



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:13 PM UTC

PDB ID : 1HXD / pdb_00001hxd
Title : CRYSTAL STRUCTURE OF E. COLI BIOTIN REPRESSOR WITH BOUND BIOTIN
Authors : Kwon, K.; Streaker, E.D.; Ruparelia, S.; Beckett, D.
Deposited on : 2001-01-12
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

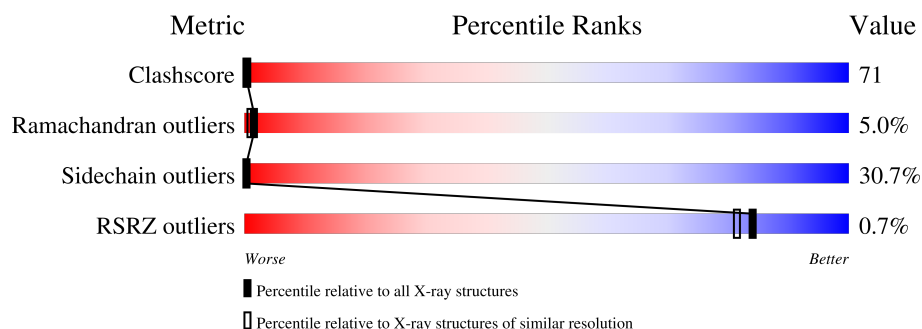
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	321	
1	B	321	

2 Entry composition [i](#)

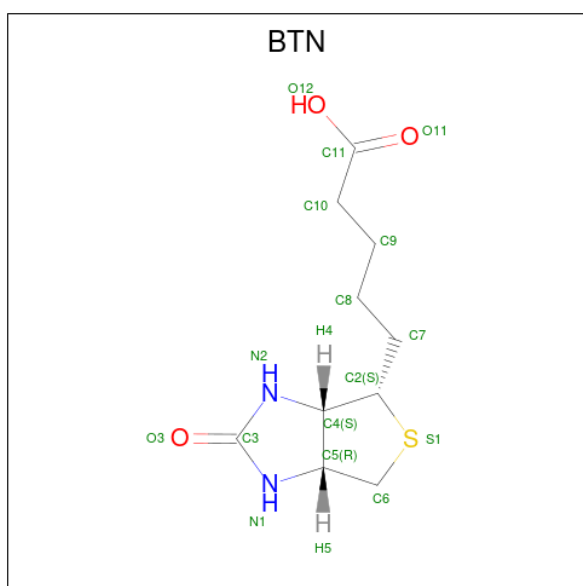
There are 3 unique types of molecules in this entry. The entry contains 4803 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BIRA BIFUNCTIONAL PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2356	1508	414	426	8			
1	B	305	Total	C	N	O	S	0	0	0
			2356	1508	414	426	8			

- Molecule 2 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

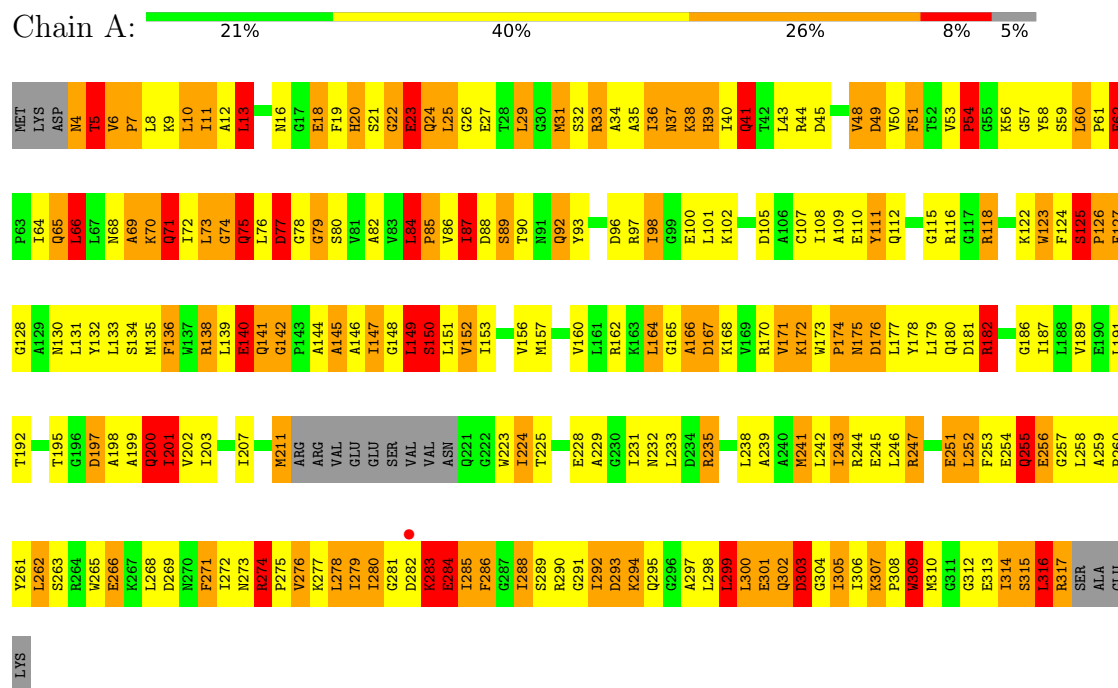
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	31	Total 31	O 31	0	0

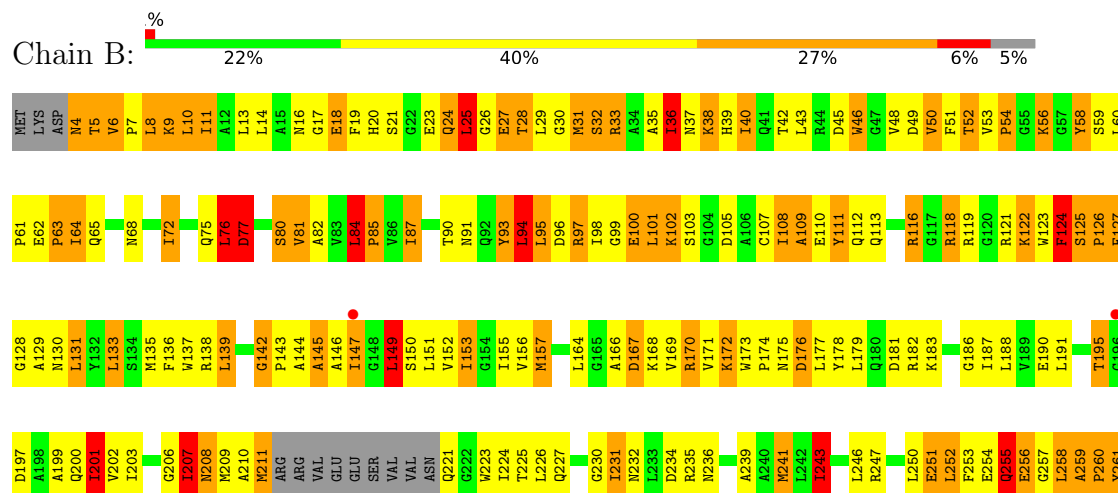
3 Residue-property plots

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: BIRA BIFUNCTIONAL PROTEIN



• Molecule 1: BIRA BIFUNCTIONAL PROTEIN



L262	S263	R264	W265	E266	K267	L268	D269	N270	F271	T272	N273	R274	P275	V276	K277	L278	T279	T280	G281	D282	K283	E284	I285	F286	G287	I288	S289	R290	G291	T292	D293	K294	Q295	G296	A297	L298	L299	L300	E301	Q302	D303	G304	I305	I306	K307	F308	W309	M310	G311	G312	E313	T314	S315	L316	R317	SER	ALA	GLU	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.90Å 108.90Å 143.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.00 – 2.40 13.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	83.0 (13.00-2.40) 81.9 (13.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.39Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.189 , (Not available) 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.168 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4803	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.53	16/2395 (0.7%)	2.10	91/3234 (2.8%)
1	B	1.53	12/2395 (0.5%)	2.06	74/3234 (2.3%)
All	All	1.53	28/4790 (0.6%)	2.08	165/6468 (2.6%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ASP	CG-OD2	7.93	1.40	1.25
1	A	100	GLU	CD-OE2	6.89	1.38	1.25
1	A	10	LEU	CA-C	-6.82	1.43	1.52
1	A	20	HIS	CA-C	-6.18	1.45	1.52
1	B	126	PRO	C-N	-6.03	1.25	1.33
1	B	299	LEU	CA-C	-6.01	1.45	1.53
1	A	111	TYR	N-CA	-5.88	1.39	1.46
1	A	66	LEU	CA-C	-5.82	1.45	1.53
1	B	127	PHE	N-CA	-5.73	1.38	1.46
1	A	271	PHE	C-N	-5.67	1.27	1.33
1	B	39	HIS	CA-C	-5.59	1.45	1.52
1	A	152	VAL	CA-C	-5.53	1.46	1.52
1	A	317	ARG	NE-CZ	5.53	1.39	1.33
1	A	20	HIS	N-CA	-5.41	1.39	1.46
1	A	187	ILE	CA-C	-5.35	1.46	1.52
1	A	105	ASP	CG-OD2	5.26	1.35	1.25
1	B	203	ILE	N-CA	-5.22	1.39	1.46
1	A	274	ARG	CA-C	-5.21	1.47	1.52
1	A	186	GLY	CA-C	-5.21	1.47	1.51
1	A	176	ASP	CG-OD2	5.19	1.35	1.25
1	B	254	GLU	CD-OE2	5.17	1.35	1.25
1	B	100	GLU	CD-OE2	5.12	1.35	1.25
1	B	93	TYR	N-CA	-5.12	1.40	1.46
1	B	282	ASP	CG-OD2	5.11	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	ILE	CA-CB	-5.11	1.48	1.54
1	B	76	LEU	CA-C	-5.03	1.47	1.53
1	B	201	ILE	N-CA	-5.03	1.40	1.46
1	A	13	LEU	C-N	-5.00	1.26	1.33

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	O-C-N	12.05	129.42	121.71
1	A	175	ASN	N-CA-C	11.14	124.53	110.61
1	B	50	VAL	CB-CA-C	10.51	125.14	110.84
1	B	280	ILE	N-CA-C	-10.28	98.59	110.21
1	B	175	ASN	N-CA-C	9.79	127.61	113.02
1	A	49	ASP	N-CA-CB	9.30	124.21	110.35
1	A	284	GLU	N-CA-C	8.99	122.88	108.41
1	B	279	ILE	N-CA-C	8.79	120.87	107.78
1	B	167	ASP	N-CA-C	8.78	122.99	111.75
1	A	243	ILE	CB-CA-C	-8.77	100.30	112.14
1	A	100	GLU	N-CA-C	-8.62	100.79	112.94
1	B	155	ILE	CB-CA-C	-8.62	100.94	111.97
1	A	84	LEU	C-N-CD	-8.27	91.09	125.00
1	A	299	LEU	CA-C-N	-8.22	110.07	122.74
1	A	299	LEU	C-N-CA	-8.22	110.07	122.74
1	B	295	GLN	N-CA-C	-8.17	102.34	112.88
1	A	202	VAL	CB-CA-C	8.12	122.30	110.77
1	A	175	ASN	CB-CA-C	-7.69	98.12	111.35
1	A	60	LEU	N-CA-CB	7.63	122.92	109.94
1	A	23	GLU	CB-CA-C	7.62	122.75	110.95
1	B	149	LEU	CB-CA-C	-7.53	95.44	110.42
1	A	77	ASP	CA-CB-CG	7.50	120.10	112.60
1	A	54	PRO	CB-CA-C	7.46	123.86	111.56
1	A	33	ARG	N-CA-C	-7.39	103.21	111.71
1	A	23	GLU	N-CA-CB	-7.23	99.49	109.98
1	A	182	ARG	CB-CA-C	7.20	123.63	109.66
1	A	303	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	274	ARG	CA-C-N	7.17	127.10	119.85
1	B	274	ARG	C-N-CA	7.17	127.10	119.85
1	A	73	LEU	O-C-N	7.15	130.34	122.11
1	A	87	ILE	CA-C-N	7.05	129.60	120.44
1	A	87	ILE	C-N-CA	7.05	129.60	120.44
1	A	127	PHE	CA-CB-CG	-7.05	106.75	113.80
1	A	232	ASN	CA-CB-CG	7.01	119.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	PHE	CB-CA-C	7.01	121.68	110.19
1	A	243	ILE	N-CA-C	6.91	117.66	110.62
1	B	307	LYS	C-N-CD	-6.89	96.73	125.00
1	A	201	ILE	N-CA-C	6.86	117.78	108.17
1	A	84	LEU	CB-CA-C	6.84	119.42	109.09
1	B	298	LEU	CB-CA-C	-6.83	98.96	109.89
1	A	126	PRO	CB-CA-C	-6.80	102.69	111.46
1	A	279	ILE	CB-CA-C	-6.78	100.16	111.29
1	A	51	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	255	GLN	N-CA-CB	6.67	120.57	110.30
1	A	233	LEU	CB-CA-C	-6.65	98.14	109.51
1	B	175	ASN	CA-C-N	-6.63	111.21	123.01
1	B	175	ASN	C-N-CA	-6.63	111.21	123.01
1	B	124	PHE	N-CA-CB	6.62	121.67	110.49
1	A	235	ARG	CA-C-N	6.58	129.10	120.28
1	A	235	ARG	C-N-CA	6.58	129.10	120.28
1	B	129	ALA	N-CA-C	6.57	121.58	112.45
1	A	62	GLU	CA-C-N	6.42	127.39	120.13
1	A	62	GLU	C-N-CA	6.42	127.39	120.13
1	B	125	SER	CA-C-N	6.33	126.67	119.83
1	B	125	SER	C-N-CA	6.33	126.67	119.83
1	A	247	ARG	N-CA-C	-6.32	103.53	111.11
1	A	274	ARG	CA-C-N	6.32	127.27	120.13
1	A	274	ARG	C-N-CA	6.32	127.27	120.13
1	A	125	SER	N-CA-CB	-6.31	101.91	110.74
1	A	39	HIS	CA-CB-CG	-6.22	107.58	113.80
1	B	36	ILE	CB-CA-C	-6.20	103.95	111.88
1	A	283	LYS	CA-C-N	6.17	130.62	122.42
1	A	283	LYS	C-N-CA	6.17	130.62	122.42
1	B	272	ILE	CB-CA-C	6.13	121.58	111.59
1	A	142	GLY	CA-C-N	6.10	127.47	119.84
1	A	142	GLY	C-N-CA	6.10	127.47	119.84
1	B	277	LYS	CA-C-N	-6.08	112.36	122.21
1	B	277	LYS	C-N-CA	-6.08	112.36	122.21
1	A	100	GLU	CA-C-O	6.03	126.60	119.48
1	B	279	ILE	CA-C-O	6.01	126.20	120.25
1	B	299	LEU	CA-C-N	-5.96	114.49	122.72
1	B	299	LEU	C-N-CA	-5.96	114.49	122.72
1	B	181	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	232	ASN	CB-CA-C	-5.95	102.01	111.17
1	A	136	PHE	CA-CB-CG	-5.92	107.88	113.80
1	B	231	ILE	CB-CA-C	-5.90	102.66	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	ILE	CB-CA-C	-5.83	103.08	111.19
1	A	77	ASP	CB-CA-C	5.83	122.02	110.42
1	A	25	LEU	N-CA-C	5.82	118.10	111.11
1	A	256	GLU	N-CA-C	5.80	122.80	114.39
1	A	69	ALA	CA-C-N	5.79	128.04	120.28
1	A	69	ALA	C-N-CA	5.79	128.04	120.28
1	B	135	MET	CA-C-N	-5.78	114.84	122.99
1	B	135	MET	C-N-CA	-5.78	114.84	122.99
1	A	192	THR	N-CA-CB	5.78	120.89	110.83
1	B	175	ASN	CB-CA-C	-5.77	100.74	110.44
1	A	244	ARG	CB-CA-C	5.72	119.77	110.96
1	A	123	TRP	N-CA-C	5.72	118.72	111.69
1	B	274	ARG	O-C-N	5.71	126.21	121.35
1	A	149	LEU	N-CA-C	-5.67	105.00	111.07
1	B	243	ILE	N-CA-CB	-5.64	103.95	110.55
1	B	125	SER	N-CA-C	5.62	119.45	108.21
1	A	315	SER	N-CA-C	-5.61	101.61	109.69
1	B	19	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	176	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	24	GLN	CB-CA-C	5.56	119.61	110.88
1	B	151	LEU	N-CA-CB	5.56	118.03	109.91
1	B	292	ILE	N-CA-C	5.54	118.09	108.95
1	A	111	TYR	N-CA-CB	-5.54	101.58	110.77
1	B	46	TRP	CB-CA-C	-5.53	99.53	110.27
1	A	22	GLY	CA-C-N	5.52	128.14	120.63
1	A	22	GLY	C-N-CA	5.52	128.14	120.63
1	A	229	ALA	O-C-N	5.49	129.48	122.39
1	A	140	GLU	N-CA-C	5.49	117.12	111.03
1	A	251	GLU	O-C-N	5.47	127.94	122.03
1	B	284	GLU	N-CA-C	5.47	118.29	110.68
1	A	224	ILE	CB-CA-C	5.45	119.51	110.30
1	A	7	PRO	CB-CA-C	5.42	120.50	111.56
1	B	84	LEU	C-N-CD	-5.42	102.79	125.00
1	B	30	GLY	N-CA-C	-5.40	107.56	115.72
1	B	56	LYS	CA-C-N	-5.39	112.55	121.12
1	B	56	LYS	C-N-CA	-5.39	112.55	121.12
1	A	142	GLY	O-C-N	5.38	127.15	121.77
1	B	251	GLU	CB-CA-C	5.35	120.52	110.63
1	A	77	ASP	N-CA-C	-5.34	99.42	110.80
1	B	170	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	A	22	GLY	CA-C-O	5.33	125.49	119.09
1	B	179	LEU	CB-CA-C	5.33	118.85	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ILE	CB-CA-C	5.32	119.91	110.71
1	A	284	GLU	CB-CA-C	-5.32	102.03	110.81
1	B	142	GLY	O-C-N	5.32	127.09	121.77
1	B	53	VAL	O-C-N	5.30	127.14	121.10
1	B	282	ASP	CA-C-N	-5.29	112.64	121.64
1	B	282	ASP	C-N-CA	-5.29	112.64	121.64
1	A	79	GLY	N-CA-C	5.29	120.71	111.46
1	A	305	ILE	N-CA-C	5.28	116.11	107.24
1	B	25	LEU	N-CA-C	5.28	117.04	111.28
1	A	288	ILE	N-CA-C	5.27	116.31	108.46
1	A	233	LEU	N-CA-C	5.27	118.69	110.32
1	A	100	GLU	CB-CA-C	5.26	119.69	110.64
1	B	261	TYR	CB-CA-C	-5.26	101.30	110.09
1	B	266	GLU	CB-CA-C	-5.26	101.74	110.68
1	B	111	TYR	N-CA-CB	-5.26	101.61	111.13
1	B	109	ALA	N-CA-C	5.24	118.13	109.85
1	B	265	TRP	CA-CB-CG	-5.24	103.64	113.60
1	A	200	GLN	CB-CA-C	5.22	118.75	110.19
1	A	256	GLU	CB-CA-C	-5.19	100.76	109.27
1	A	41	GLN	N-CA-CB	5.18	117.53	110.01
1	B	81	VAL	N-CA-C	5.17	115.72	108.17
1	B	101	LEU	CB-CA-C	-5.15	100.11	109.38
1	A	151	LEU	CA-C-O	5.14	126.00	120.55
1	B	283	LYS	CA-C-N	5.14	129.79	122.08
1	B	283	LYS	C-N-CA	5.14	129.79	122.08
1	B	39	HIS	O-C-N	5.14	129.50	122.46
1	A	37	ASN	N-CA-CB	5.13	118.23	110.28
1	A	171	VAL	N-CA-C	5.12	115.96	108.53
1	B	63	PRO	N-CA-C	-5.11	103.75	111.41
1	A	316	LEU	CB-CA-C	5.10	119.28	110.45
1	B	52	THR	N-CA-C	5.10	117.22	108.90
1	A	247	ARG	CB-CA-C	5.09	118.95	110.81
1	B	208	ASN	CA-CB-CG	-5.09	107.51	112.60
1	B	101	LEU	N-CA-C	5.08	117.77	109.59
1	B	251	GLU	N-CA-C	-5.08	105.87	111.71
1	A	96	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	176	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	280	ILE	CA-C-O	-5.07	116.51	122.13
1	A	105	ASP	O-C-N	-5.06	116.80	122.97
1	A	309	TRP	CB-CA-C	-5.05	102.86	110.24
1	B	94	LEU	N-CA-C	5.05	118.60	112.23
1	A	71	GLN	N-CA-C	-5.05	105.67	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	SER	CA-CB-OG	-5.03	101.04	111.10
1	B	46	TRP	N-CA-C	5.03	119.18	113.19
1	A	174	PRO	CB-CA-C	-5.01	99.47	112.00
1	B	306	ILE	CB-CA-C	5.01	117.88	110.77
1	A	6	VAL	O-C-N	5.00	126.80	121.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2356	0	2431	336	0
1	B	2356	0	2431	348	0
2	A	16	0	15	1	0
2	B	16	0	15	5	0
3	A	28	0	0	4	0
3	B	31	0	0	1	0
All	All	4803	0	4892	684	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

All (684) 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:262:LEU:HD22	1:B:294:LYS:HD2	1.29	1.13
1:B:8:LEU:HA	1:B:11:ILE:HG22	1.29	1.13
1:A:70:LYS:H	1:A:70:LYS:HD3	1.10	1.12
1:A:277:LYS:HE2	1:A:284:GLU:HG2	1.29	1.08
1:B:278:LEU:HB2	1:B:314:ILE:HG22	1.11	1.08
1:A:131:LEU:HD23	1:A:207:ILE:HD12	1.35	1.05
1:B:298:LEU:HD21	1:B:300:LEU:HD13	1.38	1.04
1:A:16:ASN:HD21	1:A:20:HIS:HE1	1.04	1.03
1:B:262:LEU:HD22	1:B:294:LYS:HA	1.42	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:SER:HB2	1:A:23:GLU:HG3	1.36	1.01
1:B:301:GLU:HA	1:B:306:ILE:HG13	1.42	1.00
1:B:20:HIS:HB3	1:B:25:LEU:HD21	1.44	0.97
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.45	0.97
1:A:148:GLY:HA3	1:A:258:LEU:HD21	1.44	0.96
1:A:79:GLY:HA2	1:A:247:ARG:HH12	1.31	0.95
1:A:295:GLN:HB3	1:A:310:MET:HE1	1.48	0.95
1:A:16:ASN:HD22	1:A:18:GLU:H	1.07	0.95
1:B:29:LEU:HD12	1:B:36:ILE:HD11	1.49	0.93
1:A:172:LYS:HG3	1:A:271:PHE:CE2	2.04	0.92
1:B:278:LEU:HB2	1:B:314:ILE:CG2	2.00	0.92
1:B:262:LEU:HD13	1:B:294:LYS:HG3	1.53	0.91
1:A:285:ILE:HG21	1:A:309:TRP:CH2	2.05	0.91
1:A:286:PHE:CE2	1:A:317:ARG:HD2	2.05	0.91
1:B:8:LEU:HA	1:B:11:ILE:CG2	2.01	0.90
1:B:262:LEU:CD2	1:B:294:LYS:HA	2.03	0.89
1:B:278:LEU:HA	1:B:314:ILE:HA	1.55	0.88
1:B:119:ARG:NH1	1:B:281:GLY:HA2	1.89	0.88
1:B:262:LEU:CD2	1:B:294:LYS:HD2	2.05	0.87
1:A:98:ILE:HD13	1:A:136:PHE:CE1	2.10	0.87
1:B:62:GLU:HG2	1:B:63:PRO:HD2	1.57	0.87
1:B:259:ALA:HB3	1:B:260:PRO:HD3	1.55	0.86
1:B:262:LEU:HB2	1:B:294:LYS:HE3	1.58	0.86
1:B:171:VAL:HG23	1:B:269:ASP:HA	1.58	0.85
1:B:93:TYR:CD2	1:B:94:LEU:HD23	2.12	0.85
1:A:16:ASN:ND2	1:A:18:GLU:H	1.74	0.85
1:B:301:GLU:CG	1:B:306:ILE:HD11	2.06	0.84
1:B:111:TYR:CE2	1:B:113:GLN:HG2	2.13	0.84
1:A:16:ASN:HD21	1:A:20:HIS:CE1	1.93	0.84
1:A:38:LYS:HG3	1:A:41:GLN:NE2	1.92	0.84
1:A:138:ARG:HD3	1:A:200:GLN:NE2	1.93	0.84
1:A:26:GLY:HA2	1:A:36:ILE:HD11	1.59	0.83
1:B:172:LYS:HG3	1:B:271:PHE:HE2	1.43	0.83
1:A:298:LEU:C	1:A:299:LEU:HD23	2.04	0.83
1:A:173:TRP:HB2	1:A:265:TRP:HZ2	1.42	0.83
1:A:277:LYS:HE3	1:A:286:PHE:CE1	2.14	0.83
1:A:84:LEU:O	1:A:109:ALA:HA	1.79	0.82
1:A:66:LEU:H	1:A:66:LEU:HD12	1.43	0.82
1:A:301:GLU:HB2	1:A:306:ILE:HG13	1.61	0.82
1:B:279:ILE:HG22	1:B:283:LYS:H	1.44	0.82
1:A:93:TYR:HA	1:A:97:ARG:HH12	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:HD13	1:A:136:PHE:HE1	1.41	0.81
1:B:98:ILE:HA	1:B:101:LEU:HD12	1.60	0.81
1:A:70:LYS:HD3	1:A:70:LYS:N	1.94	0.80
1:B:93:TYR:HD2	1:B:94:LEU:HD23	1.46	0.80
1:B:305:ILE:C	1:B:306:ILE:HD12	2.07	0.80
1:A:147:ILE:HG23	1:A:148:GLY:H	1.45	0.80
1:B:24:GLN:HA	1:B:27:GLU:CD	2.08	0.79
1:B:252:LEU:HD23	1:B:261:TYR:OH	1.82	0.79
1:B:272:ILE:HD12	1:B:273:ASN:N	1.98	0.79
1:A:172:LYS:HG3	1:A:271:PHE:HE2	1.46	0.79
1:A:160:VAL:O	1:A:164:LEU:HD12	1.83	0.78
1:A:68:ASN:HB3	1:A:71:GLN:HB2	1.65	0.78
1:A:295:GLN:HB3	1:A:310:MET:CE	2.12	0.78
1:B:272:ILE:HD12	1:B:273:ASN:H	1.48	0.78
1:B:211:MET:H	1:B:227:GLN:NE2	1.82	0.78
1:B:21:SER:O	1:B:25:LEU:HG	1.83	0.77
1:B:262:LEU:HD13	1:B:294:LYS:CG	2.14	0.77
1:B:10:LEU:HD12	1:B:10:LEU:H	1.50	0.77
1:A:135:MET:HE2	1:A:243:ILE:HG23	1.66	0.77
1:A:6:VAL:HB	1:A:7:PRO:HD3	1.65	0.77
1:B:139:LEU:HG	1:B:201:ILE:CD1	2.15	0.76
1:A:274:ARG:NH2	1:A:316:LEU:HD13	2.00	0.76
1:A:307:LYS:HE3	1:A:308:PRO:HD2	1.67	0.76
1:A:16:ASN:HD22	1:A:18:GLU:N	1.83	0.76
1:A:111:TYR:HB2	1:A:127:PHE:HA	1.65	0.76
1:B:123:TRP:CZ3	1:B:223:TRP:HH2	2.04	0.76
1:A:239:ALA:O	1:A:243:ILE:HD12	1.85	0.76
1:B:65:GLN:HE22	1:B:234:ASP:CG	1.94	0.76
1:A:247:ARG:O	1:A:251:GLU:HG3	1.85	0.75
1:B:26:GLY:HA2	1:B:36:ILE:HD13	1.69	0.75
1:B:298:LEU:C	1:B:299:LEU:HD23	2.11	0.75
1:A:286:PHE:HE2	1:A:317:ARG:HB2	1.52	0.75
1:B:26:GLY:HA2	1:B:36:ILE:CD1	2.15	0.75
1:B:6:VAL:HG23	1:B:7:PRO:HD2	1.69	0.75
1:A:149:LEU:HD23	1:A:150:SER:N	2.01	0.75
1:B:16:ASN:C	1:B:63:PRO:HB3	2.12	0.75
1:B:31:MET:HB2	1:B:36:ILE:CD1	2.17	0.74
1:B:62:GLU:HG2	1:B:63:PRO:CD	2.17	0.74
1:B:279:ILE:HA	1:B:283:LYS:O	1.87	0.74
1:A:149:LEU:O	1:A:153:ILE:HD12	1.85	0.74
1:B:278:LEU:CB	1:B:314:ILE:HG22	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:O	1:A:76:LEU:HD23	1.86	0.74
1:B:37:ASN:HB3	1:B:38:LYS:NZ	2.03	0.74
1:B:277:LYS:HG3	1:B:317:ARG:HG3	1.69	0.74
1:B:84:LEU:O	1:B:109:ALA:HA	1.87	0.74
1:B:48:VAL:HG12	1:B:50:VAL:HG23	1.69	0.73
1:B:262:LEU:HD23	1:B:292:ILE:HD12	1.70	0.73
1:A:243:ILE:O	1:A:247:ARG:HG3	1.87	0.73
1:A:79:GLY:HA2	1:A:247:ARG:NH1	2.01	0.73
1:B:301:GLU:CA	1:B:306:ILE:HG13	2.17	0.73
1:B:191:LEU:HD12	1:B:191:LEU:O	1.87	0.73
1:B:262:LEU:HD23	1:B:292:ILE:CD1	2.17	0.73
1:A:21:SER:HB2	1:A:23:GLU:CG	2.17	0.73
1:B:298:LEU:CD2	1:B:300:LEU:HD13	2.18	0.73
1:B:98:ILE:HD12	1:B:99:GLY:N	2.04	0.73
1:B:119:ARG:HH12	1:B:281:GLY:HA2	1.52	0.73
1:B:262:LEU:HD13	1:B:294:LYS:CD	2.19	0.73
1:B:10:LEU:HD12	1:B:10:LEU:N	2.04	0.72
1:B:285:ILE:HG21	1:B:309:TRP:CH2	2.24	0.72
1:B:262:LEU:HD22	1:B:294:LYS:CD	2.16	0.72
1:B:112:GLN:NE2	2:B:501:BTN:H62	2.04	0.72
1:B:145:ALA:HB1	1:B:253:PHE:CE2	2.24	0.72
1:B:277:LYS:HE3	1:B:317:ARG:HG3	1.71	0.72
1:A:79:GLY:CA	1:A:247:ARG:HH12	2.02	0.72
1:B:68:ASN:O	1:B:72:ILE:HD12	1.87	0.72
1:B:145:ALA:HB1	1:B:253:PHE:HE2	1.53	0.72
1:B:301:GLU:HA	1:B:306:ILE:CG1	2.19	0.72
1:B:5:THR:HA	1:B:8:LEU:HD11	1.71	0.71
1:B:316:LEU:HD12	1:B:317:ARG:H	1.54	0.71
1:A:172:LYS:HE2	1:A:314:ILE:HG22	1.72	0.71
1:B:297:ALA:HB1	1:B:309:TRP:O	1.91	0.71
1:A:148:GLY:CA	1:A:258:LEU:HD21	2.21	0.71
1:A:172:LYS:HE3	1:A:314:ILE:O	1.90	0.71
1:B:276:VAL:HA	1:B:317:ARG:HB2	1.72	0.71
1:B:299:LEU:HD23	1:B:299:LEU:N	2.06	0.71
1:A:149:LEU:O	1:A:152:VAL:HB	1.90	0.70
1:B:302:GLN:O	1:B:305:ILE:HD12	1.90	0.70
1:A:201:ILE:HG22	1:A:203:ILE:HG13	1.72	0.70
1:B:139:LEU:HG	1:B:201:ILE:HD11	1.71	0.70
1:A:253:PHE:CE1	1:A:257:GLY:HA2	2.27	0.70
1:A:93:TYR:HA	1:A:97:ARG:NH1	2.05	0.70
1:A:166:ALA:HA	1:A:231:ILE:HD13	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLU:O	1:B:27:GLU:HB3	1.92	0.69
1:B:112:GLN:HE22	2:B:501:BTN:H62	1.55	0.69
1:B:280:ILE:O	1:B:282:ASP:N	2.25	0.69
1:B:171:VAL:HG22	1:B:268:LEU:C	2.16	0.69
1:B:278:LEU:O	1:B:279:ILE:HD13	1.92	0.69
1:A:65:GLN:NE2	1:A:66:LEU:N	2.41	0.69
1:B:146:ALA:O	1:B:149:LEU:HB2	1.93	0.69
1:B:305:ILE:O	1:B:306:ILE:HD12	1.93	0.69
1:A:277:LYS:HE2	1:A:284:GLU:CG	2.17	0.69
1:B:36:ILE:HG22	1:B:37:ASN:N	2.07	0.68
1:B:91:ASN:ND2	1:B:190:GLU:OE2	2.26	0.68
1:A:147:ILE:HG23	1:A:148:GLY:N	2.08	0.68
1:B:182:ARG:HH12	1:B:221:GLN:HE21	1.41	0.68
1:B:274:ARG:HB3	1:B:275:PRO:HD2	1.74	0.68
1:A:314:ILE:HD12	1:A:315:SER:N	2.09	0.68
1:B:207:ILE:HG22	1:B:209:MET:HG3	1.75	0.68
1:A:263:SER:O	1:A:266:GLU:HG3	1.93	0.68
1:A:69:ALA:O	1:A:73:LEU:N	2.19	0.68
1:B:5:THR:HA	1:B:8:LEU:CD1	2.24	0.68
1:B:239:ALA:O	1:B:243:ILE:HD12	1.93	0.68
1:B:170:ARG:HB3	1:B:270:ASN:HB2	1.75	0.67
1:A:60:LEU:HB3	1:A:61:PRO:HD2	1.76	0.67
1:A:298:LEU:HD12	1:A:299:LEU:H	1.59	0.67
1:B:172:LYS:CG	1:B:271:PHE:HE2	2.07	0.67
1:A:65:GLN:HE21	1:A:66:LEU:H	1.40	0.67
1:A:261:TYR:O	1:A:263:SER:N	2.28	0.67
1:B:37:ASN:OD1	1:B:38:LYS:NZ	2.28	0.67
1:A:71:GLN:O	1:A:75:GLN:NE2	2.28	0.67
1:A:259:ALA:HA	1:A:262:LEU:HD11	1.77	0.67
1:B:10:LEU:HA	1:B:13:LEU:HD12	1.77	0.67
1:A:93:TYR:O	1:A:97:ARG:NH1	2.27	0.67
1:A:134:SER:HA	1:A:203:ILE:O	1.95	0.67
1:B:258:LEU:HD22	1:B:262:LEU:HD21	1.77	0.67
1:A:69:ALA:HB3	1:A:70:LYS:HD3	1.77	0.66
1:A:32:SER:OG	1:A:34:ALA:HB3	1.94	0.66
1:A:146:ALA:O	1:A:149:LEU:HB3	1.95	0.66
1:A:173:TRP:HB2	1:A:265:TRP:CZ2	2.28	0.66
1:B:262:LEU:HB2	1:B:294:LYS:CE	2.26	0.66
1:B:279:ILE:O	1:B:313:GLU:N	2.27	0.66
1:A:38:LYS:O	1:A:41:GLN:NE2	2.24	0.66
1:A:25:LEU:O	1:A:29:LEU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:PRO:O	1:B:11:ILE:HG22	1.96	0.66
1:A:172:LYS:HE2	1:A:314:ILE:CG2	2.25	0.66
1:A:299:LEU:HD23	1:A:299:LEU:N	2.11	0.65
1:B:279:ILE:HG22	1:B:280:ILE:O	1.95	0.65
1:A:252:LEU:O	1:A:252:LEU:HD12	1.96	0.65
1:B:142:GLY:O	1:B:144:ALA:N	2.29	0.65
1:B:17:GLY:N	1:B:63:PRO:HB3	2.11	0.65
1:B:262:LEU:CD1	1:B:294:LYS:HG3	2.26	0.65
1:B:258:LEU:HD22	1:B:262:LEU:CG	2.26	0.65
1:B:10:LEU:HD13	1:B:43:LEU:HD11	1.78	0.65
1:B:118:ARG:NH1	1:B:187:ILE:O	2.29	0.65
1:A:182:ARG:NH2	1:A:223:TRP:O	2.29	0.65
1:A:303:ASP:OD1	1:A:305:ILE:HD12	1.97	0.65
1:B:164:LEU:HD21	1:B:241:MET:HE3	1.78	0.65
1:B:255:GLN:O	1:B:257:GLY:N	2.30	0.65
1:B:8:LEU:CA	1:B:11:ILE:HG22	2.20	0.65
1:B:133:LEU:CD1	1:B:243:ILE:HD11	2.27	0.65
1:B:182:ARG:NH1	1:B:223:TRP:O	2.30	0.64
1:A:87:ILE:CD1	1:A:93:TYR:HB2	2.27	0.64
1:A:97:ARG:O	1:A:101:LEU:HG	1.97	0.64
1:B:302:GLN:N	1:B:305:ILE:O	2.29	0.64
1:A:9:LYS:O	1:A:13:LEU:HG	1.96	0.64
1:B:149:LEU:O	1:B:152:VAL:HB	1.98	0.64
1:B:259:ALA:O	1:B:262:LEU:HD12	1.98	0.64
1:A:22:GLY:N	1:A:23:GLU:HG2	2.12	0.64
1:A:87:ILE:HD11	1:A:93:TYR:HB2	1.79	0.64
1:A:65:GLN:HE21	1:A:66:LEU:N	1.96	0.64
1:A:182:ARG:HB2	1:A:224:ILE:CG2	2.27	0.64
1:B:279:ILE:HG12	1:B:313:GLU:O	1.98	0.64
1:A:131:LEU:HD21	1:A:242:LEU:CD1	2.27	0.63
1:B:6:VAL:HG23	1:B:7:PRO:CD	2.27	0.63
1:B:10:LEU:CD1	1:B:43:LEU:HD11	2.28	0.63
1:A:173:TRP:CD1	1:A:292:ILE:HG21	2.34	0.63
1:B:8:LEU:H	1:B:8:LEU:HD12	1.63	0.63
1:A:10:LEU:HA	1:A:13:LEU:HD11	1.80	0.63
1:A:273:ASN:OD1	1:A:290:ARG:NH1	2.31	0.63
1:B:252:LEU:HD23	1:B:261:TYR:CZ	2.33	0.63
1:B:293:ASP:OD1	1:B:294:LYS:N	2.29	0.63
1:A:69:ALA:HB3	1:A:70:LYS:CD	2.29	0.62
1:A:291:GLY:O	1:A:298:LEU:HD12	1.98	0.62
1:B:259:ALA:HB3	1:B:260:PRO:CD	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:OE2	1:A:140:GLU:HA	1.99	0.62
1:A:273:ASN:HA	1:A:290:ARG:NH1	2.15	0.62
1:B:52:THR:O	1:B:54:PRO:HD3	1.99	0.62
1:B:276:VAL:CA	1:B:317:ARG:HB2	2.29	0.62
1:A:135:MET:CE	1:A:243:ILE:HG23	2.29	0.62
1:A:279:ILE:HA	1:A:283:LYS:O	1.99	0.62
1:A:4:ASN:O	1:A:8:LEU:HD12	2.00	0.62
1:B:149:LEU:O	1:B:153:ILE:HG12	1.98	0.62
1:A:11:ILE:O	1:A:11:ILE:HD12	1.99	0.62
1:B:6:VAL:HB	1:B:7:PRO:HD3	1.82	0.62
1:B:301:GLU:CD	1:B:306:ILE:HD11	2.24	0.62
1:A:276:VAL:HB	1:A:314:ILE:HD11	1.82	0.61
1:A:303:ASP:O	1:A:305:ILE:N	2.33	0.61
1:B:211:MET:N	1:B:227:GLN:HE21	1.98	0.61
1:B:246:LEU:O	1:B:250:LEU:HG	2.00	0.61
1:A:162:ARG:HA	1:A:166:ALA:O	2.00	0.61
1:A:298:LEU:O	1:A:299:LEU:HD23	2.00	0.61
1:B:133:LEU:HD23	1:B:133:LEU:C	2.25	0.61
1:A:148:GLY:O	1:A:152:VAL:HG23	2.01	0.61
1:B:95:LEU:HD13	1:B:202:VAL:HG21	1.83	0.61
1:B:275:PRO:HB2	1:B:317:ARG:HB3	1.83	0.61
1:A:259:ALA:O	1:A:262:LEU:HD12	2.00	0.61
1:B:133:LEU:HD12	1:B:243:ILE:HD11	1.82	0.61
1:A:98:ILE:CD1	1:A:136:PHE:HE1	2.13	0.61
1:B:62:GLU:CG	1:B:63:PRO:HD2	2.30	0.61
1:A:157:MET:HE2	1:A:242:LEU:HD22	1.83	0.61
1:A:274:ARG:HH21	1:A:316:LEU:HD13	1.63	0.60
1:A:289:SER:O	1:A:290:ARG:HD3	2.01	0.60
1:B:307:LYS:HG2	1:B:308:PRO:HD2	1.83	0.60
1:A:36:ILE:O	1:A:40:ILE:HG12	2.01	0.60
1:A:10:LEU:O	1:A:13:LEU:N	2.28	0.60
1:A:49:ASP:O	1:A:61:PRO:HD3	2.02	0.60
1:A:166:ALA:CA	1:A:231:ILE:HD13	2.32	0.60
1:B:37:ASN:HB3	1:B:38:LYS:HZ3	1.65	0.60
1:A:276:VAL:HG23	1:A:277:LYS:N	2.15	0.60
1:A:37:ASN:O	1:A:40:ILE:HB	2.01	0.60
1:B:211:MET:N	1:B:227:GLN:NE2	2.50	0.60
1:B:258:LEU:O	1:B:258:LEU:HD23	2.01	0.60
1:B:152:VAL:O	1:B:156:VAL:HG23	2.01	0.60
1:A:6:VAL:HG11	1:A:39:HIS:CD2	2.36	0.59
1:A:65:GLN:NE2	1:A:66:LEU:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:H	1:A:66:LEU:CD1	2.07	0.59
1:A:80:SER:H	1:A:247:ARG:HH22	1.50	0.59
1:A:26:GLY:O	1:A:31:MET:N	2.30	0.59
1:A:274:ARG:HH21	1:A:316:LEU:CD1	2.15	0.59
1:A:274:ARG:HB3	1:A:275:PRO:HD2	1.82	0.59
1:B:7:PRO:O	1:B:10:LEU:HD12	2.01	0.59
1:A:293:ASP:CG	1:A:297:ALA:HB3	2.28	0.59
1:A:314:ILE:HD12	1:A:315:SER:O	2.02	0.59
1:B:96:ASP:C	1:B:97:ARG:HG3	2.26	0.59
1:A:112:GLN:HB2	1:A:125:SER:HB2	1.84	0.59
1:A:189:VAL:HG22	1:A:203:ILE:HG23	1.85	0.59
1:B:301:GLU:CB	1:B:306:ILE:HD11	2.33	0.59
1:B:191:LEU:HD12	1:B:191:LEU:C	2.28	0.59
1:A:76:LEU:O	1:A:77:ASP:HB3	2.01	0.59
1:B:301:GLU:HG3	1:B:306:ILE:HD11	1.83	0.58
1:A:21:SER:CB	1:A:23:GLU:HG3	2.23	0.58
1:A:111:TYR:HB3	1:A:127:PHE:CD2	2.37	0.58
1:B:87:ILE:O	1:B:112:GLN:HA	2.03	0.58
1:B:285:ILE:O	1:B:286:PHE:HD1	1.86	0.58
1:B:288:ILE:HG21	1:B:290:ARG:NH1	2.17	0.58
1:A:162:ARG:HH21	1:A:170:ARG:HG2	1.68	0.58
1:B:80:SER:H	1:B:247:ARG:HH22	1.51	0.58
1:A:86:VAL:O	1:A:87:ILE:HB	2.04	0.58
1:B:122:LYS:HG2	1:B:123:TRP:N	2.18	0.58
1:A:75:GLN:O	1:A:76:LEU:HB2	2.03	0.57
1:B:262:LEU:CG	1:B:294:LYS:HD2	2.33	0.57
1:B:211:MET:H	1:B:227:GLN:HE21	1.51	0.57
1:A:147:ILE:CG2	1:A:148:GLY:H	2.15	0.57
1:A:293:ASP:HB3	1:A:299:LEU:HD21	1.85	0.57
1:B:149:LEU:HD22	1:B:253:PHE:CE2	2.40	0.57
1:A:38:LYS:O	1:A:41:GLN:HG3	2.04	0.57
1:A:225:THR:HG23	1:A:228:GLU:OE1	2.05	0.57
1:A:7:PRO:O	1:A:11:ILE:HG22	2.05	0.56
1:A:21:SER:HA	1:A:57:GLY:HA3	1.87	0.56
1:A:265:TRP:NE1	1:A:269:ASP:OD2	2.37	0.56
1:A:6:VAL:HB	1:A:7:PRO:CD	2.36	0.56
1:A:292:ILE:HA	1:A:297:ALA:O	2.05	0.56
1:B:16:ASN:ND2	1:B:18:GLU:HB2	2.21	0.56
1:B:253:PHE:O	1:B:257:GLY:HA2	2.04	0.56
1:B:258:LEU:HD22	1:B:262:LEU:CD2	2.34	0.56
1:A:38:LYS:HG3	1:A:41:GLN:CD	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HD3	1:A:200:GLN:HE21	1.67	0.56
1:B:26:GLY:HA2	1:B:36:ILE:HD11	1.87	0.56
1:A:40:ILE:HG22	1:A:44:ARG:NH1	2.21	0.56
1:A:146:ALA:HA	1:A:149:LEU:HB3	1.87	0.56
1:B:258:LEU:HD22	1:B:262:LEU:HD11	1.87	0.56
1:A:8:LEU:O	1:A:12:ALA:HB2	2.06	0.56
1:B:122:LYS:HE2	1:B:124:PHE:HB2	1.88	0.56
1:A:77:ASP:OD1	1:A:78:GLY:N	2.30	0.55
1:A:61:PRO:CD	1:A:62:GLU:H	2.20	0.55
1:B:5:THR:O	1:B:8:LEU:HD12	2.06	0.55
1:B:62:GLU:HG2	1:B:63:PRO:N	2.19	0.55
1:B:256:GLU:HB3	1:B:260:PRO:HD3	1.87	0.55
1:B:257:GLY:O	1:B:260:PRO:HD2	2.06	0.55
1:A:146:ALA:O	1:A:149:LEU:N	2.39	0.55
1:A:298:LEU:HD12	1:A:299:LEU:N	2.21	0.55
1:A:131:LEU:HD23	1:A:207:ILE:CD1	2.24	0.55
1:B:285:ILE:HD13	1:B:309:TRP:CZ3	2.42	0.55
1:A:11:ILE:HD12	1:A:11:ILE:C	2.30	0.55
1:B:138:ARG:HD2	3:B:1635:HOH:O	2.06	0.55
1:A:32:SER:O	1:A:36:ILE:HD12	2.07	0.55
1:A:278:LEU:HD21	1:A:309:TRP:CE3	2.42	0.55
1:A:180:GLN:O	1:A:182:ARG:HG3	2.07	0.55
1:A:269:ASP:OD1	3:A:606:HOH:O	2.18	0.55
1:B:37:ASN:HB3	1:B:38:LYS:HZ1	1.71	0.55
1:B:31:MET:HB2	1:B:36:ILE:HD12	1.87	0.54
1:B:4:ASN:O	1:B:7:PRO:HD2	2.06	0.54
1:A:70:LYS:H	1:A:70:LYS:CD	1.93	0.54
1:A:72:ILE:O	1:A:75:GLN:OE1	2.26	0.54
1:B:8:LEU:CD1	1:B:8:LEU:H	2.16	0.54
1:A:40:ILE:HG22	1:A:44:ARG:CZ	2.38	0.54
1:A:258:LEU:O	1:A:261:TYR:N	2.36	0.54
1:B:278:LEU:HD23	1:B:285:ILE:HB	1.89	0.54
1:A:8:LEU:C	1:A:11:ILE:HG22	2.32	0.54
1:A:116:ARG:HG3	1:A:116:ARG:O	2.08	0.54
1:A:162:ARG:NH2	1:A:170:ARG:HG2	2.23	0.54
1:A:256:GLU:OE1	1:A:260:PRO:HG3	2.08	0.54
1:B:171:VAL:CG2	1:B:269:ASP:HA	2.36	0.54
1:A:279:ILE:HG23	1:A:283:LYS:C	2.33	0.53
1:A:251:GLU:O	1:A:254:GLU:N	2.41	0.53
1:A:309:TRP:N	1:A:309:TRP:CD1	2.75	0.53
1:B:64:ILE:HD13	1:B:65:GLN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:NH1	1:A:224:ILE:HD12	2.23	0.53
1:B:207:ILE:HG22	1:B:209:MET:CG	2.37	0.53
1:A:152:VAL:O	1:A:156:VAL:HG23	2.08	0.53
1:B:4:ASN:O	1:B:4:ASN:OD1	2.26	0.53
1:A:74:GLY:O	1:A:75:GLN:O	2.27	0.53
1:B:6:VAL:CB	1:B:7:PRO:HD3	2.39	0.53
1:B:8:LEU:HD12	1:B:8:LEU:N	2.19	0.53
1:B:137:TRP:CE3	1:B:250:LEU:HD12	2.44	0.53
1:A:87:ILE:O	1:A:112:GLN:HA	2.09	0.53
1:B:147:ILE:HD13	1:B:147:ILE:H	1.74	0.53
1:B:176:ASP:CG	1:B:183:LYS:HE3	2.33	0.52
1:B:48:VAL:CG1	1:B:50:VAL:HG23	2.37	0.52
1:A:276:VAL:CG2	1:A:314:ILE:HD11	2.39	0.52
1:A:252:LEU:HA	1:A:255:GLN:HG3	1.90	0.52
1:B:208:ASN:HD21	1:B:223:TRP:HZ3	1.56	0.52
1:A:16:ASN:ND2	1:A:18:GLU:N	2.51	0.52
1:B:68:ASN:C	1:B:72:ILE:HD12	2.35	0.52
1:B:24:GLN:O	1:B:28:THR:HG23	2.09	0.52
1:B:282:ASP:O	1:B:282:ASP:OD2	2.28	0.52
1:B:285:ILE:C	1:B:286:PHE:HD1	2.18	0.52
1:A:110:GLU:OE1	1:A:235:ARG:NH2	2.31	0.52
1:B:49:ASP:O	1:B:61:PRO:HD3	2.09	0.52
1:B:127:PHE:CD1	1:B:127:PHE:C	2.88	0.52
1:A:173:TRP:CD1	1:A:292:ILE:CG2	2.93	0.52
1:A:182:ARG:HB2	1:A:224:ILE:HG22	1.90	0.51
1:A:6:VAL:CB	1:A:7:PRO:HD3	2.39	0.51
1:A:147:ILE:CG2	1:A:148:GLY:N	2.73	0.51
1:A:300:LEU:O	1:A:302:GLN:OE1	2.28	0.51
1:A:263:SER:HA	1:A:266:GLU:CG	2.40	0.51
1:B:210:ALA:O	1:B:225:THR:HG21	2.11	0.51
1:B:170:ARG:HG3	1:B:170:ARG:NH1	2.21	0.51
1:B:265:TRP:CD1	1:B:265:TRP:C	2.89	0.51
1:A:149:LEU:HD23	1:A:149:LEU:C	2.35	0.51
1:A:223:TRP:CD1	1:A:223:TRP:N	2.78	0.51
1:A:285:ILE:HG21	1:A:309:TRP:CZ3	2.43	0.51
1:B:26:GLY:CA	1:B:36:ILE:HD13	2.39	0.51
1:A:142:GLY:C	1:A:199:ALA:HB2	2.35	0.51
1:A:257:GLY:O	1:A:260:PRO:HD2	2.11	0.51
1:A:65:GLN:NE2	1:A:66:LEU:HD12	2.25	0.51
1:A:98:ILE:HD12	1:A:200:GLN:HB2	1.92	0.51
1:A:243:ILE:O	1:A:243:ILE:HG22	2.05	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HB3	1:A:309:TRP:CZ2	2.46	0.51
1:B:123:TRP:CH2	1:B:223:TRP:CH2	2.98	0.51
1:B:280:ILE:C	1:B:282:ASP:H	2.19	0.51
1:A:153:ILE:O	1:A:157:MET:HG3	2.10	0.51
1:A:298:LEU:HG	1:A:299:LEU:N	2.26	0.51
1:B:170:ARG:HD3	1:B:268:LEU:O	2.10	0.51
1:B:314:ILE:O	1:B:315:SER:HB3	2.10	0.51
1:A:29:LEU:HB3	1:A:31:MET:HG3	1.93	0.50
1:A:131:LEU:HD22	1:A:238:LEU:HG	1.93	0.50
1:A:166:ALA:CB	1:A:231:ILE:HD13	2.41	0.50
1:B:123:TRP:CH2	1:B:223:TRP:HH2	2.28	0.50
1:A:171:VAL:HG22	1:A:268:LEU:C	2.36	0.50
1:B:276:VAL:H	1:B:317:ARG:HH11	1.59	0.50
1:A:171:VAL:HG22	1:A:268:LEU:O	2.11	0.50
1:B:77:ASP:OD1	1:B:77:ASP:O	2.29	0.50
1:B:138:ARG:C	1:B:139:LEU:HD23	2.36	0.50
1:B:58:TYR:CD1	1:B:58:TYR:N	2.80	0.50
1:B:62:GLU:HG2	1:B:63:PRO:O	2.12	0.50
1:B:97:ARG:O	1:B:101:LEU:HG	2.11	0.50
1:A:26:GLY:HA2	1:A:36:ILE:CD1	2.37	0.50
1:A:51:PHE:HD2	1:A:59:SER:HB3	1.76	0.50
1:B:51:PHE:HB3	1:B:59:SER:O	2.12	0.50
1:B:279:ILE:CG2	1:B:283:LYS:H	2.21	0.50
1:B:139:LEU:N	1:B:199:ALA:O	2.34	0.50
1:A:13:LEU:HD13	1:A:25:LEU:HD22	1.94	0.49
1:B:48:VAL:HG12	1:B:49:ASP:N	2.27	0.49
1:B:301:GLU:HB2	1:B:306:ILE:CG1	2.42	0.49
1:B:258:LEU:CD2	1:B:262:LEU:HG	2.42	0.49
1:A:201:ILE:N	1:A:201:ILE:HD12	2.27	0.49
1:B:64:ILE:CD1	1:B:65:GLN:H	2.25	0.49
1:B:81:VAL:HG12	1:B:82:ALA:N	2.25	0.49
1:B:138:ARG:O	1:B:139:LEU:HD23	2.13	0.49
1:B:316:LEU:HD12	1:B:317:ARG:N	2.26	0.49
1:A:259:ALA:HB3	1:A:260:PRO:CD	2.31	0.49
1:B:65:GLN:O	1:B:235:ARG:HD3	2.12	0.49
1:B:277:LYS:O	1:B:314:ILE:HA	2.13	0.49
1:A:40:ILE:HG23	1:A:50:VAL:HG11	1.94	0.49
1:A:82:ALA:O	1:A:107:CYS:HA	2.12	0.49
1:A:68:ASN:O	1:A:71:GLN:N	2.45	0.49
1:A:195:THR:HB	3:A:642:HOH:O	2.12	0.49
1:B:14:LEU:HA	1:B:20:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:THR:O	1:A:8:LEU:HB2	2.12	0.49
1:A:65:GLN:HE21	1:A:66:LEU:HD12	1.78	0.49
1:A:302:GLN:OE1	1:A:305:ILE:O	2.30	0.49
1:B:258:LEU:HD22	1:B:262:LEU:CD1	2.42	0.49
1:A:51:PHE:CZ	1:A:53:VAL:CG2	2.96	0.49
1:A:175:ASN:O	1:A:176:ASP:OD1	2.31	0.49
1:A:58:TYR:CD1	1:A:58:TYR:N	2.81	0.48
1:A:277:LYS:HE3	1:A:286:PHE:CD1	2.48	0.48
1:B:65:GLN:NE2	1:B:234:ASP:OD2	2.42	0.48
1:B:90:THR:O	1:B:93:TYR:HB3	2.13	0.48
1:B:210:ALA:HA	1:B:227:GLN:NE2	2.28	0.48
1:A:16:ASN:ND2	1:A:18:GLU:CB	2.76	0.48
1:B:6:VAL:O	1:B:9:LYS:HB2	2.12	0.48
1:A:128:GLY:HA2	1:A:235:ARG:NH2	2.28	0.48
1:A:259:ALA:CB	1:A:260:PRO:HD3	2.25	0.48
1:A:301:GLU:HA	1:A:305:ILE:O	2.14	0.48
1:B:262:LEU:CB	1:B:294:LYS:HD2	2.44	0.48
1:A:5:THR:C	1:A:7:PRO:HD2	2.38	0.48
1:A:85:PRO:C	1:A:86:VAL:HG23	2.38	0.48
1:B:119:ARG:CZ	1:B:281:GLY:HA2	2.43	0.48
1:A:9:LYS:O	1:A:12:ALA:HB3	2.13	0.48
1:B:307:LYS:HD3	1:B:308:PRO:O	2.14	0.48
1:B:82:ALA:O	1:B:107:CYS:HA	2.14	0.48
1:B:207:ILE:HG22	1:B:207:ILE:O	2.12	0.48
1:B:172:LYS:CG	1:B:271:PHE:CE2	2.95	0.48
1:B:285:ILE:HG21	1:B:309:TRP:CZ2	2.49	0.48
1:B:149:LEU:CD2	1:B:253:PHE:CE2	2.97	0.47
1:B:302:GLN:HE22	1:B:309:TRP:HZ2	1.61	0.47
1:B:84:LEU:HD23	1:B:87:ILE:HG13	1.96	0.47
1:B:292:ILE:HB	1:B:296:GLY:HA2	1.96	0.47
1:A:8:LEU:HA	1:A:11:ILE:CG2	2.44	0.47
1:A:10:LEU:HA	1:A:10:LEU:HD23	1.56	0.47
1:A:278:LEU:HG	1:A:285:ILE:HD12	1.96	0.47
1:B:6:VAL:CB	1:B:7:PRO:CD	2.92	0.47
1:B:144:ALA:O	1:B:145:ALA:HB2	2.15	0.47
1:B:255:GLN:C	1:B:257:GLY:H	2.22	0.47
1:B:274:ARG:HB3	1:B:275:PRO:CD	2.43	0.47
1:B:314:ILE:HB	1:B:315:SER:H	1.54	0.47
1:A:44:ARG:HA	1:A:48:VAL:O	2.14	0.47
1:A:5:THR:O	1:A:8:LEU:N	2.48	0.47
1:A:6:VAL:N	1:A:7:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLN:HB2	1:A:125:SER:CB	2.44	0.47
1:B:49:ASP:O	1:B:60:LEU:HD23	2.14	0.47
1:A:61:PRO:HD2	1:A:62:GLU:H	1.79	0.47
1:A:82:ALA:HA	3:A:638:HOH:O	2.14	0.47
1:B:277:LYS:HG2	1:B:286:PHE:CZ	2.50	0.47
1:A:252:LEU:HD12	1:A:252:LEU:C	2.37	0.47
1:B:93:TYR:HD2	1:B:94:LEU:CD2	2.22	0.47
1:B:137:TRP:CH2	1:B:250:LEU:HB2	2.50	0.47
1:A:80:SER:H	1:A:247:ARG:NH2	2.13	0.47
1:B:116:ARG:HG2	1:B:116:ARG:HH11	1.80	0.47
1:B:130:ASN:HB3	1:B:207:ILE:O	2.14	0.47
1:A:238:LEU:O	1:A:242:LEU:HG	2.15	0.47
1:A:259:ALA:N	1:A:260:PRO:CD	2.78	0.47
1:B:210:ALA:HA	1:B:227:GLN:CD	2.40	0.47
1:A:13:LEU:HG	1:A:13:LEU:H	1.54	0.46
1:B:110:GLU:O	1:B:127:PHE:HA	2.15	0.46
1:B:258:LEU:HD22	1:B:262:LEU:HG	1.96	0.46
1:B:276:VAL:N	1:B:317:ARG:HB2	2.30	0.46
1:A:10:LEU:HD23	1:A:13:LEU:HD11	1.97	0.46
1:B:207:ILE:O	1:B:209:MET:HG3	2.15	0.46
1:B:98:ILE:HD12	1:B:98:ILE:C	2.40	0.46
1:B:133:LEU:HD11	1:B:243:ILE:HD11	1.96	0.46
1:B:301:GLU:HA	1:B:306:ILE:CD1	2.46	0.46
1:A:286:PHE:CD2	1:A:317:ARG:HD2	2.50	0.46
1:B:123:TRP:CZ3	1:B:223:TRP:CH2	2.95	0.46
1:B:137:TRP:CE3	1:B:250:LEU:CD1	2.98	0.46
1:A:16:ASN:ND2	1:A:18:GLU:CG	2.79	0.46
1:A:21:SER:C	1:A:23:GLU:H	2.22	0.46
1:A:111:TYR:CB	1:A:127:PHE:CD2	2.99	0.46
1:A:223:TRP:N	1:A:223:TRP:HD1	2.13	0.46
1:B:157:MET:HB2	1:B:177:LEU:HD11	1.98	0.46
1:B:277:LYS:HB3	1:B:286:PHE:CE1	2.50	0.46
1:A:6:VAL:N	1:A:7:PRO:HD2	2.31	0.46
1:A:40:ILE:CG2	1:A:44:ARG:NH1	2.79	0.46
1:A:272:ILE:HA	1:A:289:SER:HB3	1.97	0.46
1:A:279:ILE:HG23	1:A:283:LYS:N	2.31	0.46
1:B:31:MET:CB	1:B:36:ILE:HD12	2.45	0.46
1:B:173:TRP:HA	1:B:174:PRO:HA	1.50	0.46
1:B:195:THR:C	1:B:197:ASP:N	2.74	0.46
1:B:280:ILE:C	1:B:282:ASP:N	2.74	0.46
1:A:4:ASN:HD22	1:A:4:ASN:HA	1.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LEU:HD12	1:B:11:ILE:N	2.31	0.46
1:B:259:ALA:O	1:B:261:TYR:N	2.49	0.46
1:B:278:LEU:N	1:B:285:ILE:O	2.49	0.46
1:A:89:SER:HA	1:A:112:GLN:HG2	1.98	0.46
1:A:211:MET:HG3	1:A:228:GLU:HG3	1.97	0.46
1:B:310:MET:O	1:B:311:GLY:O	2.34	0.46
1:A:166:ALA:HB2	1:A:231:ILE:HD13	1.98	0.45
1:A:279:ILE:HG13	1:A:284:GLU:HA	1.98	0.45
1:A:32:SER:OG	1:A:35:ALA:N	2.41	0.45
1:A:118:ARG:CZ	1:A:175:ASN:HB2	2.46	0.45
1:A:139:LEU:O	1:A:198:ALA:HA	2.16	0.45
1:A:277:LYS:O	1:A:314:ILE:HD13	2.17	0.45
1:B:16:ASN:HD21	1:B:18:GLU:HB2	1.78	0.45
1:B:24:GLN:HA	1:B:27:GLU:OE2	2.15	0.45
1:B:43:LEU:HD23	1:B:46:TRP:CE3	2.51	0.45
1:B:298:LEU:HG	1:B:299:LEU:N	2.32	0.45
1:A:26:GLY:CA	1:A:36:ILE:HD11	2.37	0.45
1:A:276:VAL:CB	1:A:314:ILE:HD11	2.45	0.45
1:B:182:ARG:HB2	1:B:224:ILE:CG2	2.46	0.45
1:B:188:LEU:HB2	2:B:501:BTN:H101	1.98	0.45
1:B:286:PHE:C	1:B:300:LEU:HD23	2.41	0.45
1:B:307:LYS:HG2	1:B:308:PRO:CD	2.47	0.45
1:A:11:ILE:CG2	1:A:12:ALA:N	2.80	0.45
1:A:126:PRO:HD2	1:A:132:TYR:OH	2.16	0.45
1:B:98:ILE:HG22	1:B:136:PHE:CE1	2.51	0.45
1:B:195:THR:C	1:B:197:ASP:H	2.23	0.45
1:A:41:GLN:HG3	1:A:41:GLN:H	1.70	0.45
1:A:85:PRO:O	1:A:110:GLU:HB2	2.16	0.45
1:A:130:ASN:HB3	1:A:207:ILE:O	2.16	0.45
1:B:50:VAL:HG22	1:B:60:LEU:HD21	1.99	0.45
1:B:80:SER:HB3	1:B:105:ASP:OD1	2.16	0.45
1:B:171:VAL:HG23	1:B:269:ASP:CA	2.40	0.45
1:A:303:ASP:C	1:A:305:ILE:N	2.73	0.45
1:B:7:PRO:CG	1:B:42:THR:HG21	2.46	0.45
1:B:103:SER:OG	1:B:138:ARG:HB3	2.16	0.45
1:B:171:VAL:CG2	1:B:269:ASP:N	2.80	0.45
1:A:293:ASP:OD1	1:A:297:ALA:HB3	2.16	0.45
1:B:76:LEU:HG	1:B:247:ARG:NH1	2.31	0.45
1:B:84:LEU:CD2	1:B:107:CYS:SG	3.05	0.45
1:B:262:LEU:HD13	1:B:294:LYS:CE	2.46	0.45
1:A:38:LYS:HG3	1:A:41:GLN:HE22	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:HG3	1:A:295:GLN:NE2	2.32	0.45
1:B:40:ILE:HD12	1:B:58:TYR:CG	2.52	0.45
1:B:171:VAL:HG22	1:B:269:ASP:N	2.31	0.45
1:B:5:THR:CA	1:B:8:LEU:HD11	2.44	0.44
1:B:279:ILE:HG23	1:B:283:LYS:O	2.18	0.44
1:B:7:PRO:O	1:B:10:LEU:CD1	2.66	0.44
1:B:102:LYS:HD2	1:B:102:LYS:HA	1.43	0.44
1:A:92:GLN:NE2	1:A:92:GLN:HA	2.32	0.44
1:A:173:TRP:O	1:A:314:ILE:HG21	2.17	0.44
1:B:11:ILE:HD12	1:B:11:ILE:O	2.17	0.44
1:B:186:GLY:HA3	2:B:501:BTN:O12	2.17	0.44
1:A:11:ILE:HG23	1:A:12:ALA:N	2.32	0.44
1:A:51:PHE:CD2	1:A:59:SER:HB3	2.53	0.44
1:A:60:LEU:HB3	1:A:61:PRO:CD	2.45	0.44
1:A:101:LEU:O	1:A:102:LYS:HE2	2.17	0.44
1:A:111:TYR:HB2	1:A:127:PHE:CA	2.42	0.44
1:A:141:GLN:H	1:A:141:GLN:CD	2.25	0.44
1:A:182:ARG:CZ	1:A:224:ILE:HB	2.47	0.44
1:B:227:GLN:O	1:B:230:GLY:N	2.41	0.44
1:A:298:LEU:CG	1:A:299:LEU:N	2.76	0.44
1:A:314:ILE:HD12	1:A:315:SER:H	1.82	0.44
1:A:53:VAL:HA	1:A:54:PRO:HD2	1.51	0.44
1:B:84:LEU:HD22	1:B:107:CYS:SG	2.58	0.44
1:B:133:LEU:HD11	1:B:243:ILE:CD1	2.48	0.44
1:B:191:LEU:H	1:B:191:LEU:HG	1.53	0.44
1:B:37:ASN:CB	1:B:38:LYS:NZ	2.77	0.44
1:B:300:LEU:HD12	1:B:300:LEU:HA	1.79	0.44
1:A:243:ILE:HG22	1:A:247:ARG:HG3	1.99	0.44
1:B:265:TRP:NE1	1:B:269:ASP:HB2	2.33	0.44
1:A:82:ALA:HB3	1:A:107:CYS:HB3	1.99	0.43
1:B:4:ASN:C	1:B:6:VAL:N	2.75	0.43
1:B:146:ALA:HB1	1:B:147:ILE:HD13	2.00	0.43
1:B:208:ASN:ND2	1:B:223:TRP:CZ3	2.83	0.43
1:A:93:TYR:CA	1:A:97:ARG:NH1	2.79	0.43
1:B:166:ALA:O	1:B:169:VAL:HG23	2.18	0.43
1:A:115:GLY:N	3:A:604:HOH:O	2.44	0.43
1:B:170:ARG:HG2	1:B:268:LEU:O	2.18	0.43
1:A:8:LEU:HA	1:A:11:ILE:HG21	1.99	0.43
1:A:73:LEU:O	1:A:74:GLY:O	2.35	0.43
1:A:90:THR:OG1	2:A:500:BTN:H62	2.19	0.43
1:B:32:SER:OG	1:B:35:ALA:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ILE:O	1:B:247:ARG:HG3	2.18	0.43
1:A:298:LEU:CD1	1:A:299:LEU:N	2.81	0.43
1:A:19:PHE:C	1:A:20:HIS:ND1	2.77	0.43
1:A:65:GLN:O	1:A:235:ARG:NH1	2.48	0.43
1:B:4:ASN:HA	1:B:6:VAL:HG23	2.00	0.43
1:B:182:ARG:HH11	1:B:221:GLN:HB3	1.84	0.43
1:B:277:LYS:HA	1:B:286:PHE:CD1	2.53	0.43
1:A:173:TRP:HA	1:A:174:PRO:HA	1.82	0.43
1:A:29:LEU:HD13	1:A:29:LEU:HA	1.31	0.43
1:A:145:ALA:O	1:A:146:ALA:HB3	2.19	0.43
1:A:299:LEU:HD22	1:A:299:LEU:HA	1.72	0.43
1:A:302:GLN:O	1:A:305:ILE:HB	2.18	0.43
1:B:76:LEU:HD12	1:B:76:LEU:HA	1.70	0.43
1:B:122:LYS:CE	1:B:124:PHE:HB2	2.48	0.43
1:B:178:TYR:HA	1:B:182:ARG:O	2.19	0.43
1:B:182:ARG:NH1	1:B:221:GLN:HE21	2.14	0.43
1:B:5:THR:C	1:B:8:LEU:HD12	2.44	0.43
1:B:10:LEU:CD1	1:B:11:ILE:N	2.82	0.43
1:A:21:SER:C	1:A:23:GLU:N	2.77	0.42
1:B:226:LEU:HD23	1:B:226:LEU:HA	1.81	0.42
1:A:8:LEU:O	1:A:11:ILE:HG22	2.19	0.42
1:A:24:GLN:O	1:A:27:GLU:HG2	2.19	0.42
1:A:26:GLY:CA	1:A:36:ILE:CD1	2.96	0.42
1:B:94:LEU:C	1:B:96:ASP:N	2.75	0.42
1:B:98:ILE:HD12	1:B:99:GLY:H	1.79	0.42
1:B:264:ARG:O	1:B:268:LEU:HD12	2.19	0.42
1:B:288:ILE:HG22	1:B:289:SER:O	2.20	0.42
1:A:65:GLN:HE21	1:A:65:GLN:HA	1.84	0.42
1:B:164:LEU:CD2	1:B:241:MET:HE3	2.48	0.42
1:B:236:ASN:HD22	1:B:236:ASN:N	2.17	0.42
1:A:75:GLN:C	1:A:77:ASP:H	2.27	0.42
1:B:48:VAL:CG1	1:B:49:ASP:N	2.81	0.42
1:B:112:GLN:CD	2:B:501:BTN:H62	2.45	0.42
1:B:262:LEU:HD13	1:B:294:LYS:HE3	2.01	0.42
1:B:272:ILE:HD11	1:B:290:ARG:HA	2.02	0.42
1:A:307:LYS:HD2	1:A:307:LYS:HA	1.85	0.42
1:B:125:SER:HA	1:B:126:PRO:HD2	1.93	0.42
1:A:80:SER:N	1:A:247:ARG:HH22	2.16	0.42
1:A:167:ASP:OD2	1:A:167:ASP:N	2.29	0.42
1:A:274:ARG:HB3	1:A:275:PRO:CD	2.50	0.42
1:B:6:VAL:CG2	1:B:7:PRO:CD	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:GLU:O	1:B:255:GLN:NE2	2.53	0.42
1:B:279:ILE:C	1:B:313:GLU:H	2.27	0.42
1:A:166:ALA:HA	1:A:231:ILE:CD1	2.47	0.42
1:A:278:LEU:HG	1:A:285:ILE:CD1	2.50	0.42
1:B:149:LEU:HD12	1:B:153:ILE:HD11	2.02	0.42
1:B:259:ALA:CB	1:B:260:PRO:CD	2.92	0.42
1:A:258:LEU:C	1:A:260:PRO:HD2	2.44	0.42
1:A:280:ILE:HD12	1:A:281:GLY:N	2.35	0.42
1:B:7:PRO:HG3	1:B:42:THR:HG21	2.02	0.42
1:B:136:PHE:C	1:B:136:PHE:CD2	2.97	0.42
1:B:280:ILE:HG23	1:B:281:GLY:N	2.34	0.42
1:A:123:TRP:O	1:A:124:PHE:HB3	2.20	0.42
1:A:259:ALA:CB	1:A:260:PRO:CD	2.95	0.42
1:B:33:ARG:H	1:B:33:ARG:HG2	1.50	0.42
1:A:280:ILE:HD13	1:A:312:GLY:HA2	2.00	0.41
1:A:138:ARG:HG2	1:A:198:ALA:HB1	2.02	0.41
1:B:289:SER:HA	1:B:300:LEU:HD12	2.02	0.41
1:A:69:ALA:HB3	1:A:70:LYS:HD2	2.01	0.41
1:A:149:LEU:C	1:A:153:ILE:HD12	2.45	0.41
1:A:164:LEU:HD21	1:A:241:MET:HE3	2.02	0.41
1:A:177:LEU:C	1:A:178:TYR:CD1	2.99	0.41
1:B:111:TYR:HE2	1:B:113:GLN:HG2	1.76	0.41
1:B:119:ARG:HH12	1:B:281:GLY:CA	2.26	0.41
1:B:262:LEU:HD21	1:B:294:LYS:HA	1.94	0.41
1:B:40:ILE:HD12	1:B:58:TYR:CD2	2.55	0.41
1:B:170:ARG:NH1	1:B:170:ARG:CG	2.75	0.41
1:B:293:ASP:HB3	1:B:297:ALA:H	1.85	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.91	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.90	0.41
1:A:288:ILE:HG22	1:A:289:SER:N	2.34	0.41
1:B:84:LEU:HA	1:B:85:PRO:HD3	1.69	0.41
1:A:43:LEU:C	1:A:45:ASP:N	2.75	0.41
1:B:110:GLU:OE1	1:B:128:GLY:HA2	2.21	0.41
1:B:131:LEU:O	1:B:206:GLY:HA2	2.20	0.41
1:B:262:LEU:CB	1:B:294:LYS:CE	2.98	0.41
1:B:272:ILE:HD13	1:B:291:GLY:N	2.36	0.41
1:A:165:GLY:O	1:A:167:ASP:N	2.54	0.41
1:A:283:LYS:HB3	1:A:283:LYS:HE2	1.75	0.41
1:A:314:ILE:HD12	1:A:314:ILE:C	2.40	0.41
1:B:25:LEU:HB2	1:B:36:ILE:HG12	2.03	0.41
1:B:293:ASP:CG	1:B:294:LYS:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HB3	1:A:31:MET:CG	2.51	0.41
1:A:68:ASN:O	1:A:69:ALA:C	2.63	0.41
1:A:263:SER:HA	1:A:266:GLU:CD	2.46	0.41
1:A:277:LYS:HE2	1:A:284:GLU:OE2	2.20	0.41
1:B:111:TYR:CE2	1:B:113:GLN:CG	2.97	0.41
1:A:6:VAL:CB	1:A:7:PRO:CD	2.97	0.40
1:A:75:GLN:OE1	1:A:76:LEU:HD23	2.21	0.40
1:A:238:LEU:HD12	1:A:238:LEU:C	2.45	0.40
1:B:147:ILE:HD13	1:B:147:ILE:N	2.35	0.40
1:B:7:PRO:HA	1:B:10:LEU:HD11	2.03	0.40
1:B:149:LEU:O	1:B:152:VAL:N	2.54	0.40
1:A:10:LEU:C	1:A:12:ALA:N	2.79	0.40
1:A:51:PHE:CD2	1:A:51:PHE:C	2.99	0.40
1:A:144:ALA:O	1:A:145:ALA:HB2	2.22	0.40
1:A:179:LEU:C	1:A:181:ASP:N	2.79	0.40
1:A:307:LYS:CE	1:A:308:PRO:HD2	2.46	0.40
1:A:60:LEU:CB	1:A:61:PRO:CD	2.99	0.40
1:A:252:LEU:HD11	1:A:256:GLU:OE2	2.22	0.40
1:B:288:ILE:CG2	1:B:290:ARG:NH1	2.84	0.40

There are no symmetry-related clashes.

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	301/321 (94%)	249 (83%)	39 (13%)	13 (4%)	2	1
1	B	301/321 (94%)	249 (83%)	35 (12%)	17 (6%)	1	1
All	All	602/642 (94%)	498 (83%)	74 (12%)	30 (5%)	1	1

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	54	PRO
1	A	75	GLN
1	A	145	ALA
1	A	147	ILE
1	A	166	ALA
1	A	262	LEU
1	B	124	PHE
1	B	143	PRO
1	B	145	ALA
1	B	256	GLU
1	B	259	ALA
1	B	281	GLY
1	B	315	SER
1	B	316	LEU
1	A	74	GLY
1	A	77	ASP
1	A	85	PRO
1	A	304	GLY
1	B	85	PRO
1	B	255	GLN
1	B	311	GLY
1	A	197	ASP
1	B	54	PRO
1	B	153	ILE
1	B	314	ILE
1	B	77	ASP
1	B	260	PRO
1	A	303	ASP
1	B	308	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	243/258 (94%)	167 (69%)	76 (31%)	0 0
1	B	243/258 (94%)	170 (70%)	73 (30%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	486/516 (94%)	337 (69%)	149 (31%)	0 0

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	5	THR
1	A	11	ILE
1	A	13	LEU
1	A	18	GLU
1	A	23	GLU
1	A	24	GLN
1	A	29	LEU
1	A	31	MET
1	A	33	ARG
1	A	36	ILE
1	A	38	LYS
1	A	41	GLN
1	A	48	VAL
1	A	56	LYS
1	A	62	GLU
1	A	64	ILE
1	A	65	GLN
1	A	66	LEU
1	A	70	LYS
1	A	71	GLN
1	A	75	GLN
1	A	77	ASP
1	A	84	LEU
1	A	87	ILE
1	A	88	ASP
1	A	89	SER
1	A	92	GLN
1	A	98	ILE
1	A	108	ILE
1	A	118	ARG
1	A	122	LYS
1	A	125	SER
1	A	133	LEU
1	A	138	ARG
1	A	140	GLU
1	A	141	GLN

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Mol	Chain	Res	Type
1	A	149	LEU
1	A	150	SER
1	A	164	LEU
1	A	167	ASP
1	A	168	LYS
1	A	172	LYS
1	A	182	ARG
1	A	191	LEU
1	A	197	ASP
1	A	200	GLN
1	A	201	ILE
1	A	211	MET
1	A	241	MET
1	A	245	GLU
1	A	252	LEU
1	A	255	GLN
1	A	266	GLU
1	A	274	ARG
1	A	276	VAL
1	A	278	LEU
1	A	280	ILE
1	A	282	ASP
1	A	283	LYS
1	A	284	GLU
1	A	285	ILE
1	A	286	PHE
1	A	292	ILE
1	A	293	ASP
1	A	294	LYS
1	A	299	LEU
1	A	300	LEU
1	A	301	GLU
1	A	302	GLN
1	A	303	ASP
1	A	307	LYS
1	A	309	TRP
1	A	313	GLU
1	A	314	ILE
1	A	316	LEU
1	B	4	ASN
1	B	5	THR
1	B	6	VAL

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Mol	Chain	Res	Type
1	B	8	LEU
1	B	9	LYS
1	B	10	LEU
1	B	11	ILE
1	B	18	GLU
1	B	25	LEU
1	B	27	GLU
1	B	28	THR
1	B	31	MET
1	B	32	SER
1	B	33	ARG
1	B	36	ILE
1	B	38	LYS
1	B	40	ILE
1	B	45	ASP
1	B	56	LYS
1	B	58	TYR
1	B	64	ILE
1	B	72	ILE
1	B	75	GLN
1	B	76	LEU
1	B	77	ASP
1	B	80	SER
1	B	84	LEU
1	B	87	ILE
1	B	94	LEU
1	B	95	LEU
1	B	97	ARG
1	B	100	GLU
1	B	102	LYS
1	B	108	ILE
1	B	116	ARG
1	B	118	ARG
1	B	121	ARG
1	B	122	LYS
1	B	131	LEU
1	B	133	LEU
1	B	139	LEU
1	B	147	ILE
1	B	149	LEU
1	B	150	SER
1	B	157	MET

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Mol	Chain	Res	Type
1	B	167	ASP
1	B	168	LYS
1	B	172	LYS
1	B	195	THR
1	B	200	GLN
1	B	201	ILE
1	B	207	ILE
1	B	211	MET
1	B	231	ILE
1	B	241	MET
1	B	243	ILE
1	B	252	LEU
1	B	255	GLN
1	B	258	LEU
1	B	272	ILE
1	B	276	VAL
1	B	278	LEU
1	B	279	ILE
1	B	280	ILE
1	B	283	LYS
1	B	285	ILE
1	B	292	ILE
1	B	300	LEU
1	B	302	GLN
1	B	303	ASP
1	B	305	ILE
1	B	313	GLU
1	B	314	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	16	ASN
1	A	39	HIS
1	A	65	GLN
1	A	113	GLN
1	A	200	GLN
1	A	227	GLN
1	A	295	GLN
1	B	4	ASN
1	B	16	ASN

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Mol	Chain	Res	Type
1	B	141	GLN
1	B	180	GLN
1	B	221	GLN
1	B	227	GLN
1	B	273	ASN
1	B	302	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BTN	B	501	-	17,17,17	0.71	0	23,23,23	1.69	4 (17%)
2	BTN	A	500	-	17,17,17	0.64	0	23,23,23	1.43	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BTN	B	501	-	-	2/7/28/28	0/2/2/2
2	BTN	A	500	-	-	2/7/28/28	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	BTN	C2-C4-N2	-4.81	108.25	113.34
2	B	501	BTN	C2-C4-N2	4.16	117.75	113.34
2	B	501	BTN	C6-S1-C2	3.93	98.15	89.98
2	B	501	BTN	C9-C10-C11	-2.62	107.68	114.51
2	A	500	BTN	C6-C5-N1	-2.61	109.81	113.18
2	B	501	BTN	C6-C5-N1	-2.03	110.56	113.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	BTN	C9-C10-C11-O11
2	A	500	BTN	C9-C10-C11-O12
2	B	501	BTN	C9-C10-C11-O11
2	B	501	BTN	C9-C10-C11-O12

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	BTN	5	0
2	A	500	BTN	1	0

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 [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	305/321 (95%)	-0.65	1 (0%) 90 88	13, 37, 88, 99	0
1	B	305/321 (95%)	-0.62	3 (0%) 79 76	14, 36, 83, 100	0
All	All	610/642 (95%)	-0.64	4 (0%) 84 81	13, 36, 86, 100	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	ASP	3.6
1	A	282	ASP	2.2
1	B	147	ILE	2.1
1	B	196	GLY	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BTN	B	501	16/16	0.98	0.06	1,23,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BTN	A	500	16/16	0.99	0.04	2,18,60,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.