



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:15 AM UTC

PDB ID : 2D4A / pdb_00002d4a
Title : Structure of the malate dehydrogenase from *Aeropyrum pernix*
Authors : Kawakami, R.; Sakuraba, H.; Tsuge, H.; Ohshima, T.
Deposited on : 2005-10-12
Resolution : 2.87 Å(reported)

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

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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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

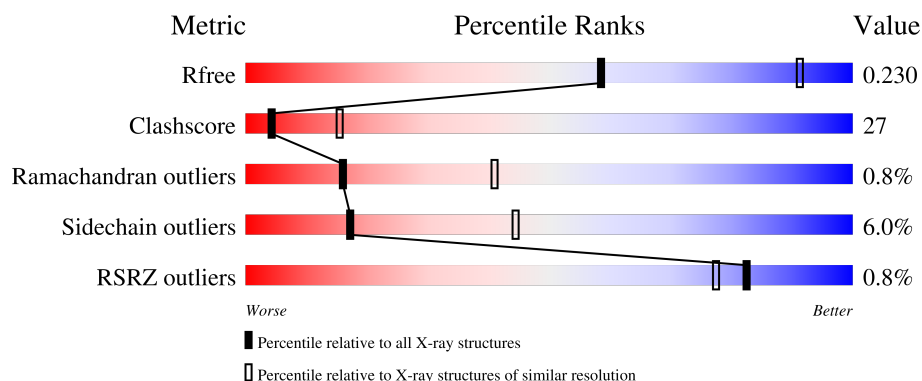
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	308	% 52% 35% 10% ..
1	B	308	54% 31% 12% ..
1	C	308	% 48% 37% 11% ..
1	D	308	2% 52% 38% 9% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9292 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	301	Total	C	N	O	S	0	0	0
			2289	1455	383	438	13			
1	D	308	Total	C	N	O	S	0	0	0
			2346	1489	397	446	14			
1	C	299	Total	C	N	O	S	0	0	0
			2274	1446	384	431	13			
1	A	298	Total	C	N	O	S	0	0	0
			2262	1440	379	430	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9YEA1
B	1	MET	-	initiating methionine	UNP Q9YEA1
C	1	MET	-	initiating methionine	UNP Q9YEA1
D	1	MET	-	initiating methionine	UNP Q9YEA1

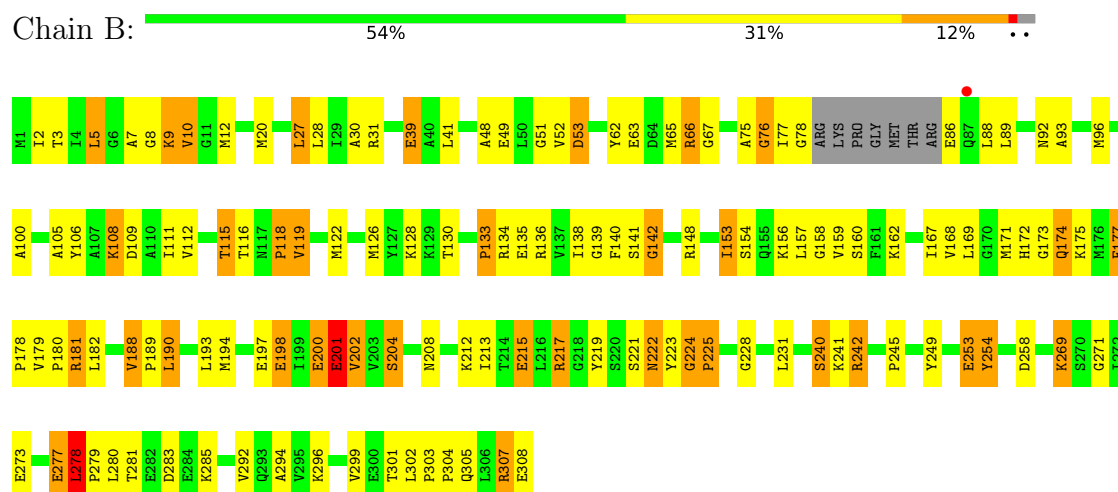
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	42	Total	O	0	0
			42	42		
2	D	34	Total	O	0	0
			34	34		
2	C	17	Total	O	0	0
			17	17		
2	A	28	Total	O	0	0
			28	28		

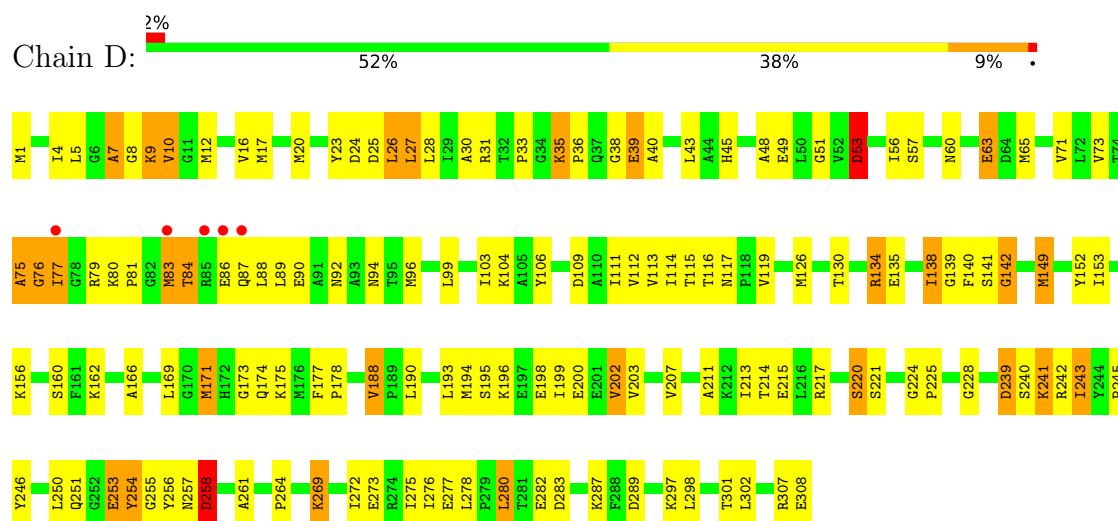
3 Residue-property plots

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

• Molecule 1: Malate dehydrogenase

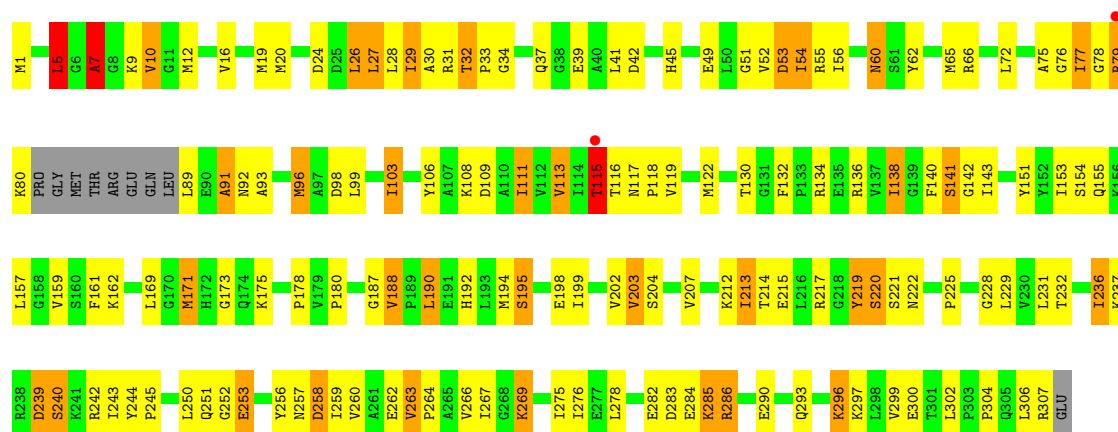


• Molecule 1: Malate dehydrogenase

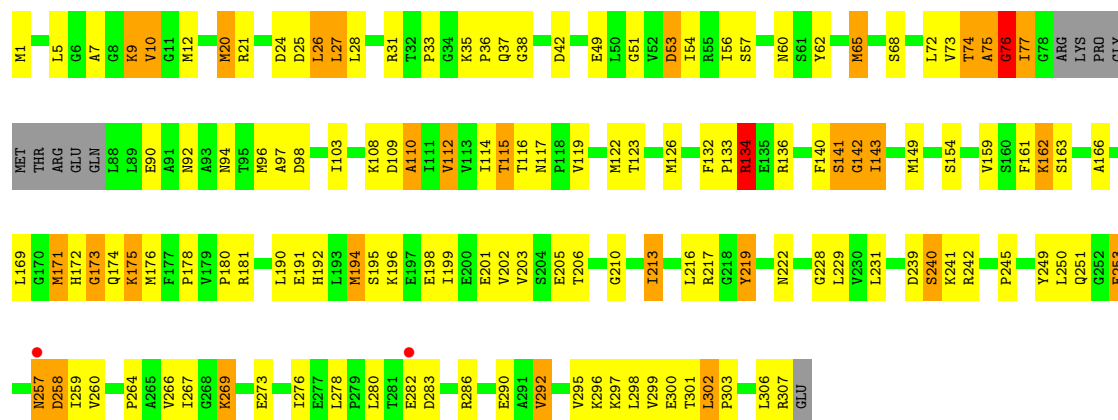


• Molecule 1: Malate dehydrogenase





● Molecule 1: Malate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.17Å 84.01Å 216.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.87 19.92 – 2.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.92-2.87) 81.7 (19.92-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.240 0.195 , 0.230	Depositor DCC
R_{free} test set	2707 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.85 , 112.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9292	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.98	15/2295 (0.7%)	1.50	54/3100 (1.7%)
1	B	1.29	30/2322 (1.3%)	1.77	89/3136 (2.8%)
1	C	1.04	21/2307 (0.9%)	1.51	50/3114 (1.6%)
1	D	0.90	16/2381 (0.7%)	1.37	43/3215 (1.3%)
All	All	1.06	82/9305 (0.9%)	1.54	236/12565 (1.9%)

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	3
1	B	0	3
1	C	0	4
1	D	0	2
All	All	0	12

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	TYR	C-N	12.44	1.50	1.33
1	C	253	GLU	C-N	-12.39	1.16	1.33
1	A	134	ARG	C-O	-12.12	1.08	1.24
1	C	258	ASP	C-N	11.75	1.49	1.33
1	B	67	GLY	C-N	11.42	1.48	1.33
1	B	52	VAL	C-N	-11.35	1.18	1.33
1	D	254	TYR	C-N	11.29	1.48	1.33
1	D	135	GLU	C-N	-11.28	1.17	1.33
1	B	240	SER	C-N	-11.17	1.18	1.33
1	C	9	LYS	C-N	-10.99	1.20	1.33
1	D	258	ASP	C-N	10.88	1.48	1.33
1	A	257	ASN	C-N	-10.84	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	200	GLU	C-N	10.72	1.48	1.34
1	B	197	GLU	C-N	10.40	1.46	1.33
1	A	123	THR	C-N	-10.34	1.20	1.33
1	B	188	VAL	C-N	-10.26	1.21	1.33
1	B	217	ARG	C-N	-9.74	1.19	1.33
1	C	115	THR	C-N	9.53	1.46	1.33
1	A	112	VAL	C-N	-9.51	1.21	1.33
1	C	219	TYR	C-N	-9.49	1.20	1.33
1	D	38	GLY	C-N	-9.44	1.20	1.33
1	C	284	GLU	C-N	9.36	1.47	1.33
1	A	292	VAL	C-N	-9.36	1.21	1.34
1	C	5	LEU	C-N	9.32	1.47	1.33
1	C	54	ILE	C-N	8.95	1.46	1.33
1	C	7	ALA	C-N	8.92	1.46	1.33
1	B	8	GLY	C-N	8.74	1.45	1.33
1	B	179	VAL	C-O	8.64	1.35	1.24
1	C	195	SER	C-O	8.62	1.35	1.23
1	B	119	VAL	N-CA	-8.57	1.34	1.46
1	A	57	SER	C-N	8.57	1.43	1.33
1	B	202	VAL	C-N	-8.53	1.22	1.33
1	B	108	LYS	C-N	-8.50	1.22	1.33
1	C	256	TYR	C-N	-8.39	1.22	1.33
1	B	254	TYR	C-N	8.14	1.43	1.33
1	A	240	SER	C-N	8.08	1.45	1.33
1	D	39	GLU	C-N	-8.05	1.23	1.34
1	C	99	LEU	C-N	7.92	1.44	1.34
1	A	290	GLU	C-N	7.69	1.43	1.33
1	C	203	VAL	C-N	7.68	1.44	1.33
1	B	139	GLY	C-N	7.52	1.44	1.33
1	A	21	ARG	C-N	-7.51	1.23	1.33
1	B	292	VAL	C-N	7.49	1.44	1.34
1	C	29	ILE	C-N	7.33	1.42	1.33
1	C	32	THR	C-N	7.20	1.42	1.33
1	A	38	GLY	C-N	-7.12	1.23	1.33
1	B	27	LEU	C-N	-7.03	1.24	1.33
1	B	201	GLU	C-N	-6.93	1.25	1.34
1	B	174	GLN	C-N	-6.87	1.23	1.33
1	B	2	ILE	C-N	-6.73	1.24	1.33
1	D	243	ILE	C-N	-6.71	1.25	1.33
1	B	141	SER	C-N	-6.70	1.24	1.33
1	A	65	MET	C-N	6.67	1.43	1.33
1	C	240	SER	C-N	-6.61	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	ARG	CA-C	-6.52	1.44	1.52
1	C	10	VAL	C-N	-6.48	1.25	1.33
1	C	141	SER	C-N	6.45	1.42	1.33
1	B	109	ASP	N-CA	6.38	1.53	1.46
1	C	55	ARG	C-N	-6.36	1.25	1.33
1	D	297	LYS	C-N	6.14	1.42	1.33
1	D	111	ILE	C-N	6.03	1.45	1.33
1	D	298	LEU	C-N	6.01	1.41	1.33
1	A	133	PRO	C-N	5.82	1.41	1.33
1	B	51	GLY	C-N	-5.82	1.27	1.33
1	A	142	GLY	C-N	-5.82	1.26	1.34
1	D	188	VAL	C-N	5.79	1.40	1.33
1	D	283	ASP	C-N	-5.69	1.26	1.34
1	D	240	SER	C-N	5.67	1.41	1.33
1	B	136	ARG	C-N	-5.52	1.26	1.33
1	D	241	LYS	C-N	5.50	1.41	1.33
1	A	90	GLU	C-N	-5.49	1.26	1.33
1	C	286	ARG	C-N	5.34	1.41	1.33
1	D	253	GLU	C-N	5.32	1.41	1.33
1	B	158	GLY	C-N	5.20	1.40	1.33
1	B	242	ARG	C-N	5.19	1.40	1.33
1	B	197	GLU	C-O	5.18	1.30	1.24
1	C	296	LYS	C-O	5.18	1.30	1.24
1	B	156	LYS	C-N	5.17	1.40	1.33
1	B	118	PRO	C-O	-5.14	1.12	1.23
1	D	255	GLY	C-N	-5.12	1.26	1.33
1	D	239	ASP	C-N	5.10	1.41	1.33
1	B	118	PRO	C-N	-5.02	1.27	1.33

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	134	ARG	O-C-N	16.16	139.25	122.12
1	C	219	TYR	O-C-N	-16.08	103.66	123.44
1	C	7	ALA	O-C-N	-15.85	101.64	122.40
1	B	201	GLU	O-C-N	-15.71	103.84	122.22
1	C	115	THR	O-C-N	-15.43	103.06	122.34
1	C	240	SER	O-C-N	-14.82	104.88	122.22
1	A	196	LYS	O-C-N	14.78	137.90	122.08
1	B	217	ARG	O-C-N	-12.97	105.66	122.39
1	B	106	TYR	O-C-N	-12.66	106.78	122.35
1	B	254	TYR	O-C-N	-11.60	107.16	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	VAL	CA-C-N	-11.42	103.78	121.02
1	B	202	VAL	C-N-CA	-11.42	103.78	121.02
1	D	258	ASP	O-C-N	-11.15	109.48	122.86
1	D	135	GLU	O-C-N	-11.12	107.64	122.43
1	B	197	GLU	O-C-N	10.98	133.38	122.07
1	A	38	GLY	O-C-N	-10.83	110.76	122.24
1	C	219	TYR	CA-C-N	10.83	142.22	121.54
1	C	219	TYR	C-N-CA	10.83	142.22	121.54
1	A	162	LYS	O-C-N	10.54	133.30	122.12
1	C	195	SER	O-C-N	-10.44	110.89	122.79
1	B	307	ARG	O-C-N	-10.23	111.39	122.03
1	A	134	ARG	O-C-N	-10.09	109.17	122.59
1	D	77	ILE	O-C-N	-10.08	112.30	123.18
1	B	179	VAL	O-C-N	9.93	132.42	121.10
1	C	213	ILE	CA-C-N	-9.90	107.57	120.44
1	C	213	ILE	C-N-CA	-9.90	107.57	120.44
1	C	115	THR	CA-C-O	9.79	130.80	119.35
1	B	142	GLY	N-CA-C	9.69	124.65	112.83
1	B	224	GLY	CA-C-N	-9.64	107.79	119.84
1	B	224	GLY	C-N-CA	-9.64	107.79	119.84
1	C	258	ASP	O-C-N	-9.59	109.84	122.40
1	C	98	ASP	CA-C-N	9.47	133.92	120.28
1	C	98	ASP	C-N-CA	9.47	133.92	120.28
1	A	10	VAL	O-C-N	9.46	134.78	121.82
1	C	32	THR	O-C-N	9.22	131.92	121.32
1	B	52	VAL	CA-C-N	9.14	137.99	120.99
1	B	52	VAL	C-N-CA	9.14	137.99	120.99
1	C	98	ASP	O-C-N	-9.05	112.31	122.09
1	C	240	SER	CA-C-N	9.01	135.50	122.35
1	C	240	SER	C-N-CA	9.01	135.50	122.35
1	B	253	GLU	O-C-N	8.90	134.21	122.82
1	A	10	VAL	CA-C-N	-8.88	108.94	120.22
1	A	10	VAL	C-N-CA	-8.88	108.94	120.22
1	D	135	GLU	CA-C-N	8.51	135.60	122.08
1	D	135	GLU	C-N-CA	8.51	135.60	122.08
1	B	119	VAL	O-C-N	8.44	133.38	121.82
1	A	175	LYS	O-C-N	-8.39	112.03	122.35
1	A	175	LYS	CA-C-O	8.35	129.71	119.78
1	A	196	LYS	CA-C-N	-8.10	109.91	120.44
1	A	196	LYS	C-N-CA	-8.10	109.91	120.44
1	D	134	ARG	CA-C-N	-8.09	105.95	120.99
1	D	134	ARG	C-N-CA	-8.09	105.95	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	GLY	CA-C-N	-8.03	108.34	120.94
1	B	67	GLY	C-N-CA	-8.03	108.34	120.94
1	A	163	SER	O-C-N	-7.90	110.70	122.39
1	B	254	TYR	CA-C-N	7.89	134.99	120.87
1	B	254	TYR	C-N-CA	7.89	134.99	120.87
1	A	163	SER	CA-C-N	7.88	134.18	122.91
1	A	163	SER	C-N-CA	7.88	134.18	122.91
1	A	27	LEU	O-C-N	-7.77	114.18	123.27
1	B	52	VAL	O-C-N	-7.76	113.54	122.62
1	B	111	ILE	O-C-N	-7.73	111.39	122.76
1	B	119	VAL	CA-C-N	-7.67	108.65	120.31
1	B	119	VAL	C-N-CA	-7.67	108.65	120.31
1	C	5	LEU	CA-C-N	-7.66	106.39	121.41
1	C	5	LEU	C-N-CA	-7.66	106.39	121.41
1	D	139	GLY	O-C-N	-7.61	117.72	123.35
1	C	91	ALA	N-CA-C	-7.61	103.73	113.16
1	B	283	ASP	CA-C-N	7.54	131.00	120.29
1	B	283	ASP	C-N-CA	7.54	131.00	120.29
1	A	194	MET	CA-C-N	-7.49	109.38	122.64
1	A	194	MET	C-N-CA	-7.49	109.38	122.64
1	B	225	PRO	CA-N-CD	-7.48	101.53	112.00
1	D	258	ASP	CA-C-O	7.43	130.89	122.27
1	B	180	PRO	O-C-N	-7.39	112.66	122.64
1	C	113	VAL	CA-C-N	7.27	132.21	122.90
1	C	113	VAL	C-N-CA	7.27	132.21	122.90
1	B	278	LEU	O-C-N	-7.24	113.56	121.53
1	B	217	ARG	CA-C-O	7.18	128.12	119.43
1	A	258	ASP	CA-C-N	7.15	134.83	121.97
1	A	258	ASP	C-N-CA	7.15	134.83	121.97
1	B	179	VAL	CA-C-O	-7.10	110.44	119.95
1	C	113	VAL	O-C-N	-7.09	115.68	123.20
1	D	283	ASP	O-C-N	7.08	129.74	122.09
1	A	219	TYR	O-C-N	7.07	131.72	123.17
1	C	9	LYS	O-C-N	6.97	129.54	122.08
1	B	105	ALA	CA-C-O	6.96	127.27	119.41
1	B	180	PRO	CA-C-N	6.94	134.80	121.54
1	B	180	PRO	C-N-CA	6.94	134.80	121.54
1	D	53	ASP	O-C-N	-6.87	113.46	122.59
1	D	297	LYS	CA-C-N	6.85	129.46	120.28
1	D	297	LYS	C-N-CA	6.85	129.46	120.28
1	B	212	LYS	O-C-N	6.83	129.94	122.15
1	C	213	ILE	O-C-N	6.82	128.86	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	PRO	O-C-N	6.81	131.43	123.06
1	B	10	VAL	CA-C-N	6.80	127.49	119.94
1	B	10	VAL	C-N-CA	6.80	127.49	119.94
1	D	240	SER	CA-C-N	-6.78	112.86	122.63
1	D	240	SER	C-N-CA	-6.78	112.86	122.63
1	C	258	ASP	CA-C-O	6.78	129.40	121.54
1	B	197	GLU	CA-C-N	-6.68	111.51	120.79
1	B	197	GLU	C-N-CA	-6.68	111.51	120.79
1	C	204	SER	O-C-N	6.64	129.26	122.09
1	B	174	GLN	O-C-N	6.62	130.41	122.27
1	A	110	ALA	N-CA-C	6.62	119.48	110.55
1	B	215	GLU	CA-C-N	-6.58	109.73	120.71
1	B	215	GLU	C-N-CA	-6.58	109.73	120.71
1	D	141	SER	CA-C-N	6.57	127.27	119.98
1	D	141	SER	C-N-CA	6.57	127.27	119.98
1	D	141	SER	O-C-N	-6.51	113.93	122.59
1	D	83	MET	N-CA-C	6.50	120.12	109.72
1	A	75	ALA	N-CA-C	6.49	118.44	111.36
1	B	307	ARG	CA-C-N	6.45	133.30	121.70
1	B	307	ARG	C-N-CA	6.45	133.30	121.70
1	B	75	ALA	N-CA-C	6.44	120.60	112.87
1	B	202	VAL	O-C-N	6.44	129.59	122.12
1	D	7	ALA	CA-C-N	6.43	130.98	122.75
1	D	7	ALA	C-N-CA	6.43	130.98	122.75
1	D	138	ILE	N-CA-C	6.38	117.05	107.80
1	C	195	SER	CA-C-N	6.38	129.69	120.38
1	C	195	SER	C-N-CA	6.38	129.69	120.38
1	B	201	GLU	CA-C-N	6.35	131.39	121.35
1	B	201	GLU	C-N-CA	6.35	131.39	121.35
1	B	204	SER	CA-C-O	6.35	127.28	120.24
1	B	148	ARG	O-C-N	-6.29	115.59	122.07
1	B	53	ASP	CA-CB-CG	6.28	118.88	112.60
1	B	224	GLY	C-N-CD	6.25	150.65	125.00
1	A	216	LEU	N-CA-C	6.23	118.16	111.36
1	C	111	ILE	O-C-N	-6.17	115.91	122.95
1	A	192	HIS	CB-CG-CD2	-6.17	123.17	131.20
1	A	123	THR	O-C-N	-6.15	115.02	122.22
1	C	60	ASN	N-CA-C	-6.15	105.06	113.30
1	B	212	LYS	CA-C-N	-6.13	109.75	120.29
1	B	212	LYS	C-N-CA	-6.13	109.75	120.29
1	A	143	ILE	O-C-N	6.10	127.87	121.89
1	C	115	THR	CA-C-N	6.09	130.13	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	THR	C-N-CA	6.09	130.13	121.42
1	A	74	THR	CA-C-O	6.06	127.28	119.95
1	B	138	ILE	N-CA-C	6.06	117.02	108.36
1	A	38	GLY	CA-C-N	6.05	130.97	120.68
1	A	38	GLY	C-N-CA	6.05	130.97	120.68
1	A	142	GLY	N-CA-C	6.05	119.52	112.50
1	D	254	TYR	CA-C-N	6.04	132.75	120.80
1	D	254	TYR	C-N-CA	6.04	132.75	120.80
1	A	162	LYS	CA-C-N	-5.92	110.09	121.94
1	A	162	LYS	C-N-CA	-5.92	110.09	121.94
1	C	138	ILE	N-CA-C	5.92	116.39	108.11
1	C	253	GLU	O-C-N	-5.89	115.78	122.97
1	A	123	THR	CA-C-N	5.88	128.44	120.44
1	A	123	THR	C-N-CA	5.88	128.44	120.44
1	B	215	GLU	O-C-N	5.87	128.34	122.12
1	A	134	ARG	CA-C-N	5.87	132.97	122.06
1	A	134	ARG	C-N-CA	5.87	132.97	122.06
1	B	115	THR	CA-C-O	5.85	125.33	118.90
1	C	141	SER	CA-C-N	5.84	126.59	119.99
1	C	141	SER	C-N-CA	5.84	126.59	119.99
1	C	9	LYS	N-CA-C	5.79	118.08	111.02
1	C	141	SER	O-C-N	-5.79	116.12	121.79
1	B	141	SER	O-C-N	-5.78	114.90	122.59
1	B	222	ASN	CA-C-O	5.78	126.28	119.06
1	D	7	ALA	O-C-N	-5.74	111.26	122.11
1	B	109	ASP	CA-C-O	5.74	126.72	119.95
1	D	177	PHE	CA-C-N	5.74	126.91	120.66
1	D	177	PHE	C-N-CA	5.74	126.91	120.66
1	B	177	PHE	CA-C-N	5.72	126.18	120.52
1	B	177	PHE	C-N-CA	5.72	126.18	120.52
1	D	297	LYS	O-C-N	-5.70	116.08	122.12
1	D	51	GLY	CA-C-N	-5.68	115.69	122.22
1	D	51	GLY	C-N-CA	-5.68	115.69	122.22
1	B	188	VAL	CA-C-N	5.68	125.86	119.90
1	B	188	VAL	C-N-CA	5.68	125.86	119.90
1	B	204	SER	CA-CB-OG	5.68	122.46	111.10
1	B	142	GLY	O-C-N	5.66	127.66	122.17
1	A	194	MET	O-C-N	5.62	130.65	123.11
1	B	222	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	253	GLU	O-C-N	-5.58	115.68	122.82
1	C	285	LYS	CA-C-O	5.58	126.23	119.31
1	B	53	ASP	N-CA-C	5.54	119.51	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	GLY	N-CA-C	5.54	119.37	112.73
1	A	192	HIS	CA-CB-CG	5.53	119.33	113.80
1	D	253	GLU	O-C-N	5.53	129.90	122.82
1	C	253	GLU	CA-C-N	5.49	131.67	123.05
1	C	253	GLU	C-N-CA	5.49	131.67	123.05
1	B	133	PRO	CA-C-N	5.47	128.16	120.28
1	B	133	PRO	C-N-CA	5.47	128.16	120.28
1	A	98	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	240	SER	N-CA-C	5.45	119.55	113.01
1	D	254	TYR	O-C-N	-5.44	111.82	122.11
1	A	20	MET	O-C-N	-5.44	116.47	122.07
1	B	253	GLU	CA-C-N	-5.43	111.16	121.54
1	B	253	GLU	C-N-CA	-5.43	111.16	121.54
1	B	198	GLU	N-CA-C	5.43	117.64	111.02
1	C	54	ILE	O-C-N	-5.42	115.93	122.59
1	A	134	ARG	CA-C-O	5.41	128.25	120.51
1	D	10	VAL	O-C-N	5.40	128.96	121.84
1	B	240	SER	N-CA-C	5.38	118.95	112.38
1	A	26	LEU	CB-CA-C	5.38	119.22	109.37
1	B	134	ARG	CA-C-N	5.38	128.24	120.38
1	B	134	ARG	C-N-CA	5.38	128.24	120.38
1	B	76	GLY	N-CA-C	5.38	119.46	112.25
1	A	73	VAL	O-C-N	5.38	129.44	122.77
1	C	96	MET	N-CA-C	-5.37	105.51	111.36
1	B	174	GLN	N-CA-C	5.36	118.04	111.82
1	D	51	GLY	O-C-N	5.35	128.96	122.32
1	A	115	THR	N-CA-C	-5.35	107.41	114.04
1	D	115	THR	N-CA-C	-5.35	107.41	114.04
1	C	263	VAL	CA-C-N	5.33	125.09	119.76
1	C	263	VAL	C-N-CA	5.33	125.09	119.76
1	B	303	PRO	N-CA-C	-5.32	104.21	110.70
1	C	188	VAL	N-CA-C	5.30	114.15	108.95
1	B	200	GLU	CA-C-N	5.28	127.88	120.28
1	B	200	GLU	C-N-CA	5.28	127.88	120.28
1	B	8	GLY	O-C-N	5.28	128.20	122.77
1	A	173	GLY	CA-C-N	5.27	128.32	120.31
1	A	173	GLY	C-N-CA	5.27	128.32	120.31
1	D	220	SER	N-CA-C	5.26	117.07	110.24
1	D	75	ALA	N-CA-C	5.24	119.15	112.87
1	A	73	VAL	CA-C-N	-5.24	114.27	122.49
1	A	73	VAL	C-N-CA	-5.24	114.27	122.49
1	B	136	ARG	O-C-N	-5.23	116.03	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	TYR	CA-C-N	5.21	132.72	123.34
1	B	106	TYR	C-N-CA	5.21	132.72	123.34
1	B	158	GLY	CA-C-O	5.17	125.92	119.88
1	C	10	VAL	CA-C-N	5.16	125.67	120.00
1	C	10	VAL	C-N-CA	5.16	125.67	120.00
1	B	100	ALA	O-C-N	-5.14	116.67	122.12
1	D	84	THR	N-CA-C	5.14	116.69	108.41
1	D	280	LEU	N-CA-C	5.13	118.10	109.95
1	C	239	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	153	ILE	CB-CA-C	-5.11	105.33	112.02
1	A	301	THR	N-CA-C	-5.10	106.22	112.90
1	D	253	GLU	CA-C-N	-5.08	114.68	122.61
1	D	253	GLU	C-N-CA	-5.08	114.68	122.61
1	B	225	PRO	N-CA-CB	5.05	108.55	103.25
1	A	98	ASP	O-C-N	5.01	127.44	122.03
1	A	192	HIS	N-CA-C	-5.01	107.22	113.38

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain
1	A	194	MET	Mainchain
1	A	76	GLY	Mainchain
1	B	201	GLU	Mainchain
1	B	202	VAL	Mainchain
1	B	278	LEU	Mainchain
1	C	115	THR	Mainchain
1	C	219	TYR	Mainchain
1	C	258	ASP	Mainchain
1	C	7	ALA	Mainchain
1	D	258	ASP	Mainchain
1	D	8	GLY	Mainchain

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	2262	0	2337	120	1
1	B	2289	0	2356	129	2
1	C	2274	0	2350	153	0
1	D	2346	0	2422	139	1
2	A	28	0	0	1	0
2	B	42	0	0	1	0
2	C	17	0	0	0	0
2	D	34	0	0	1	0
All	All	9292	0	9465	504	3

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 27.

All (504) 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:174:GLN:NE2	1:B:175:LYS:HZ2	1.34	1.24
1:B:174:GLN:NE2	1:B:175:LYS:NZ	1.93	1.17
1:B:76:GLY:HA3	1:B:116:THR:HG23	1.32	1.09
1:A:76:GLY:HA3	1:A:116:THR:HG23	1.33	1.06
1:A:259:ILE:HD13	1:A:292:VAL:HG13	1.44	1.00
1:B:242:ARG:NH2	1:D:53:ASP:OD1	1.95	0.98
1:D:80:LYS:O	1:D:83:MET:HB2	1.63	0.96
1:B:118:PRO:O	1:B:122:MET:HG2	1.68	0.93
1:A:149:MET:HE2	1:A:166:ALA:HB1	1.51	0.91
1:D:134:ARG:HH11	1:D:251:GLN:NE2	1.67	0.91
1:D:84:THR:HB	1:D:87:GLN:HB2	1.50	0.91
1:D:84:THR:HB	1:D:87:GLN:CB	2.04	0.88
1:B:96:MET:CG	1:B:122:MET:HE3	2.04	0.88
1:D:243:ILE:HD13	1:D:276:ILE:CD1	2.03	0.87
1:C:232:THR:O	1:C:236:ILE:HD13	1.73	0.87
1:C:53:ASP:OD1	1:A:242:ARG:HD2	1.75	0.87
1:B:153:ILE:CD1	1:B:190:LEU:HD11	2.05	0.87
1:B:154:SER:HB2	1:B:159:VAL:O	1.76	0.86
1:A:195:SER:OG	1:A:198:GLU:HG3	1.76	0.86
1:D:26:LEU:HD21	1:D:56:ILE:HG12	1.59	0.85
1:B:153:ILE:HD13	1:B:190:LEU:HD11	1.59	0.84
1:D:134:ARG:HH11	1:D:251:GLN:HE21	1.24	0.84
1:D:140:PHE:CZ	1:D:228:GLY:HA3	2.11	0.84
1:B:77:ILE:HG22	1:B:92:ASN:OD1	1.76	0.84
1:C:296:LYS:O	1:C:300:GLU:HG3	1.79	0.83
1:B:174:GLN:HE21	1:B:175:LYS:NZ	1.67	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:LYS:HB3	1:C:297:LYS:NZ	1.95	0.82
1:C:142:GLY:HA3	1:C:245:PRO:HG2	1.62	0.81
1:B:174:GLN:HE21	1:B:175:LYS:HZ2	0.82	0.81
1:B:96:MET:HG2	1:B:122:MET:HE3	1.61	0.80
1:C:143:ILE:HD11	1:C:244:TYR:HB3	1.63	0.80
1:D:134:ARG:HD2	1:D:251:GLN:CD	2.07	0.80
1:A:75:ALA:O	1:A:76:GLY:O	1.99	0.79
1:B:12:MET:SD	1:B:39:GLU:HG2	2.22	0.79
1:A:303:PRO:HD2	1:A:306:LEU:HD12	1.62	0.79
1:D:171:MET:HE1	1:D:173:GLY:C	2.08	0.79
1:A:76:GLY:HA3	1:A:116:THR:CG2	2.12	0.79
1:A:259:ILE:HD12	1:A:296:LYS:HG3	1.63	0.79
1:C:236:ILE:HD11	1:C:267:ILE:CD1	2.13	0.79
1:C:269:LYS:HB3	1:C:269:LYS:NZ	1.95	0.79
1:B:204:SER:O	1:B:208:ASN:HB2	1.82	0.79
1:B:171:MET:HE2	1:B:173:GLY:N	1.96	0.79
1:C:154:SER:HB2	1:C:159:VAL:O	1.83	0.79
1:A:171:MET:HE2	1:A:175:LYS:H	1.46	0.79
1:A:9:LYS:HB2	1:A:9:LYS:NZ	1.98	0.78
1:D:213:ILE:HD11	1:D:221:SER:HB2	1.64	0.78
1:A:266:VAL:HG23	1:A:276:ILE:HD11	1.65	0.78
1:D:138:ILE:HG13	1:D:272:ILE:HD11	1.65	0.77
1:A:117:ASN:OD1	1:A:119:VAL:HG23	1.84	0.77
1:B:9:LYS:HD3	1:B:219:TYR:CE1	2.19	0.77
1:B:76:GLY:CA	1:B:116:THR:HG23	2.13	0.77
1:D:117:ASN:OD1	1:D:119:VAL:HG23	1.85	0.77
1:D:153:ILE:HG23	1:D:194:MET:HE1	1.67	0.76
1:C:239:ASP:HB2	1:C:269:LYS:HB2	1.66	0.76
1:B:92:ASN:HB3	1:B:122:MET:HE2	1.68	0.76
1:C:77:ILE:HD13	1:C:78:GLY:N	2.01	0.75
1:B:174:GLN:NE2	1:B:175:LYS:HZ1	1.85	0.74
1:D:239:ASP:OD1	1:D:241:LYS:NZ	2.15	0.73
1:C:140:PHE:CE2	1:C:225:PRO:HA	2.23	0.73
1:A:115:THR:HG21	1:A:229:LEU:HD11	1.71	0.73
1:B:213:ILE:O	1:B:217:ARG:HG2	1.89	0.73
1:C:140:PHE:CZ	1:C:228:GLY:HA3	2.24	0.73
1:D:140:PHE:CE1	1:D:228:GLY:HA3	2.24	0.73
1:B:63:GLU:O	1:B:66:ARG:HG3	1.89	0.72
1:C:169:LEU:HD11	1:C:278:LEU:HD12	1.70	0.72
1:B:53:ASP:OD2	1:A:162:LYS:HG3	1.89	0.71
1:D:153:ILE:HG23	1:D:194:MET:CE	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:MET:CE	1:A:175:LYS:H	2.02	0.71
1:D:80:LYS:HG2	1:D:81:PRO:HD2	1.73	0.71
1:A:1:MET:HA	1:A:24:ASP:OD2	1.90	0.71
1:B:96:MET:HG3	1:B:122:MET:HE3	1.72	0.71
1:C:103:ILE:HD11	1:C:130:THR:HG22	1.71	0.71
1:A:154:SER:HB2	1:A:159:VAL:O	1.90	0.71
1:C:269:LYS:HB3	1:C:269:LYS:HZ3	1.57	0.70
1:B:171:MET:HE2	1:B:173:GLY:CA	2.21	0.70
1:C:141:SER:HB2	1:C:262:GLU:OE1	1.92	0.69
1:B:93:ALA:N	1:B:122:MET:HE1	2.07	0.69
1:A:171:MET:HE1	1:A:173:GLY:C	2.18	0.69
1:A:249:TYR:CZ	1:A:258:ASP:HA	2.29	0.68
1:C:77:ILE:HG22	1:C:92:ASN:OD1	1.93	0.68
1:A:134:ARG:HH12	1:A:253:GLU:CD	2.01	0.68
1:D:79:ARG:HE	1:D:83:MET:HB3	1.59	0.68
1:D:171:MET:HE3	1:D:171:MET:O	1.94	0.68
1:A:115:THR:CG2	1:A:229:LEU:HD11	2.24	0.68
1:C:140:PHE:CE1	1:C:228:GLY:HA3	2.29	0.68
1:A:171:MET:HE2	1:A:175:LYS:N	2.09	0.68
1:C:79:ARG:HH11	1:C:79:ARG:HB2	1.58	0.68
1:C:297:LYS:HB3	1:C:297:LYS:HZ3	1.59	0.68
1:A:210:GLY:HA2	1:A:213:ILE:HD11	1.76	0.67
1:A:286:ARG:HB3	1:A:286:ARG:NH1	2.09	0.67
1:B:304:PRO:HA	1:B:307:ARG:HG2	1.76	0.67
1:D:152:TYR:HB3	1:D:202:VAL:HG12	1.77	0.66
1:C:213:ILE:HD11	1:C:221:SER:HB2	1.76	0.66
1:D:195:SER:OG	1:D:198:GLU:HG3	1.96	0.66
1:B:92:ASN:C	1:B:122:MET:HE1	2.20	0.66
1:A:282:GLU:HG3	1:A:283:ASP:N	2.11	0.66
1:A:178:PRO:HG3	1:A:203:VAL:HG22	1.77	0.66
1:C:199:ILE:O	1:C:203:VAL:HG23	1.96	0.65
1:A:199:ILE:O	1:A:203:VAL:HG23	1.96	0.65
1:B:242:ARG:CZ	1:D:53:ASP:OD1	2.43	0.65
1:B:307:ARG:O	1:B:308:GLU:HB2	1.95	0.65
1:B:174:GLN:HE22	1:B:175:LYS:NZ	1.91	0.65
1:D:196:LYS:O	1:D:200:GLU:HG3	1.96	0.65
1:A:240:SER:OG	1:A:242:ARG:HD3	1.96	0.65
1:D:89:LEU:HG	1:D:302:LEU:HD11	1.78	0.65
1:C:293:GLN:O	1:C:296:LYS:HB3	1.97	0.65
1:B:162:LYS:HD3	1:A:53:ASP:OD1	1.96	0.65
1:C:79:ARG:HG2	1:C:214:THR:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TYR:N	1:B:277:GLU:OE1	2.28	0.64
1:D:71:VAL:HG11	1:D:103:ILE:CD1	2.27	0.64
1:C:169:LEU:HD21	1:C:264:PRO:HD3	1.80	0.64
1:D:253:GLU:HG2	1:D:275:ILE:HB	1.80	0.64
1:B:181:ARG:NH1	1:B:182:LEU:HD21	2.12	0.64
1:D:269:LYS:NZ	1:D:269:LYS:HB3	2.13	0.64
1:B:217:ARG:HH22	1:B:222:ASN:N	1.95	0.64
1:B:181:ARG:O	1:B:182:LEU:HD23	1.98	0.63
1:D:243:ILE:HD13	1:D:276:ILE:HD13	1.80	0.63
1:A:134:ARG:NH1	1:A:253:GLU:OE1	2.31	0.63
1:D:162:LYS:HG3	1:C:53:ASP:OD2	1.97	0.63
1:C:7:ALA:HA	1:C:12:MET:CE	2.29	0.62
1:A:259:ILE:CD1	1:A:292:VAL:HG13	2.25	0.62
1:A:282:GLU:HG3	1:A:283:ASP:H	1.64	0.62
1:B:167:ILE:HD11	1:C:187:GLY:HA2	1.80	0.62
1:A:72:LEU:HD22	1:A:229:LEU:HD22	1.82	0.62
1:D:84:THR:HB	1:D:87:GLN:HB3	1.82	0.62
1:A:269:LYS:NZ	1:A:269:LYS:HB3	2.14	0.62
1:B:231:LEU:HD11	1:A:49:GLU:O	2.00	0.62
1:D:241:LYS:NZ	1:D:273:GLU:OE2	2.31	0.62
1:B:213:ILE:HD11	1:B:221:SER:HB2	1.80	0.62
1:D:241:LYS:CD	1:D:273:GLU:OE2	2.47	0.62
1:B:188:VAL:HG22	1:C:278:LEU:HD23	1.82	0.61
1:D:71:VAL:HG11	1:D:103:ILE:HD11	1.82	0.61
1:D:169:LEU:HD11	1:D:278:LEU:HD12	1.82	0.61
1:A:9:LYS:HB2	1:A:9:LYS:HZ2	1.65	0.61
1:C:118:PRO:O	1:C:122:MET:HG2	2.00	0.61
1:B:135:GLU:O	1:B:271:GLY:HA3	2.00	0.61
1:D:138:ILE:CG1	1:D:272:ILE:HD11	2.30	0.61
1:D:250:LEU:HD11	1:D:261:ALA:HB3	1.81	0.61
1:A:149:MET:HE2	1:A:166:ALA:CB	2.29	0.61
1:A:9:LYS:HD3	1:A:219:TYR:CE1	2.36	0.61
1:B:140:PHE:CZ	1:B:228:GLY:HA3	2.35	0.61
1:B:162:LYS:CD	1:A:53:ASP:OD1	2.49	0.60
1:B:217:ARG:NH2	1:B:221:SER:HA	2.16	0.60
1:B:222:ASN:C	1:B:225:PRO:HD2	2.26	0.60
1:A:134:ARG:HD2	1:A:251:GLN:NE2	2.15	0.60
1:A:142:GLY:HA3	1:A:245:PRO:HG2	1.83	0.60
1:C:236:ILE:HD11	1:C:267:ILE:HD11	1.84	0.60
1:C:236:ILE:HD11	1:C:267:ILE:HD13	1.82	0.60
1:B:49:GLU:O	1:A:231:LEU:HD11	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:LEU:HD23	1:C:113:VAL:HG22	1.83	0.60
1:D:24:ASP:OD1	1:D:25:ASP:N	2.33	0.59
1:A:7:ALA:HA	1:A:12:MET:HE3	1.84	0.59
1:B:242:ARG:NE	1:D:53:ASP:OD1	2.34	0.59
1:C:92:ASN:O	1:C:96:MET:HG2	2.02	0.59
1:C:66:ARG:HG3	1:C:66:ARG:HH11	1.67	0.59
1:D:199:ILE:O	1:D:203:VAL:HG23	2.03	0.59
1:C:293:GLN:OE1	1:C:296:LYS:HD2	2.03	0.59
1:B:217:ARG:HH22	1:B:222:ASN:H	1.50	0.58
1:A:171:MET:HE1	1:A:174:GLN:N	2.18	0.58
1:A:276:ILE:HD12	1:A:276:ILE:N	2.17	0.58
1:A:201:GLU:O	1:A:205:GLU:HG2	2.03	0.58
1:A:269:LYS:HB3	1:A:269:LYS:HZ3	1.68	0.58
1:A:140:PHE:CZ	1:A:228:GLY:HA3	2.39	0.58
1:B:77:ILE:HG22	1:B:92:ASN:CG	2.28	0.58
1:D:7:ALA:HB3	1:D:30:ALA:HB2	1.84	0.58
1:C:195:SER:OG	1:C:198:GLU:HG3	2.04	0.58
1:D:301:THR:HG22	1:D:301:THR:O	2.03	0.58
1:B:160:SER:OG	1:A:53:ASP:OD2	2.22	0.58
1:B:12:MET:HE1	1:B:28:LEU:CD1	2.34	0.57
1:C:194:MET:HB2	1:C:199:ILE:HD11	1.86	0.57
1:B:281:THR:O	1:B:285:LYS:HD3	2.05	0.57
1:C:213:ILE:O	1:C:217:ARG:HG2	2.03	0.57
1:A:296:LYS:O	1:A:300:GLU:HG3	2.04	0.57
1:B:142:GLY:HA3	1:B:245:PRO:HG2	1.85	0.57
1:B:201:GLU:HB3	2:B:338:HOH:O	2.05	0.57
1:B:86:GLU:OE2	1:B:301:THR:HG21	2.05	0.57
1:C:259:ILE:HG13	1:C:260:VAL:H	1.70	0.57
1:A:171:MET:HE1	1:A:173:GLY:CA	2.34	0.57
1:C:297:LYS:NZ	1:C:297:LYS:CB	2.66	0.57
1:D:217:ARG:CD	1:C:39:GLU:HG3	2.34	0.56
1:D:302:LEU:O	1:D:307:ARG:NH1	2.38	0.56
1:C:79:ARG:HB3	1:C:220:SER:HB3	1.87	0.56
1:C:7:ALA:HA	1:C:12:MET:HE3	1.86	0.56
1:A:68:SER:O	1:A:110:ALA:HB2	2.05	0.56
1:C:199:ILE:O	1:C:202:VAL:HG22	2.04	0.56
1:D:134:ARG:NH1	1:D:251:GLN:HE21	1.98	0.56
1:B:96:MET:HE3	1:B:116:THR:HG21	1.88	0.56
1:D:156:LYS:HE3	1:D:198:GLU:OE1	2.06	0.56
1:C:79:ARG:HG3	1:C:80:LYS:H	1.71	0.56
1:D:138:ILE:N	1:D:138:ILE:HD12	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:MET:HB3	1:C:198:GLU:HB2	1.87	0.55
1:C:250:LEU:O	1:C:257:ASN:HA	2.06	0.55
1:B:162:LYS:HD2	1:A:51:GLY:O	2.05	0.55
1:D:89:LEU:HG	1:D:302:LEU:CD1	2.36	0.55
1:C:293:GLN:CD	1:C:296:LYS:HD2	2.32	0.55
1:B:217:ARG:NH2	1:B:222:ASN:OD1	2.40	0.55
1:A:134:ARG:HD2	1:A:251:GLN:CD	2.32	0.55
1:D:213:ILE:HG22	1:C:41:LEU:HD23	1.89	0.55
1:C:157:LEU:HG	1:C:194:MET:HE3	1.88	0.55
1:D:26:LEU:CD2	1:D:56:ILE:HG12	2.34	0.55
1:D:188:VAL:HB	1:D:193:LEU:HD11	1.87	0.55
1:D:257:ASN:O	1:D:258:ASP:C	2.49	0.55
1:A:202:VAL:HG23	1:A:203:VAL:N	2.22	0.54
1:C:259:ILE:HG13	1:C:260:VAL:N	2.23	0.54
1:A:286:ARG:HB3	1:A:286:ARG:HH11	1.72	0.54
1:C:89:LEU:C	1:C:91:ALA:H	2.15	0.54
1:A:92:ASN:O	1:A:96:MET:HG2	2.07	0.54
1:C:169:LEU:CD2	1:C:264:PRO:HD3	2.36	0.54
1:A:33:PRO:HA	1:A:60:ASN:OD1	2.06	0.54
1:D:80:LYS:HD2	1:D:81:PRO:O	2.07	0.54
1:B:222:ASN:O	1:B:225:PRO:HD2	2.07	0.54
1:D:134:ARG:HD2	1:D:251:GLN:NE2	2.22	0.54
1:D:307:ARG:O	1:D:308:GLU:HB2	2.07	0.54
1:A:114:ILE:HD11	1:A:126:MET:HG2	1.90	0.54
1:D:7:ALA:HA	1:D:12:MET:HE3	1.90	0.54
1:B:93:ALA:CA	1:B:122:MET:HE1	2.37	0.54
1:D:171:MET:HE1	1:D:173:GLY:CA	2.38	0.54
1:C:153:ILE:HD13	1:C:202:VAL:HG11	1.88	0.53
1:C:253:GLU:HG2	1:C:275:ILE:HB	1.91	0.53
1:B:169:LEU:HD11	1:B:278:LEU:HD12	1.90	0.53
1:D:190:LEU:HD11	1:D:194:MET:HE3	1.88	0.53
1:B:7:ALA:HA	1:B:12:MET:CE	2.39	0.53
1:C:66:ARG:HG3	1:C:66:ARG:NH1	2.23	0.53
1:C:108:LYS:HA	1:C:132:PHE:CZ	2.44	0.53
1:C:293:GLN:NE2	1:C:296:LYS:HD2	2.22	0.53
1:C:7:ALA:HB3	1:C:30:ALA:HB2	1.91	0.53
1:A:77:ILE:O	1:A:77:ILE:CG2	2.57	0.53
1:D:162:LYS:HD3	1:C:51:GLY:O	2.09	0.53
1:D:269:LYS:HB3	1:D:269:LYS:HZ3	1.73	0.53
1:A:302:LEU:O	1:A:307:ARG:NH1	2.42	0.53
1:D:149:MET:HG2	1:D:166:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:HH11	1:C:79:ARG:CB	2.20	0.52
1:C:142:GLY:CA	1:C:245:PRO:HG2	2.37	0.52
1:C:171:MET:CE	1:C:175:LYS:H	2.22	0.52
1:B:62:TYR:O	1:B:65:MET:HG2	2.09	0.52
1:B:217:ARG:NH2	1:B:222:ASN:N	2.58	0.52
1:B:53:ASP:OD2	1:A:162:LYS:CG	2.56	0.52
1:C:115:THR:HG23	1:C:225:PRO:HB3	1.91	0.52
1:B:12:MET:HE1	1:B:28:LEU:HD11	1.91	0.52
1:B:116:THR:O	1:B:119:VAL:HG12	2.10	0.52
1:D:90:GLU:O	1:D:94:ASN:ND2	2.43	0.52
1:D:65:MET:SD	1:D:103:ILE:HD13	2.49	0.52
1:D:77:ILE:HG22	1:D:92:ASN:OD1	2.09	0.52
1:C:134:ARG:HH22	1:C:253:GLU:CD	2.18	0.52
1:D:171:MET:HE3	1:D:171:MET:C	2.34	0.52
1:B:171:MET:CE	1:B:173:GLY:HA3	2.39	0.52
1:B:299:VAL:O	1:B:302:LEU:HB2	2.10	0.52
1:D:307:ARG:O	1:D:308:GLU:CB	2.57	0.52
1:A:5:LEU:HD21	1:A:103:ILE:HD11	1.92	0.52
1:B:88:LEU:HG	1:B:92:ASN:ND2	2.25	0.51
1:B:153:ILE:HD11	1:B:190:LEU:HD11	1.87	0.51
1:C:282:GLU:HG3	1:C:283:ASP:N	2.25	0.51
1:B:7:ALA:HA	1:B:12:MET:HE2	1.91	0.51
1:B:167:ILE:CD1	1:C:187:GLY:HA2	2.41	0.51
1:D:243:ILE:CD1	1:D:276:ILE:CD1	2.84	0.51
1:C:62:TYR:O	1:C:65:MET:HG2	2.10	0.51
1:A:213:ILE:O	1:A:217:ARG:HG2	2.11	0.51
1:C:1:MET:HA	1:C:24:ASP:OD2	2.10	0.51
1:C:171:MET:HE1	1:C:173:GLY:C	2.36	0.51
1:C:26:LEU:HD22	1:C:54:ILE:HD12	1.93	0.51
1:D:4:ILE:HB	1:D:28:LEU:HD13	1.93	0.51
1:C:142:GLY:HA3	1:C:245:PRO:CG	2.39	0.51
1:B:93:ALA:HA	1:B:122:MET:HE1	1.92	0.51
1:A:176:MET:HE1	1:A:206:THR:CG2	2.41	0.51
1:D:1:MET:HA	1:D:24:ASP:OD2	2.09	0.51
1:D:79:ARG:HD2	1:D:83:MET:HE2	1.93	0.50
1:A:75:ALA:C	1:A:76:GLY:O	2.54	0.50
1:D:20:MET:HB2	1:C:20:MET:HE2	1.94	0.50
1:D:134:ARG:CD	1:D:251:GLN:NE2	2.74	0.50
1:D:217:ARG:HD3	1:C:39:GLU:HG3	1.93	0.50
1:D:75:ALA:O	1:D:76:GLY:O	2.29	0.50
1:D:199:ILE:O	1:D:202:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:ARG:HD2	1:C:39:GLU:HG3	1.92	0.50
1:A:142:GLY:C	1:A:245:PRO:HG2	2.37	0.50
1:D:243:ILE:CD1	1:D:276:ILE:HD11	2.42	0.50
1:C:10:VAL:HA	1:C:222:ASN:HB2	1.93	0.50
1:B:20:MET:HB2	1:A:20:MET:HE2	1.94	0.50
1:B:269:LYS:NZ	1:B:269:LYS:HB3	2.27	0.50
1:C:92:ASN:HB3	1:C:116:THR:HG21	1.94	0.50
1:B:89:LEU:HD11	1:B:302:LEU:HD11	1.94	0.50
1:D:171:MET:HE2	1:D:175:LYS:C	2.37	0.50
1:C:190:LEU:HD13	1:C:199:ILE:HD12	1.93	0.50
1:A:9:LYS:HB2	1:A:9:LYS:HZ3	1.72	0.50
1:D:113:VAL:HA	1:D:138:ILE:O	2.12	0.49
1:C:198:GLU:O	1:C:202:VAL:HG13	2.12	0.49
1:D:254:TYR:CZ	1:D:277:GLU:HA	2.47	0.49
1:C:203:VAL:O	1:C:207:VAL:HG23	2.12	0.49
1:C:286:ARG:NH1	1:C:290:GLU:OE2	2.44	0.49
1:D:7:ALA:HA	1:D:12:MET:CE	2.42	0.49
1:B:62:TYR:HB3	1:B:65:MET:HE3	1.95	0.49
1:D:76:GLY:HA3	1:D:116:THR:HG23	1.94	0.49
1:B:171:MET:CE	1:B:173:GLY:N	2.71	0.49
1:C:194:MET:HB2	1:C:199:ILE:CD1	2.43	0.49
1:D:195:SER:O	1:D:199:ILE:HG13	2.12	0.49
1:A:75:ALA:O	1:A:76:GLY:C	2.54	0.49
1:A:117:ASN:HA	1:A:119:VAL:N	2.28	0.49
1:B:278:LEU:HD23	1:C:188:VAL:HG22	1.95	0.49
1:B:171:MET:CE	1:B:173:GLY:CA	2.91	0.49
1:B:194:MET:HG2	1:B:198:GLU:OE1	2.13	0.49
1:D:160:SER:HB2	1:A:240:SER:O	2.12	0.49
1:C:253:GLU:CD	1:C:253:GLU:H	2.21	0.49
1:D:27:LEU:HD22	1:D:28:LEU:N	2.27	0.48
1:D:117:ASN:HA	1:D:119:VAL:N	2.28	0.48
1:C:34:GLY:H	1:C:60:ASN:HD21	1.59	0.48
1:C:113:VAL:HA	1:C:138:ILE:O	2.13	0.48
1:B:77:ILE:HG13	1:B:78:GLY:N	2.28	0.48
1:D:48:ALA:HA	1:C:161:PHE:CE1	2.48	0.48
1:A:12:MET:HE1	1:A:28:LEU:CD1	2.44	0.48
1:B:48:ALA:HA	1:A:161:PHE:CE1	2.48	0.48
1:D:92:ASN:O	1:D:96:MET:HG2	2.14	0.48
1:D:213:ILE:CG2	1:C:41:LEU:HD23	2.42	0.48
1:B:41:LEU:HD23	1:A:213:ILE:HG23	1.95	0.48
1:D:214:THR:OG1	1:D:220:SER:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:CD2	1:C:54:ILE:HD12	2.43	0.48
1:B:168:VAL:HA	1:B:178:PRO:HA	1.95	0.48
1:B:181:ARG:NH2	1:B:279:PRO:O	2.47	0.48
1:D:79:ARG:NH2	1:D:83:MET:O	2.45	0.48
1:D:241:LYS:CE	1:D:273:GLU:OE2	2.62	0.48
1:C:66:ARG:NH2	1:C:106:TYR:HD1	2.12	0.48
1:C:79:ARG:HG3	1:C:80:LYS:N	2.28	0.48
1:C:27:LEU:HD22	1:C:29:ILE:HG13	1.96	0.48
1:C:171:MET:HE2	1:C:175:LYS:N	2.29	0.48
1:C:12:MET:HE1	1:C:28:LEU:CD1	2.44	0.47
1:D:7:ALA:HB3	1:D:30:ALA:CB	2.43	0.47
1:D:35:LYS:HB3	1:D:36:PRO:HD3	1.95	0.47
1:B:269:LYS:NZ	1:B:269:LYS:CB	2.77	0.47
1:D:142:GLY:HA3	1:D:245:PRO:HG2	1.96	0.47
1:D:169:LEU:CD2	1:D:264:PRO:HD3	2.44	0.47
1:C:243:ILE:CD1	1:C:266:VAL:HG22	2.44	0.47
1:B:223:TYR:O	1:B:224:GLY:C	2.57	0.47
1:D:63:GLU:HG3	1:D:106:TYR:CZ	2.48	0.47
1:C:153:ILE:HD11	1:C:202:VAL:HG21	1.97	0.47
1:B:167:ILE:HD12	1:B:182:LEU:CB	2.45	0.47
1:C:109:ASP:HA	1:C:136:ARG:NH1	2.30	0.47
1:D:269:LYS:NZ	1:D:269:LYS:CB	2.78	0.47
1:C:5:LEU:HD12	1:C:29:ILE:HB	1.97	0.47
1:B:92:ASN:C	1:B:122:MET:CE	2.87	0.47
1:B:307:ARG:O	1:B:308:GLU:CB	2.61	0.47
1:C:245:PRO:HA	1:C:263:VAL:O	2.15	0.47
1:A:24:ASP:OD1	1:A:25:ASP:N	2.42	0.47
1:D:213:ILE:HD12	1:C:42:ASP:HB2	1.96	0.47
1:D:256:TYR:OH	1:D:289:ASP:OD1	2.28	0.47
1:C:111:ILE:HD12	1:C:111:ILE:N	2.30	0.46
1:C:117:ASN:HA	1:C:118:PRO:C	2.39	0.46
1:A:5:LEU:CD2	1:A:103:ILE:HD11	2.46	0.46
1:A:65:MET:HE1	1:A:103:ILE:HD13	1.96	0.46
1:C:117:ASN:HA	1:C:119:VAL:N	2.30	0.46
1:D:196:LYS:HE3	1:D:200:GLU:OE2	2.15	0.46
1:C:113:VAL:HG12	1:C:138:ILE:HB	1.97	0.46
1:C:171:MET:HE2	1:C:175:LYS:CA	2.45	0.46
1:B:171:MET:HE2	1:B:173:GLY:HA3	1.97	0.46
1:B:175:LYS:HE2	1:B:294:ALA:HB2	1.98	0.46
1:B:181:ARG:HH12	1:B:182:LEU:HD21	1.79	0.46
1:B:188:VAL:HG11	1:B:193:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ALA:HA	1:A:12:MET:CE	2.46	0.46
1:A:140:PHE:CE1	1:A:228:GLY:HA3	2.51	0.46
1:B:174:GLN:HE22	1:B:175:LYS:HZ1	1.56	0.46
1:D:35:LYS:HB3	1:D:36:PRO:CD	2.45	0.46
1:D:45:HIS:O	1:D:49:GLU:HG3	2.15	0.46
1:C:7:ALA:HB3	1:C:30:ALA:CB	2.46	0.46
1:C:239:ASP:CB	1:C:269:LYS:HB2	2.43	0.46
1:B:115:THR:HG23	1:B:225:PRO:HB3	1.97	0.45
1:B:269:LYS:HB3	1:B:269:LYS:HZ3	1.81	0.45
1:D:71:VAL:HG11	1:D:103:ILE:HD12	1.97	0.45
1:A:9:LYS:CD	1:A:219:TYR:CE1	2.99	0.45
1:B:140:PHE:CE1	1:B:228:GLY:HA3	2.51	0.45
1:C:269:LYS:NZ	1:C:269:LYS:CB	2.73	0.45
1:A:171:MET:O	1:A:176:MET:HB2	2.15	0.45
1:D:80:LYS:HD2	1:D:80:LYS:C	2.41	0.45
1:C:243:ILE:HG13	1:C:276:ILE:HD11	1.98	0.45
1:C:299:VAL:O	1:C:302:LEU:HB2	2.16	0.45
1:D:211:ALA:O	1:D:215:GLU:HG2	2.16	0.45
1:C:12:MET:O	1:C:16:VAL:HG23	2.16	0.45
1:A:26:LEU:CD2	1:A:54:ILE:HD12	2.46	0.45
1:A:141:SER:HB2	1:A:172:HIS:HB2	1.99	0.45
1:D:79:ARG:HD2	1:D:79:ARG:HA	1.83	0.45
1:C:79:ARG:CB	1:C:220:SER:HB3	2.47	0.45
1:A:191:GLU:HG3	2:A:319:HOH:O	2.16	0.45
1:D:140:PHE:CE1	1:D:228:GLY:CA	2.97	0.45
1:B:240:SER:OG	1:B:242:ARG:HG3	2.17	0.45
1:B:304:PRO:O	1:B:305:GLN:C	2.59	0.45
1:D:10:VAL:HG12	2:D:317:HOH:O	2.16	0.45
1:D:1:MET:SD	1:D:27:LEU:HB2	2.57	0.45
1:D:198:GLU:O	1:D:202:VAL:HG22	2.16	0.45
1:A:94:ASN:O	1:A:97:ALA:HB3	2.17	0.45
1:B:3:THR:HG22	1:B:5:LEU:HD13	1.99	0.45
1:D:80:LYS:O	1:D:83:MET:CB	2.52	0.45
1:C:293:GLN:HE22	1:C:296:LYS:HD2	1.82	0.45
1:A:142:GLY:CA	1:A:245:PRO:HG2	2.46	0.45
1:A:202:VAL:CG2	1:A:203:VAL:N	2.80	0.45
1:C:115:THR:OG1	1:C:229:LEU:HD11	2.16	0.44
1:C:171:MET:CE	1:C:175:LYS:N	2.80	0.44
1:B:213:ILE:CD1	1:B:221:SER:HB2	2.46	0.44
1:A:259:ILE:HG12	1:A:260:VAL:N	2.32	0.44
1:D:86:GLU:OE2	1:D:301:THR:HG21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:MET:O	1:D:16:VAL:HG23	2.17	0.44
1:C:299:VAL:O	1:C:307:ARG:HD3	2.18	0.44
1:A:169:LEU:CD2	1:A:264:PRO:HD3	2.48	0.44
1:A:278:LEU:O	1:A:280:LEU:HD13	2.18	0.44
1:B:188:VAL:HA	1:B:189:PRO:HD3	1.76	0.44
1:B:241:LYS:HD2	1:B:273:GLU:OE1	2.18	0.44
1:D:79:ARG:HG2	1:D:88:LEU:HD22	1.99	0.44
1:D:203:VAL:O	1:D:207:VAL:HG23	2.18	0.44
1:C:19:MET:O	1:C:52:VAL:HG11	2.18	0.44
1:C:269:LYS:HB3	1:C:269:LYS:HZ2	1.80	0.44
1:B:242:ARG:HE	1:C:162:LYS:HD3	1.83	0.44
1:D:39:GLU:O	1:D:40:ALA:C	2.60	0.44
1:C:26:LEU:CD2	1:C:56:ILE:HG12	2.48	0.44
1:C:171:MET:HE2	1:C:175:LYS:H	1.83	0.44
1:C:178:PRO:O	1:C:180:PRO:HD3	2.17	0.44
1:C:304:PRO:HA	1:C:307:ARG:HG3	1.98	0.44
1:B:66:ARG:NH1	1:B:66:ARG:HG2	2.32	0.43
1:B:253:GLU:H	1:B:253:GLU:CD	2.26	0.43
1:D:71:VAL:HB	1:D:112:VAL:HG12	2.00	0.43
1:C:178:PRO:HG3	1:C:203:VAL:HG22	2.00	0.43
1:C:297:LYS:CB	1:C:297:LYS:HZ2	2.29	0.43
1:A:9:LYS:HG2	1:A:222:ASN:ND2	2.33	0.43
1:A:65:MET:SD	1:A:103:ILE:HD13	2.58	0.43
1:B:115:THR:CG2	1:B:225:PRO:HB3	2.47	0.43
1:A:36:PRO:HG2	1:A:37:GLN:OE1	2.18	0.43
1:D:188:VAL:HG22	1:A:278:LEU:HD23	2.01	0.43
1:A:241:LYS:NZ	1:A:273:GLU:OE2	2.35	0.43
1:C:26:LEU:HD23	1:C:26:LEU:H	1.82	0.43
1:C:37:GLN:HE22	1:C:60:ASN:ND2	2.16	0.43
1:C:103:ILE:HD11	1:C:130:THR:CG2	2.44	0.43
1:A:1:MET:CA	1:A:24:ASP:OD2	2.64	0.43
1:A:20:MET:HE3	1:A:20:MET:HB3	1.88	0.43
1:A:199:ILE:O	1:A:202:VAL:HG22	2.19	0.43
1:C:151:TYR:O	1:C:155:GLN:HG2	2.19	0.43
1:A:250:LEU:O	1:A:257:ASN:HA	2.19	0.43
1:B:171:MET:CE	1:B:172:HIS:C	2.92	0.43
1:B:241:LYS:HE2	1:B:273:GLU:OE2	2.19	0.43
1:C:45:HIS:O	1:C:49:GLU:HG3	2.19	0.43
1:A:176:MET:HE1	1:A:206:THR:HG22	2.00	0.43
1:A:239:ASP:HB2	1:A:269:LYS:HB2	2.00	0.43
1:B:162:LYS:HD2	1:A:53:ASP:OD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ASP:OD2	1:D:109:ASP:N	2.52	0.42
1:D:134:ARG:NH2	1:D:275:ILE:HD13	2.34	0.42
1:D:224:GLY:O	1:D:225:PRO:C	2.61	0.42
1:C:242:ARG:C	1:C:243:ILE:HD12	2.44	0.42
1:A:176:MET:CE	1:A:206:THR:HG22	2.49	0.42
1:A:286:ARG:CZ	1:A:286:ARG:CB	2.97	0.42
1:A:295:VAL:O	1:A:299:VAL:HG23	2.20	0.42
1:C:169:LEU:HD11	1:C:278:LEU:CD1	2.46	0.42
1:A:10:VAL:HG13	1:A:74:THR:HB	2.01	0.42
1:A:178:PRO:O	1:A:180:PRO:HD3	2.19	0.42
1:D:84:THR:O	1:D:87:GLN:N	2.53	0.42
1:B:77:ILE:HG23	1:B:88:LEU:HD12	2.00	0.42
1:C:77:ILE:HD13	1:C:77:ILE:C	2.45	0.42
1:D:23:TYR:O	1:D:24:ASP:HB2	2.19	0.42
1:D:308:GLU:OE1	1:D:308:GLU:HA	2.19	0.42
1:C:240:SER:OG	1:C:242:ARG:HG3	2.19	0.42
1:D:73:VAL:HB	1:D:114:ILE:HD13	2.02	0.42
1:B:20:MET:HE2	1:A:20:MET:HB2	2.01	0.42
1:C:243:ILE:HD11	1:C:266:VAL:HG22	2.01	0.42
1:D:49:GLU:O	1:C:231:LEU:HD11	2.20	0.42
1:D:17:MET:HE2	1:C:16:VAL:HG13	2.02	0.42
1:A:169:LEU:HD11	1:A:278:LEU:HD12	2.02	0.42
1:D:27:LEU:HD23	1:D:57:SER:HB2	2.01	0.41
1:D:43:LEU:HD23	1:D:56:ILE:HG21	2.01	0.41
1:B:128:LYS:HD2	1:B:308:GLU:HG2	2.00	0.41
1:C:212:LYS:O	1:C:215:GLU:HB3	2.20	0.41
1:C:242:ARG:O	1:C:266:VAL:HA	2.20	0.41
1:B:96:MET:HG2	1:B:122:MET:CE	2.42	0.41
1:B:249:TYR:OH	1:B:258:ASP:HA	2.19	0.41
1:D:33:PRO:HA	1:D:60:ASN:HD21	1.86	0.41
1:C:76:GLY:HA3	1:C:116:THR:HG23	2.01	0.41
1:A:96:MET:HG3	1:A:122:MET:SD	2.60	0.41
1:C:32:THR:HA	1:C:33:PRO:HD3	1.94	0.41
1:D:126:MET:O	1:D:130:THR:HG23	2.20	0.41
1:D:138:ILE:CG2	1:D:246:TYR:CD1	3.03	0.41
1:D:253:GLU:H	1:D:253:GLU:CD	2.28	0.41
1:C:236:ILE:CD1	1:C:236:ILE:N	2.82	0.41
1:A:108:LYS:O	1:A:136:ARG:NH1	2.49	0.41
1:B:66:ARG:CG	1:B:66:ARG:HH11	2.33	0.41
1:C:134:ARG:HH21	1:C:251:GLN:N	2.19	0.41
1:C:252:GLY:N	1:C:257:ASN:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LYS:HB3	1:A:36:PRO:CD	2.50	0.41
1:A:297:LYS:HB3	1:A:297:LYS:HE2	1.71	0.41
1:B:9:LYS:NZ	1:B:9:LYS:HB2	2.35	0.41
1:D:142:GLY:C	1:D:245:PRO:HG2	2.46	0.41
1:C:93:ALA:HB1	1:C:306:LEU:HD13	2.03	0.41
1:A:171:MET:HE2	1:A:175:LYS:CA	2.51	0.41
1:B:88:LEU:HG	1:B:92:ASN:HD22	1.85	0.41
1:B:126:MET:O	1:B:130:THR:HG23	2.21	0.41
1:B:217:ARG:NH1	1:A:42:ASP:OD2	2.54	0.41
1:D:9:LYS:HB2	1:D:9:LYS:NZ	2.35	0.41
1:D:12:MET:HE1	1:D:28:LEU:HG	2.03	0.41
1:C:252:GLY:H	1:C:257:ASN:HB3	1.86	0.41
1:C:140:PHE:HZ	1:C:228:GLY:HA3	1.83	0.40
1:A:108:LYS:HA	1:A:132:PHE:CZ	2.55	0.40
1:D:27:LEU:HD22	1:D:27:LEU:C	2.46	0.40
1:C:72:LEU:HD23	1:C:113:VAL:CG2	2.51	0.40
1:A:24:ASP:CG	1:A:25:ASP:N	2.79	0.40
1:B:7:ALA:HB3	1:B:30:ALA:HB2	2.02	0.40
1:B:157:LEU:HD21	1:B:194:MET:HE2	2.02	0.40
1:C:52:VAL:HG12	1:C:54:ILE:HG23	2.03	0.40
1:C:171:MET:HE1	1:C:175:LYS:H	1.86	0.40
1:C:192:HIS:O	1:C:192:HIS:CG	2.75	0.40
1:B:177:PHE:HA	1:B:178:PRO:HD2	1.91	0.40
1:B:249:TYR:CZ	1:B:258:ASP:HA	2.56	0.40
1:B:278:LEU:HB2	1:B:280:LEU:CD1	2.51	0.40
1:B:301:THR:HG22	1:B:301:THR:O	2.22	0.40
1:A:62:TYR:O	1:A:65:MET:HG2	2.21	0.40

All (3) 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:B:108:LYS:NZ	1:B:200:GLU:OE1[4_557]	1.86	0.34
1:B:133:PRO:CA	1:B:215:GLU:OE1[4_557]	1.99	0.21
1:D:87:GLN:NE2	1:A:181:ARG:NH1[3_756]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/308 (96%)	276 (94%)	15 (5%)	3 (1%)	12	35
1	B	297/308 (96%)	280 (94%)	16 (5%)	1 (0%)	36	62
1	C	295/308 (96%)	279 (95%)	13 (4%)	3 (1%)	12	35
1	D	306/308 (99%)	287 (94%)	17 (6%)	2 (1%)	18	44
All	All	1192/1232 (97%)	1122 (94%)	61 (5%)	9 (1%)	16	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	53	ASP
1	C	220	SER
1	B	181	ARG
1	C	53	ASP
1	C	75	ALA
1	A	53	ASP
1	A	76	GLY
1	A	141	SER
1	D	76	GLY

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	241/250 (96%)	226 (94%)	15 (6%)	16	43
1	B	244/250 (98%)	232 (95%)	12 (5%)	22	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	242/250 (97%)	229 (95%)	13 (5%)	20	49
1	D	250/250 (100%)	231 (92%)	19 (8%)	12	33
All	All	977/1000 (98%)	918 (94%)	59 (6%)	17	44

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	LEU
1	B	9	LYS
1	B	10	VAL
1	B	27	LEU
1	B	31	ARG
1	B	39	GLU
1	B	66	ARG
1	B	112	VAL
1	B	190	LEU
1	B	269	LYS
1	B	277	GLU
1	B	296	LYS
1	D	5	LEU
1	D	9	LYS
1	D	26	LEU
1	D	27	LEU
1	D	31	ARG
1	D	35	LYS
1	D	63	GLU
1	D	99	LEU
1	D	104	LYS
1	D	149	MET
1	D	171	MET
1	D	174	GLN
1	D	178	PRO
1	D	202	VAL
1	D	242	ARG
1	D	269	LYS
1	D	280	LEU
1	D	282	GLU
1	D	287	LYS
1	C	5	LEU
1	C	26	LEU
1	C	27	LEU

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Mol	Chain	Res	Type
1	C	31	ARG
1	C	77	ILE
1	C	79	ARG
1	C	103	ILE
1	C	171	MET
1	C	190	LEU
1	C	236	ILE
1	C	237	LYS
1	C	269	LYS
1	C	285	LYS
1	A	9	LYS
1	A	27	LEU
1	A	31	ARG
1	A	56	ILE
1	A	77	ILE
1	A	109	ASP
1	A	112	VAL
1	A	143	ILE
1	A	171	MET
1	A	190	LEU
1	A	213	ILE
1	A	267	ILE
1	A	269	LYS
1	A	298	LEU
1	A	302	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	ASN
1	B	165	ASN
1	B	172	HIS
1	B	174	GLN
1	B	251	GLN
1	D	45	HIS
1	D	60	ASN
1	D	94	ASN
1	D	174	GLN
1	D	208	ASN
1	D	251	GLN
1	D	293	GLN
1	C	45	HIS

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Mol	Chain	Res	Type
1	C	60	ASN
1	C	165	ASN
1	C	251	GLN
1	A	165	ASN
1	A	251	GLN

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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	C	2
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	219:TYR	C	220:SER	N	1.20
1	A	123:THR	C	124:TYR	N	1.20
1	B	217:ARG	C	218:GLY	N	1.19
1	B	52:VAL	C	53:ASP	N	1.18
1	B	240:SER	C	241:LYS	N	1.18
1	D	135:GLU	C	136:ARG	N	1.17
1	C	253:GLU	C	254:TYR	N	1.16

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	298/308 (96%)	-0.75	2 (0%) 84 80	21, 35, 58, 74	0
1	B	301/308 (97%)	-0.64	1 (0%) 90 87	18, 34, 53, 79	0
1	C	299/308 (97%)	-0.74	2 (0%) 84 80	23, 39, 62, 82	0
1	D	308/308 (100%)	-0.81	5 (1%) 70 63	20, 34, 59, 71	0
All	All	1206/1232 (97%)	-0.74	10 (0%) 82 77	18, 35, 59, 82	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	GLN	5.6
1	D	85	ARG	3.8
1	D	87	GLN	3.3
1	A	282	GLU	3.2
1	D	86	GLU	2.7
1	C	79	ARG	2.7
1	D	77	ILE	2.1
1	A	257	ASN	2.1
1	D	83	MET	2.0
1	C	115	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.