLY:HA2	2.49	0.48
1:C:129:ILE:HG12	1:C:129:ILE:O	2.14	0.48
1:B:63:PRO:O	1:B:65:GLN:N	2.47	0.48
1:B:279:ASN:C	1:B:281:THR:H	2.22	0.48
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.96	0.48
1:C:216:PHE:O	1:C:217:SER:C	2.56	0.48
1:A:187:HIS:HA	1:A:190:ILE:HD11	1.96	0.47
1:B:19:GLN:HB3	1:B:141:HIS:CE1	2.49	0.47
1:B:312:HIS:HD1	1:C:187:HIS:HD1	1.61	0.47
1:C:265:TYR:CE1	1:C:305:GLY:HA2	2.49	0.47
1:A:192:THR:HG22	1:A:193:LEU:HD12	1.95	0.47
1:A:150:LYS:C	1:A:152:LEU:H	2.21	0.47
1:A:188:TYR:OH	1:C:317:ASP:HA	2.14	0.47
1:B:100:ASP:OD1	1:B:100:ASP:C	2.57	0.47
1:B:129:ILE:HG12	1:B:129:ILE:O	2.14	0.47
1:C:19:GLN:HB3	1:C:141:HIS:CE1	2.49	0.47
1:B:68:LYS:NZ	1:B:138:GLY:H	2.13	0.47
1:B:100:ASP:OD1	1:B:102:SER:N	2.42	0.47
1:C:150:LYS:C	1:C:152:LEU:H	2.21	0.47
1:C:170:SER:C	1:C:172:LYS:H	2.22	0.47
1:A:19:GLN:HB3	1:A:141:HIS:CE1	2.50	0.47
1:A:100:ASP:C	1:A:100:ASP:OD1	2.57	0.47
1:A:124:ASP:OD1	1:A:125:ALA:N	2.47	0.47
1:B:192:THR:HG22	1:B:193:LEU:HD12	1.95	0.47
1:C:68:LYS:NZ	1:C:138:GLY:H	2.13	0.47
1:A:265:TYR:CE1	1:A:305:GLY:HA2	2.49	0.47
1:B:141:HIS:CD2	1:B:141:HIS:C	2.91	0.47
1:A:68:LYS:NZ	1:A:138:GLY:H	2.13	0.47
1:A:201:THR:HB	1:C:262:GLU:OE1	2.15	0.47
1:B:6:LYS:HE3	1:B:91:GLY:O	2.14	0.47
1:B:150:LYS:C	1:B:152:LEU:H	2.21	0.47
1:B:212:MET:HE2	1:B:260:ILE:HG23	1.95	0.47
1:B:270:LEU:HD23	1:B:304:PHE:CE1	2.50	0.47
1:C:100:ASP:C	1:C:100:ASP:OD1	2.57	0.47
1:C:124:ASP:OD1	1:C:125:ALA:N	2.47	0.47
1:C:171:ALA:HB1	1:C:195:ILE:HG12	1.97	0.47
1:C:187:HIS:HA	1:C:190:ILE:HD11	1.96	0.47
1:C:212:MET:HE2	1:C:260:ILE:HG23	1.95	0.47
1:C:235:GLY:O	1:C:252:LEU:HD12	2.15	0.47
1:A:8:ILE:CD1	1:A:93:ILE:HB	2.43	0.47
1:A:110:GLY:HA2	1:A:113:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ILE:HG23	1:A:186:GLU:HG2	1.97	0.47
1:B:171:ALA:HB1	1:B:195:ILE:HG12	1.97	0.47
1:C:63:PRO:O	1:C:65:GLN:N	2.47	0.47
1:C:279:ASN:C	1:C:281:THR:H	2.22	0.47
1:A:170:SER:C	1:A:172:LYS:H	2.23	0.47
1:A:270:LEU:HD23	1:A:304:PHE:CE1	2.50	0.47
1:B:187:HIS:HA	1:B:190:ILE:HD11	1.96	0.47
1:A:201:THR:CG2	1:C:308:ARG:HB2	2.42	0.46
1:A:258:LEU:HD23	1:A:299:LEU:CD2	2.43	0.46
1:B:124:ASP:OD1	1:B:125:ALA:N	2.47	0.46
1:B:170:SER:C	1:B:172:LYS:H	2.23	0.46
1:B:235:GLY:O	1:B:252:LEU:HD12	2.15	0.46
1:C:79:GLN:O	1:C:83:VAL:HG23	2.15	0.46
1:C:8:ILE:CD1	1:C:93:ILE:HB	2.43	0.46
1:C:110:GLY:HA2	1:C:113:ARG:HD2	1.97	0.46
1:A:26:LYS:HD2	1:A:281:THR:CG2	2.46	0.46
1:B:16:SER:CB	1:B:24:VAL:HG23	2.45	0.46
1:B:254:TYR:CZ	1:B:258:LEU:HD11	2.50	0.46
1:B:312:HIS:HD2	1:C:188:TYR:HD1	1.63	0.46
1:B:207:GLY:O	1:B:208:ILE:C	2.58	0.46
1:C:129:ILE:HG23	1:C:186:GLU:HG2	1.97	0.46
1:C:207:GLY:O	1:C:208:ILE:C	2.58	0.46
1:A:254:TYR:CZ	1:A:258:LEU:HD11	2.50	0.46
1:B:216:PHE:O	1:B:217:SER:C	2.56	0.46
1:C:100:ASP:OD1	1:C:102:SER:N	2.42	0.46
1:C:254:TYR:CZ	1:C:258:LEU:HD11	2.50	0.46
1:B:197:TYR:CD1	1:B:197:TYR:C	2.94	0.46
1:B:207:GLY:O	1:B:209:GLY:N	2.49	0.46
1:B:287:GLU:OE2	1:B:291:ARG:NE	2.44	0.46
1:C:207:GLY:O	1:C:209:GLY:N	2.49	0.46
1:A:164:TRP:CH2	1:A:165:VAL:HG22	2.51	0.46
1:B:263:GLU:O	1:B:267:THR:HG23	2.16	0.46
1:C:16:SER:CB	1:C:24:VAL:HG23	2.45	0.46
1:C:164:TRP:CH2	1:C:165:VAL:HG22	2.51	0.46
1:A:16:SER:CB	1:A:24:VAL:HG23	2.45	0.46
1:B:152:LEU:HA	1:B:155:LYS:HG3	1.97	0.46
1:B:260:ILE:O	1:B:261:THR:C	2.58	0.46
1:A:81:ALA:O	1:A:110:GLY:HA3	2.16	0.46
1:C:81:ALA:O	1:C:110:GLY:HA3	2.16	0.46
1:C:263:GLU:O	1:C:267:THR:HG23	2.16	0.46
1:A:79:GLN:O	1:A:83:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HA	1:A:155:LYS:HG3	1.97	0.45
1:C:197:TYR:CD1	1:C:197:TYR:C	2.94	0.45
1:C:270:LEU:HD23	1:C:304:PHE:CE1	2.50	0.45
1:B:26:LYS:HD2	1:B:281:THR:CG2	2.46	0.45
1:A:9:GLU:OE2	1:A:87:THR:HG21	2.17	0.45
1:A:235:GLY:O	1:A:252:LEU:HD12	2.15	0.45
1:A:171:ALA:HB1	1:A:195:ILE:HG12	1.97	0.45
1:A:207:GLY:O	1:A:208:ILE:C	2.58	0.45
1:A:244:THR:CG2	1:A:245:GLY:H	2.21	0.45
1:B:9:GLU:OE2	1:B:87:THR:HG21	2.17	0.45
1:B:81:ALA:O	1:B:110:GLY:HA3	2.16	0.45
1:A:100:ASP:OD1	1:A:102:SER:N	2.42	0.45
1:A:207:GLY:O	1:A:209:GLY:N	2.49	0.45
1:B:180:ARG:HB3	1:B:200:MET:HG2	1.99	0.45
1:C:152:LEU:HA	1:C:155:LYS:HG3	1.97	0.45
1:C:260:ILE:O	1:C:261:THR:C	2.58	0.45
1:A:147:PHE:CD1	1:A:147:PHE:N	2.85	0.45
1:B:129:ILE:HG23	1:B:186:GLU:HG2	1.97	0.45
1:C:180:ARG:HB3	1:C:200:MET:HG2	1.99	0.45
1:A:287:GLU:OE2	1:A:291:ARG:NE	2.44	0.45
1:B:79:GLN:O	1:B:83:VAL:HG23	2.15	0.45
1:B:147:PHE:CD1	1:B:147:PHE:N	2.85	0.45
1:C:237:ASP:N	1:C:252:LEU:O	2.49	0.45
1:B:135:THR:HG21	1:B:143:GLN:HE21	1.82	0.45
1:B:164:TRP:CH2	1:B:165:VAL:HG22	2.51	0.45
1:C:26:LYS:HD2	1:C:281:THR:CG2	2.46	0.45
1:C:100:ASP:O	1:C:276:MET:HE3	2.17	0.45
1:A:78:GLU:HB2	1:A:164:TRP:CE2	2.52	0.45
1:C:290:THR:O	1:C:294:ASN:ND2	2.50	0.45
1:A:290:THR:O	1:A:294:ASN:ND2	2.50	0.44
1:C:147:PHE:CD1	1:C:147:PHE:N	2.85	0.44
1:A:197:TYR:C	1:A:197:TYR:CD1	2.94	0.44
1:A:263:GLU:O	1:A:267:THR:HG23	2.16	0.44
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.99	0.44
1:B:110:GLY:HA2	1:B:113:ARG:HD2	1.97	0.44
1:C:19:GLN:HB2	1:C:20:PRO:HD2	1.99	0.44
1:C:78:GLU:HB2	1:C:164:TRP:CE2	2.52	0.44
1:B:78:GLU:HB2	1:B:164:TRP:CE2	2.52	0.44
1:B:100:ASP:O	1:B:276:MET:HE3	2.17	0.44
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.99	0.44
1:B:290:THR:O	1:B:294:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HG21	1:A:143:GLN:HE21	1.82	0.44
1:A:214:GLU:O	1:A:215:THR:C	2.60	0.44
1:B:192:THR:C	1:B:194:GLY:H	2.26	0.44
1:B:212:MET:HA	1:B:215:THR:OG1	2.18	0.44
1:A:180:ARG:HB3	1:A:200:MET:HG2	1.99	0.44
1:A:212:MET:HA	1:A:215:THR:OG1	2.18	0.44
1:A:291:ARG:O	1:A:295:THR:CG2	2.66	0.44
1:C:205:LYS:HE3	1:C:206:LEU:CD2	2.48	0.44
1:C:293:VAL:O	1:C:296:ALA:HB3	2.18	0.44
1:A:118:LEU:C	1:A:118:LEU:CD1	2.91	0.43
1:B:205:LYS:HE3	1:B:206:LEU:CD2	2.48	0.43
1:B:308:ARG:NH1	1:C:204:ASP:OD2	2.45	0.43
1:C:84:VAL:HG21	1:C:107:SER:HA	2.00	0.43
1:A:100:ASP:O	1:A:276:MET:HE3	2.17	0.43
1:A:197:TYR:C	1:A:197:TYR:HD1	2.26	0.43
1:B:26:LYS:O	1:B:29:ALA:HB3	2.18	0.43
1:B:291:ARG:O	1:B:295:THR:CG2	2.66	0.43
1:B:293:VAL:O	1:B:296:ALA:HB3	2.18	0.43
1:C:9:GLU:OE2	1:C:87:THR:HG21	2.17	0.43
1:C:137:SER:OG	1:C:139:ASN:ND2	2.51	0.43
1:C:192:THR:C	1:C:194:GLY:H	2.26	0.43
1:C:291:ARG:O	1:C:295:THR:CG2	2.66	0.43
1:A:137:SER:OG	1:A:139:ASN:ND2	2.51	0.43
1:A:180:ARG:HG3	1:A:248:VAL:CG1	2.48	0.43
1:A:208:ILE:HD11	1:A:260:ILE:CD1	2.47	0.43
1:B:66:ILE:O	1:B:67:VAL:C	2.61	0.43
1:B:137:SER:OG	1:B:139:ASN:ND2	2.51	0.43
1:C:26:LYS:O	1:C:29:ALA:HB3	2.19	0.43
1:C:159:VAL:HA	1:C:160:PRO:HD3	1.93	0.43
1:C:197:TYR:C	1:C:197:TYR:HD1	2.26	0.43
1:C:212:MET:HA	1:C:215:THR:OG1	2.18	0.43
1:A:26:LYS:O	1:A:29:ALA:HB3	2.18	0.43
1:A:205:LYS:HE3	1:A:206:LEU:CD2	2.48	0.43
1:B:214:GLU:O	1:B:215:THR:C	2.61	0.43
1:A:66:ILE:O	1:A:67:VAL:C	2.62	0.43
1:A:123:VAL:HA	1:A:177:ILE:O	2.19	0.43
1:B:118:LEU:C	1:B:118:LEU:CD1	2.91	0.43
1:B:197:TYR:C	1:B:197:TYR:HD1	2.26	0.43
1:C:180:ARG:HG3	1:C:248:VAL:CG1	2.48	0.43
1:C:214:GLU:O	1:C:215:THR:C	2.60	0.43
1:B:85:ALA:HB2	1:B:113:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ARG:HD2	1:C:200:MET:HE2	2.00	0.43
1:C:71:ARG:HG3	1:C:71:ARG:HH11	1.84	0.43
1:C:118:LEU:C	1:C:118:LEU:CD1	2.91	0.43
1:A:32:ARG:C	1:A:34:ALA:N	2.77	0.43
1:B:150:LYS:C	1:B:152:LEU:N	2.77	0.43
1:A:85:ALA:HB2	1:A:113:ARG:HD2	2.00	0.43
1:A:110:GLY:O	1:A:113:ARG:HB2	2.19	0.43
1:A:192:THR:C	1:A:194:GLY:H	2.26	0.43
1:A:84:VAL:HG21	1:A:107:SER:HA	2.00	0.43
1:B:180:ARG:HG3	1:B:248:VAL:CG1	2.48	0.43
1:C:66:ILE:O	1:C:67:VAL:C	2.61	0.43
1:C:150:LYS:C	1:C:152:LEU:N	2.77	0.43
1:A:260:ILE:O	1:A:261:THR:C	2.58	0.43
1:A:164:TRP:CZ3	1:A:165:VAL:HG22	2.54	0.42
1:A:293:VAL:O	1:A:296:ALA:HB3	2.18	0.42
1:B:157:PRO:O	1:B:158:ASP:C	2.62	0.42
1:B:310:GLY:O	1:C:187:HIS:CD2	2.72	0.42
1:C:123:VAL:HA	1:C:177:ILE:O	2.18	0.42
1:C:164:TRP:CZ3	1:C:165:VAL:HG22	2.54	0.42
1:A:71:ARG:HG3	1:A:71:ARG:HH11	1.84	0.42
1:A:150:LYS:C	1:A:152:LEU:N	2.77	0.42
1:A:237:ASP:N	1:A:252:LEU:O	2.49	0.42
1:B:208:ILE:HD11	1:B:260:ILE:CD1	2.47	0.42
1:A:265:TYR:CD2	1:A:265:TYR:C	2.97	0.42
1:B:123:VAL:HA	1:B:177:ILE:O	2.18	0.42
1:B:280:PRO:HA	1:B:289:VAL:HG13	2.01	0.42
1:C:85:ALA:HB2	1:C:113:ARG:HD2	2.00	0.42
1:C:265:TYR:CD2	1:C:265:TYR:C	2.97	0.42
1:A:169:ILE:N	1:A:169:ILE:CD1	2.82	0.42
1:B:32:ARG:C	1:B:34:ALA:N	2.77	0.42
1:B:84:VAL:HG21	1:B:107:SER:HA	2.00	0.42
1:B:110:GLY:O	1:B:113:ARG:HB2	2.19	0.42
1:B:193:LEU:O	1:B:194:GLY:C	2.62	0.42
1:C:135:THR:HG21	1:C:143:GLN:HE21	1.82	0.42
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.84	0.42
1:B:131:THR:C	1:B:133:LEU:N	2.77	0.42
1:A:71:ARG:HG3	1:A:71:ARG:NH1	2.35	0.42
1:A:236:LEU:HA	1:A:252:LEU:HB2	2.01	0.42
1:B:169:ILE:N	1:B:169:ILE:CD1	2.82	0.42
1:A:207:GLY:C	1:A:209:GLY:N	2.77	0.42
1:A:280:PRO:HA	1:A:289:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LEU:HA	1:C:252:LEU:HB2	2.01	0.42
1:A:64:PHE:O	1:A:65:GLN:HB2	2.19	0.42
1:B:62:SER:HA	1:B:63:PRO:HD3	1.86	0.42
1:B:125:ALA:CB	1:B:234:ASP:OD1	2.68	0.42
1:C:64:PHE:O	1:C:65:GLN:HB2	2.19	0.42
1:C:157:PRO:O	1:C:158:ASP:C	2.63	0.42
1:B:219:LEU:C	1:B:220:LEU:HD23	2.45	0.42
1:C:193:LEU:O	1:C:194:GLY:C	2.62	0.42
1:A:103:MET:HB2	1:A:276:MET:HE1	2.02	0.41
1:A:131:THR:C	1:A:133:LEU:N	2.77	0.41
1:A:193:LEU:O	1:A:194:GLY:C	2.62	0.41
1:A:219:LEU:C	1:A:220:LEU:HD23	2.45	0.41
1:B:103:MET:HB2	1:B:276:MET:HE1	2.02	0.41
1:B:164:TRP:CZ3	1:B:165:VAL:HG22	2.54	0.41
1:C:151:GLU:OE2	1:C:170:SER:HB2	2.20	0.41
1:C:208:ILE:HD12	1:C:208:ILE:HA	1.94	0.41
1:C:110:GLY:O	1:C:113:ARG:HB2	2.19	0.41
1:C:125:ALA:HB3	1:C:234:ASP:OD1	2.21	0.41
1:C:280:PRO:HA	1:C:289:VAL:HG13	2.01	0.41
1:A:80:LEU:O	1:A:81:ALA:C	2.63	0.41
1:B:64:PHE:O	1:B:65:GLN:HB2	2.19	0.41
1:B:131:THR:C	1:B:133:LEU:H	2.28	0.41
1:B:207:GLY:C	1:B:209:GLY:N	2.77	0.41
1:B:236:LEU:HA	1:B:252:LEU:HB2	2.01	0.41
1:B:284:LYS:C	1:B:285:THR:CG2	2.93	0.41
1:C:32:ARG:C	1:C:34:ALA:N	2.77	0.41
1:C:125:ALA:CB	1:C:234:ASP:OD1	2.68	0.41
1:C:198:PHE:CG	1:C:211:VAL:HG13	2.56	0.41
1:C:219:LEU:C	1:C:220:LEU:HD23	2.45	0.41
1:C:313:LYS:HA	1:C:314:PRO:HD3	1.92	0.41
1:A:131:THR:C	1:A:133:LEU:H	2.28	0.41
1:A:157:PRO:O	1:A:158:ASP:C	2.62	0.41
1:A:198:PHE:CG	1:A:211:VAL:HG13	2.55	0.41
1:C:93:ILE:HG23	1:C:271:SER:O	2.20	0.41
1:C:207:GLY:C	1:C:209:GLY:N	2.77	0.41
1:A:125:ALA:CB	1:A:234:ASP:OD1	2.68	0.41
1:A:151:GLU:OE2	1:A:170:SER:HB2	2.20	0.41
1:A:159:VAL:HA	1:A:160:PRO:HD3	1.93	0.41
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.35	0.41
1:B:232:ASP:OD2	1:B:234:ASP:OD2	2.39	0.41
1:C:71:ARG:HG3	1:C:71:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HG23	1:A:271:SER:O	2.20	0.41
1:C:131:THR:C	1:C:133:LEU:H	2.28	0.41
1:B:80:LEU:O	1:B:81:ALA:C	2.63	0.41
1:B:237:ASP:N	1:B:252:LEU:O	2.49	0.41
1:C:232:ASP:OD2	1:C:234:ASP:OD2	2.39	0.41
1:A:232:ASP:OD2	1:A:234:ASP:OD2	2.39	0.41
1:B:125:ALA:HB3	1:B:234:ASP:OD1	2.21	0.41
1:C:103:MET:HB2	1:C:276:MET:HE1	2.02	0.41
1:B:86:GLU:O	1:B:89:LYS:HB3	2.21	0.41
1:C:80:LEU:O	1:C:81:ALA:C	2.63	0.41
1:C:180:ARG:HG3	1:C:248:VAL:HG12	2.03	0.41
1:C:284:LYS:C	1:C:285:THR:CG2	2.93	0.41
1:A:284:LYS:C	1:A:285:THR:CG2	2.93	0.40
1:B:93:ILE:HG23	1:B:271:SER:O	2.20	0.40
1:C:131:THR:C	1:C:133:LEU:N	2.77	0.40
1:C:174:ILE:HG12	1:C:175:VAL:N	2.35	0.40
1:B:265:TYR:CD2	1:B:265:TYR:C	2.97	0.40
1:C:37:VAL:O	1:C:38:GLU:C	2.64	0.40
1:B:174:ILE:HG12	1:B:175:VAL:N	2.35	0.40
1:B:259:TYR:HE1	1:C:205:LYS:HB2	1.80	0.40
1:C:270:LEU:HD23	1:C:304:PHE:HE1	1.87	0.40
1:A:125:ALA:HB3	1:A:234:ASP:OD1	2.21	0.40
1:B:198:PHE:CG	1:B:211:VAL:HG13	2.56	0.40
1:C:140:LEU:O	1:C:142:GLY:N	2.54	0.40
1:C:166:THR:O	1:C:167:PRO:C	2.64	0.40
1:B:68:LYS:C	1:B:70:PRO:HD3	2.47	0.40
1:B:151:GLU:OE2	1:B:170:SER:HB2	2.20	0.40
1:C:62:SER:HA	1:C:63:PRO:HD3	1.86	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	312/323 (97%)	245 (78%)	54 (17%)	13 (4%)	2	7
1	B	312/323 (97%)	244 (78%)	55 (18%)	13 (4%)	2	7
1	C	312/323 (97%)	245 (78%)	54 (17%)	13 (4%)	2	7
All	All	936/969 (97%)	734 (78%)	163 (17%)	39 (4%)	2	7

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PHE
1	A	143	GLN
1	B	64	PHE
1	B	143	GLN
1	C	64	PHE
1	C	143	GLN
1	A	14	PRO
1	A	171	ALA
1	A	280	PRO
1	B	14	PRO
1	B	171	ALA
1	B	280	PRO
1	C	14	PRO
1	C	171	ALA
1	C	280	PRO
1	A	135	THR
1	A	139	ASN
1	B	135	THR
1	B	139	ASN
1	C	135	THR
1	C	139	ASN
1	A	222	ARG
1	B	222	ARG
1	C	222	ARG
1	A	69	ASN
1	A	163	SER
1	B	69	ASN
1	B	163	SER
1	C	69	ASN
1	C	163	SER
1	A	65	GLN
1	B	65	GLN
1	C	65	GLN
1	A	208	ILE

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Mol	Chain	Res	Type
1	B	208	ILE
1	C	208	ILE
1	A	167	PRO
1	B	167	PRO
1	C	167	PRO

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	264/273 (97%)	244 (92%)	20 (8%)	12	36
1	B	264/273 (97%)	244 (92%)	20 (8%)	12	36
1	C	264/273 (97%)	244 (92%)	20 (8%)	12	36
All	All	792/819 (97%)	732 (92%)	60 (8%)	12	36

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	47	VAL
1	A	118	LEU
1	A	123	VAL
1	A	127	THR
1	A	135	THR
1	A	144	PRO
1	A	169	ILE
1	A	197	TYR
1	A	201	THR
1	A	225	ARG
1	A	233	VAL
1	A	238	PRO
1	A	239	VAL
1	A	246	THR
1	A	264	ILE
1	A	273	LEU

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Mol	Chain	Res	Type
1	A	285	THR
1	A	287	GLU
1	A	295	THR
1	B	24	VAL
1	B	47	VAL
1	B	118	LEU
1	B	123	VAL
1	B	127	THR
1	B	135	THR
1	B	144	PRO
1	B	169	ILE
1	B	197	TYR
1	B	201	THR
1	B	225	ARG
1	B	233	VAL
1	B	238	PRO
1	B	239	VAL
1	B	246	THR
1	B	264	ILE
1	B	273	LEU
1	B	285	THR
1	B	287	GLU
1	B	295	THR
1	C	24	VAL
1	C	47	VAL
1	C	118	LEU
1	C	123	VAL
1	C	127	THR
1	C	135	THR
1	C	144	PRO
1	C	169	ILE
1	C	197	TYR
1	C	201	THR
1	C	225	ARG
1	C	233	VAL
1	C	238	PRO
1	C	239	VAL
1	C	246	THR
1	C	264	ILE
1	C	273	LEU
1	C	285	THR
1	C	287	GLU

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Mol	Chain	Res	Type
1	C	295	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	69	ASN
1	A	79	GLN
1	A	88	GLN
1	A	90	ASN
1	A	115	HIS
1	A	139	ASN
1	A	143	GLN
1	A	294	ASN
1	A	311	ASN
1	B	65	GLN
1	B	69	ASN
1	B	79	GLN
1	B	88	GLN
1	B	90	ASN
1	B	115	HIS
1	B	139	ASN
1	B	143	GLN
1	B	294	ASN
1	B	311	ASN
1	C	65	GLN
1	C	69	ASN
1	C	79	GLN
1	C	88	GLN
1	C	115	HIS
1	C	139	ASN
1	C	143	GLN
1	C	294	ASN
1	C	311	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
3	NNH	A	901	2	8,11,11	2.30	2 (25%)	8,13,13	1.68	1 (12%)
3	NNH	B	902	2	8,11,11	2.30	2 (25%)	8,13,13	1.68	1 (12%)
3	NNH	C	903	2	8,11,11	2.29	2 (25%)	8,13,13	1.67	1 (12%)

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
3	NNH	A	901	2	-	1/10/12/12	-
3	NNH	B	902	2	-	1/10/12/12	-
3	NNH	C	903	2	-	1/10/12/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	NNH	CE-NH1	4.35	1.44	1.34
3	A	901	NNH	CE-NH1	4.34	1.44	1.34
3	C	903	NNH	CE-NH1	4.33	1.44	1.34
3	B	902	NNH	OH1-NH1	-4.10	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NNH	OH1-NH1	-4.10	1.30	1.40
3	C	903	NNH	OH1-NH1	-4.10	1.30	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	NNH	CG-ND-CE	3.38	129.66	123.46
3	C	903	NNH	CG-ND-CE	3.38	129.66	123.46
3	B	902	NNH	CG-ND-CE	3.37	129.65	123.46

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	NNH	CA-CB-CG-ND
3	B	902	NNH	CA-CB-CG-ND
3	C	903	NNH	CA-CB-CG-ND

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.