



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:35 PM UTC

PDB ID : 1LBI / pdb_00001lbi
Title : LAC REPRESSOR
Authors : Lewis, M.; Chang, G.; Horton, N.C.; Kercher, M.A.; Pace, H.C.; Lu, P.
Deposited on : 1996-02-17
Resolution : 2.70 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

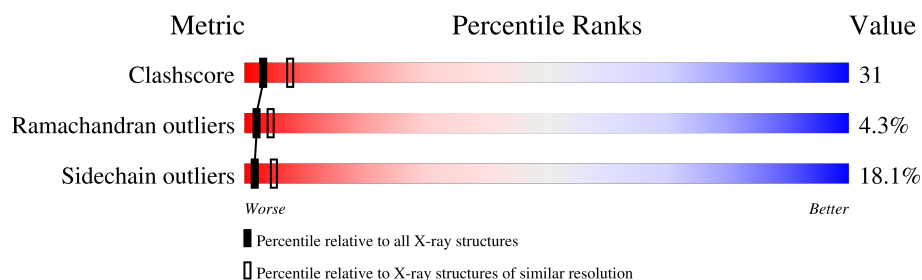
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	360	27% 39% 14% • 18%
1	B	360	29% 39% 12% • 18%
1	C	360	32% 34% 13% • 18%
1	D	360	31% 40% 10% • 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8872 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 LAC REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	B	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	C	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	D	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			

There are 8 discrepancies between the modelled and reference sequences:

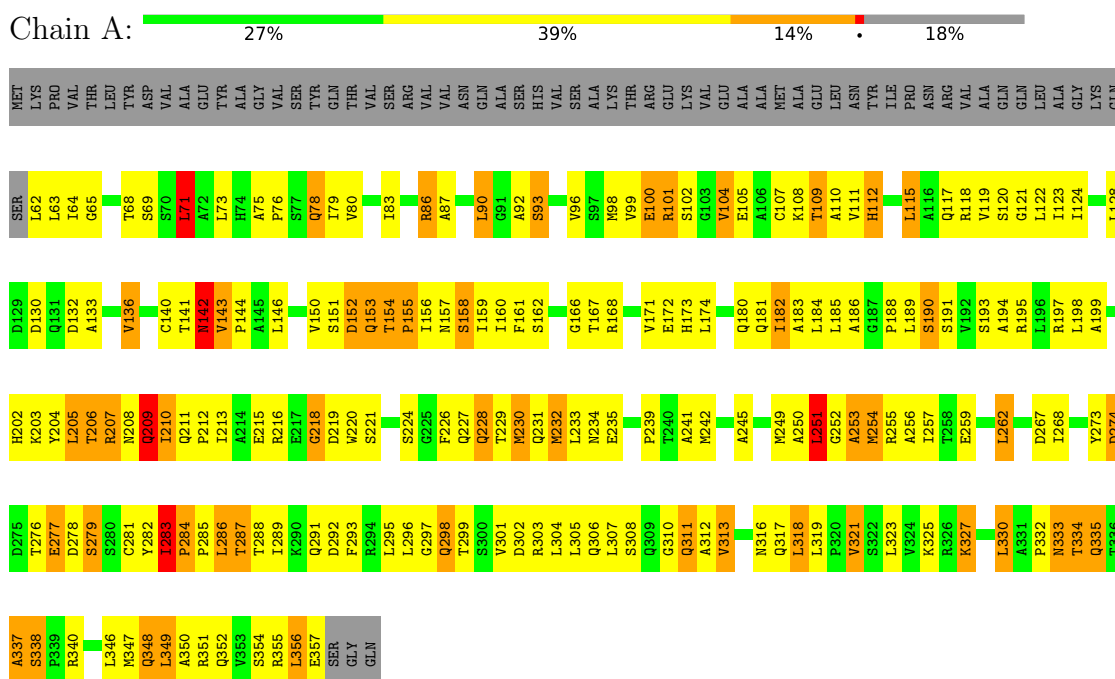
Chain	Residue	Modelled	Actual	Comment	Reference
A	109	THR	ALA	conflict	UNP P03023
A	286	LEU	SER	conflict	UNP P03023
B	109	THR	ALA	conflict	UNP P03023
B	286	LEU	SER	conflict	UNP P03023
C	109	THR	ALA	conflict	UNP P03023
C	286	LEU	SER	conflict	UNP P03023
D	109	THR	ALA	conflict	UNP P03023
D	286	LEU	SER	conflict	UNP P03023

3 Residue-property plots

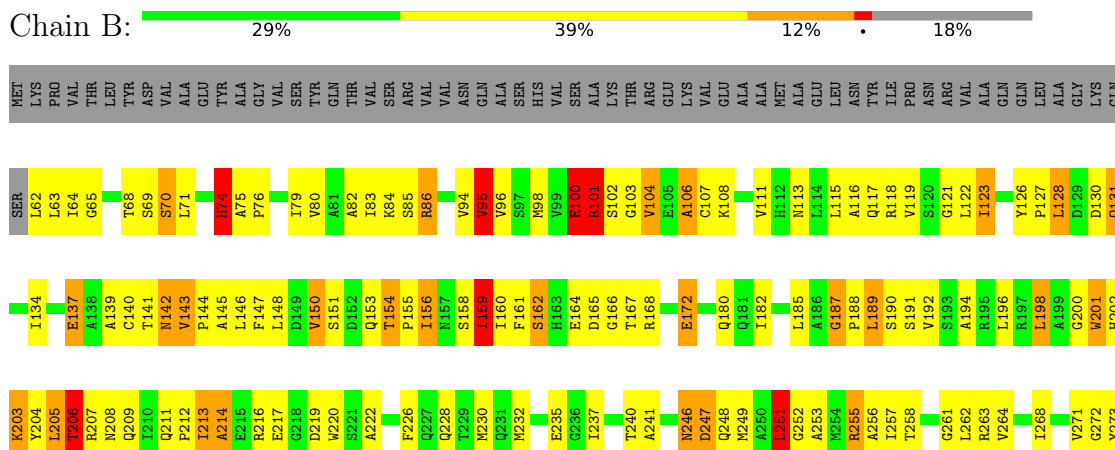
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

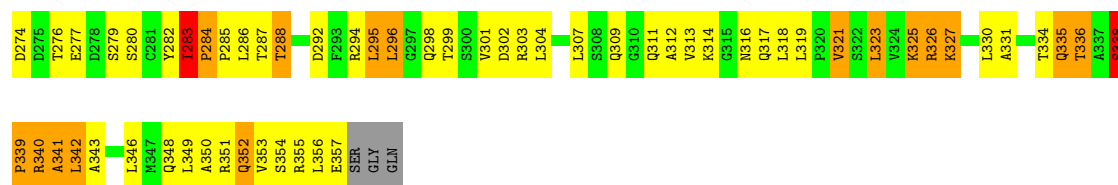
Note EDS was not executed.

• Molecule 1: LAC REPRESSOR



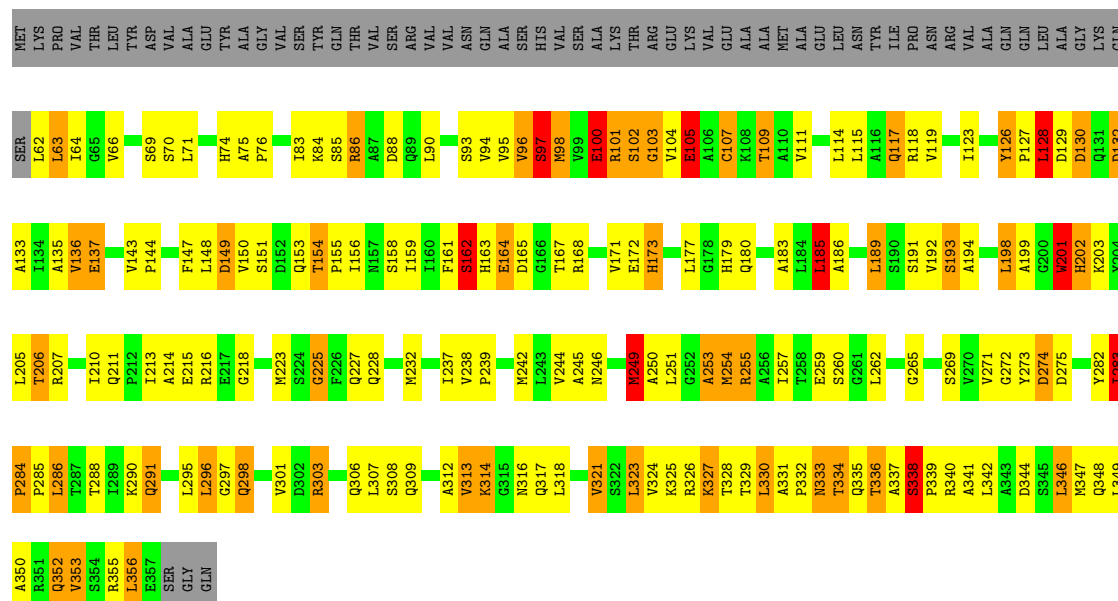
• Molecule 1: LAC REPRESSOR





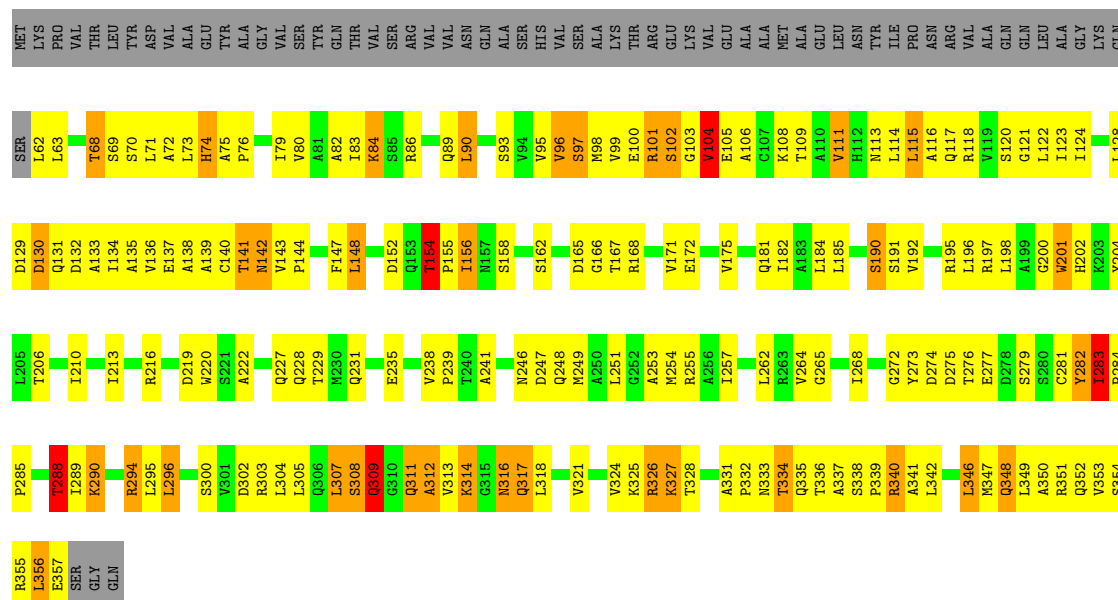
• Molecule 1: LAC REPRESSOR

Chain C: 32% 34% 13% 18%



• Molecule 1: LAC REPRESSOR

Chain D: 31% 40% 10% 18%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.30 Å 73.30 Å 147.80 Å 90.00° 120.30° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.250 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8872	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.07	2/2247 (0.1%)	1.51	44/3055 (1.4%)
1	B	1.10	6/2247 (0.3%)	1.93	49/3055 (1.6%)
1	C	1.13	6/2247 (0.3%)	1.59	45/3055 (1.5%)
1	D	1.10	1/2247 (0.0%)	1.45	29/3055 (0.9%)
All	All	1.10	15/8988 (0.2%)	1.63	167/12220 (1.4%)

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	C	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	230	MET	SD-CE	7.92	1.99	1.79
1	C	249	MET	SD-CE	-7.81	1.60	1.79
1	A	254	MET	SD-CE	-7.57	1.60	1.79
1	B	336	THR	CA-C	6.47	1.59	1.52
1	C	66	VAL	CA-CB	6.03	1.61	1.54
1	A	96	VAL	CA-CB	5.89	1.62	1.54
1	C	254	MET	SD-CE	-5.87	1.64	1.79
1	B	336	THR	CA-CB	5.84	1.63	1.53
1	C	333	ASN	CA-C	5.70	1.60	1.52
1	C	284	PRO	CA-C	5.44	1.57	1.52
1	B	271	VAL	CA-CB	5.36	1.61	1.54
1	B	95	VAL	CA-CB	5.20	1.61	1.54
1	D	124	ILE	CA-CB	5.16	1.59	1.53
1	B	206	THR	CA-CB	5.10	1.62	1.53
1	C	96	VAL	CA-CB	5.07	1.60	1.54

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ILE	CA-C-N	43.52	165.20	120.38
1	B	283	ILE	C-N-CA	43.52	165.20	120.38
1	C	283	ILE	CA-C-N	-18.83	100.98	120.38
1	C	283	ILE	C-N-CA	-18.83	100.98	120.38
1	D	283	ILE	CA-C-N	-14.72	105.21	120.38
1	D	283	ILE	C-N-CA	-14.72	105.21	120.38
1	C	309	GLN	N-CA-C	-13.36	96.71	111.14
1	B	154	THR	CA-C-N	12.87	135.93	119.84
1	B	154	THR	C-N-CA	12.87	135.93	119.84
1	B	334	THR	N-CA-C	-11.83	98.23	112.89
1	C	284	PRO	N-CA-C	-11.82	96.28	110.70
1	B	283	ILE	C-N-CD	-11.61	77.40	125.00
1	A	283	ILE	CA-C-N	-10.14	109.93	120.38
1	A	283	ILE	C-N-CA	-10.14	109.93	120.38
1	C	353	VAL	N-CA-C	-9.59	101.52	110.82
1	B	286	LEU	N-CA-C	9.50	124.21	109.96
1	A	152	ASP	N-CA-C	-9.31	101.18	112.54
1	C	245	ALA	N-CA-C	9.31	122.41	111.71
1	C	63	LEU	N-CA-C	9.17	123.63	109.96
1	B	336	THR	N-CA-C	-9.12	93.13	108.26
1	C	314	LYS	N-CA-C	9.11	124.55	110.42
1	B	103	GLY	N-CA-C	8.87	123.14	110.46
1	B	235	GLU	N-CA-C	-8.75	102.60	113.28
1	D	113	ASN	N-CA-C	-8.75	100.61	111.11
1	A	154	THR	CA-C-N	8.68	130.69	119.84
1	A	154	THR	C-N-CA	8.68	130.69	119.84
1	C	336	THR	N-CA-C	-8.65	101.68	113.18
1	C	201	TRP	N-CA-C	-8.63	101.84	111.07
1	A	327	LYS	N-CA-C	8.62	122.58	112.93
1	D	190	SER	N-CA-C	-8.61	102.21	112.89
1	B	335	GLN	N-CA-C	8.29	128.46	110.80
1	A	92	ALA	N-CA-C	8.21	121.12	110.53
1	D	282	TYR	N-CA-C	-8.17	99.74	110.53
1	A	100	GLU	N-CA-C	-8.15	98.41	110.48
1	A	334	THR	N-CA-C	8.10	123.17	113.28
1	B	104	VAL	CB-CA-C	-8.09	103.75	111.44
1	C	333	ASN	N-CA-C	8.09	128.03	110.80
1	B	240	THR	N-CA-C	-8.05	103.25	113.23
1	B	255	ARG	N-CA-C	-7.92	102.72	111.36
1	A	140	CYS	N-CA-C	-7.87	97.93	109.11
1	B	327	LYS	N-CA-C	7.86	121.68	112.72
1	A	209	GLN	N-CA-C	7.66	121.96	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	LEU	N-CA-C	-7.55	102.98	111.14
1	C	218	GLY	N-CA-C	-7.50	102.46	112.81
1	B	283	ILE	N-CA-C	7.31	124.66	108.88
1	C	286	LEU	N-CA-C	7.26	121.03	110.28
1	C	74	HIS	N-CA-C	7.25	118.83	111.07
1	A	104	VAL	CB-CA-C	-7.23	100.55	112.26
1	A	87	ALA	N-CA-C	-7.14	103.10	111.03
1	A	279	SER	N-CA-C	7.05	119.87	111.33
1	C	132	ASP	N-CA-C	-7.03	102.82	111.40
1	D	314	LYS	N-CA-C	6.95	120.76	110.48
1	C	327	LYS	N-CA-C	6.88	122.63	112.94
1	B	277	GLU	N-CA-C	6.86	119.63	111.33
1	A	205	LEU	N-CA-C	-6.84	103.75	111.14
1	A	253	ALA	N-CA-C	-6.80	103.80	111.07
1	C	238	VAL	CA-C-N	6.69	127.23	120.14
1	C	238	VAL	C-N-CA	6.69	127.23	120.14
1	B	208	ASN	N-CA-C	-6.68	102.45	111.87
1	B	251	LEU	N-CA-C	-6.66	103.11	111.11
1	A	208	ASN	N-CA-C	-6.58	106.00	112.97
1	B	341	ALA	N-CA-C	6.57	118.44	111.28
1	B	319	LEU	N-CA-C	-6.52	101.91	110.39
1	A	256	ALA	N-CA-C	-6.42	104.14	112.23
1	C	105	GLU	N-CA-C	6.42	118.15	111.03
1	B	287	THR	N-CA-C	-6.41	99.44	109.25
1	C	296	LEU	N-CA-C	-6.40	104.23	111.07
1	D	68	THR	N-CA-C	6.39	119.42	109.52
1	C	282	TYR	N-CA-C	-6.38	101.94	110.55
1	A	195	ARG	N-CA-C	-6.38	104.69	113.18
1	B	279	SER	N-CA-C	6.35	124.33	110.80
1	A	71	LEU	N-CA-C	6.34	124.30	110.80
1	A	182	ILE	N-CA-C	6.34	117.24	107.99
1	B	352	GLN	N-CA-C	-6.33	104.30	111.14
1	C	341	ALA	N-CA-C	-6.33	104.00	111.03
1	B	212	PRO	N-CA-C	6.30	121.53	111.26
1	B	284	PRO	CA-N-CD	-6.30	103.19	112.00
1	C	338	SER	N-CA-C	6.29	123.71	109.81
1	C	128	LEU	N-CA-C	6.28	118.86	109.25
1	A	286	LEU	N-CA-C	6.26	119.72	109.76
1	A	287	THR	N-CA-C	-6.26	100.31	110.20
1	C	253	ALA	N-CA-C	-6.24	104.59	111.82
1	A	65	GLY	N-CA-C	-6.23	99.62	110.71
1	D	307	LEU	N-CA-C	-6.22	104.61	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	VAL	N-CA-C	-6.21	96.42	109.34
1	D	154	THR	N-CA-C	6.16	117.56	109.93
1	B	247	ASP	N-CA-C	6.12	120.01	112.54
1	B	338	SER	N-CA-C	6.08	123.26	109.81
1	A	190	SER	N-CA-C	-6.05	100.55	109.62
1	A	319	LEU	CA-C-N	6.02	125.98	119.78
1	A	319	LEU	C-N-CA	6.02	125.98	119.78
1	A	228	GLN	N-CA-C	-6.01	104.64	111.14
1	B	205	LEU	N-CA-C	-6.00	104.66	111.14
1	C	83	ILE	N-CA-C	-6.00	104.46	111.00
1	A	218	GLY	N-CA-C	-5.99	104.37	112.57
1	A	110	ALA	N-CA-C	-5.98	104.88	111.82
1	A	160	ILE	N-CA-C	5.94	117.24	108.45
1	C	338	SER	CA-C-N	5.93	125.80	119.28
1	C	338	SER	C-N-CA	5.93	125.80	119.28
1	B	340	ARG	N-CA-C	-5.92	105.91	113.01
1	C	149	ASP	N-CA-C	5.87	118.45	110.06
1	C	100	GLU	N-CA-C	-5.87	101.59	110.28
1	C	162	SER	N-CA-C	5.82	117.52	109.15
1	D	96	VAL	N-CA-C	5.81	117.14	108.54
1	C	225	GLY	N-CA-C	-5.80	105.77	112.50
1	B	282	TYR	N-CA-C	-5.76	101.76	110.28
1	B	101	ARG	N-CA-C	5.75	123.06	110.80
1	D	84	LYS	N-CA-C	-5.72	105.12	111.36
1	B	211	GLN	CA-C-N	5.72	126.05	119.93
1	B	211	GLN	C-N-CA	5.72	126.05	119.93
1	C	173	HIS	N-CA-C	-5.71	104.51	112.45
1	C	260	SER	N-CA-C	-5.70	106.55	112.93
1	D	104	VAL	N-CA-C	5.70	121.19	109.34
1	C	202	HIS	N-CA-C	5.69	117.17	110.97
1	B	68	THR	N-CA-C	5.69	115.92	108.07
1	B	164	GLU	N-CA-C	-5.69	105.06	112.23
1	D	75	ALA	CA-C-N	-5.66	113.84	119.56
1	D	75	ALA	C-N-CA	-5.66	113.84	119.56
1	D	72	ALA	N-CA-C	5.66	119.38	111.74
1	C	137	GLU	N-CA-C	-5.65	105.03	111.14
1	A	143	VAL	CA-C-N	5.65	125.97	119.93
1	A	143	VAL	C-N-CA	5.65	125.97	119.93
1	A	136	VAL	N-CA-C	-5.64	104.86	110.62
1	D	210	ILE	N-CA-C	5.63	117.10	108.71
1	A	251	LEU	N-CA-C	-5.57	105.21	111.28
1	C	255	ARG	N-CA-C	-5.57	105.11	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	352	GLN	N-CA-C	-5.53	107.54	114.56
1	B	96	VAL	N-CA-C	5.49	117.22	108.87
1	D	281	CYS	N-CA-C	5.48	119.27	112.59
1	D	283	ILE	CB-CA-C	5.48	121.33	111.36
1	B	70	SER	N-CA-C	-5.45	99.20	110.80
1	D	290	LYS	N-CA-C	5.44	117.59	109.59
1	A	102	SER	N-CA-C	5.43	116.83	109.11
1	B	209	GLN	N-CA-C	5.41	118.85	111.39
1	C	185	LEU	N-CA-C	-5.40	97.45	107.71
1	B	134	ILE	N-CA-C	-5.39	105.12	110.62
1	B	301	VAL	N-CA-C	-5.38	104.71	110.36
1	C	97	SER	N-CA-C	-5.37	101.14	109.72
1	B	162	SER	N-CA-C	5.36	116.86	109.15
1	B	284	PRO	CA-C-N	5.33	125.64	119.93
1	B	284	PRO	C-N-CA	5.33	125.64	119.93
1	A	158	SER	N-CA-C	5.31	117.06	108.41
1	D	74	HIS	N-CA-C	5.31	117.14	111.36
1	B	123	ILE	N-CA-C	-5.28	99.35	106.85
1	D	295	LEU	N-CA-C	-5.27	105.53	111.28
1	C	199	ALA	N-CA-C	-5.27	105.43	111.07
1	D	97	SER	N-CA-C	-5.26	101.13	109.76
1	C	164	GLU	N-CA-C	-5.24	105.25	111.69
1	B	74	HIS	N-CA-C	5.24	117.39	111.11
1	C	331	ALA	N-CA-C	-5.21	103.38	110.36
1	B	187	GLY	N-CA-C	-5.19	105.95	112.23
1	D	73	LEU	N-CA-C	-5.18	101.25	109.96
1	B	302	ASP	N-CA-C	5.18	116.61	111.07
1	A	232	MET	CA-C-N	5.18	127.53	120.54
1	A	232	MET	C-N-CA	5.18	127.53	120.54
1	A	112	HIS	CB-CA-C	-5.17	102.20	110.79
1	A	73	LEU	N-CA-C	-5.14	102.87	110.48
1	D	311	GLN	N-CA-C	5.14	116.85	108.63
1	A	227	GLN	N-CA-C	5.13	118.00	111.69
1	D	238	VAL	CA-C-N	5.05	124.95	119.85
1	D	238	VAL	C-N-CA	5.05	124.95	119.85
1	D	288	THR	N-CA-C	5.05	117.09	109.41
1	D	197	ARG	N-CA-C	-5.04	105.86	111.36
1	A	284	PRO	N-CA-C	-5.03	104.57	110.70
1	B	106	ALA	N-CA-C	-5.02	104.81	112.04
1	C	318	LEU	N-CA-C	5.01	117.06	107.75
1	C	98	MET	N-CA-C	5.01	117.13	109.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	126	TYR	Sidechain

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	2218	0	2269	166	0
1	B	2218	0	2269	147	0
1	C	2218	0	2269	150	0
1	D	2218	0	2269	149	0
All	All	8872	0	9076	565	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 31.

All (565) 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:A:144:PRO:HG2	1:A:308:SER:HA	1.24	1.13
1:A:115:LEU:HD11	1:A:143:VAL:HG11	1.18	1.10
1:C:283:ILE:HG22	1:C:284:PRO:HD3	1.43	1.01
1:B:189:LEU:HD13	1:B:217:GLU:HG3	1.40	0.99
1:A:144:PRO:HB3	1:A:307:LEU:HD22	1.44	0.98
1:C:97:SER:HB2	1:C:114:LEU:HD21	1.48	0.95
1:B:216:ARG:HB3	1:B:228:GLN:HE21	1.30	0.94
1:C:254:MET:HE2	1:C:286:LEU:HD13	1.52	0.91
1:D:138:ALA:HA	1:D:141:THR:HG23	1.52	0.90
1:C:107:CYS:O	1:C:111:VAL:HG23	1.73	0.88
1:B:338:SER:O	1:B:342:LEU:HD12	1.73	0.88
1:D:105:GLU:O	1:D:109:THR:HG23	1.73	0.87
1:B:214:ALA:HB2	1:B:237:ILE:HG21	1.55	0.87
1:B:339:PRO:HA	1:D:357:GLU:OE1	1.76	0.85
1:A:104:VAL:HG13	1:A:132:ASP:HB3	1.55	0.85
1:C:104:VAL:HG21	1:C:135:ALA:HB3	1.57	0.85
1:B:115:LEU:HG	1:B:143:VAL:HG21	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:LEU:HG	1:C:119:VAL:HG12	1.59	0.84
1:D:71:LEU:HD11	1:D:101:ARG:HG3	1.60	0.84
1:A:245:ALA:O	1:A:273:TYR:HB3	1.76	0.83
1:B:113:ASN:O	1:B:117:GLN:HG2	1.79	0.83
1:B:115:LEU:HD11	1:B:122:LEU:HD21	1.59	0.82
1:C:349:LEU:HD13	1:D:346:LEU:HD23	1.61	0.82
1:B:222:ALA:HA	1:B:248:GLN:O	1.79	0.81
1:B:108:LYS:NZ	1:B:139:ALA:HB2	1.94	0.81
1:B:216:ARG:HH11	1:B:228:GLN:NE2	1.78	0.80
1:B:86:ARG:HG3	1:B:298:GLN:HA	1.63	0.79
1:C:283:ILE:HG22	1:C:284:PRO:CD	2.13	0.79
1:C:342:LEU:HD21	1:D:352:GLN:HB3	1.64	0.79
1:A:253:ALA:O	1:A:257:ILE:HG12	1.82	0.79
1:C:312:ALA:HB1	1:C:314:LYS:NZ	1.97	0.79
1:C:147:PHE:CD2	1:C:156:ILE:HD12	2.16	0.79
1:B:168:ARG:O	1:B:172:GLU:HB2	1.83	0.78
1:D:254:MET:HE3	1:D:284:PRO:HD2	1.66	0.77
1:B:350:ALA:HA	1:D:346:LEU:HD12	1.67	0.77
1:A:239:PRO:O	1:A:268:ILE:HG12	1.85	0.77
1:B:76:PRO:O	1:B:80:VAL:HG23	1.85	0.77
1:A:283:ILE:HG22	1:A:284:PRO:HD3	1.65	0.77
1:A:63:LEU:HD23	1:A:119:VAL:HA	1.66	0.76
1:C:202:HIS:O	1:C:206:THR:HG23	1.84	0.76
1:C:246:ASN:OD1	1:C:249:MET:HB2	1.85	0.76
1:C:353:VAL:O	1:C:356:LEU:HB2	1.86	0.76
1:C:117:GLN:O	1:C:118:ARG:HD2	1.85	0.76
1:B:150:VAL:HG21	1:B:156:ILE:HD11	1.68	0.75
1:A:346:LEU:HD23	1:B:349:LEU:HD13	1.67	0.75
1:A:347:MET:O	1:A:351:ARG:HG3	1.87	0.75
1:A:168:ARG:O	1:A:172:GLU:HG3	1.86	0.75
1:A:206:THR:HB	1:A:211:GLN:HE22	1.51	0.74
1:D:86:ARG:HG3	1:D:86:ARG:O	1.85	0.74
1:C:334:THR:C	1:C:336:THR:H	1.95	0.74
1:D:348:GLN:O	1:D:352:GLN:HG2	1.86	0.74
1:C:323:LEU:HD21	1:C:325:LYS:HG2	1.67	0.73
1:B:64:ILE:HD11	1:B:94:VAL:HG22	1.70	0.73
1:D:348:GLN:HG3	1:D:351:ARG:HH21	1.53	0.73
1:C:126:TYR:CD1	1:C:127:PRO:HD2	2.23	0.73
1:A:63:LEU:HD12	1:A:93:SER:HB3	1.70	0.73
1:A:191:SER:HB3	1:A:194:ALA:HB3	1.71	0.73
1:C:216:ARG:HB3	1:C:228:GLN:HE21	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD21	1:B:140:CYS:HA	1.71	0.71
1:C:168:ARG:O	1:C:172:GLU:HG2	1.89	0.71
1:B:346:LEU:HD12	1:D:350:ALA:HA	1.71	0.71
1:C:312:ALA:HB1	1:C:314:LYS:HZ3	1.54	0.71
1:A:64:ILE:HG13	1:A:304:LEU:HD23	1.72	0.71
1:C:70:SER:HB2	1:D:84:LYS:HG2	1.72	0.70
1:A:316:ASN:HD21	1:A:318:LEU:HD12	1.55	0.70
1:B:108:LYS:HZ2	1:B:139:ALA:HB2	1.54	0.70
1:A:250:ALA:O	1:A:254:MET:HG3	1.91	0.69
1:A:203:LYS:O	1:A:207:ARG:HD3	1.92	0.69
1:B:339:PRO:HA	1:D:357:GLU:CD	2.17	0.69
1:C:306:GLN:OE1	1:C:313:VAL:HG11	1.92	0.69
1:D:123:ILE:CG2	1:D:148:LEU:HD22	2.22	0.69
1:C:183:ALA:HB1	1:C:232:MET:HE1	1.73	0.69
1:A:144:PRO:CG	1:A:308:SER:HA	2.14	0.69
1:B:188:PRO:HD3	1:B:219:ASP:HA	1.74	0.69
1:A:146:LEU:HD11	1:A:159:ILE:HG13	1.76	0.68
1:A:104:VAL:HG12	1:A:136:VAL:CG2	2.24	0.68
1:D:216:ARG:HH11	1:D:228:GLN:NE2	1.91	0.68
1:D:97:SER:HB2	1:D:114:LEU:HG	1.75	0.67
1:A:283:ILE:HG22	1:A:284:PRO:CD	2.24	0.67
1:A:79:ILE:HG22	1:A:83:ILE:HD13	1.76	0.67
1:B:213:ILE:HG13	1:B:213:ILE:O	1.95	0.67
1:D:181:GLN:HG2	1:D:213:ILE:HD13	1.75	0.67
1:B:216:ARG:HB3	1:B:228:GLN:NE2	2.05	0.67
1:A:98:MET:O	1:B:84:LYS:HE3	1.93	0.67
1:A:62:LEU:N	1:A:120:SER:HG	1.93	0.67
1:A:356:LEU:HD13	1:B:342:LEU:CD1	2.25	0.67
1:B:246:ASN:OD1	1:B:249:MET:HG3	1.95	0.67
1:C:126:TYR:CG	1:C:127:PRO:HD2	2.30	0.66
1:C:63:LEU:CG	1:C:119:VAL:HG12	2.26	0.66
1:A:146:LEU:HD21	1:A:159:ILE:HD12	1.78	0.66
1:B:357:GLU:OE2	1:D:340:ARG:HA	1.96	0.66
1:C:144:PRO:HG3	1:C:308:SER:HB3	1.77	0.66
1:C:254:MET:CE	1:C:286:LEU:HD13	2.26	0.65
1:C:273:TYR:O	1:C:274:ASP:HB2	1.95	0.65
1:A:203:LYS:O	1:A:207:ARG:HB2	1.96	0.65
1:C:332:PRO:O	1:C:333:ASN:HB2	1.95	0.65
1:A:348:GLN:O	1:A:352:GLN:HG3	1.96	0.65
1:A:104:VAL:HG12	1:A:136:VAL:HG23	1.78	0.65
1:A:104:VAL:CG1	1:A:132:ASP:HB3	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:LEU:CD1	1:D:140:CYS:HB2	2.26	0.65
1:D:191:SER:O	1:D:195:ARG:HB2	1.97	0.64
1:B:160:ILE:HG22	1:B:161:PHE:O	1.98	0.64
1:C:323:LEU:CD2	1:C:325:LYS:HG2	2.27	0.64
1:D:132:ASP:O	1:D:136:VAL:HG23	1.98	0.64
1:D:339:PRO:C	1:D:341:ALA:H	2.05	0.64
1:A:86:ARG:NH2	1:A:90:LEU:HD13	2.12	0.64
1:B:338:SER:HB2	1:B:342:LEU:HD12	1.79	0.64
1:A:186:ALA:HA	1:A:245:ALA:HB2	1.80	0.63
1:B:283:ILE:O	1:B:283:ILE:HG22	1.97	0.63
1:A:352:GLN:HB2	1:B:342:LEU:HD21	1.79	0.63
1:D:324:VAL:HG11	1:D:326:ARG:NH1	2.13	0.63
1:B:338:SER:HB2	1:B:342:LEU:CD1	2.29	0.63
1:D:275:ASP:HB3	1:D:290:LYS:HG3	1.81	0.63
1:D:71:LEU:HD11	1:D:101:ARG:CG	2.29	0.62
1:D:90:LEU:HD23	1:D:305:LEU:HD11	1.82	0.62
1:B:104:VAL:O	1:B:108:LYS:HG2	1.99	0.62
1:D:168:ARG:HH11	1:D:168:ARG:HG2	1.64	0.62
1:A:69:SER:O	1:A:98:MET:HE2	1.99	0.62
1:B:216:ARG:NH1	1:B:228:GLN:NE2	2.48	0.62
1:A:283:ILE:O	1:A:285:PRO:N	2.33	0.61
1:A:356:LEU:HD13	1:B:342:LEU:HD13	1.82	0.61
1:C:290:LYS:O	1:C:321:VAL:HG22	2.00	0.61
1:A:226:PHE:HA	1:A:252:GLY:O	2.00	0.61
1:A:109:THR:HA	1:A:112:HIS:CD2	2.35	0.61
1:B:311:GLN:O	1:B:313:VAL:HG23	2.01	0.61
1:C:185:LEU:HB3	1:C:244:VAL:HG13	1.80	0.61
1:C:313:VAL:HG22	1:C:313:VAL:O	2.00	0.61
1:A:346:LEU:HD12	1:C:350:ALA:HA	1.83	0.61
1:B:207:ARG:O	1:B:207:ARG:HG2	2.00	0.61
1:C:162:SER:HB3	1:C:165:ASP:HB2	1.83	0.61
1:A:150:VAL:HG11	1:A:156:ILE:HD11	1.83	0.61
1:A:283:ILE:CG2	1:A:284:PRO:HD3	2.31	0.61
1:A:104:VAL:O	1:A:108:LYS:HG2	2.01	0.60
1:B:111:VAL:O	1:B:115:LEU:HD13	2.01	0.60
1:B:146:LEU:HD13	1:B:307:LEU:HD11	1.82	0.60
1:C:70:SER:HB3	1:C:98:MET:HB3	1.82	0.60
1:A:152:ASP:HA	1:A:316:ASN:OD1	2.01	0.60
1:D:70:SER:HB3	1:D:98:MET:HB3	1.83	0.60
1:A:142:ASN:ND2	1:A:143:VAL:N	2.48	0.60
1:C:97:SER:HB2	1:C:114:LEU:CD2	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLU:CD	1:D:340:ARG:HA	2.25	0.60
1:A:202:HIS:O	1:A:206:THR:HG23	2.01	0.60
1:B:148:LEU:HD12	1:B:159:ILE:CG2	2.32	0.60
1:B:222:ALA:O	1:B:252:GLY:HA3	2.01	0.60
1:C:86:ARG:HD2	1:C:298:GLN:HB2	1.83	0.59
1:C:336:THR:C	1:C:338:SER:H	2.10	0.59
1:D:90:LEU:HD23	1:D:305:LEU:CD1	2.31	0.59
1:C:333:ASN:HB3	1:C:336:THR:OG1	2.02	0.59
1:C:336:THR:O	1:D:356:LEU:HD22	2.02	0.59
1:C:183:ALA:HB3	1:C:242:MET:HG2	1.83	0.59
1:C:215:GLU:C	1:C:216:ARG:HD2	2.28	0.59
1:D:227:GLN:O	1:D:231:GLN:HG3	2.02	0.59
1:D:103:GLY:O	1:D:105:GLU:N	2.36	0.59
1:D:104:VAL:HG23	1:D:136:VAL:CG2	2.32	0.59
1:C:114:LEU:O	1:C:119:VAL:HG22	2.02	0.59
1:A:205:LEU:HD12	1:A:212:PRO:HG3	1.85	0.59
1:B:323:LEU:HD23	1:B:325:LYS:HG3	1.85	0.59
1:C:126:TYR:O	1:C:149:ASP:HB3	2.03	0.59
1:A:288:THR:HG22	1:A:289:ILE:N	2.16	0.58
1:C:342:LEU:CD2	1:D:352:GLN:HB3	2.32	0.58
1:C:118:ARG:HH22	1:D:118:ARG:HE	1.51	0.58
1:D:222:ALA:HA	1:D:248:GLN:O	2.03	0.58
1:B:122:LEU:HD23	1:B:140:CYS:HB3	1.85	0.58
1:A:281:CYS:O	1:B:251:LEU:HD22	2.04	0.58
1:C:128:LEU:HD21	1:C:136:VAL:HG21	1.86	0.58
1:A:115:LEU:HD13	1:A:122:LEU:HD11	1.84	0.58
1:B:330:LEU:HD12	1:B:331:ALA:H	1.67	0.58
1:D:111:VAL:CG2	1:D:140:CYS:HB3	2.33	0.58
1:A:255:ARG:NH1	1:B:280:SER:O	2.37	0.58
1:C:133:ALA:HB1	1:C:156:ILE:HD13	1.85	0.58
1:A:295:LEU:O	1:A:299:THR:HG23	2.04	0.58
1:B:202:HIS:O	1:B:206:THR:HG23	2.04	0.57
1:C:95:VAL:HG13	1:D:95:VAL:HG22	1.86	0.57
1:D:111:VAL:HG21	1:D:140:CYS:HB3	1.86	0.57
1:D:138:ALA:HA	1:D:141:THR:CG2	2.31	0.57
1:A:347:MET:HG2	1:C:347:MET:HG2	1.86	0.57
1:C:346:LEU:HD13	1:D:349:LEU:HD13	1.85	0.57
1:C:117:GLN:HG3	1:D:117:GLN:NE2	2.20	0.57
1:C:167:THR:HA	1:C:201:TRP:CZ3	2.38	0.57
1:A:157:ASN:HD22	1:A:307:LEU:HD11	1.70	0.57
1:D:171:VAL:O	1:D:175:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD12	1:A:267:ASP:HB3	1.86	0.57
1:D:111:VAL:O	1:D:115:LEU:HB2	2.04	0.57
1:A:193:SER:O	1:A:197:ARG:HB2	2.05	0.57
1:A:183:ALA:HB3	1:A:242:MET:HG2	1.86	0.57
1:D:312:ALA:C	1:D:314:LYS:N	2.62	0.57
1:A:273:TYR:N	1:A:288:THR:HG23	2.20	0.56
1:B:108:LYS:HZ1	1:B:139:ALA:HB2	1.69	0.56
1:C:118:ARG:HH22	1:D:118:ARG:NE	2.02	0.56
1:B:64:ILE:CD1	1:B:94:VAL:HG22	2.35	0.56
1:B:148:LEU:HD12	1:B:159:ILE:HG23	1.86	0.56
1:B:167:THR:HA	1:B:201:TRP:CZ3	2.41	0.56
1:B:216:ARG:HH11	1:B:228:GLN:HE22	1.50	0.56
1:D:332:PRO:C	1:D:334:THR:H	2.14	0.56
1:C:255:ARG:O	1:C:259:GLU:HG3	2.05	0.56
1:A:273:TYR:O	1:A:274:ASP:HB2	2.06	0.56
1:C:214:ALA:HB2	1:C:237:ILE:HD13	1.88	0.56
1:A:219:ASP:O	1:A:220:TRP:HB2	2.04	0.56
1:C:161:PHE:CG	1:C:291:GLN:HG2	2.41	0.56
1:A:232:MET:HE1	1:A:242:MET:SD	2.45	0.56
1:C:104:VAL:CG2	1:C:136:VAL:HG23	2.35	0.56
1:A:283:ILE:O	1:A:284:PRO:C	2.49	0.55
1:C:223:MET:O	1:C:227:GLN:HG3	2.05	0.55
1:D:265:GLY:HA2	1:D:328:THR:O	2.05	0.55
1:D:337:ALA:O	1:D:338:SER:C	2.49	0.55
1:A:267:ASP:OD1	1:A:333:ASN:ND2	2.39	0.55
1:D:121:GLY:HA3	1:D:304:LEU:HD21	1.87	0.55
1:D:102:SER:HB2	1:D:106:ALA:HB2	1.87	0.55
1:D:254:MET:CE	1:D:284:PRO:HD2	2.36	0.55
1:B:119:VAL:HG23	1:B:143:VAL:HG11	1.88	0.55
1:B:75:ALA:HB3	1:B:76:PRO:HD3	1.88	0.55
1:A:228:GLN:OE1	1:A:228:GLN:HA	2.06	0.55
1:B:253:ALA:O	1:B:257:ILE:HG13	2.07	0.55
1:D:347:MET:O	1:D:350:ALA:HB3	2.07	0.55
1:B:102:SER:HA	1:B:126:TYR:OH	2.07	0.54
1:D:86:ARG:HE	1:D:89:GLN:NE2	2.04	0.54
1:B:100:GLU:H	1:B:100:GLU:CD	2.16	0.54
1:B:159:ILE:HD11	1:B:299:THR:CG2	2.36	0.54
1:C:123:ILE:HG23	1:C:148:LEU:CD1	2.36	0.54
1:D:122:LEU:HD13	1:D:140:CYS:HB2	1.89	0.54
1:A:303:ARG:O	1:A:307:LEU:HB2	2.07	0.54
1:A:357:GLU:HB2	1:C:339:PRO:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:NH1	1:B:228:GLN:HE22	2.05	0.54
1:A:174:LEU:HD22	1:A:241:ALA:HB1	1.88	0.54
1:C:329:THR:O	1:C:330:LEU:HD22	2.08	0.54
1:D:99:VAL:HG13	1:D:106:ALA:O	2.08	0.54
1:D:108:LYS:HE2	1:D:139:ALA:HB2	1.89	0.54
1:A:206:THR:HB	1:A:211:GLN:NE2	2.22	0.54
1:C:101:ARG:HD3	1:C:102:SER:N	2.23	0.54
1:D:192:VAL:O	1:D:196:LEU:HD12	2.08	0.54
1:C:150:VAL:HG21	1:C:156:ILE:HD11	1.90	0.54
1:C:283:ILE:O	1:C:285:PRO:HD3	2.08	0.54
1:A:98:MET:HB2	1:B:84:LYS:HG2	1.89	0.53
1:C:185:LEU:HD11	1:C:225:GLY:HA2	1.90	0.53
1:B:263:ARG:NH2	1:B:336:THR:HB	2.22	0.53
1:B:346:LEU:HD21	1:C:346:LEU:HG	1.90	0.53
1:C:192:VAL:HG13	1:C:193:SER:N	2.24	0.53
1:C:273:TYR:O	1:C:274:ASP:CB	2.56	0.53
1:D:283:ILE:O	1:D:285:PRO:HD3	2.08	0.53
1:A:76:PRO:O	1:A:80:VAL:HG23	2.08	0.53
1:C:75:ALA:HB3	1:C:76:PRO:HD3	1.89	0.53
1:A:298:GLN:O	1:A:302:ASP:HB2	2.07	0.53
1:C:85:SER:O	1:C:88:ASP:HB2	2.09	0.53
1:A:146:LEU:HD21	1:A:159:ILE:CD1	2.39	0.53
1:A:287:THR:HG23	1:A:325:LYS:HA	1.90	0.53
1:A:311:GLN:O	1:A:313:VAL:HG22	2.09	0.53
1:D:144:PRO:HG2	1:D:308:SER:HA	1.89	0.53
1:B:159:ILE:HD11	1:B:299:THR:HG22	1.91	0.53
1:B:343:ALA:HB2	1:D:354:SER:HB3	1.91	0.53
1:A:133:ALA:HB1	1:A:156:ILE:CD1	2.39	0.53
1:C:186:ALA:N	1:C:216:ARG:O	2.42	0.53
1:D:327:LYS:NZ	1:D:327:LYS:HB3	2.23	0.53
1:A:161:PHE:HZ	1:A:292:ASP:O	1.91	0.53
1:D:253:ALA:O	1:D:257:ILE:HG13	2.09	0.53
1:A:332:PRO:O	1:A:334:THR:N	2.42	0.53
1:D:168:ARG:O	1:D:172:GLU:HG3	2.09	0.53
1:D:235:GLU:O	1:D:235:GLU:HG2	2.08	0.53
1:C:297:GLY:O	1:C:301:VAL:HG23	2.08	0.52
1:B:146:LEU:HD13	1:B:307:LEU:CD1	2.40	0.52
1:D:162:SER:HA	1:D:318:LEU:HD12	1.91	0.52
1:B:86:ARG:O	1:B:86:ARG:HD3	2.09	0.52
1:C:84:LYS:HD3	1:D:98:MET:HB2	1.91	0.52
1:D:200:GLY:O	1:D:201:TRP:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ALA:O	1:A:273:TYR:CB	2.55	0.52
1:B:226:PHE:HA	1:B:252:GLY:O	2.09	0.52
1:C:104:VAL:HG22	1:C:136:VAL:HG23	1.90	0.52
1:A:231:GLN:O	1:A:235:GLU:HB2	2.10	0.52
1:C:103:GLY:C	1:C:105:GLU:H	2.17	0.52
1:C:333:ASN:HB3	1:C:336:THR:CB	2.40	0.52
1:D:104:VAL:HG23	1:D:136:VAL:HG22	1.91	0.52
1:D:141:THR:C	1:D:143:VAL:H	2.18	0.52
1:A:283:ILE:O	1:A:285:PRO:CD	2.58	0.51
1:A:350:ALA:CB	1:C:347:MET:HG3	2.40	0.51
1:C:284:PRO:HB2	1:C:328:THR:HG22	1.91	0.51
1:C:103:GLY:C	1:C:105:GLU:N	2.67	0.51
1:D:168:ARG:HG2	1:D:168:ARG:NH1	2.26	0.51
1:C:118:ARG:O	1:C:118:ARG:HG2	2.11	0.51
1:B:296:LEU:O	1:B:296:LEU:HD22	2.10	0.51
1:C:333:ASN:OD1	1:C:335:GLN:N	2.42	0.51
1:D:86:ARG:HH21	1:D:89:GLN:NE2	2.09	0.51
1:D:133:ALA:O	1:D:137:GLU:HB2	2.11	0.51
1:B:131:GLN:CD	1:B:131:GLN:H	2.19	0.51
1:A:233:LEU:HD11	1:A:257:ILE:HD13	1.93	0.51
1:C:333:ASN:OD1	1:C:334:THR:N	2.43	0.51
1:D:116:ALA:C	1:D:118:ARG:H	2.19	0.51
1:D:141:THR:C	1:D:142:ASN:ND2	2.69	0.51
1:A:207:ARG:C	1:A:209:GLN:H	2.19	0.50
1:C:86:ARG:HG2	1:C:301:VAL:HB	1.92	0.50
1:C:154:THR:HG23	1:C:156:ILE:HG12	1.93	0.50
1:D:165:ASP:O	1:D:166:GLY:C	2.54	0.50
1:D:247:ASP:OD1	1:D:288:THR:HG21	2.11	0.50
1:A:86:ARG:NH1	1:A:302:ASP:OD1	2.44	0.50
1:B:64:ILE:CG1	1:B:94:VAL:HG22	2.41	0.50
1:B:158:SER:OG	1:B:316:ASN:HB3	2.11	0.50
1:C:173:HIS:CE1	1:C:177:LEU:HD11	2.46	0.50
1:B:115:LEU:CD1	1:B:122:LEU:HD21	2.36	0.50
1:B:202:HIS:C	1:B:206:THR:HG23	2.36	0.50
1:B:340:ARG:O	1:B:343:ALA:HB3	2.12	0.50
1:C:307:LEU:HD23	1:C:313:VAL:HG13	1.94	0.50
1:C:336:THR:O	1:C:338:SER:N	2.43	0.50
1:B:70:SER:HA	1:B:98:MET:HE2	1.93	0.50
1:A:117:GLN:HB3	1:B:117:GLN:OE1	2.11	0.50
1:C:98:MET:O	1:D:84:LYS:HE3	2.10	0.50
1:A:83:ILE:HD12	1:A:297:GLY:HA2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLY:C	1:B:288:THR:HG22	2.37	0.50
1:C:147:PHE:CG	1:C:156:ILE:HD12	2.46	0.50
1:D:272:GLY:C	1:D:288:THR:HG22	2.37	0.50
1:B:191:SER:O	1:B:194:ALA:HB3	2.12	0.49
1:A:337:ALA:O	1:A:338:SER:HB2	2.10	0.49
1:D:219:ASP:O	1:D:220:TRP:HB2	2.12	0.49
1:A:199:ALA:O	1:A:202:HIS:HB2	2.11	0.49
1:A:204:TYR:HA	1:A:207:ARG:HB2	1.95	0.49
1:C:158:SER:O	1:C:303:ARG:NH2	2.45	0.49
1:D:129:ASP:O	1:D:131:GLN:N	2.45	0.49
1:A:133:ALA:HB1	1:A:156:ILE:HD13	1.94	0.49
1:B:115:LEU:HG	1:B:143:VAL:CG2	2.37	0.49
1:B:191:SER:HB3	1:B:194:ALA:CB	2.42	0.49
1:B:191:SER:HB3	1:B:194:ALA:HB2	1.93	0.49
1:B:201:TRP:HA	1:B:201:TRP:HE3	1.77	0.49
1:A:86:ARG:HG2	1:A:298:GLN:HA	1.93	0.49
1:B:127:PRO:O	1:B:128:LEU:HD13	2.13	0.49
1:D:182:ILE:HA	1:D:241:ALA:O	2.12	0.49
1:A:229:THR:HG23	1:A:232:MET:CE	2.43	0.49
1:C:95:VAL:HG13	1:D:95:VAL:CG2	2.42	0.49
1:C:269:SER:HA	1:C:328:THR:O	2.11	0.49
1:C:312:ALA:HB1	1:C:314:LYS:HZ2	1.77	0.49
1:B:303:ARG:HE	1:B:317:GLN:NE2	2.11	0.49
1:A:352:GLN:CB	1:B:342:LEU:HD21	2.43	0.48
1:B:74:HIS:ND1	1:B:74:HIS:N	2.61	0.48
1:C:326:ARG:C	1:C:327:LYS:HD2	2.38	0.48
1:A:75:ALA:HB3	1:A:76:PRO:HD3	1.95	0.48
1:A:79:ILE:O	1:A:83:ILE:HD13	2.13	0.48
1:A:184:LEU:HG	1:A:212:PRO:HB3	1.95	0.48
1:B:350:ALA:CA	1:D:346:LEU:HD12	2.38	0.48
1:B:116:ALA:C	1:B:118:ARG:H	2.21	0.48
1:B:343:ALA:CB	1:D:354:SER:HB3	2.43	0.48
1:A:167:THR:O	1:A:171:VAL:HG23	2.13	0.48
1:D:148:LEU:HD11	1:D:300:SER:HB3	1.94	0.48
1:B:285:PRO:HB2	1:B:326:ARG:HG2	1.94	0.48
1:A:105:GLU:O	1:A:109:THR:HG22	2.13	0.48
1:C:84:LYS:HE2	1:C:88:ASP:OD1	2.14	0.48
1:C:334:THR:C	1:C:336:THR:N	2.66	0.48
1:C:105:GLU:O	1:C:109:THR:HG22	2.13	0.48
1:A:254:MET:CE	1:A:286:LEU:HD13	2.44	0.48
1:B:201:TRP:HA	1:B:201:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:SER:HB3	1:B:341:ALA:HB3	1.96	0.48
1:C:100:GLU:CD	1:C:100:GLU:H	2.22	0.47
1:D:147:PHE:O	1:D:158:SER:HA	2.13	0.47
1:B:137:GLU:HB3	1:B:147:PHE:CZ	2.48	0.47
1:B:219:ASP:O	1:B:220:TRP:HB2	2.14	0.47
1:C:203:LYS:O	1:C:207:ARG:HD3	2.14	0.47
1:D:356:LEU:O	1:D:357:GLU:HB3	2.14	0.47
1:A:181:GLN:NE2	1:A:213:ILE:HG21	2.28	0.47
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.75	0.47
1:D:339:PRO:C	1:D:341:ALA:N	2.72	0.47
1:B:63:LEU:HB3	1:B:119:VAL:HA	1.96	0.47
1:A:283:ILE:HG22	1:A:284:PRO:N	2.29	0.47
1:A:288:THR:CG2	1:A:289:ILE:N	2.77	0.47
1:A:313:VAL:HG23	1:A:313:VAL:O	2.14	0.47
1:A:166:GLY:CA	1:A:321:VAL:HG11	2.45	0.47
1:B:304:LEU:HA	1:B:307:LEU:HD12	1.96	0.47
1:D:331:ALA:C	1:D:333:ASN:H	2.21	0.47
1:A:276:THR:O	1:A:278:ASP:N	2.48	0.47
1:C:344:ASP:O	1:C:348:GLN:HG3	2.15	0.47
1:D:303:ARG:NH1	1:D:317:GLN:HB2	2.29	0.47
1:C:118:ARG:NH2	1:D:118:ARG:NE	2.62	0.46
1:D:141:THR:O	1:D:142:ASN:CG	2.58	0.46
1:A:78:GLN:HE21	1:A:293:PHE:HD2	1.63	0.46
1:A:221:SER:O	1:A:249:MET:HG2	2.14	0.46
1:B:232:MET:HG2	1:B:237:ILE:HB	1.96	0.46
1:A:142:ASN:CG	1:A:143:VAL:N	2.73	0.46
1:A:151:SER:HB3	1:A:154:THR:OG1	2.15	0.46
1:A:337:ALA:O	1:A:338:SER:CB	2.63	0.46
1:B:202:HIS:O	1:B:204:TYR:N	2.48	0.46
1:C:123:ILE:HG23	1:C:148:LEU:HD13	1.96	0.46
1:C:290:LYS:HB2	1:C:324:VAL:CG2	2.46	0.46
1:C:70:SER:CB	1:C:98:MET:HB3	2.44	0.46
1:C:101:ARG:NH1	1:C:102:SER:O	2.48	0.46
1:A:254:MET:HE2	1:A:286:LEU:HD13	1.98	0.46
1:D:82:ALA:O	1:D:294:ARG:NH2	2.49	0.46
1:D:99:VAL:HG13	1:D:106:ALA:C	2.39	0.46
1:D:220:TRP:CZ3	1:D:246:ASN:HB3	2.51	0.46
1:C:86:ARG:NH1	1:C:90:LEU:HD11	2.30	0.46
1:D:216:ARG:NH1	1:D:228:GLN:NE2	2.60	0.46
1:C:126:TYR:HD2	1:C:128:LEU:HD13	1.80	0.46
1:C:272:GLY:HA3	1:C:288:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ASP:OD2	1:D:279:SER:OG	2.25	0.46
1:A:173:HIS:CG	1:A:323:LEU:HD21	2.51	0.46
1:C:213:ILE:HD11	1:C:239:PRO:HB3	1.97	0.46
1:D:201:TRP:CE3	1:D:201:TRP:HA	2.51	0.46
1:D:202:HIS:O	1:D:206:THR:HG23	2.15	0.46
1:D:282:TYR:O	1:D:283:ILE:O	2.34	0.46
1:B:142:ASN:O	1:B:143:VAL:C	2.59	0.46
1:A:182:ILE:N	1:A:182:ILE:HD12	2.31	0.45
1:B:137:GLU:HB3	1:B:147:PHE:CE1	2.50	0.45
1:B:160:ILE:HG22	1:B:161:PHE:N	2.31	0.45
1:D:167:THR:O	1:D:171:VAL:HG23	2.16	0.45
1:B:151:SER:C	1:B:153:GLN:H	2.23	0.45
1:C:64:ILE:HG12	1:C:94:VAL:HG22	1.99	0.45
1:D:296:LEU:HD22	1:D:296:LEU:O	2.16	0.45
1:A:213:ILE:HD11	1:A:239:PRO:HB3	1.99	0.45
1:A:332:PRO:C	1:A:334:THR:N	2.74	0.45
1:B:182:ILE:HA	1:B:241:ALA:O	2.15	0.45
1:D:97:SER:CB	1:D:114:LEU:HG	2.45	0.45
1:D:349:LEU:O	1:D:353:VAL:HG23	2.17	0.45
1:A:273:TYR:O	1:A:274:ASP:CB	2.64	0.45
1:B:146:LEU:HD11	1:B:303:ARG:HD3	1.98	0.45
1:C:180:GLN:HG2	1:C:210:ILE:HD11	1.99	0.45
1:A:68:THR:O	1:A:98:MET:HA	2.16	0.45
1:B:253:ALA:O	1:B:256:ALA:HB3	2.17	0.45
1:C:107:CYS:HB3	1:C:136:VAL:HG21	1.99	0.45
1:D:100:GLU:HA	1:D:101:ARG:HH21	1.81	0.45
1:B:142:ASN:O	1:B:144:PRO:N	2.50	0.45
1:D:273:TYR:CE2	1:D:289:ILE:HG21	2.52	0.45
1:C:161:PHE:CD2	1:C:291:GLN:HG2	2.52	0.45
1:B:121:GLY:HA3	1:B:304:LEU:HD21	1.99	0.45
1:C:250:ALA:O	1:C:254:MET:HG3	2.17	0.45
1:A:171:VAL:HG21	1:A:204:TYR:HB2	1.99	0.44
1:A:197:ARG:NH2	1:A:273:TYR:CE1	2.85	0.44
1:A:355:ARG:HH22	1:B:261:GLY:HA3	1.82	0.44
1:B:160:ILE:O	1:B:318:LEU:HA	2.16	0.44
1:C:307:LEU:CD2	1:C:313:VAL:HG13	2.47	0.44
1:D:309:GLN:NE2	1:D:311:GLN:HE22	2.15	0.44
1:A:158:SER:O	1:A:316:ASN:HA	2.17	0.44
1:A:231:GLN:HG2	1:A:235:GLU:OE1	2.16	0.44
1:D:114:LEU:HD13	1:D:122:LEU:CD2	2.47	0.44
1:B:154:THR:HA	1:B:155:PRO:HD3	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:O	1:B:353:VAL:HG23	2.16	0.44
1:B:65:GLY:HA2	1:B:95:VAL:O	2.18	0.44
1:D:284:PRO:O	1:D:285:PRO:C	2.59	0.44
1:D:167:THR:HA	1:D:201:TRP:CZ3	2.52	0.44
1:D:352:GLN:OE1	1:D:352:GLN:HA	2.16	0.44
1:B:202:HIS:O	1:B:205:LEU:N	2.50	0.44
1:D:71:LEU:HD21	1:D:101:ARG:HG2	1.99	0.44
1:D:141:THR:O	1:D:142:ASN:ND2	2.51	0.44
1:D:201:TRP:HA	1:D:201:TRP:HE3	1.82	0.44
1:D:264:VAL:HB	1:D:284:PRO:HG2	1.98	0.44
1:A:121:GLY:HA2	1:A:143:VAL:CG2	2.48	0.44
1:B:101:ARG:HD3	1:B:101:ARG:C	2.43	0.44
1:C:275:ASP:HB3	1:C:290:LYS:HG3	1.99	0.44
1:D:137:GLU:HG3	1:D:156:ILE:HG22	1.99	0.44
1:A:143:VAL:HA	1:A:144:PRO:HD3	1.86	0.44
1:A:205:LEU:HB3	1:A:210:ILE:O	2.17	0.44
1:A:230:MET:O	1:A:234:ASN:HB2	2.17	0.44
1:C:163:HIS:CD2	1:C:163:HIS:H	2.36	0.44
1:C:273:TYR:CD1	1:C:291:GLN:NE2	2.86	0.44
1:D:123:ILE:HG23	1:D:148:LEU:HD22	1.96	0.44
1:D:309:GLN:HB3	1:D:311:GLN:OE1	2.18	0.44
1:C:96:VAL:HB	1:D:96:VAL:HB	2.00	0.43
1:C:189:LEU:HD21	1:C:198:LEU:HD12	2.00	0.43
1:A:349:LEU:HD13	1:B:342:LEU:HD23	1.99	0.43
1:B:264:VAL:HA	1:B:268:ILE:O	2.18	0.43
1:D:282:TYR:O	1:D:283:ILE:C	2.59	0.43
1:A:104:VAL:HG13	1:A:132:ASP:CB	2.38	0.43
1:A:306:GLN:O	1:A:307:LEU:C	2.61	0.43
1:A:348:GLN:NE2	1:B:258:THR:O	2.51	0.43
1:D:76:PRO:O	1:D:80:VAL:HG23	2.19	0.43
1:A:188:PRO:C	1:A:190:SER:H	2.27	0.43
1:C:70:SER:HB2	1:D:84:LYS:CG	2.44	0.43
1:D:115:LEU:HD13	1:D:122:LEU:HD11	2.00	0.43
1:A:174:LEU:HD22	1:A:241:ALA:CB	2.47	0.43
1:D:264:VAL:CG1	1:D:328:THR:HG22	2.48	0.43
1:D:325:LYS:C	1:D:326:ARG:HG2	2.43	0.43
1:A:283:ILE:O	1:A:285:PRO:HD3	2.18	0.43
1:A:330:LEU:HD11	1:A:340:ARG:NH1	2.34	0.43
1:B:104:VAL:C	1:B:106:ALA:H	2.27	0.43
1:B:202:HIS:O	1:B:203:LYS:C	2.61	0.43
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HA	1:A:306:GLN:HE21	1.84	0.43
1:B:166:GLY:CA	1:B:321:VAL:HG11	2.49	0.43
1:C:128:LEU:HG	1:C:132:ASP:HB3	2.01	0.43
1:D:111:VAL:CG1	1:D:140:CYS:HB3	2.48	0.43
1:D:264:VAL:HG12	1:D:328:THR:HG22	2.00	0.43
1:A:142:ASN:ND2	1:A:142:ASN:C	2.76	0.43
1:C:101:ARG:HH11	1:C:102:SER:C	2.26	0.43
1:C:129:ASP:O	1:C:132:ASP:HB2	2.19	0.43
1:C:206:THR:HG22	1:C:211:GLN:OE1	2.19	0.43
1:C:265:GLY:HA2	1:C:328:THR:O	2.19	0.43
1:A:301:VAL:O	1:A:305:LEU:HG	2.19	0.43
1:B:79:ILE:O	1:B:83:ILE:HG13	2.19	0.43
1:A:206:THR:CB	1:A:211:GLN:HE22	2.27	0.42
1:A:251:LEU:HA	1:A:254:MET:HE3	2.01	0.42
1:B:285:PRO:CB	1:B:326:ARG:HG2	2.49	0.42
1:D:140:CYS:O	1:D:140:CYS:SG	2.76	0.42
1:A:183:ALA:HB2	1:A:239:PRO:HB3	2.01	0.42
1:B:187:GLY:O	1:B:188:PRO:C	2.61	0.42
1:C:62:LEU:HB3	1:C:63:LEU:H	1.56	0.42
1:C:286:LEU:HG	1:C:288:THR:HG23	2.01	0.42
1:D:216:ARG:HB3	1:D:228:GLN:NE2	2.34	0.42
1:B:166:GLY:HA2	1:B:321:VAL:HG11	2.00	0.42
1:C:167:THR:HA	1:C:201:TRP:HZ3	1.82	0.42
1:C:273:TYR:CE1	1:C:291:GLN:NE2	2.88	0.42
1:A:350:ALA:HB3	1:C:347:MET:HG3	2.01	0.42
1:D:168:ARG:HD3	1:D:204:TYR:CE1	2.54	0.42
1:A:122:LEU:HD22	1:A:124:ILE:HD11	2.01	0.42
1:B:273:TYR:N	1:B:288:THR:HG22	2.34	0.42
1:C:154:THR:HA	1:C:155:PRO:HD2	1.87	0.42
1:D:154:THR:HA	1:D:155:PRO:HD3	1.80	0.42
1:A:111:VAL:HG21	1:A:136:VAL:HG13	2.01	0.42
1:C:102:SER:O	1:C:103:GLY:O	2.37	0.42
1:C:123:ILE:HG23	1:C:148:LEU:HD11	2.01	0.42
1:B:330:LEU:HD12	1:B:331:ALA:N	2.33	0.42
1:D:239:PRO:O	1:D:268:ILE:HG12	2.20	0.42
1:A:218:GLY:HA2	1:A:224:SER:HB2	2.00	0.42
1:A:349:LEU:HD22	1:A:349:LEU:HA	1.75	0.42
1:C:265:GLY:O	1:C:330:LEU:HB2	2.19	0.42
1:C:327:LYS:HG3	1:C:340:ARG:NH1	2.35	0.42
1:B:192:VAL:HG22	1:B:196:LEU:HD11	2.01	0.42
1:A:99:VAL:HG12	1:A:100:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ALA:CB	1:C:232:MET:HE1	2.47	0.41
1:D:141:THR:HB	1:D:142:ASN:H	1.63	0.41
1:D:229:THR:OG1	1:D:253:ALA:HA	2.20	0.41
1:A:86:ARG:HB3	1:A:301:VAL:HG21	2.02	0.41
1:A:307:LEU:O	1:A:310:GLY:N	2.53	0.41
1:B:62:LEU:HG	1:B:63:LEU:N	2.35	0.41
1:D:104:VAL:O	1:D:108:LYS:HG3	2.20	0.41
1:B:82:ALA:O	1:B:85:SER:HB2	2.20	0.41
1:D:144:PRO:HB2	1:D:304:LEU:HD11	2.03	0.41
1:D:246:ASN:OD1	1:D:249:MET:HG3	2.20	0.41
1:A:283:ILE:HA	1:B:255:ARG:HG2	2.03	0.41
1:B:162:SER:OG	1:B:165:ASP:HB2	2.20	0.41
1:B:167:THR:HG21	1:B:200:GLY:HA3	2.01	0.41
1:C:191:SER:HB3	1:C:194:ALA:HB2	2.02	0.41
1:C:210:ILE:HD12	1:C:210:ILE:HG23	1.77	0.41
1:D:86:ARG:HD3	1:D:302:ASP:OD1	2.20	0.41
1:D:120:SER:O	1:D:144:PRO:HD2	2.21	0.41
1:A:143:VAL:HG13	1:A:143:VAL:O	2.20	0.41
1:A:184:LEU:O	1:A:215:GLU:HA	2.21	0.41
1:B:86:ARG:CG	1:B:298:GLN:HA	2.40	0.41
1:D:152:ASP:HB2	1:D:316:ASN:ND2	2.36	0.41
1:A:274:ASP:OD1	1:A:291:GLN:NE2	2.52	0.41
1:A:327:LYS:HA	1:A:340:ARG:HH22	1.85	0.41
1:B:292:ASP:HB3	1:B:295:LEU:HB3	2.02	0.41
1:B:247:ASP:OD1	1:B:288:THR:HG21	2.20	0.41
1:D:332:PRO:C	1:D:334:THR:N	2.76	0.41
1:A:104:VAL:HG23	1:A:105:GLU:N	2.34	0.41
1:A:115:LEU:CD1	1:A:122:LEU:HD11	2.50	0.41
1:A:284:PRO:O	1:A:285:PRO:C	2.61	0.41
1:A:349:LEU:HD22	1:B:342:LEU:HD23	2.03	0.41
1:B:213:ILE:O	1:B:213:ILE:CG1	2.66	0.41
1:B:222:ALA:CA	1:B:248:GLN:O	2.61	0.41
1:C:290:LYS:HB2	1:C:324:VAL:HG23	2.01	0.41
1:C:350:ALA:C	1:C:352:GLN:H	2.29	0.41
1:D:79:ILE:O	1:D:83:ILE:HG13	2.21	0.41
1:B:122:LEU:O	1:B:145:ALA:HA	2.21	0.41
1:A:245:ALA:HB3	1:A:249:MET:HE1	2.04	0.40
1:A:255:ARG:O	1:A:259:GLU:HG3	2.20	0.40
1:C:153:GLN:H	1:C:153:GLN:HG2	1.64	0.40
1:D:104:VAL:HG21	1:D:135:ALA:HB3	2.04	0.40
1:B:352:GLN:O	1:B:355:ARG:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ARG:HD3	1:B:86:ARG:C	2.45	0.40
1:C:63:LEU:CD1	1:C:119:VAL:HG12	2.50	0.40
1:C:179:HIS:CE1	1:C:332:PRO:HD3	2.56	0.40
1:C:253:ALA:O	1:C:257:ILE:HG13	2.21	0.40
1:D:148:LEU:HD11	1:D:300:SER:CB	2.52	0.40
1:A:150:VAL:CG2	1:A:158:SER:CB	3.00	0.40
1:A:151:SER:C	1:A:153:GLN:N	2.77	0.40
1:A:205:LEU:CD1	1:A:212:PRO:HG3	2.50	0.40
1:A:254:MET:HE1	1:A:282:TYR:HD2	1.87	0.40
1:B:220:TRP:CE3	1:B:249:MET:HE2	2.56	0.40
1:B:338:SER:HA	1:B:339:PRO:HD2	1.69	0.40
1:A:107:CYS:O	1:A:111:VAL:HG23	2.22	0.40
1:B:198:LEU:HD23	1:B:201:TRP:HD1	1.86	0.40
1:C:353:VAL:HG22	1:D:342:LEU:HD13	2.04	0.40
1:D:275:ASP:CB	1:D:290:LYS:HG3	2.49	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	294/360 (82%)	244 (83%)	32 (11%)	18 (6%)	1	2
1	B	294/360 (82%)	247 (84%)	31 (10%)	16 (5%)	1	2
1	C	294/360 (82%)	260 (88%)	26 (9%)	8 (3%)	4	10
1	D	294/360 (82%)	247 (84%)	38 (13%)	9 (3%)	3	8
All	All	1176/1440 (82%)	998 (85%)	127 (11%)	51 (4%)	2	4

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	THR
1	A	142	ASN
1	A	162	SER
1	A	274	ASP
1	A	277	GLU
1	A	283	ILE
1	A	311	GLN
1	A	338	SER
1	B	69	SER
1	B	101	ARG
1	B	141	THR
1	B	159	ILE
1	B	214	ALA
1	B	283	ILE
1	B	284	PRO
1	B	335	GLN
1	B	339	PRO
1	C	274	ASP
1	C	337	ALA
1	D	104	VAL
1	D	130	ASP
1	D	312	ALA
1	A	101	ARG
1	A	312	ALA
1	A	333	ASN
1	A	335	GLN
1	A	356	LEU
1	B	203	LYS
1	B	274	ASP
1	B	312	ALA
1	C	103	GLY
1	C	130	ASP
1	C	159	ILE
1	C	338	SER
1	D	274	ASP
1	A	71	LEU
1	A	337	ALA
1	B	130	ASP
1	B	314	LYS
1	D	63	LEU
1	D	283	ILE
1	A	155	PRO
1	B	100	GLU

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Mol	Chain	Res	Type
1	C	283	ILE
1	D	102	SER
1	A	130	ASP
1	A	189	LEU
1	C	189	LEU
1	D	141	THR
1	D	309	GLN
1	B	150	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/295 (82%)	206 (85%)	37 (15%)	3	7
1	B	243/295 (82%)	199 (82%)	44 (18%)	2	5
1	C	243/295 (82%)	194 (80%)	49 (20%)	1	4
1	D	243/295 (82%)	197 (81%)	46 (19%)	1	4
All	All	972/1180 (82%)	796 (82%)	176 (18%)	2	5

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	78	GLN
1	A	86	ARG
1	A	90	LEU
1	A	93	SER
1	A	101	ARG
1	A	109	THR
1	A	115	LEU
1	A	118	ARG
1	A	123	ILE
1	A	128	LEU
1	A	142	ASN
1	A	153	GLN

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Mol	Chain	Res	Type
1	A	155	PRO
1	A	180	GLN
1	A	185	LEU
1	A	198	LEU
1	A	206	THR
1	A	207	ARG
1	A	209	GLN
1	A	210	ILE
1	A	216	ARG
1	A	230	MET
1	A	251	LEU
1	A	262	LEU
1	A	277	GLU
1	A	279	SER
1	A	296	LEU
1	A	298	GLN
1	A	317	GLN
1	A	318	LEU
1	A	321	VAL
1	A	330	LEU
1	A	335	GLN
1	A	348	GLN
1	A	349	LEU
1	A	354	SER
1	B	71	LEU
1	B	74	HIS
1	B	86	ARG
1	B	95	VAL
1	B	100	GLU
1	B	101	ARG
1	B	107	CYS
1	B	123	ILE
1	B	128	LEU
1	B	131	GLN
1	B	137	GLU
1	B	142	ASN
1	B	143	VAL
1	B	156	ILE
1	B	159	ILE
1	B	172	GLU
1	B	180	GLN
1	B	185	LEU

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Mol	Chain	Res	Type
1	B	189	LEU
1	B	190	SER
1	B	198	LEU
1	B	201	TRP
1	B	206	THR
1	B	213	ILE
1	B	246	ASN
1	B	251	LEU
1	B	262	LEU
1	B	276	THR
1	B	288	THR
1	B	294	ARG
1	B	295	LEU
1	B	296	LEU
1	B	309	GLN
1	B	321	VAL
1	B	323	LEU
1	B	325	LYS
1	B	326	ARG
1	B	327	LYS
1	B	338	SER
1	B	342	LEU
1	B	348	GLN
1	B	351	ARG
1	B	354	SER
1	B	356	LEU
1	C	69	SER
1	C	71	LEU
1	C	86	ARG
1	C	93	SER
1	C	97	SER
1	C	100	GLU
1	C	101	ARG
1	C	102	SER
1	C	105	GLU
1	C	107	CYS
1	C	109	THR
1	C	115	LEU
1	C	117	GLN
1	C	128	LEU
1	C	130	ASP
1	C	136	VAL

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Mol	Chain	Res	Type
1	C	137	GLU
1	C	143	VAL
1	C	151	SER
1	C	154	THR
1	C	162	SER
1	C	164	GLU
1	C	171	VAL
1	C	185	LEU
1	C	193	SER
1	C	198	LEU
1	C	201	TRP
1	C	206	THR
1	C	249	MET
1	C	251	LEU
1	C	262	LEU
1	C	271	VAL
1	C	283	ILE
1	C	291	GLN
1	C	295	LEU
1	C	296	LEU
1	C	298	GLN
1	C	303	ARG
1	C	313	VAL
1	C	316	ASN
1	C	317	GLN
1	C	321	VAL
1	C	323	LEU
1	C	330	LEU
1	C	334	THR
1	C	338	SER
1	C	346	LEU
1	C	355	ARG
1	C	356	LEU
1	D	62	LEU
1	D	68	THR
1	D	69	SER
1	D	74	HIS
1	D	90	LEU
1	D	93	SER
1	D	101	ARG
1	D	104	VAL
1	D	111	VAL

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Mol	Chain	Res	Type
1	D	115	LEU
1	D	128	LEU
1	D	130	ASP
1	D	134	ILE
1	D	142	ASN
1	D	148	LEU
1	D	154	THR
1	D	156	ILE
1	D	184	LEU
1	D	185	LEU
1	D	190	SER
1	D	198	LEU
1	D	201	TRP
1	D	251	LEU
1	D	255	ARG
1	D	262	LEU
1	D	276	THR
1	D	277	GLU
1	D	288	THR
1	D	294	ARG
1	D	296	LEU
1	D	307	LEU
1	D	308	SER
1	D	309	GLN
1	D	313	VAL
1	D	316	ASN
1	D	317	GLN
1	D	321	VAL
1	D	326	ARG
1	D	327	LYS
1	D	334	THR
1	D	335	GLN
1	D	336	THR
1	D	340	ARG
1	D	348	GLN
1	D	355	ARG
1	D	356	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS

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Mol	Chain	Res	Type
1	A	113	ASN
1	A	142	ASN
1	A	157	ASN
1	A	180	GLN
1	A	181	GLN
1	A	202	HIS
1	A	234	ASN
1	A	291	GLN
1	A	306	GLN
1	A	311	GLN
1	A	316	ASN
1	A	333	ASN
1	B	113	ASN
1	B	125	ASN
1	B	142	ASN
1	B	157	ASN
1	B	228	GLN
1	B	291	GLN
1	B	317	GLN
1	C	78	GLN
1	C	163	HIS
1	C	202	HIS
1	C	228	GLN
1	C	234	ASN
1	C	291	GLN
1	C	298	GLN
1	D	89	GLN
1	D	112	HIS
1	D	113	ASN
1	D	142	ASN
1	D	208	ASN
1	D	228	GLN
1	D	234	ASN
1	D	309	GLN
1	D	333	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](#)

There are no ligands in this entry.

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.