



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:01 AM UTC

PDB ID : 2ETN / pdb_00002etn
Title : Crystal structure of Thermus aquaticus Gfh1
Authors : Lamour, V.; Hogan, B.P.; Erie, D.A.; Darst, S.A.
Deposited on : 2005-10-27
Resolution : 3.30 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)	:	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

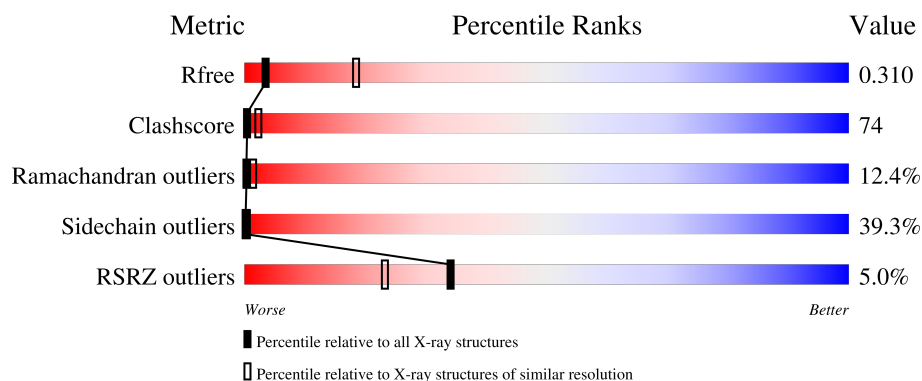
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

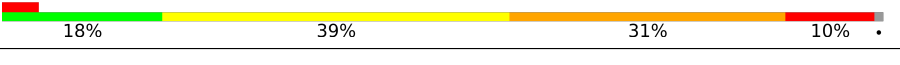
The reported resolution of this entry is 3.30 Å.

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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	157	
1	B	157	
1	C	157	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3550 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.

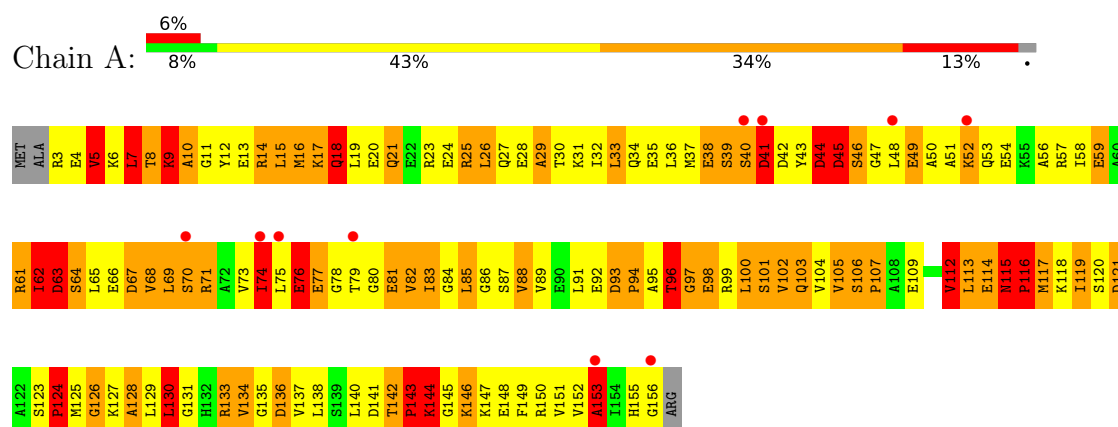
- Molecule 1 is a protein called anti-cleavage anti-GreA transcription factor Gfh1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1180	728	206	242	4			
1	B	155	Total	C	N	O	S	0	0	0
			1185	731	207	243	4			
1	C	155	Total	C	N	O	S	0	0	0
			1185	731	207	243	4			

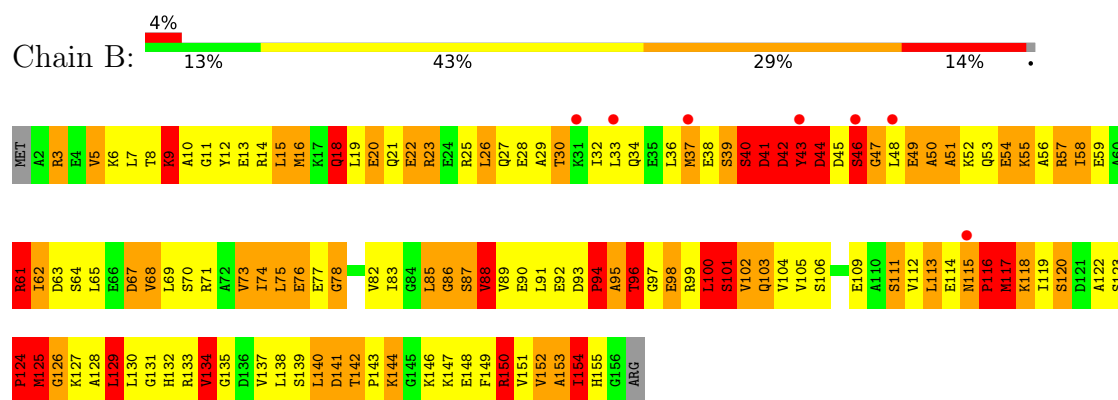
3 Residue-property plots

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.

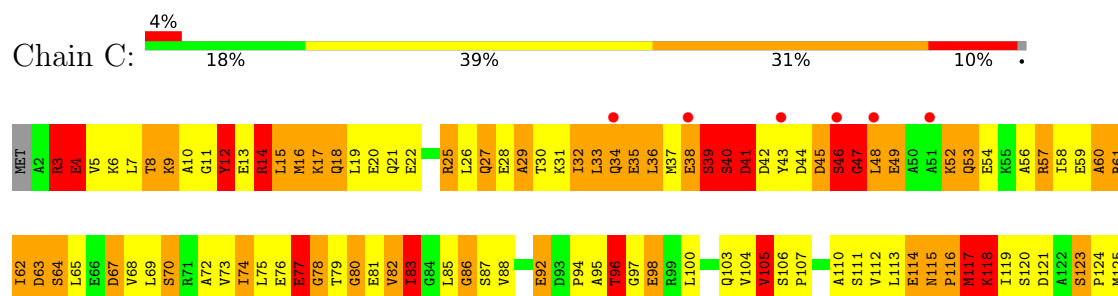
- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1



- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1



- Molecule 1: anti-cleavage anti-GreA transcription factor Gfh1



G126	K127	A128	L129	L130	R133	V134	G135	D136	V137	L138	T142	P143	K144	G145	K146	K147	E148	F149	R150	V151	V152	A153	I154	H155	G156	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.20Å 76.40Å 53.10Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.00-3.30) 92.3 (30.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.250 , 0.325 0.262 , 0.310	Depositor DCC
R_{free} test set	1113 reflections (8.89%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3550	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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	1.74	14/1189 (1.2%)	2.04	43/1597 (2.7%)
1	B	1.93	20/1194 (1.7%)	2.24	49/1604 (3.1%)
1	C	2.11	24/1194 (2.0%)	2.16	46/1604 (2.9%)
All	All	1.93	58/3577 (1.6%)	2.15	138/4805 (2.9%)

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	B	0	3
1	C	0	5
All	All	0	8

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	GLY	N-CA	28.29	1.86	1.45
1	B	44	ASP	C-O	18.52	1.45	1.24
1	B	101	SER	N-CA	17.67	1.67	1.46
1	C	78	GLY	N-CA	16.47	1.69	1.45
1	B	16	MET	SD-CE	14.99	2.17	1.79
1	C	16	MET	SD-CE	12.74	2.11	1.79
1	A	46	SER	N-CA	-12.32	1.31	1.46
1	C	154	ILE	N-CA	12.11	1.61	1.46
1	B	41	ASP	C-O	-11.83	1.09	1.24
1	A	16	MET	SD-CE	11.65	2.08	1.79
1	C	118	LYS	N-CA	-11.06	1.31	1.46
1	C	45	ASP	N-CA	9.41	1.59	1.46
1	B	73	VAL	CA-CB	-9.13	1.42	1.54
1	C	112	VAL	CA-CB	-8.32	1.45	1.54
1	A	138	LEU	CA-C	-8.27	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	44	ASP	N-CA	8.22	1.56	1.46
1	A	115	ASN	CA-C	-8.11	1.42	1.52
1	C	40	SER	CB-OG	7.96	1.58	1.42
1	C	105	VAL	N-CA	-7.63	1.37	1.46
1	A	74	ILE	CG1-CD1	7.40	1.80	1.51
1	B	88	VAL	CA-CB	-7.34	1.45	1.54
1	C	153	ALA	CA-C	7.19	1.62	1.52
1	C	29	ALA	CA-CB	-7.01	1.42	1.53
1	B	85	LEU	CA-CB	-7.01	1.44	1.53
1	C	115	ASN	CA-C	-6.95	1.44	1.52
1	A	117	MET	CA-C	-6.84	1.44	1.52
1	B	118	LYS	N-CA	-6.70	1.38	1.46
1	C	29	ALA	CA-C	-6.34	1.44	1.53
1	B	133	ARG	CA-C	-6.19	1.45	1.52
1	A	29	ALA	CA-CB	-6.12	1.44	1.53
1	A	97	GLY	N-CA	6.10	1.54	1.45
1	B	42	ASP	C-N	6.04	1.42	1.33
1	A	62	ILE	CA-C	-5.93	1.45	1.52
1	C	127	LYS	CA-C	-5.90	1.44	1.52
1	C	92	GLU	CA-C	5.87	1.60	1.52
1	A	155	HIS	CB-CG	5.82	1.58	1.50
1	C	4	GLU	N-CA	5.78	1.53	1.46
1	B	16	MET	CA-C	-5.72	1.45	1.52
1	C	5	VAL	N-CA	-5.68	1.39	1.46
1	B	129	LEU	CG-CD2	-5.65	1.33	1.52
1	C	16	MET	CA-C	-5.64	1.45	1.52
1	B	15	LEU	CA-C	-5.63	1.45	1.52
1	C	98	GLU	CA-CB	5.56	1.59	1.52
1	A	124	PRO	CA-CB	-5.50	1.46	1.53
1	C	72	ALA	CA-C	-5.50	1.45	1.52
1	C	74	ILE	CA-CB	-5.44	1.48	1.54
1	A	18	GLN	CA-C	-5.37	1.45	1.52
1	B	23	ARG	CA-C	-5.31	1.46	1.52
1	B	150	ARG	N-CA	-5.31	1.39	1.46
1	B	46	SER	CB-OG	5.30	1.52	1.42
1	B	120	SER	CA-C	-5.26	1.46	1.52
1	A	150	ARG	N-CA	-5.19	1.39	1.46
1	A	112	VAL	CA-CB	-5.16	1.48	1.54
1	C	72	ALA	CA-CB	-5.09	1.44	1.53
1	C	14	ARG	NE-CZ	5.08	1.38	1.33
1	B	61	ARG	CA-C	-5.06	1.46	1.52
1	B	18	GLN	N-CA	-5.05	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	ALA	CA-CB	-5.01	1.45	1.53

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	SER	N-CA-C	-21.53	78.61	111.56
1	B	117	MET	CA-C-N	20.95	153.20	122.41
1	B	117	MET	C-N-CA	20.95	153.20	122.41
1	B	154	ILE	N-CA-CB	-16.23	88.17	110.56
1	B	118	LYS	N-CA-CB	14.51	131.97	110.35
1	B	116	PRO	CA-N-CD	-12.97	93.85	112.00
1	B	100	LEU	CA-C-N	-12.35	100.20	121.94
1	B	100	LEU	C-N-CA	-12.35	100.20	121.94
1	C	83	ILE	N-CA-CB	12.19	131.34	111.23
1	C	4	GLU	CA-C-N	11.70	139.48	123.10
1	C	4	GLU	C-N-CA	11.70	139.48	123.10
1	C	117	MET	CA-C-N	11.36	143.23	121.54
1	C	117	MET	C-N-CA	11.36	143.23	121.54
1	A	43	TYR	CA-C-N	11.09	136.54	120.90
1	A	43	TYR	C-N-CA	11.09	136.54	120.90
1	B	73	VAL	CB-CA-C	-11.05	94.20	110.33
1	B	44	ASP	O-C-N	-11.01	109.34	122.11
1	C	5	VAL	N-CA-C	10.39	121.61	106.85
1	B	61	ARG	N-CA-C	-10.32	99.57	111.03
1	C	47	GLY	N-CA-C	9.77	136.34	113.18
1	A	71	ARG	N-CA-C	-9.74	101.15	113.23
1	B	154	ILE	N-CA-C	9.73	123.67	108.87
1	C	78	GLY	N-CA-C	9.69	136.14	113.18
1	C	45	ASP	N-CA-C	-9.63	88.64	107.62
1	C	118	LYS	N-CA-CB	9.63	126.77	110.49
1	A	44	ASP	N-CA-C	9.61	123.79	110.24
1	A	41	ASP	N-CA-C	-9.08	91.47	110.80
1	C	44	ASP	CA-C-N	-8.68	110.30	123.14
1	C	44	ASP	C-N-CA	-8.68	110.30	123.14
1	B	86	GLY	CA-C-N	-8.62	107.99	122.64
1	B	86	GLY	C-N-CA	-8.62	107.99	122.64
1	C	92	GLU	N-CA-C	8.57	121.54	108.52
1	C	154	ILE	N-CA-CB	8.49	125.24	111.23
1	C	3	ARG	N-CA-C	-8.42	92.87	110.80
1	A	80	GLY	N-CA-C	8.40	123.02	110.75
1	B	44	ASP	CA-C-O	-8.36	112.02	120.80
1	C	104	VAL	CA-C-N	-8.36	108.78	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	VAL	C-N-CA	-8.36	108.78	122.57
1	B	76	GLU	N-CA-C	-8.27	99.49	110.24
1	C	41	ASP	CA-C-N	8.25	134.51	122.63
1	C	41	ASP	C-N-CA	8.25	134.51	122.63
1	A	46	SER	N-CA-CB	8.22	122.96	110.14
1	B	37	MET	N-CA-C	-8.13	101.48	111.40
1	B	42	ASP	CA-C-N	8.12	137.04	121.54
1	B	42	ASP	C-N-CA	8.12	137.04	121.54
1	A	151	VAL	N-CA-C	-8.06	95.90	108.23
1	C	40	SER	N-CA-C	7.96	127.76	110.80
1	B	42	ASP	CA-C-O	7.87	131.76	120.51
1	B	41	ASP	CA-C-N	7.71	136.26	121.54
1	B	41	ASP	C-N-CA	7.71	136.26	121.54
1	C	152	VAL	CB-CA-C	-7.39	99.17	111.29
1	A	128	ALA	N-CA-C	7.29	118.87	111.07
1	C	83	ILE	N-CA-C	-7.08	94.60	109.34
1	A	150	ARG	N-CA-C	-7.01	99.91	110.28
1	B	41	ASP	CA-C-O	6.88	130.35	120.51
1	B	88	VAL	N-CA-C	6.87	117.76	107.80
1	B	39	SER	N-CA-C	-6.87	102.15	112.04
1	C	45	ASP	N-CA-CB	6.77	121.91	110.46
1	C	137	VAL	CB-CA-C	-6.73	101.21	110.77
1	C	41	ASP	N-CA-C	6.68	125.03	110.80
1	C	40	SER	CA-C-N	6.64	134.22	121.54
1	C	40	SER	C-N-CA	6.64	134.22	121.54
1	C	77	GLU	CA-C-N	-6.61	108.45	121.41
1	C	77	GLU	C-N-CA	-6.61	108.45	121.41
1	A	5	VAL	CA-C-N	-6.53	113.47	122.93
1	A	5	VAL	C-N-CA	-6.53	113.47	122.93
1	A	41	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	45	ASP	CA-CB-CG	-6.33	106.27	112.60
1	A	7	LEU	N-CA-C	6.33	118.58	109.14
1	A	81	GLU	N-CA-C	-6.30	101.78	110.35
1	A	41	ASP	CB-CA-C	6.28	122.92	110.42
1	C	154	ILE	N-CA-C	-6.27	96.31	109.34
1	A	20	GLU	N-CA-C	-6.25	104.53	111.71
1	B	78	GLY	N-CA-C	-6.20	104.22	114.76
1	B	73	VAL	CA-C-N	-6.20	113.73	122.34
1	B	73	VAL	C-N-CA	-6.20	113.73	122.34
1	A	75	LEU	N-CA-C	6.12	119.52	108.69
1	A	41	ASP	O-C-N	6.07	130.66	122.59
1	B	43	TYR	N-CA-C	6.02	123.63	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ILE	N-CA-C	5.97	118.36	109.17
1	C	27	GLN	N-CA-C	-5.95	104.70	111.07
1	A	68	VAL	CB-CA-C	5.91	119.20	111.81
1	C	12	TYR	CA-CB-CG	5.89	124.50	113.90
1	C	16	MET	N-CA-C	-5.87	105.78	113.12
1	C	136	ASP	N-CA-C	-5.86	100.73	110.17
1	C	81	GLU	N-CA-C	-5.80	105.46	112.54
1	B	94	PRO	CA-N-CD	-5.77	103.93	112.00
1	C	153	ALA	N-CA-C	5.74	123.02	110.80
1	B	16	MET	N-CA-C	-5.73	105.56	113.18
1	A	63	ASP	N-CA-C	-5.70	104.93	112.34
1	C	88	VAL	CB-CA-C	-5.65	105.04	111.59
1	B	102	VAL	CB-CA-C	-5.63	100.79	110.30
1	B	125	MET	N-CA-CB	5.60	118.13	110.01
1	B	75	LEU	N-CA-C	5.60	118.08	109.07
1	A	143	PRO	CB-CA-C	-5.59	102.34	111.56
1	C	61	ARG	CG-CD-NE	-5.58	99.73	112.00
1	A	150	ARG	CA-C-N	5.58	129.34	122.37
1	A	150	ARG	C-N-CA	5.58	129.34	122.37
1	A	152	VAL	CB-CA-C	-5.57	102.16	111.29
1	B	124	PRO	CA-C-N	-5.53	113.25	120.44
1	B	124	PRO	C-N-CA	-5.53	113.25	120.44
1	A	140	LEU	CA-C-N	-5.48	114.91	122.30
1	A	140	LEU	C-N-CA	-5.48	114.91	122.30
1	B	102	VAL	CA-C-N	-5.48	113.86	122.73
1	B	102	VAL	C-N-CA	-5.48	113.86	122.73
1	A	52	LYS	N-CA-C	-5.47	105.32	111.28
1	A	39	SER	CA-C-N	5.46	130.12	121.99
1	A	39	SER	C-N-CA	5.46	130.12	121.99
1	B	152	VAL	CB-CA-C	-5.44	102.36	111.29
1	B	82	VAL	N-CA-C	5.39	116.35	108.53
1	B	95	ALA	N-CA-C	-5.39	103.86	110.65
1	B	5	VAL	N-CA-C	-5.38	100.66	108.36
1	C	112	VAL	N-CA-C	-5.38	107.12	113.42
1	C	110	ALA	N-CA-C	5.37	118.98	109.96
1	A	103	GLN	N-CA-C	5.35	117.95	109.50
1	A	130	LEU	N-CA-C	5.34	116.95	108.67
1	B	23	ARG	CB-CA-C	-5.32	101.81	110.85
1	A	76	GLU	N-CA-C	-5.32	102.03	109.96
1	B	85	LEU	N-CA-C	5.31	119.27	111.04
1	C	14	ARG	N-CA-C	-5.30	105.91	112.38
1	C	41	ASP	O-C-N	5.26	129.59	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ASN	CA-C-N	-5.24	113.29	119.84
1	A	115	ASN	C-N-CA	-5.24	113.29	119.84
1	C	68	VAL	CB-CA-C	-5.23	105.12	111.87
1	B	9	LYS	CA-C-N	5.23	127.60	120.54
1	B	9	LYS	C-N-CA	5.23	127.60	120.54
1	A	77	GLU	N-CA-C	5.21	117.05	110.33
1	A	141	ASP	N-CA-C	5.20	117.22	108.96
1	B	97	GLY	CA-C-N	5.16	128.10	120.82
1	B	97	GLY	C-N-CA	5.16	128.10	120.82
1	A	153	ALA	CA-C-N	5.11	131.17	121.97
1	A	153	ALA	C-N-CA	5.11	131.17	121.97
1	B	140	LEU	CB-CA-C	-5.10	102.91	110.62
1	A	116	PRO	CB-CA-C	5.08	119.95	111.56
1	A	59	GLU	N-CA-C	-5.05	105.04	111.11
1	C	29	ALA	N-CA-C	-5.05	104.76	112.04
1	C	42	ASP	CA-CB-CG	-5.05	107.55	112.60
1	C	60	ALA	N-CA-C	-5.00	105.50	112.45

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	SER	Peptide
1	B	41	ASP	Mainchain
1	B	44	ASP	Mainchain
1	C	153	ALA	Peptide
1	C	39	SER	Peptide
1	C	40	SER	Peptide
1	C	46	SER	Peptide
1	C	77	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1180	0	1201	180	0
1	B	1185	0	1205	203	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1185	0	1206	162	0
All	All	3550	0	3612	529	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 74.

All (529) 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:74:ILE:CD1	1:A:74:ILE:CG1	1.80	1.59
1:C:78:GLY:N	1:C:78:GLY:CA	1.69	1.56
1:A:16:MET:SD	1:A:16:MET:CE	2.08	1.42
1:C:16:MET:SD	1:C:16:MET:CE	2.11	1.36
1:C:47:GLY:CA	1:C:47:GLY:N	1.86	1.36
1:B:16:MET:SD	1:B:16:MET:CE	2.17	1.33
1:B:129:LEU:H	1:B:129:LEU:CD1	1.24	1.28
1:B:129:LEU:HD12	1:B:129:LEU:N	1.16	1.27
1:B:96:THR:HG21	1:B:98:GLU:HG3	1.19	1.18
1:A:85:LEU:N	1:A:85:LEU:HD12	1.42	1.17
1:A:28:GLU:HB2	1:C:25:ARG:HG2	1.20	1.16
1:B:129:LEU:CD1	1:B:129:LEU:N	1.84	1.12
1:A:85:LEU:H	1:A:85:LEU:CD1	1.62	1.11
1:C:8:THR:HG22	1:C:135:GLY:O	1.47	1.11
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.09	1.10
1:B:83:ILE:HG12	1:B:154:ILE:CD1	1.82	1.10
1:A:113:LEU:HD23	1:A:113:LEU:N	1.52	1.10
1:C:96:THR:HG23	1:C:96:THR:O	1.49	1.10
1:C:80:GLY:HA2	1:C:133:ARG:HG2	1.22	1.10
1:B:129:LEU:H	1:B:129:LEU:HD13	1.09	1.07
1:B:54:GLU:OE1	1:B:54:GLU:CA	2.00	1.07
1:A:115:ASN:HB3	1:A:116:PRO:HD2	1.33	1.06
1:B:112:VAL:HG12	1:B:117:MET:HE2	1.38	1.05
1:B:112:VAL:CB	1:B:117:MET:HE2	1.84	1.05
1:A:85:LEU:HD12	1:A:85:LEU:H	0.96	1.05
1:A:95:ALA:O	1:A:96:THR:HB	1.51	1.05
1:A:115:ASN:O	1:A:116:PRO:C	1.99	1.03
1:A:85:LEU:N	1:A:85:LEU:CD1	2.17	1.03
1:B:96:THR:CG2	1:B:98:GLU:HG3	1.89	1.03
1:C:80:GLY:CA	1:C:133:ARG:HG2	1.89	1.02
1:B:51:ALA:O	1:B:54:GLU:HB2	1.59	1.02
1:B:112:VAL:CG1	1:B:117:MET:HE2	1.89	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:THR:O	1:C:96:THR:CG2	2.04	1.01
1:A:115:ASN:HB3	1:A:116:PRO:CD	1.91	1.01
1:B:112:VAL:HB	1:B:117:MET:CE	1.92	1.00
1:C:115:ASN:HB3	1:C:116:PRO:CD	1.94	0.98
1:A:145:GLY:C	1:A:146:LYS:HD3	1.88	0.98
1:A:88:VAL:HG13	1:A:103:GLN:HB2	1.42	0.97
1:B:114:GLU:OE1	1:B:118:LYS:HE3	1.64	0.97
1:C:134:VAL:CG1	1:C:153:ALA:H	1.76	0.97
1:C:107:PRO:HD3	1:C:121:ASP:OD1	1.62	0.97
1:B:3:ARG:HG3	1:B:71:ARG:HH12	1.31	0.96
1:A:82:VAL:HG12	1:A:83:ILE:H	1.30	0.94
1:B:44:ASP:O	1:B:45:ASP:HB2	1.67	0.94
1:B:16:MET:HG2	1:B:69:LEU:HD21	1.50	0.93
1:B:112:VAL:CB	1:B:117:MET:CE	2.44	0.93
1:C:3:ARG:O	1:C:4:GLU:CB	2.15	0.93
1:B:54:GLU:OE1	1:B:54:GLU:HA	1.12	0.93
1:B:40:SER:C	1:B:42:ASP:H	1.76	0.92
1:C:105:VAL:HG21	1:C:118:LYS:HB3	1.48	0.92
1:C:38:GLU:O	1:C:40:SER:HB3	1.70	0.91
1:C:125:MET:O	1:C:129:LEU:HD12	1.70	0.90
1:B:125:MET:O	1:B:129:LEU:HD13	1.71	0.90
1:C:3:ARG:O	1:C:4:GLU:HB2	1.69	0.90
1:C:134:VAL:HG13	1:C:153:ALA:H	1.36	0.89
1:C:105:VAL:CG2	1:C:118:LYS:HB3	2.01	0.89
1:A:61:ARG:HH11	1:A:61:ARG:CG	1.84	0.89
1:B:42:ASP:N	1:B:42:ASP:OD2	2.04	0.89
1:B:12:TYR:O	1:B:16:MET:HG3	1.73	0.89
1:A:100:LEU:HD12	1:A:101:SER:N	1.88	0.88
1:A:121:ASP:C	1:A:121:ASP:OD1	2.16	0.88
1:C:77:GLU:C	1:C:78:GLY:CA	2.46	0.88
1:A:87:SER:HA	1:A:156:GLY:O	1.75	0.86
1:A:113:LEU:N	1:A:113:LEU:CD2	2.31	0.86
1:B:6:LYS:HD3	1:B:75:LEU:HD11	1.57	0.85
1:B:3:ARG:HG3	1:B:71:ARG:NH1	1.92	0.85
1:A:112:VAL:C	1:A:113:LEU:HD23	2.01	0.84
1:B:34:GLN:NE2	1:B:55:LYS:HZ2	1.77	0.83
1:C:115:ASN:HB3	1:C:116:PRO:HD2	1.60	0.83
1:C:64:SER:O	1:C:67:ASP:HB3	1.77	0.83
1:C:15:LEU:HD12	1:C:137:VAL:HG11	1.62	0.82
1:B:83:ILE:HG12	1:B:154:ILE:HD12	1.58	0.82
1:A:24:GLU:HG3	1:C:25:ARG:HD2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:CA	1:B:117:MET:HE2	2.10	0.82
1:B:128:ALA:C	1:B:129:LEU:HD12	2.04	0.82
1:C:53:GLN:HA	1:C:53:GLN:OE1	1.79	0.81
1:C:62:ILE:HG22	1:C:63:ASP:N	1.91	0.81
1:A:5:VAL:HB	1:A:71:ARG:HB3	1.62	0.81
1:B:34:GLN:NE2	1:B:55:LYS:NZ	2.29	0.81
1:A:61:ARG:HG2	1:A:61:ARG:NH1	1.91	0.81
1:B:96:THR:CG2	1:B:98:GLU:CG	2.59	0.80
1:C:7:LEU:O	1:C:75:LEU:HG	1.81	0.80
1:B:143:PRO:HG3	1:C:114:GLU:HG3	1.63	0.80
1:C:38:GLU:O	1:C:40:SER:CB	2.29	0.80
1:B:92:GLU:O	1:B:94:PRO:CD	2.30	0.79
1:C:10:ALA:O	1:C:14:ARG:HB2	1.82	0.79
1:C:8:THR:CG2	1:C:135:GLY:O	2.31	0.79
1:B:16:MET:C	1:B:18:GLN:H	1.89	0.78
1:B:112:VAL:HA	1:B:117:MET:HG2	1.67	0.77
1:B:96:THR:HG21	1:B:98:GLU:CG	2.07	0.77
1:A:88:VAL:HG13	1:A:103:GLN:CB	2.14	0.76
1:A:19:LEU:HD21	1:A:66:GLU:HG2	1.66	0.76
1:C:45:ASP:O	1:C:47:GLY:N	2.18	0.76
1:B:92:GLU:C	1:B:94:PRO:HD3	2.10	0.75
1:B:40:SER:C	1:B:42:ASP:N	2.43	0.75
1:B:50:ALA:O	1:B:51:ALA:C	2.31	0.74
1:B:92:GLU:O	1:B:94:PRO:HD3	1.87	0.74
1:C:83:ILE:HG22	1:C:130:LEU:HD12	1.69	0.74
1:B:74:ILE:CG2	1:B:75:LEU:N	2.50	0.74
1:B:22:GLU:OE2	1:B:61:ARG:HD3	1.88	0.73
1:B:112:VAL:HA	1:B:117:MET:HE2	1.71	0.73
1:A:100:LEU:HD12	1:A:101:SER:H	1.54	0.72
1:C:26:LEU:HD12	1:C:26:LEU:O	1.88	0.72
1:C:33:LEU:O	1:C:36:LEU:N	2.22	0.72
1:B:43:TYR:HA	1:B:48:LEU:HD12	1.72	0.72
1:C:82:VAL:HG12	1:C:83:ILE:N	2.03	0.72
1:A:28:GLU:HB2	1:C:25:ARG:CG	2.10	0.72
1:A:38:GLU:C	1:A:40:SER:H	1.96	0.72
1:B:85:LEU:O	1:B:87:SER:N	2.22	0.72
1:A:16:MET:O	1:A:18:GLN:N	2.22	0.72
1:C:115:ASN:O	1:C:116:PRO:C	2.32	0.72
1:A:24:GLU:HG2	1:C:21:GLN:HG2	1.72	0.71
1:A:115:ASN:CB	1:A:116:PRO:CD	2.64	0.71
1:B:112:VAL:CA	1:B:117:MET:CE	2.67	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:O	1:B:126:GLY:C	2.28	0.71
1:A:49:GLU:HG3	1:A:53:GLN:NE2	2.05	0.71
1:A:119:ILE:CD1	1:A:125:MET:HG2	2.21	0.71
1:C:57:ARG:O	1:C:61:ARG:HB2	1.91	0.71
1:A:4:GLU:OE2	1:A:6:LYS:HE3	1.90	0.71
1:A:49:GLU:O	1:A:50:ALA:C	2.34	0.70
1:C:82:VAL:CG1	1:C:83:ILE:H	2.04	0.70
1:B:83:ILE:HB	1:B:131:GLY:H	1.56	0.70
1:B:112:VAL:HB	1:B:117:MET:HE3	1.71	0.70
1:A:67:ASP:C	1:A:67:ASP:OD1	2.35	0.69
1:B:92:GLU:O	1:B:94:PRO:HD2	1.92	0.69
1:B:16:MET:C	1:B:18:GLN:N	2.46	0.69
1:B:83:ILE:HG12	1:B:154:ILE:HD11	1.71	0.69
1:C:82:VAL:HG12	1:C:83:ILE:H	1.56	0.69
1:A:147:LYS:HB3	1:A:149:PHE:CE1	2.27	0.69
1:A:82:VAL:HG12	1:A:83:ILE:N	2.07	0.69
1:B:51:ALA:O	1:B:54:GLU:N	2.26	0.69
1:C:134:VAL:HG13	1:C:153:ALA:N	2.06	0.69
1:A:49:GLU:HA	1:A:49:GLU:OE1	1.92	0.68
1:C:34:GLN:O	1:C:38:GLU:HB2	1.94	0.68
1:A:124:PRO:O	1:A:128:ALA:N	2.24	0.68
1:B:83:ILE:CG1	1:B:154:ILE:CD1	2.69	0.68
1:B:74:ILE:HG23	1:B:75:LEU:N	2.09	0.67
1:B:114:GLU:HG2	1:C:143:PRO:HG3	1.74	0.67
1:B:141:ASP:HB3	1:B:146:LYS:HG2	1.76	0.67
1:C:95:ALA:O	1:C:96:THR:HB	1.95	0.67
1:B:88:VAL:O	1:B:154:ILE:HA	1.95	0.67
1:C:48:LEU:HD11	1:C:52:LYS:HB2	1.77	0.66
1:A:87:SER:CA	1:A:156:GLY:O	2.43	0.66
1:B:125:MET:HA	1:B:128:ALA:HB3	1.77	0.66
1:B:74:ILE:HG23	1:B:75:LEU:H	1.61	0.66
1:B:88:VAL:HG23	1:B:155:HIS:O	1.96	0.66
1:B:104:VAL:HG11	1:B:130:LEU:HD13	1.78	0.66
1:C:48:LEU:HD12	1:C:48:LEU:O	1.94	0.66
1:C:56:ALA:HA	1:C:59:GLU:HB2	1.76	0.66
1:A:93:ASP:O	1:A:97:GLY:N	2.20	0.66
1:B:95:ALA:O	1:B:96:THR:HB	1.95	0.66
1:A:96:THR:HG21	1:A:98:GLU:OE1	1.96	0.66
1:A:17:LYS:O	1:A:21:GLN:HB2	1.97	0.65
1:C:4:GLU:HA	1:C:4:GLU:OE1	1.95	0.65
1:A:15:LEU:HD13	1:A:137:VAL:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:HIS:CG	1:B:138:LEU:HD11	2.31	0.65
1:C:95:ALA:O	1:C:96:THR:CB	2.43	0.65
1:B:114:GLU:CG	1:C:143:PRO:HG3	2.27	0.65
1:A:115:ASN:O	1:A:116:PRO:O	2.14	0.65
1:A:56:ALA:O	1:A:57:ARG:C	2.36	0.65
1:A:133:ARG:O	1:A:136:ASP:HB2	1.96	0.65
1:B:26:LEU:HG	1:B:26:LEU:O	1.97	0.65
1:B:20:GLU:HA	1:B:20:GLU:OE1	1.96	0.64
1:C:82:VAL:CG1	1:C:83:ILE:N	2.59	0.64
1:C:8:THR:O	1:C:9:LYS:C	2.37	0.64
1:C:37:MET:O	1:C:40:SER:HB3	1.97	0.64
1:B:112:VAL:O	1:B:117:MET:HE3	1.98	0.64
1:A:35:GLU:HA	1:A:38:GLU:OE1	1.97	0.64
1:C:22:GLU:CD	1:C:61:ARG:NH1	2.56	0.63
1:B:112:VAL:HG12	1:B:117:MET:CE	2.21	0.63
1:C:48:LEU:CD1	1:C:52:LYS:HB2	2.29	0.63
1:A:12:TYR:CD1	1:A:69:LEU:HD23	2.34	0.63
1:A:142:THR:HG22	1:A:145:GLY:N	2.13	0.63
1:A:15:LEU:HD11	1:A:94:PRO:HG2	1.80	0.63
1:C:17:LYS:O	1:C:21:GLN:HB2	1.99	0.63
1:C:69:LEU:H	1:C:69:LEU:HD12	1.64	0.62
1:C:96:THR:O	1:C:98:GLU:N	2.31	0.62
1:C:115:ASN:CB	1:C:116:PRO:CD	2.72	0.62
1:B:55:LYS:O	1:B:59:GLU:HB3	2.00	0.62
1:A:142:THR:HG22	1:A:145:GLY:C	2.23	0.62
1:A:145:GLY:CA	1:A:146:LYS:HD3	2.28	0.62
1:A:12:TYR:CE1	1:A:69:LEU:HD23	2.35	0.61
1:A:61:ARG:CG	1:A:61:ARG:NH1	2.50	0.61
1:B:33:LEU:O	1:B:37:MET:HB2	1.99	0.61
1:B:89:VAL:CG1	1:B:91:LEU:HD21	2.30	0.61
1:C:64:SER:OG	1:C:65:LEU:N	2.32	0.61
1:B:112:VAL:CG1	1:B:117:MET:CE	2.72	0.61
1:A:16:MET:C	1:A:18:GLN:H	2.09	0.61
1:B:64:SER:O	1:B:67:ASP:HB3	2.01	0.61
1:A:24:GLU:O	1:C:25:ARG:HG3	2.00	0.61
1:B:96:THR:CG2	1:B:98:GLU:CB	2.79	0.61
1:A:76:GLU:HA	1:A:76:GLU:OE1	2.00	0.60
1:B:125:MET:O	1:B:126:GLY:O	2.19	0.60
1:A:7:LEU:HD22	1:A:135:GLY:O	2.01	0.60
1:A:8:THR:HG22	1:A:135:GLY:O	2.02	0.60
1:B:134:VAL:HG13	1:B:153:ALA:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:O	1:A:10:ALA:C	2.44	0.60
1:A:28:GLU:CB	1:C:25:ARG:HG2	2.14	0.59
1:B:44:ASP:OD1	1:B:46:SER:OG	2.19	0.59
1:B:54:GLU:O	1:B:56:ALA:N	2.35	0.59
1:C:62:ILE:HG22	1:C:63:ASP:H	1.66	0.59
1:A:121:ASP:OD1	1:A:121:ASP:O	2.20	0.59
1:B:116:PRO:O	1:B:117:MET:C	2.44	0.59
1:B:114:GLU:OE1	1:B:118:LYS:CE	2.45	0.59
1:B:26:LEU:HB2	1:B:58:ILE:HG21	1.84	0.59
1:A:14:ARG:NH1	1:A:137:VAL:O	2.36	0.58
1:B:61:ARG:HG2	1:B:61:ARG:HH11	1.68	0.58
1:B:117:MET:HE1	1:C:117:MET:HE1	1.85	0.58
1:C:142:THR:HG23	1:C:143:PRO:HD2	1.84	0.58
1:B:117:MET:HE1	1:C:117:MET:CE	2.33	0.58
1:B:83:ILE:CG1	1:B:154:ILE:HD11	2.31	0.58
1:C:19:LEU:O	1:C:20:GLU:C	2.45	0.58
1:B:96:THR:CG2	1:B:98:GLU:HB2	2.34	0.58
1:C:7:LEU:HD21	1:C:150:ARG:HD2	1.86	0.58
1:B:67:ASP:O	1:B:68:VAL:C	2.46	0.58
1:B:115:ASN:HB2	1:B:116:PRO:HD2	1.86	0.58
1:B:13:GLU:HA	1:B:16:MET:HE2	1.85	0.58
1:A:91:LEU:O	1:A:99:ARG:HA	2.03	0.57
1:A:143:PRO:C	1:A:145:GLY:H	2.12	0.57
1:B:12:TYR:CB	1:B:74:ILE:HD11	2.33	0.57
1:C:37:MET:O	1:C:40:SER:CB	2.51	0.57
1:A:74:ILE:CD1	1:A:74:ILE:CB	2.78	0.57
1:B:32:ILE:O	1:B:36:LEU:N	2.30	0.57
1:C:16:MET:O	1:C:17:LYS:C	2.46	0.57
1:C:33:LEU:O	1:C:35:GLU:N	2.36	0.57
1:B:62:ILE:O	1:B:64:SER:N	2.38	0.57
1:A:100:LEU:HD12	1:A:100:LEU:C	2.21	0.57
1:B:112:VAL:HA	1:B:117:MET:CE	2.31	0.57
1:B:125:MET:O	1:B:129:LEU:CD1	2.50	0.57
1:C:62:ILE:CG2	1:C:63:ASP:N	2.60	0.57
1:C:18:GLN:NE2	1:C:148:GLU:HG3	2.20	0.57
1:C:115:ASN:HB3	1:C:116:PRO:HD3	1.84	0.57
1:A:44:ASP:N	1:A:44:ASP:OD1	2.35	0.57
1:A:100:LEU:C	1:A:100:LEU:CD1	2.76	0.57
1:B:51:ALA:O	1:B:54:GLU:CB	2.45	0.57
1:A:142:THR:HG23	1:A:144:LYS:N	2.20	0.56
1:A:16:MET:HG3	1:A:69:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:MET:HA	1:A:128:ALA:HB3	1.87	0.56
1:B:62:ILE:O	1:B:63:ASP:C	2.45	0.56
1:B:91:LEU:HD12	1:B:100:LEU:HD23	1.86	0.56
1:A:25:ARG:HG2	1:C:28:GLU:OE1	2.06	0.56
1:B:137:VAL:O	1:B:138:LEU:HD23	2.06	0.56
1:C:92:GLU:O	1:C:94:PRO:HD3	2.06	0.56
1:A:84:GLY:C	1:A:85:LEU:HD12	2.23	0.56
1:A:93:ASP:C	1:A:93:ASP:OD2	2.49	0.56
1:B:128:ALA:HB3	1:B:129:LEU:CD1	2.36	0.56
1:C:28:GLU:O	1:C:32:ILE:HG13	2.06	0.55
1:C:105:VAL:O	1:C:121:ASP:N	2.38	0.55
1:A:58:ILE:O	1:A:59:GLU:C	2.46	0.55
1:B:96:THR:HG23	1:B:98:GLU:CG	2.36	0.55
1:B:115:ASN:CB	1:B:116:PRO:HD2	2.37	0.55
1:B:16:MET:O	1:B:18:GLN:N	2.40	0.55
1:B:150:ARG:O	1:B:152:VAL:HG23	2.07	0.55
1:B:105:VAL:HG11	1:B:118:LYS:HD3	1.89	0.55
1:C:35:GLU:HA	1:C:39:SER:HB2	1.88	0.54
1:A:130:LEU:C	1:A:130:LEU:HD12	2.32	0.54
1:B:12:TYR:HB3	1:B:74:ILE:HD11	1.88	0.54
1:B:83:ILE:HD12	1:B:129:LEU:O	2.07	0.54
1:B:139:SER:HB3	1:B:148:GLU:HG2	1.88	0.54
1:C:3:ARG:O	1:C:4:GLU:HB3	2.06	0.54
1:B:54:GLU:C	1:B:56:ALA:N	2.66	0.54
1:C:19:LEU:C	1:C:21:GLN:N	2.62	0.54
1:B:89:VAL:HG11	1:B:91:LEU:HD21	1.88	0.54
1:A:13:GLU:O	1:A:17:LYS:HG2	2.08	0.54
1:C:33:LEU:O	1:C:34:GLN:C	2.51	0.54
1:A:120:SER:O	1:A:123:SER:OG	2.26	0.53
1:B:44:ASP:OD1	1:B:46:SER:CB	2.56	0.53
1:C:45:ASP:C	1:C:47:GLY:N	2.65	0.53
1:A:6:LYS:HG3	1:A:73:VAL:HB	1.90	0.53
1:B:114:GLU:OE1	1:B:118:LYS:HG3	2.08	0.53
1:A:68:VAL:O	1:A:70:SER:N	2.40	0.53
1:C:12:TYR:O	1:C:16:MET:HG3	2.08	0.53
1:C:92:GLU:O	1:C:149:PHE:HA	2.09	0.53
1:A:4:GLU:CD	1:A:6:LYS:HE3	2.32	0.53
1:C:53:GLN:OE1	1:C:53:GLN:CA	2.56	0.53
1:A:77:GLU:C	1:A:79:THR:H	2.17	0.53
1:A:49:GLU:CD	1:A:53:GLN:NE2	2.66	0.53
1:A:9:LYS:O	1:A:11:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ARG:O	1:C:62:ILE:C	2.51	0.53
1:A:8:THR:OG1	1:A:9:LYS:N	2.40	0.52
1:A:124:PRO:O	1:A:128:ALA:CB	2.57	0.52
1:A:83:ILE:HB	1:A:131:GLY:H	1.74	0.52
1:C:11:GLY:O	1:C:15:LEU:N	2.43	0.52
1:C:142:THR:CG2	1:C:143:PRO:N	2.72	0.52
1:A:96:THR:CG2	1:A:98:GLU:OE1	2.58	0.52
1:B:28:GLU:O	1:B:32:ILE:HG12	2.09	0.52
1:B:120:SER:HB3	1:B:123:SER:HB3	1.91	0.52
1:B:134:VAL:HA	1:B:151:VAL:HG12	1.90	0.52
1:A:16:MET:C	1:A:18:GLN:N	2.63	0.52
1:B:92:GLU:C	1:B:94:PRO:CD	2.78	0.52
1:C:96:THR:HG22	1:C:98:GLU:H	1.73	0.52
1:A:28:GLU:HG3	1:A:28:GLU:O	2.10	0.52
1:A:87:SER:N	1:A:156:GLY:O	2.43	0.52
1:B:41:ASP:HA	1:B:42:ASP:OD2	2.09	0.52
1:B:138:LEU:O	1:B:149:PHE:N	2.35	0.52
1:C:67:ASP:OD1	1:C:67:ASP:C	2.52	0.52
1:A:56:ALA:O	1:A:59:GLU:N	2.43	0.52
1:B:152:VAL:O	1:B:152:VAL:HG12	2.10	0.52
1:A:130:LEU:HD12	1:A:131:GLY:N	2.25	0.52
1:C:80:GLY:HA3	1:C:133:ARG:HG2	1.86	0.51
1:A:5:VAL:HB	1:A:71:ARG:CB	2.38	0.51
1:B:126:GLY:O	1:B:127:LYS:C	2.54	0.51
1:B:34:GLN:NE2	1:B:55:LYS:HZ1	2.08	0.51
1:B:54:GLU:O	1:B:57:ARG:N	2.44	0.51
1:B:50:ALA:O	1:B:52:LYS:N	2.43	0.51
1:A:49:GLU:CG	1:A:53:GLN:NE2	2.72	0.51
1:C:16:MET:O	1:C:19:LEU:N	2.42	0.50
1:C:16:MET:C	1:C:18:GLN:N	2.64	0.50
1:B:26:LEU:HB2	1:B:58:ILE:CG2	2.41	0.50
1:B:95:ALA:O	1:B:96:THR:CB	2.60	0.50
1:A:16:MET:O	1:A:19:LEU:N	2.43	0.50
1:A:65:LEU:O	1:A:66:GLU:C	2.52	0.50
1:B:92:GLU:OE2	1:B:150:ARG:NH1	2.45	0.50
1:B:44:ASP:C	1:B:46:SER:H	2.19	0.50
1:A:5:VAL:HG12	1:A:5:VAL:O	2.10	0.50
1:A:82:VAL:HG22	1:A:133:ARG:NH1	2.27	0.50
1:B:87:SER:O	1:B:103:GLN:HB2	2.12	0.50
1:B:89:VAL:HG12	1:B:91:LEU:CD2	2.41	0.50
1:C:22:GLU:OE1	1:C:61:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:O	1:A:29:ALA:HB3	2.11	0.50
1:C:49:GLU:HA	1:C:49:GLU:OE1	2.11	0.50
1:C:58:ILE:HA	1:C:61:ARG:HB2	1.93	0.50
1:A:25:ARG:O	1:C:28:GLU:HG2	2.12	0.49
1:B:19:LEU:CD1	1:B:62:ILE:HG23	2.42	0.49
1:C:38:GLU:O	1:C:39:SER:C	2.55	0.49
1:A:14:ARG:HD3	1:A:148:GLU:OE2	2.12	0.49
1:C:13:GLU:C	1:C:15:LEU:N	2.68	0.49
1:B:57:ARG:O	1:B:61:ARG:HB2	2.12	0.49
1:A:105:VAL:CG2	1:A:119:ILE:O	2.61	0.49
1:B:14:ARG:C	1:B:16:MET:H	2.19	0.49
1:B:89:VAL:HG12	1:B:91:LEU:HD21	1.93	0.49
1:B:132:HIS:CD2	1:B:138:LEU:HD11	2.47	0.49
1:C:6:LYS:HB3	1:C:75:LEU:HD21	1.94	0.49
1:B:105:VAL:HG23	1:B:106:SER:O	2.13	0.49
1:B:44:ASP:O	1:B:45:ASP:CB	2.47	0.49
1:B:44:ASP:OD1	1:B:46:SER:HB3	2.13	0.49
1:C:92:GLU:O	1:C:94:PRO:CD	2.61	0.49
1:A:88:VAL:CG1	1:A:103:GLN:HB2	2.29	0.49
1:B:85:LEU:C	1:B:87:SER:N	2.71	0.49
1:B:47:GLY:HA2	1:B:50:ALA:CB	2.42	0.49
1:B:125:MET:O	1:B:128:ALA:HB3	2.13	0.49
1:C:105:VAL:HG22	1:C:118:LYS:HB3	1.90	0.48
1:A:18:GLN:O	1:A:21:GLN:HB3	2.13	0.48
1:A:19:LEU:HD11	1:A:62:ILE:HG23	1.94	0.48
1:A:29:ALA:O	1:A:30:THR:C	2.55	0.48
1:A:119:ILE:HD11	1:A:125:MET:HG2	1.95	0.48
1:B:83:ILE:HD13	1:B:89:VAL:HG21	1.94	0.48
1:A:29:ALA:O	1:A:32:ILE:HB	2.14	0.48
1:A:113:LEU:O	1:A:114:GLU:C	2.53	0.48
1:A:44:ASP:HB3	1:A:48:LEU:HG	1.95	0.48
1:B:29:ALA:O	1:B:30:THR:C	2.57	0.48
1:B:28:GLU:OE1	1:B:28:GLU:HA	2.13	0.48
1:C:92:GLU:O	1:C:150:ARG:N	2.42	0.48
1:C:67:ASP:O	1:C:70:SER:HB3	2.14	0.48
1:C:18:GLN:O	1:C:22:GLU:HG2	2.13	0.48
1:C:39:SER:C	1:C:40:SER:HG	2.22	0.48
1:A:49:GLU:HG3	1:A:53:GLN:HE22	1.77	0.48
1:B:67:ASP:OD1	1:B:67:ASP:C	2.56	0.48
1:A:101:SER:C	1:A:102:VAL:HG12	2.39	0.47
1:A:126:GLY:O	1:A:127:LYS:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:LEU:CD1	1:C:137:VAL:HG11	2.39	0.47
1:B:85:LEU:O	1:B:104:VAL:O	2.32	0.47
1:B:142:THR:CG2	1:B:143:PRO:N	2.76	0.47
1:B:102:VAL:HB	1:B:119:ILE:HD13	1.97	0.47
1:C:138:LEU:O	1:C:149:PHE:N	2.34	0.47
1:C:62:ILE:O	1:C:64:SER:N	2.48	0.47
1:B:34:GLN:O	1:B:37:MET:HB3	2.14	0.47
1:C:39:SER:O	1:C:40:SER:OG	2.29	0.47
1:A:105:VAL:HG21	1:A:118:LYS:HB3	1.96	0.47
1:B:59:GLU:O	1:B:63:ASP:N	2.28	0.47
1:B:105:VAL:HG21	1:B:109:GLU:O	2.15	0.47
1:C:119:ILE:HD13	1:C:125:MET:HG2	1.96	0.47
1:B:49:GLU:OE1	1:B:49:GLU:HA	2.15	0.46
1:B:61:ARG:O	1:B:62:ILE:C	2.57	0.46
1:C:47:GLY:C	1:C:49:GLU:N	2.71	0.46
1:B:112:VAL:CA	1:B:117:MET:HE3	2.44	0.46
1:B:134:VAL:HG13	1:B:153:ALA:N	2.30	0.46
1:A:66:GLU:O	1:A:67:ASP:C	2.58	0.46
1:C:47:GLY:O	1:C:49:GLU:N	2.48	0.46
1:C:114:GLU:OE1	1:C:118:LYS:HD2	2.15	0.46
1:A:96:THR:HG21	1:A:98:GLU:CD	2.40	0.46
1:B:89:VAL:O	1:B:101:SER:HA	2.16	0.46
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.43	0.46
1:C:120:SER:HB3	1:C:123:SER:HB3	1.97	0.46
1:C:142:THR:HG23	1:C:143:PRO:CD	2.45	0.46
1:B:47:GLY:O	1:B:50:ALA:N	2.49	0.46
1:C:111:SER:H	1:C:118:LYS:HB2	1.81	0.46
1:A:103:GLN:HG2	1:A:105:VAL:HG13	1.98	0.46
1:A:100:LEU:O	1:A:100:LEU:HG	2.12	0.46
1:B:6:LYS:O	1:B:135:GLY:HA2	2.16	0.46
1:C:29:ALA:O	1:C:30:THR:C	2.59	0.46
1:C:126:GLY:C	1:C:128:ALA:N	2.71	0.46
1:A:119:ILE:HD12	1:A:125:MET:HG2	1.94	0.46
1:B:61:ARG:HG2	1:B:61:ARG:NH1	2.29	0.45
1:A:6:LYS:O	1:A:135:GLY:CA	2.63	0.45
1:A:124:PRO:O	1:A:128:ALA:HB2	2.17	0.45
1:C:13:GLU:HA	1:C:16:MET:HE2	1.98	0.45
1:C:16:MET:O	1:C:18:GLN:N	2.50	0.45
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.29	0.45
1:C:54:GLU:OE2	1:C:58:ILE:HD11	2.17	0.45
1:C:80:GLY:CA	1:C:133:ARG:CG	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HG3	1:A:95:ALA:HB1	1.99	0.45
1:A:85:LEU:O	1:A:86:GLY:C	2.60	0.45
1:C:33:LEU:C	1:C:35:GLU:N	2.75	0.45
1:C:38:GLU:C	1:C:40:SER:HB3	2.39	0.45
1:A:6:LYS:O	1:A:135:GLY:HA3	2.17	0.45
1:A:27:GLN:O	1:A:28:GLU:C	2.53	0.45
1:C:114:GLU:OE1	1:C:118:LYS:HG3	2.17	0.45
1:A:23:ARG:C	1:A:25:ARG:H	2.25	0.45
1:A:74:ILE:H	1:A:74:ILE:HG13	1.60	0.45
1:A:142:THR:CG2	1:A:144:LYS:C	2.90	0.45
1:B:16:MET:O	1:B:19:LEU:N	2.50	0.45
1:A:15:LEU:O	1:A:16:MET:C	2.58	0.45
1:A:48:LEU:O	1:A:52:LYS:HB2	2.17	0.45
1:C:61:ARG:NH1	1:C:61:ARG:HG2	2.32	0.45
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.77	0.44
1:A:103:GLN:CG	1:A:104:VAL:N	2.73	0.44
1:A:105:VAL:HG22	1:A:119:ILE:O	2.17	0.44
1:C:83:ILE:CG2	1:C:130:LEU:HD12	2.44	0.44
1:C:85:LEU:N	1:C:85:LEU:HD12	2.32	0.44
1:A:62:ILE:C	1:A:64:SER:N	2.74	0.44
1:B:8:THR:O	1:B:9:LYS:C	2.60	0.44
1:C:96:THR:CG2	1:C:98:GLU:H	2.29	0.44
1:A:63:ASP:OD1	1:A:63:ASP:C	2.59	0.44
1:A:24:GLU:CG	1:C:21:GLN:HG2	2.46	0.44
1:A:119:ILE:HD12	1:A:125:MET:CG	2.47	0.44
1:B:96:THR:HG22	1:B:98:GLU:HB2	2.00	0.44
1:A:16:MET:O	1:A:17:LYS:C	2.61	0.44
1:A:16:MET:HG3	1:A:69:LEU:HD22	1.98	0.44
1:A:82:VAL:CG1	1:A:83:ILE:H	2.16	0.44
1:B:10:ALA:O	1:B:14:ARG:HB2	2.17	0.44
1:A:6:LYS:CG	1:A:73:VAL:HB	2.47	0.44
1:A:49:GLU:C	1:A:51:ALA:N	2.75	0.44
1:B:44:ASP:H	1:B:48:LEU:HD12	1.82	0.44
1:C:32:ILE:O	1:C:35:GLU:HB3	2.18	0.44
1:B:61:ARG:HG2	1:B:95:ALA:HB1	1.99	0.44
1:B:77:GLU:HG3	1:B:78:GLY:H	1.83	0.44
1:C:22:GLU:CD	1:C:61:ARG:HH12	2.25	0.44
1:C:119:ILE:CD1	1:C:125:MET:HG2	2.48	0.44
1:B:45:ASP:C	1:B:47:GLY:N	2.72	0.44
1:C:27:GLN:O	1:C:28:GLU:C	2.61	0.44
1:A:28:GLU:OE2	1:C:54:GLU:OE2	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLY:O	1:B:12:TYR:C	2.61	0.43
1:C:142:THR:HG22	1:C:144:LYS:N	2.32	0.43
1:A:25:ARG:O	1:A:26:LEU:C	2.59	0.43
1:B:14:ARG:C	1:B:16:MET:N	2.77	0.43
1:B:85:LEU:HA	1:B:85:LEU:HD12	1.25	0.43
1:B:147:LYS:HB2	1:B:149:PHE:HE1	1.83	0.43
1:A:9:LYS:C	1:A:11:GLY:N	2.76	0.43
1:A:66:GLU:O	1:A:69:LEU:N	2.51	0.43
1:A:101:SER:C	1:A:102:VAL:CG1	2.86	0.43
1:B:25:ARG:C	1:B:27:GLN:N	2.73	0.43
1:B:37:MET:O	1:B:40:SER:CB	2.66	0.43
1:B:54:GLU:HB3	1:B:55:LYS:H	1.51	0.43
1:B:125:MET:CA	1:B:128:ALA:HB3	2.45	0.43
1:B:102:VAL:CB	1:B:119:ILE:HD13	2.48	0.43
1:B:129:LEU:HD11	1:B:140:LEU:HD21	2.01	0.43
1:A:45:ASP:O	1:A:49:GLU:CB	2.66	0.43
1:A:106:SER:HA	1:A:107:PRO:HD3	1.83	0.43
1:B:114:GLU:HG3	1:C:143:PRO:HD3	2.00	0.43
1:C:69:LEU:HD12	1:C:69:LEU:N	2.32	0.43
1:C:76:GLU:O	1:C:76:GLU:HG3	2.19	0.43
1:A:23:ARG:C	1:A:25:ARG:N	2.77	0.43
1:A:36:LEU:C	1:A:38:GLU:N	2.75	0.43
1:A:47:GLY:O	1:A:51:ALA:HB3	2.19	0.43
1:C:96:THR:O	1:C:96:THR:HG22	2.08	0.43
1:C:114:GLU:O	1:C:117:MET:HG3	2.18	0.43
1:B:67:ASP:O	1:B:70:SER:N	2.51	0.42
1:A:77:GLU:C	1:A:79:THR:N	2.75	0.42
1:A:98:GLU:HG2	1:A:98:GLU:O	2.19	0.42
1:B:64:SER:O	1:B:65:LEU:C	2.61	0.42
1:C:115:ASN:O	1:C:117:MET:N	2.51	0.42
1:A:49:GLU:O	1:A:51:ALA:N	2.52	0.42
1:B:102:VAL:HG21	1:B:119:ILE:CD1	2.48	0.42
1:B:112:VAL:C	1:B:117:MET:HE3	2.44	0.42
1:B:138:LEU:O	1:B:148:GLU:HA	2.20	0.42
1:C:126:GLY:O	1:C:127:LYS:C	2.62	0.42
1:A:143:PRO:C	1:A:145:GLY:N	2.78	0.42
1:C:8:THR:HG22	1:C:135:GLY:C	2.35	0.42
1:A:15:LEU:HD11	1:A:94:PRO:CG	2.46	0.42
1:A:83:ILE:O	1:A:130:LEU:CD1	2.67	0.42
1:C:19:LEU:O	1:C:21:GLN:N	2.53	0.42
1:B:100:LEU:HD12	1:B:101:SER:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:HG21	1:B:119:ILE:HD13	2.01	0.42
1:A:115:ASN:O	1:A:117:MET:N	2.50	0.42
1:B:93:ASP:O	1:B:96:THR:HG22	2.19	0.42
1:A:14:ARG:HA	1:A:17:LYS:HG3	2.02	0.42
1:A:68:VAL:C	1:A:70:SER:H	2.26	0.42
1:B:34:GLN:HE21	1:B:55:LYS:HZ2	1.59	0.42
1:B:87:SER:O	1:B:103:GLN:CB	2.68	0.42
1:C:60:ALA:O	1:C:61:ARG:C	2.63	0.42
1:A:67:ASP:OD1	1:A:67:ASP:O	2.38	0.42
1:A:114:GLU:OE1	1:A:118:LYS:HD2	2.20	0.42
1:C:11:GLY:HA2	1:C:137:VAL:HG23	2.02	0.42
1:B:115:ASN:CB	1:B:116:PRO:CD	2.97	0.41
1:C:62:ILE:O	1:C:63:ASP:C	2.62	0.41
1:A:134:VAL:HG13	1:A:153:ALA:H	1.85	0.41
1:B:44:ASP:CG	1:B:46:SER:HB3	2.45	0.41
1:B:142:THR:HG22	1:B:144:LYS:N	2.34	0.41
1:C:125:MET:O	1:C:129:LEU:CD1	2.54	0.41
1:A:62:ILE:HG22	1:A:63:ASP:N	2.34	0.41
1:B:7:LEU:HA	1:B:135:GLY:O	2.20	0.41
1:C:38:GLU:O	1:C:40:SER:OG	2.38	0.41
1:B:33:LEU:HD23	1:B:34:GLN:HG2	2.02	0.41
1:B:125:MET:HB3	1:B:125:MET:HE3	1.74	0.41
1:A:6:LYS:O	1:A:7:LEU:HD23	2.21	0.41
1:A:33:LEU:HD21	1:A:37:MET:HE3	2.02	0.41
1:A:109:GLU:H	1:A:109:GLU:HG2	1.65	0.41
1:B:152:VAL:O	1:B:153:ALA:HB3	2.20	0.41
1:A:37:MET:O	1:A:40:SER:HB2	2.21	0.41
1:A:102:VAL:HG23	1:A:103:GLN:N	2.34	0.41
1:B:41:ASP:CA	1:B:42:ASP:OD2	2.68	0.41
1:B:111:SER:OG	1:B:113:LEU:HB2	2.21	0.41
1:C:36:LEU:O	1:C:40:SER:HA	2.21	0.41
1:C:85:LEU:O	1:C:86:GLY:C	2.63	0.41
1:A:45:ASP:O	1:A:49:GLU:HB2	2.21	0.41
1:C:45:ASP:O	1:C:47:GLY:CA	2.68	0.40
1:C:78:GLY:HA2	1:C:133:ARG:HH12	1.85	0.40
1:A:40:SER:O	1:A:41:ASP:HB3	2.21	0.40
1:C:15:LEU:HD23	1:C:69:LEU:HD11	2.02	0.40
1:A:51:ALA:O	1:A:52:LYS:C	2.63	0.40
1:C:125:MET:HE3	1:C:125:MET:HB2	1.75	0.40
1:A:16:MET:CG	1:A:69:LEU:HD22	2.51	0.40
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HD13	1:B:83:ILE:HG21	1.60	0.40
1:B:124:PRO:O	1:B:125:MET:C	2.61	0.40
1:C:129:LEU:HD12	1:C:129:LEU:H	1.86	0.40
1:B:52:LYS:C	1:B:54:GLU:H	2.30	0.40
1:B:56:ALA:O	1:B:57:ARG:C	2.64	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ASP:OD2	1:B:44:ASP:OD2[2_556]	1.87	0.33

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	152/157 (97%)	110 (72%)	26 (17%)	16 (10%)	0	2
1	B	153/157 (98%)	102 (67%)	32 (21%)	19 (12%)	0	1
1	C	153/157 (98%)	104 (68%)	27 (18%)	22 (14%)	0	1
All	All	458/471 (97%)	316 (69%)	85 (19%)	57 (12%)	0	1

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	17	LYS
1	A	41	ASP
1	A	45	ASP
1	A	116	PRO
1	B	40	SER
1	B	42	ASP

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Mol	Chain	Res	Type
1	B	43	TYR
1	B	50	ALA
1	B	55	LYS
1	B	96	THR
1	C	4	GLU
1	C	33	LEU
1	C	43	TYR
1	C	46	SER
1	C	62	ILE
1	C	63	ASP
1	C	82	VAL
1	C	96	THR
1	C	97	GLY
1	C	116	PRO
1	A	49	GLU
1	A	96	THR
1	A	144	LYS
1	B	68	VAL
1	B	117	MET
1	C	9	LYS
1	C	34	GLN
1	C	40	SER
1	C	47	GLY
1	C	117	MET
1	A	69	LEU
1	A	115	ASN
1	B	41	ASP
1	B	51	ALA
1	B	67	ASP
1	B	100	LEU
1	C	3	ARG
1	C	80	GLY
1	A	153	ALA
1	C	38	GLU
1	C	41	ASP
1	C	118	LYS
1	A	10	ALA
1	A	143	PRO
1	B	30	THR
1	B	153	ALA
1	A	126	GLY
1	B	115	ASN

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Mol	Chain	Res	Type
1	B	134	VAL
1	A	82	VAL
1	B	126	GLY
1	A	78	GLY
1	B	86	GLY
1	C	86	GLY
1	B	47	GLY
1	C	143	PRO

5.3.2 Protein sidechains [i](#)

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	129/131 (98%)	69 (54%)	60 (46%)	0	0
1	B	129/131 (98%)	83 (64%)	46 (36%)	0	1
1	C	129/131 (98%)	83 (64%)	46 (36%)	0	1
All	All	387/393 (98%)	235 (61%)	152 (39%)	0	0

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	5	VAL
1	A	7	LEU
1	A	8	THR
1	A	9	LYS
1	A	14	ARG
1	A	15	LEU
1	A	18	GLN
1	A	21	GLN
1	A	25	ARG
1	A	26	LEU
1	A	31	LYS
1	A	33	LEU
1	A	34	GLN

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Mol	Chain	Res	Type
1	A	38	GLU
1	A	39	SER
1	A	40	SER
1	A	42	ASP
1	A	44	ASP
1	A	46	SER
1	A	54	GLU
1	A	61	ARG
1	A	62	ILE
1	A	63	ASP
1	A	64	SER
1	A	67	ASP
1	A	70	SER
1	A	74	ILE
1	A	76	GLU
1	A	81	GLU
1	A	83	ILE
1	A	85	LEU
1	A	88	VAL
1	A	89	VAL
1	A	92	GLU
1	A	93	ASP
1	A	94	PRO
1	A	96	THR
1	A	98	GLU
1	A	100	LEU
1	A	101	SER
1	A	102	VAL
1	A	105	VAL
1	A	106	SER
1	A	107	PRO
1	A	112	VAL
1	A	113	LEU
1	A	114	GLU
1	A	116	PRO
1	A	119	ILE
1	A	121	ASP
1	A	124	PRO
1	A	129	LEU
1	A	130	LEU
1	A	133	ARG
1	A	134	VAL

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Mol	Chain	Res	Type
1	A	136	ASP
1	A	142	THR
1	A	144	LYS
1	A	146	LYS
1	B	3	ARG
1	B	5	VAL
1	B	9	LYS
1	B	18	GLN
1	B	20	GLU
1	B	21	GLN
1	B	22	GLU
1	B	23	ARG
1	B	26	LEU
1	B	38	GLU
1	B	39	SER
1	B	41	ASP
1	B	42	ASP
1	B	44	ASP
1	B	46	SER
1	B	49	GLU
1	B	53	GLN
1	B	54	GLU
1	B	57	ARG
1	B	58	ILE
1	B	61	ARG
1	B	62	ILE
1	B	73	VAL
1	B	76	GLU
1	B	87	SER
1	B	88	VAL
1	B	90	GLU
1	B	94	PRO
1	B	96	THR
1	B	98	GLU
1	B	99	ARG
1	B	101	SER
1	B	103	GLN
1	B	111	SER
1	B	113	LEU
1	B	116	PRO
1	B	117	MET
1	B	124	PRO

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Mol	Chain	Res	Type
1	B	125	MET
1	B	129	LEU
1	B	134	VAL
1	B	141	ASP
1	B	142	THR
1	B	144	LYS
1	B	150	ARG
1	B	154	ILE
1	C	4	GLU
1	C	8	THR
1	C	12	TYR
1	C	14	ARG
1	C	15	LEU
1	C	17	LYS
1	C	18	GLN
1	C	25	ARG
1	C	31	LYS
1	C	32	ILE
1	C	35	GLU
1	C	36	LEU
1	C	39	SER
1	C	41	ASP
1	C	46	SER
1	C	48	LEU
1	C	49	GLU
1	C	52	LYS
1	C	53	GLN
1	C	57	ARG
1	C	64	SER
1	C	67	ASP
1	C	70	SER
1	C	73	VAL
1	C	74	ILE
1	C	79	THR
1	C	83	ILE
1	C	87	SER
1	C	96	THR
1	C	100	LEU
1	C	103	GLN
1	C	105	VAL
1	C	106	SER
1	C	113	LEU

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Mol	Chain	Res	Type
1	C	114	GLU
1	C	118	LYS
1	C	123	SER
1	C	124	PRO
1	C	129	LEU
1	C	133	ARG
1	C	134	VAL
1	C	136	ASP
1	C	138	LEU
1	C	142	THR
1	C	146	LYS
1	C	152	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	34	GLN
1	A	53	GLN
1	A	132	HIS
1	A	155	HIS
1	B	34	GLN
1	C	132	HIS

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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	154/157 (98%)	0.39	10 (6%) 25 17	51, 95, 194, 253	0
1	B	155/157 (98%)	0.28	7 (4%) 38 25	41, 79, 215, 265	0
1	C	155/157 (98%)	0.39	6 (3%) 43 29	57, 92, 183, 226	0
All	All	464/471 (98%)	0.35	23 (4%) 34 23	41, 90, 198, 265	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	GLN	3.2
1	C	38	GLU	3.1
1	A	40	SER	2.8
1	C	51	ALA	2.8
1	A	41	ASP	2.8
1	C	46	SER	2.8
1	A	75	LEU	2.7
1	C	48	LEU	2.6
1	B	115	ASN	2.5
1	B	33	LEU	2.5
1	C	43	TYR	2.5
1	A	70	SER	2.5
1	B	31	LYS	2.4
1	A	79	THR	2.4
1	B	48	LEU	2.3
1	A	156	GLY	2.1
1	B	43	TYR	2.1
1	A	52	LYS	2.1
1	A	74	ILE	2.1
1	B	37	MET	2.1
1	B	46	SER	2.0
1	A	153	ALA	2.0
1	A	48	LEU	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.