



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:28 PM UTC

PDB ID : 4BEJ / pdb_00004bej
Title : Nucleotide-free Dynamin 1-like protein (DNM1L, DRP1, DLP1)
Authors : Froehlich, C.; Schwefel, D.; Faelber, K.; Daumke, O.
Deposited on : 2013-03-11
Resolution : 3.48 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

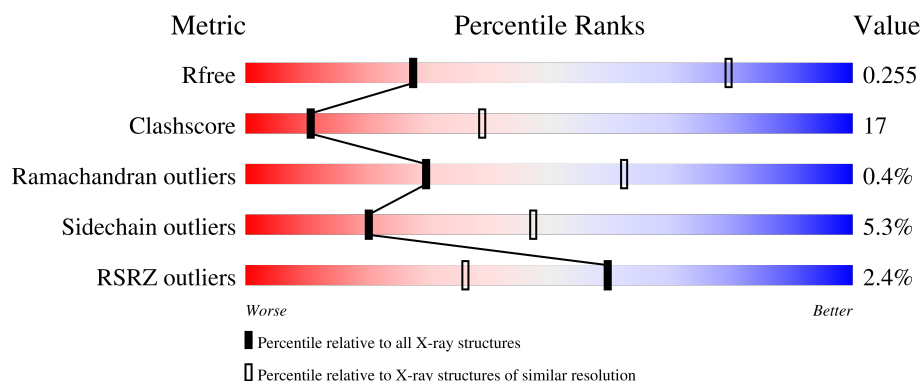
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	617	0% 53% 31% • 12%
1	B	617	2% 52% 33% • 11%
1	C	617	3% 49% 32% 5% 13%
1	D	617	2% 52% 30% • • 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17076 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 DYNAMIN 1-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4263	2701	740	801	21			
1	B	547	Total	C	N	O	S	0	0	0
			4313	2728	755	810	20			
1	C	534	Total	C	N	O	S	0	0	0
			4218	2678	736	785	19			
1	D	540	Total	C	N	O	S	0	0	0
			4282	2717	748	797	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP O00429
A	-5	PRO	-	expression tag	UNP O00429
A	-4	HIS	-	expression tag	UNP O00429
A	-3	MET	-	expression tag	UNP O00429
A	-2	GLY	-	expression tag	UNP O00429
A	-1	GLY	-	expression tag	UNP O00429
A	0	SER	-	expression tag	UNP O00429
A	401	ALA	GLY	engineered mutation	UNP O00429
A	402	ALA	PRO	engineered mutation	UNP O00429
A	403	ALA	ARG	engineered mutation	UNP O00429
A	404	ALA	PRO	engineered mutation	UNP O00429
B	-6	GLY	-	expression tag	UNP O00429
B	-5	PRO	-	expression tag	UNP O00429
B	-4	HIS	-	expression tag	UNP O00429
B	-3	MET	-	expression tag	UNP O00429
B	-2	GLY	-	expression tag	UNP O00429
B	-1	GLY	-	expression tag	UNP O00429
B	0	SER	-	expression tag	UNP O00429
B	401	ALA	GLY	engineered mutation	UNP O00429
B	402	ALA	PRO	engineered mutation	UNP O00429
B	403	ALA	ARG	engineered mutation	UNP O00429

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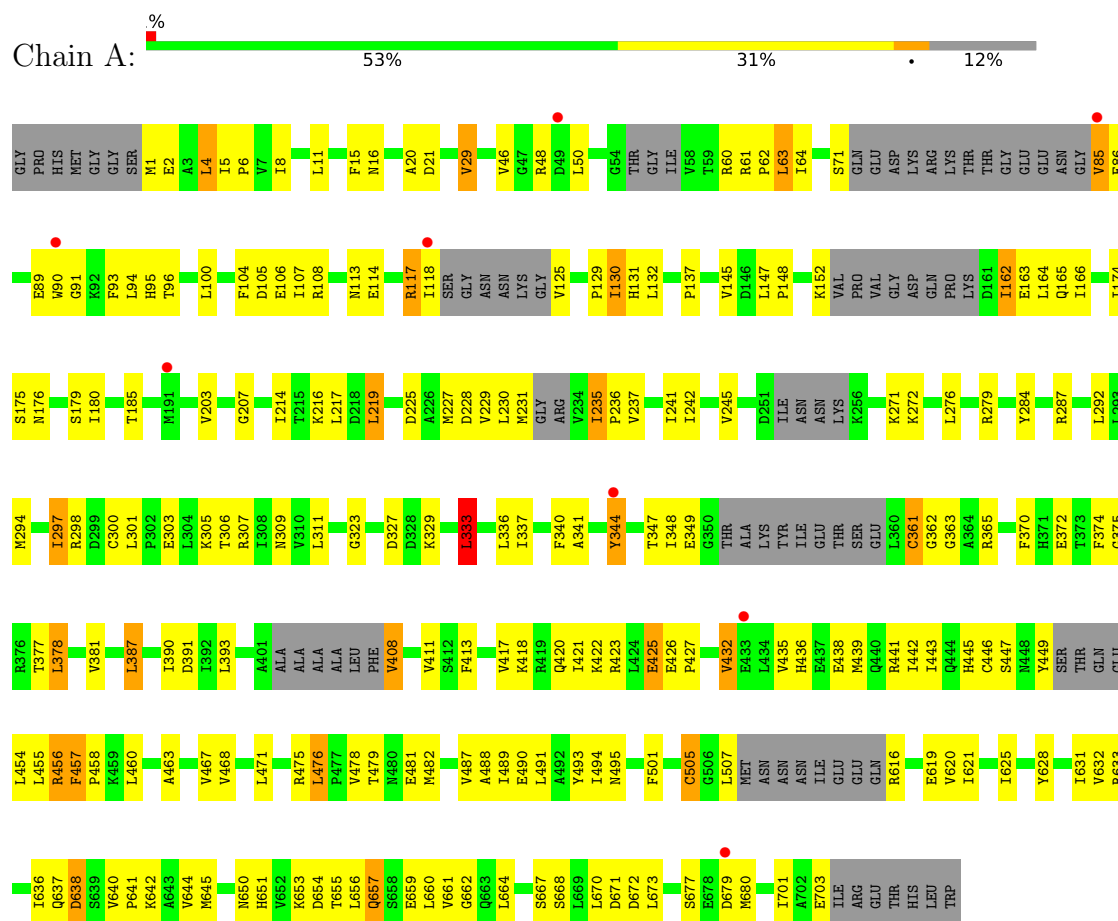
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Chain	Residue	Modelled	Actual	Comment	Reference
B	404	ALA	PRO	engineered mutation	UNP O00429
C	-6	GLY	-	expression tag	UNP O00429
C	-5	PRO	-	expression tag	UNP O00429
C	-4	HIS	-	expression tag	UNP O00429
C	-3	MET	-	expression tag	UNP O00429
C	-2	GLY	-	expression tag	UNP O00429
C	-1	GLY	-	expression tag	UNP O00429
C	0	SER	-	expression tag	UNP O00429
C	401	ALA	GLY	engineered mutation	UNP O00429
C	402	ALA	PRO	engineered mutation	UNP O00429
C	403	ALA	ARG	engineered mutation	UNP O00429
C	404	ALA	PRO	engineered mutation	UNP O00429
D	-6	GLY	-	expression tag	UNP O00429
D	-5	PRO	-	expression tag	UNP O00429
D	-4	HIS	-	expression tag	UNP O00429
D	-3	MET	-	expression tag	UNP O00429
D	-2	GLY	-	expression tag	UNP O00429
D	-1	GLY	-	expression tag	UNP O00429
D	0	SER	-	expression tag	UNP O00429
D	401	ALA	GLY	engineered mutation	UNP O00429
D	402	ALA	PRO	engineered mutation	UNP O00429
D	403	ALA	ARG	engineered mutation	UNP O00429
D	404	ALA	PRO	engineered mutation	UNP O00429

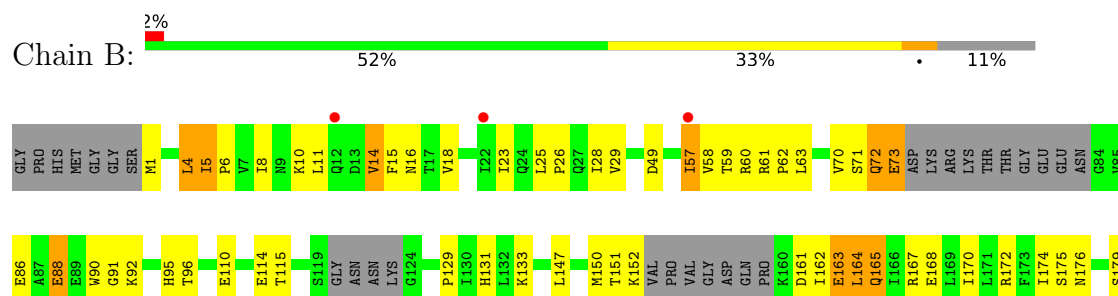
3 Residue-property plots

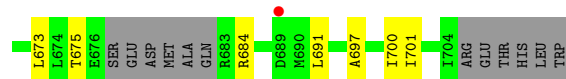
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DYNAMIN 1-LIKE PROTEIN

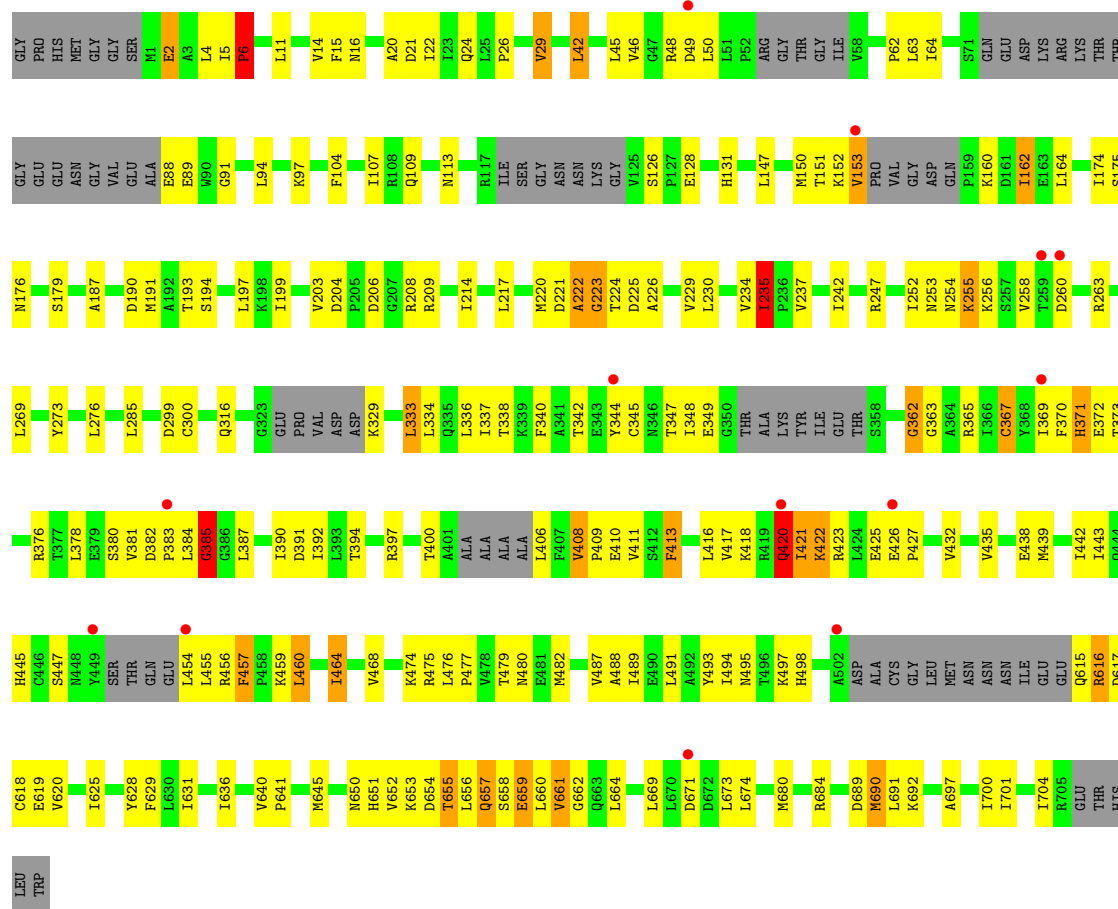


• Molecule 1: DYNAMIN 1-LIKE PROTEIN





● Molecule 1: DYNAMIN 1-LIKE PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.47Å 80.77Å 208.27Å 90.00° 93.45° 90.00°	Depositor
Resolution (Å)	47.57 – 3.48 47.57 – 3.48	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.57-3.48) 97.3 (47.57-3.48)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.276 (Not available) , 0.255	Depositor DCC
R_{free} test set	2124 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	17076	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/4314	1.19	40/5830 (0.7%)
1	B	0.46	0/4366	1.25	47/5900 (0.8%)
1	C	0.51	4/4271 (0.1%)	1.26	47/5771 (0.8%)
1	D	0.46	1/4335 (0.0%)	1.22	45/5855 (0.8%)
All	All	0.47	5/17286 (0.0%)	1.23	179/23356 (0.8%)

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	1
1	C	0	2
1	D	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	LYS	CA-CB	7.00	1.65	1.53
1	C	160	LYS	CB-CG	6.43	1.71	1.52
1	D	6	PRO	CG-CD	6.30	1.72	1.50
1	C	160	LYS	CA-C	5.54	1.60	1.52
1	C	160	LYS	CD-CE	5.53	1.69	1.52

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	THR	N-CA-C	-11.64	93.25	110.48
1	C	664	LEU	N-CA-C	11.46	123.85	111.36
1	B	18	VAL	N-CA-C	11.23	124.00	113.10
1	A	664	LEU	N-CA-C	10.83	123.16	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	GLN	N-CA-C	-9.76	100.64	111.28
1	B	664	LEU	N-CA-C	9.55	121.45	111.14
1	B	329	LYS	N-CA-C	9.54	121.68	111.28
1	D	385	GLY	CA-C-N	9.03	137.95	121.70
1	D	385	GLY	C-N-CA	9.03	137.95	121.70
1	D	6	PRO	CA-N-CD	-8.91	99.52	112.00
1	D	373	THR	N-CA-C	8.88	120.65	110.97
1	A	425	GLU	N-CA-C	8.76	120.45	111.07
1	D	616	ARG	N-CA-C	-8.74	98.75	110.55
1	A	457	PHE	CA-C-N	8.62	128.62	119.05
1	A	457	PHE	C-N-CA	8.62	128.62	119.05
1	B	413	PHE	N-CA-C	8.58	120.63	111.28
1	C	229	VAL	N-CA-C	8.53	120.30	111.00
1	B	324	GLU	CA-C-N	-8.46	111.07	119.87
1	B	324	GLU	C-N-CA	-8.46	111.07	119.87
1	D	420	GLN	N-CA-C	-8.27	101.31	111.40
1	D	253	ASN	N-CA-C	-8.21	99.47	110.55
1	D	370	PHE	CA-C-N	-8.17	109.06	122.54
1	D	370	PHE	C-N-CA	-8.17	109.06	122.54
1	D	460	LEU	N-CA-C	-8.12	101.49	111.40
1	C	408	VAL	CA-C-N	7.98	127.91	119.05
1	C	408	VAL	C-N-CA	7.98	127.91	119.05
1	D	664	LEU	N-CA-C	7.88	119.95	111.36
1	C	163	GLU	CB-CG-CD	-7.74	99.45	112.60
1	C	439	MET	N-CA-C	-7.71	100.93	112.04
1	C	91	GLY	N-CA-C	7.67	123.00	111.18
1	D	371	HIS	CA-C-N	-7.65	106.75	122.58
1	D	371	HIS	C-N-CA	-7.65	106.75	122.58
1	C	160	LYS	N-CA-C	-7.63	103.43	112.89
1	C	159	PRO	CA-C-N	7.62	134.47	121.14
1	C	159	PRO	C-N-CA	7.62	134.47	121.14
1	B	204	ASP	CA-C-N	7.60	126.87	118.97
1	B	204	ASP	C-N-CA	7.60	126.87	118.97
1	C	4	LEU	N-CA-C	7.60	119.64	111.36
1	B	91	GLY	N-CA-C	7.53	122.77	111.18
1	A	162	ILE	N-CA-C	-7.50	103.63	111.58
1	C	163	GLU	N-CA-C	7.25	119.18	111.28
1	B	5	ILE	CA-C-N	7.24	127.09	119.05
1	B	5	ILE	C-N-CA	7.24	127.09	119.05
1	B	16	ASN	N-CA-C	7.24	120.08	111.33
1	B	225	ASP	N-CA-C	-7.23	101.20	110.53
1	D	4	LEU	N-CA-C	7.20	119.21	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	ILE	CA-C-N	7.15	128.78	119.84
1	D	235	ILE	C-N-CA	7.15	128.78	119.84
1	C	160	LYS	CA-CB-CG	7.14	128.38	114.10
1	A	235	ILE	N-CA-C	7.07	113.99	107.56
1	C	2	GLU	CA-C-N	6.99	129.64	120.28
1	C	2	GLU	C-N-CA	6.99	129.64	120.28
1	A	2	GLU	CA-C-N	6.98	130.33	120.28
1	A	2	GLU	C-N-CA	6.98	130.33	120.28
1	D	457	PHE	CA-C-N	6.97	126.79	119.05
1	D	457	PHE	C-N-CA	6.97	126.79	119.05
1	B	662	GLY	N-CA-C	6.91	120.52	112.50
1	B	408	VAL	CA-C-N	6.84	126.64	119.05
1	B	408	VAL	C-N-CA	6.84	126.64	119.05
1	D	255	LYS	N-CA-C	6.84	120.82	108.17
1	C	235	ILE	CA-C-N	6.81	128.35	119.84
1	C	235	ILE	C-N-CA	6.81	128.35	119.84
1	C	620	VAL	N-CA-C	6.81	117.42	110.82
1	D	413	PHE	N-CA-C	6.75	118.64	111.28
1	C	160	LYS	CG-CD-CE	-6.69	95.91	111.30
1	B	367	CYS	N-CA-C	-6.68	104.00	111.28
1	A	91	GLY	N-CA-C	6.64	121.41	111.18
1	C	413	PHE	N-CA-C	6.63	118.51	111.28
1	D	91	GLY	N-CA-C	6.63	121.39	111.18
1	B	331	ALA	N-CA-C	6.61	118.48	111.28
1	A	344	TYR	N-CA-C	6.60	121.26	111.96
1	A	90	TRP	N-CA-C	6.58	118.86	108.79
1	B	425	GLU	N-CA-C	6.54	118.07	111.07
1	D	162	ILE	N-CA-C	-6.52	104.67	111.58
1	A	654	ASP	CA-C-N	6.47	129.79	120.79
1	A	654	ASP	C-N-CA	6.47	129.79	120.79
1	D	654	ASP	CA-C-N	6.47	129.78	120.79
1	D	654	ASP	C-N-CA	6.47	129.78	120.79
1	A	662	GLY	N-CA-C	6.46	120.00	112.50
1	D	447	SER	N-CA-C	-6.46	104.44	112.90
1	C	164	LEU	CA-CB-CG	-6.43	93.78	116.30
1	A	375	GLY	N-CA-C	6.40	120.23	112.49
1	A	660	LEU	N-CA-C	-6.39	104.23	111.14
1	D	204	ASP	CA-C-N	6.39	125.62	118.97
1	D	204	ASP	C-N-CA	6.39	125.62	118.97
1	C	457	PHE	CA-C-N	6.38	126.59	119.32
1	C	457	PHE	C-N-CA	6.38	126.59	119.32
1	B	90	TRP	N-CA-C	6.34	118.49	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	162	ILE	CA-CB-CG1	6.30	121.11	110.40
1	A	447	SER	N-CA-C	-6.27	104.68	112.90
1	C	660	LEU	N-CA-C	-6.27	104.37	111.14
1	A	408	VAL	CA-C-N	6.23	126.14	119.28
1	A	408	VAL	C-N-CA	6.23	126.14	119.28
1	C	116	GLU	N-CA-C	6.21	118.05	111.28
1	B	4	LEU	N-CA-C	6.21	118.05	111.28
1	C	160	LYS	CB-CG-CD	6.21	125.58	111.30
1	C	164	LEU	CD1-CG-CD2	6.18	124.40	110.80
1	A	413	PHE	N-CA-C	6.18	118.01	111.28
1	D	371	HIS	N-CA-C	6.15	120.92	113.17
1	B	655	THR	N-CA-C	6.13	118.50	111.02
1	C	662	GLY	N-CA-C	6.11	119.59	112.50
1	C	344	TYR	N-CA-C	6.10	120.57	111.96
1	B	447	SER	N-CA-C	-6.08	104.94	112.90
1	B	656	LEU	CA-C-N	6.05	128.39	120.28
1	B	656	LEU	C-N-CA	6.05	128.39	120.28
1	D	254	ASN	N-CA-C	-6.02	103.10	111.52
1	A	219	LEU	N-CA-C	-5.99	105.89	112.72
1	B	14	VAL	CA-C-N	5.97	130.82	120.68
1	B	14	VAL	C-N-CA	5.97	130.82	120.68
1	A	1	MET	CA-C-N	5.91	128.47	120.38
1	A	1	MET	C-N-CA	5.91	128.47	120.38
1	B	333	LEU	CA-C-N	5.89	128.77	120.28
1	B	333	LEU	C-N-CA	5.89	128.77	120.28
1	C	382	ASP	C-N-CD	-5.82	107.79	120.60
1	D	362	GLY	N-CA-C	5.81	121.43	113.99
1	D	387	LEU	CA-CB-CG	5.80	136.61	116.30
1	D	97	LYS	CB-CA-C	-5.79	109.36	117.23
1	A	165	GLN	N-CA-C	-5.77	104.99	111.28
1	D	659	GLU	N-CA-C	-5.75	105.53	112.54
1	A	659	GLU	N-CA-C	-5.66	105.63	112.54
1	B	15	PHE	N-CA-C	5.65	119.35	112.23
1	C	8	ILE	N-CA-C	-5.64	105.01	110.42
1	C	367	CYS	N-CA-C	-5.63	105.14	111.28
1	C	382	ASP	CA-C-N	5.62	140.48	127.00
1	C	382	ASP	C-N-CA	5.62	140.48	127.00
1	B	227	MET	CA-C-N	5.61	128.36	120.28
1	B	227	MET	C-N-CA	5.61	128.36	120.28
1	A	4	LEU	N-CA-C	5.59	117.38	111.28
1	A	361	CYS	CA-C-N	5.58	131.74	121.70
1	A	361	CYS	C-N-CA	5.58	131.74	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	654	ASP	CA-C-N	5.57	128.53	120.79
1	C	654	ASP	C-N-CA	5.57	128.53	120.79
1	B	334	LEU	CA-CB-CG	-5.55	96.86	116.30
1	C	176	ASN	CA-C-N	5.55	125.21	119.05
1	C	176	ASN	C-N-CA	5.55	125.21	119.05
1	D	6	PRO	CB-CG-CD	-5.55	88.34	106.10
1	D	2	GLU	CA-C-N	5.55	127.71	120.28
1	D	2	GLU	C-N-CA	5.55	127.71	120.28
1	C	51	LEU	N-CA-C	-5.53	103.10	110.07
1	A	329	LYS	N-CA-C	5.46	117.23	111.28
1	C	323	GLY	N-CA-C	5.44	119.47	112.18
1	A	333	LEU	CA-C-N	5.41	128.07	120.28
1	A	333	LEU	C-N-CA	5.41	128.07	120.28
1	B	428	SER	N-CA-C	-5.41	105.07	110.97
1	D	421	ILE	CA-C-N	5.40	128.06	120.28
1	D	421	ILE	C-N-CA	5.40	128.06	120.28
1	C	382	ASP	N-CA-C	5.38	121.70	109.81
1	A	347	THR	N-CA-C	5.37	117.22	111.36
1	D	662	GLY	N-CA-C	5.33	118.68	112.50
1	B	18	VAL	N-CA-CB	-5.28	105.49	112.36
1	C	488	ALA	N-CA-C	5.27	118.50	111.75
1	C	631	ILE	N-CA-C	-5.25	105.42	110.72
1	B	372	GLU	CA-C-N	-5.24	113.89	122.79
1	B	372	GLU	C-N-CA	-5.24	113.89	122.79
1	C	656	LEU	N-CA-C	5.24	118.45	111.75
1	B	164	LEU	N-CA-C	-5.23	105.75	111.82
1	B	165	GLN	N-CA-C	-5.21	105.60	111.28
1	B	309	ASN	N-CA-C	5.20	116.64	111.07
1	A	228	ASP	N-CA-C	5.19	116.93	111.28
1	D	223	GLY	N-CA-C	-5.18	108.10	115.30
1	D	655	THR	N-CA-C	5.18	117.34	111.02
1	B	655	THR	CA-C-N	5.17	127.92	120.38
1	B	655	THR	C-N-CA	5.17	127.92	120.38
1	A	476	LEU	CA-C-N	-5.16	113.39	119.84
1	A	476	LEU	C-N-CA	-5.16	113.39	119.84
1	A	297	ILE	N-CA-C	5.15	115.37	110.53
1	D	6	PRO	CA-CB-CG	-5.15	94.72	104.50
1	B	488	ALA	N-CA-C	5.13	118.32	111.75
1	A	294	MET	N-CA-C	5.13	116.56	111.07
1	B	385	GLY	N-CA-C	-5.12	105.21	112.37
1	A	638	ASP	N-CA-C	-5.11	107.12	113.55
1	B	370	PHE	CA-C-N	-5.08	114.16	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	PHE	C-N-CA	-5.08	114.16	122.54
1	A	372	GLU	CA-C-N	-5.04	113.13	122.60
1	A	372	GLU	C-N-CA	-5.04	113.13	122.60
1	D	658	SER	CA-C-N	-5.01	112.35	120.72
1	D	658	SER	C-N-CA	-5.01	112.35	120.72
1	C	343	GLU	N-CA-C	-5.00	107.01	113.01
1	D	367	CYS	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	LEU	Peptide
1	C	361	CYS	Peptide
1	C	381	VAL	Peptide
1	D	385	GLY	Peptide

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	4263	0	4407	149	0
1	B	4313	0	4462	153	0
1	C	4218	0	4382	168	0
1	D	4282	0	4448	138	0
All	All	17076	0	17699	582	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 17.

All (582) 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:616:ARG:HB2	1:A:619:GLU:HB2	1.43	0.99
1:B:249:GLN:HA	1:B:252:ILE:HB	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ILE:HG13	1:A:241:ILE:HD11	1.54	0.89
1:B:175:SER:HA	1:B:203:VAL:HG11	1.62	0.81
1:A:113:ASN:ND2	1:C:231:MET:O	2.13	0.80
1:C:175:SER:HA	1:C:203:VAL:HG11	1.65	0.78
1:A:11:LEU:HD11	1:A:701:ILE:HD11	1.67	0.76
1:A:61:ARG:NH1	1:A:114:GLU:OE2	2.19	0.76
1:B:324:GLU:OE2	1:B:456:ARG:NE	2.18	0.75
1:D:616:ARG:HB3	1:D:619:GLU:HB2	1.67	0.74
1:B:468:VAL:HG22	1:B:656:LEU:HD11	1.70	0.72
1:C:447:SER:HB2	1:C:461:HIS:NE2	2.04	0.72
1:A:494:ILE:HG13	1:A:628:TYR:CE2	2.24	0.72
1:A:422:LYS:HG2	1:A:491:LEU:HD21	1.71	0.72
1:B:251:ASP:OD1	1:B:251:ASP:N	2.21	0.71
1:A:284:TYR:HD1	1:A:287:ARG:HH21	1.36	0.71
1:A:216:LYS:HB3	1:A:219:LEU:HD13	1.73	0.70
1:D:160:LYS:HG3	1:D:162:ILE:H	1.55	0.70
1:D:422:LYS:HG2	1:D:491:LEU:HD21	1.73	0.70
1:A:217:LEU:HB2	1:A:245:VAL:HG13	1.74	0.70
1:A:207:GLY:HA3	1:A:237:VAL:HA	1.73	0.70
1:B:494:ILE:HG13	1:B:628:TYR:CE2	2.27	0.69
1:C:4:LEU:HD22	1:C:297:ILE:HG22	1.74	0.69
1:C:191:MET:HE1	1:C:229:VAL:HG11	1.75	0.69
1:C:235:ILE:HD11	1:C:241:ILE:HG12	1.74	0.69
1:C:394:THR:O	1:C:398:ASN:ND2	2.26	0.69
1:C:337:ILE:HD11	1:C:661:VAL:HG23	1.75	0.68
1:B:61:ARG:NH1	1:B:114:GLU:OE2	2.26	0.68
1:C:61:ARG:HD3	1:C:126:SER:HB3	1.74	0.68
1:C:494:ILE:HG13	1:C:628:TYR:CE2	2.29	0.68
1:D:175:SER:HA	1:D:203:VAL:HG11	1.77	0.67
1:C:152:LYS:HE2	1:C:195:GLU:HG2	1.76	0.67
1:A:175:SER:HA	1:A:203:VAL:HG11	1.75	0.66
1:B:174:ILE:HD11	1:B:181:ILE:HD13	1.77	0.66
1:B:382:ASP:O	1:B:423:ARG:NH2	2.28	0.66
1:C:61:ARG:NH2	1:C:114:GLU:O	2.26	0.66
1:B:129:PRO:HG2	1:B:131:HIS:HE1	1.60	0.66
1:D:362:GLY:HA3	1:D:442:ILE:HD11	1.77	0.66
1:A:16:ASN:HD22	1:A:94:LEU:HD23	1.61	0.66
1:C:620:VAL:HG22	1:C:624:LEU:HD11	1.77	0.66
1:C:163:GLU:HA	1:C:166:ILE:HD12	1.77	0.65
1:A:348:ILE:HD11	1:A:653:LYS:HE2	1.79	0.65
1:B:225:ASP:HB2	1:B:226:ALA:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HG2	1:C:294:MET:HG2	1.79	0.65
1:A:176:ASN:HB3	1:A:179:SER:HB3	1.78	0.65
1:A:231:MET:SD	1:A:276:LEU:HD21	2.37	0.65
1:C:4:LEU:HD11	1:C:298:ARG:HB3	1.79	0.65
1:A:230:LEU:O	1:A:279:ARG:NH2	2.29	0.64
1:C:620:VAL:O	1:C:624:LEU:HD13	1.97	0.64
1:C:378:LEU:HA	1:C:381:VAL:HG23	1.80	0.64
1:A:378:LEU:O	1:A:381:VAL:HG12	1.97	0.64
1:A:468:VAL:HG22	1:A:656:LEU:HD11	1.80	0.64
1:C:49:ASP:OD1	1:C:247:ARG:NH2	2.31	0.64
1:B:362:GLY:HA3	1:B:364:ALA:H	1.62	0.63
1:B:1:MET:HA	1:B:4:LEU:HD13	1.78	0.63
1:C:348:ILE:HD11	1:C:653:LYS:HE2	1.81	0.63
1:C:443:ILE:HD11	1:C:465:VAL:HA	1.81	0.63
1:A:361:CYS:HB3	1:A:363:GLY:H	1.64	0.63
1:B:348:ILE:HD11	1:B:653:LYS:HE2	1.80	0.62
1:C:93:PHE:HB3	1:C:95:HIS:CD2	2.34	0.62
1:D:468:VAL:HG22	1:D:656:LEU:HD11	1.80	0.62
1:C:153:VAL:HG11	1:C:159:PRO:HD2	1.79	0.62
1:B:482:MET:HE3	1:B:486:LEU:HG	1.82	0.62
1:B:336:LEU:HD21	1:B:455:LEU:HD22	1.81	0.62
1:A:271:LYS:HG3	1:A:272:LYS:H	1.64	0.62
1:A:361:CYS:HB3	1:A:363:GLY:N	2.15	0.62
1:C:620:VAL:HG22	1:C:624:LEU:CD1	2.29	0.62
1:B:337:ILE:HG22	1:B:464:ILE:HD11	1.82	0.62
1:A:642:LYS:NZ	1:B:490:GLU:HA	2.15	0.61
1:C:161:ASP:OD1	1:C:162:ILE:N	2.34	0.61
1:B:273:TYR:HB3	1:B:276:LEU:HD12	1.82	0.61
1:A:667:SER:HA	1:A:670:LEU:HD13	1.83	0.61
1:B:420:GLN:OE1	1:B:423:ARG:NH1	2.32	0.61
1:C:129:PRO:HG2	1:C:131:HIS:HE1	1.65	0.61
1:B:365:ARG:NH1	1:B:438:GLU:HB2	2.16	0.61
1:C:207:GLY:HA3	1:C:237:VAL:HA	1.82	0.60
1:C:160:LYS:HA	1:C:164:LEU:HD12	1.83	0.60
1:D:382:ASP:OD2	1:D:423:ARG:NH2	2.35	0.60
1:D:494:ILE:HG13	1:D:628:TYR:CE2	2.37	0.60
1:A:64:ILE:HD12	1:A:131:HIS:CE1	2.37	0.59
1:B:423:ARG:HD2	1:C:372:GLU:CD	2.27	0.59
1:C:95:HIS:HE1	1:C:110:GLU:OE2	1.85	0.59
1:A:105:ASP:OD1	1:A:108:ARG:NH1	2.36	0.59
1:B:503:ASP:HB3	1:B:504:ALA:C	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HD23	1:A:637:GLN:HB3	1.85	0.59
1:A:61:ARG:HD2	1:A:118:ILE:HG12	1.86	0.58
1:D:29:VAL:HG21	1:D:174:ILE:HG22	1.85	0.58
1:A:336:LEU:HD21	1:A:455:LEU:HD21	1.86	0.58
1:A:421:ILE:HD12	1:A:632:VAL:HG11	1.86	0.58
1:C:185:THR:HG21	1:C:191:MET:HG2	1.85	0.58
1:C:618:CYS:HA	1:C:621:ILE:HG12	1.86	0.58
1:D:26:PRO:HB3	1:D:300:CYS:SG	2.43	0.58
1:D:697:ALA:HA	1:D:700:ILE:HD12	1.85	0.58
1:D:247:ARG:NH1	1:D:252:ILE:HG12	2.19	0.58
1:A:677:SER:HB3	1:A:680:MET:HG2	1.85	0.58
1:C:163:GLU:O	1:C:166:ILE:HB	2.04	0.58
1:D:16:ASN:HD22	1:D:94:LEU:HD23	1.69	0.57
1:A:501:PHE:O	1:A:505:CYS:HB2	2.03	0.57
1:C:174:ILE:HD11	1:C:181:ILE:HD13	1.86	0.57
1:D:179:SER:O	1:D:209:ARG:NH1	2.35	0.57
1:C:482:MET:HE3	1:C:486:LEU:HG	1.86	0.57
1:C:464:ILE:HG23	1:C:660:LEU:HD11	1.86	0.57
1:A:456:ARG:HG2	1:A:680:MET:HE1	1.85	0.57
1:D:488:ALA:HA	1:D:491:LEU:HD13	1.86	0.57
1:C:621:ILE:HG13	1:C:622:GLU:N	2.20	0.57
1:A:117:ARG:HB2	1:A:117:ARG:NH1	2.20	0.56
1:D:340:PHE:HZ	1:D:443:ILE:HG23	1.70	0.56
1:A:642:LYS:HZ2	1:B:490:GLU:HA	1.70	0.56
1:B:456:ARG:O	1:B:458:PRO:HD3	2.05	0.56
1:A:117:ARG:HB2	1:A:117:ARG:HH11	1.70	0.56
1:B:221:ASP:C	1:B:223:GLY:HA3	2.30	0.56
1:B:489:ILE:HG13	1:B:490:GLU:OE1	2.05	0.56
1:D:247:ARG:HE	1:D:258:VAL:HG22	1.69	0.56
1:D:187:ALA:HA	1:D:191:MET:CE	2.36	0.56
1:D:94:LEU:HB2	1:D:131:HIS:HB2	1.87	0.56
1:A:60:ARG:HB3	1:A:125:VAL:HA	1.86	0.56
1:B:503:ASP:HA	1:B:504:ALA:HB3	1.86	0.56
1:A:29:VAL:HG21	1:A:174:ILE:HG22	1.87	0.55
1:A:8:ILE:HG13	1:A:297:ILE:HD13	1.88	0.55
1:B:658:SER:HA	1:B:661:VAL:HG13	1.87	0.55
1:C:103:ASP:O	1:C:106:GLU:HG2	2.07	0.55
1:D:260:ASP:OD1	1:D:263:ARG:NH2	2.39	0.55
1:B:409:PRO:O	1:B:412:SER:OG	2.19	0.55
1:B:476:LEU:O	1:B:480:ASN:ND2	2.40	0.55
1:A:645:MET:HG3	1:B:493:TYR:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:LEU:HD21	1:C:622:GLU:HG3	1.89	0.55
1:A:488:ALA:HA	1:A:491:LEU:HD13	1.88	0.55
1:C:382:ASP:OD2	1:C:423:ARG:NH2	2.34	0.55
1:C:96:THR:HG21	1:C:101:TYR:HE1	1.70	0.54
1:B:163:GLU:OE2	1:B:167:ARG:NH1	2.40	0.54
1:A:340:PHE:HE1	1:A:446:CYS:HB2	1.72	0.54
1:C:383:PRO:HB3	1:C:629:PHE:CD1	2.43	0.54
1:A:63:LEU:HA	1:A:130:ILE:HG23	1.89	0.54
1:B:229:VAL:HG23	1:B:234:VAL:O	2.08	0.54
1:A:489:ILE:HD12	1:B:482:MET:HE2	1.90	0.54
1:B:488:ALA:HA	1:B:491:LEU:HD13	1.90	0.54
1:A:417:VAL:HG11	1:A:628:TYR:HD2	1.72	0.54
1:B:162:ILE:O	1:B:165:GLN:HB2	2.08	0.54
1:D:413:PHE:O	1:D:417:VAL:HG12	2.07	0.54
1:D:247:ARG:HE	1:D:258:VAL:CG2	2.21	0.54
1:B:92:LYS:HE3	1:B:133:LYS:HD2	1.90	0.54
1:D:435:VAL:O	1:D:439:MET:HG3	2.08	0.54
1:A:176:ASN:HD22	1:A:179:SER:N	2.06	0.53
1:A:305:LYS:NZ	1:A:309:ASN:OD1	2.38	0.53
1:B:471:LEU:HA	1:B:474:LYS:HD3	1.89	0.53
1:C:160:LYS:HA	1:C:164:LEU:CD1	2.38	0.53
1:B:377:THR:HG22	1:C:380:SER:HB2	1.90	0.53
1:B:418:LYS:HD2	1:B:491:LEU:HA	1.91	0.53
1:B:418:LYS:NZ	1:B:490:GLU:O	2.42	0.53
1:D:378:LEU:HA	1:D:381:VAL:HG23	1.89	0.53
1:A:645:MET:O	1:A:650:ASN:HB2	2.08	0.53
1:B:26:PRO:HB2	1:B:297:ILE:HG22	1.90	0.53
1:B:250:LEU:HD23	1:B:253:ASN:HD21	1.74	0.53
1:D:22:ILE:HB	1:D:690:MET:HE1	1.91	0.53
1:A:85:VAL:N	1:A:86:GLU:HA	2.23	0.53
1:B:170:ILE:O	1:B:174:ILE:HG22	2.09	0.53
1:D:206:ASP:OD2	1:D:208:ARG:NH2	2.42	0.53
1:A:478:VAL:O	1:A:481:GLU:HG2	2.08	0.53
1:B:667:SER:HA	1:B:670:LEU:HD13	1.90	0.53
1:A:95:HIS:CD2	1:A:96:THR:HG23	2.44	0.53
1:B:49:ASP:HB3	1:B:247:ARG:NH2	2.24	0.53
1:A:305:LYS:HD3	1:A:701:ILE:HG21	1.90	0.52
1:A:361:CYS:CB	1:A:363:GLY:H	2.23	0.52
1:B:129:PRO:HG2	1:B:131:HIS:CE1	2.43	0.52
1:B:652:VAL:HA	1:B:655:THR:OG1	2.09	0.52
1:D:221:ASP:OD1	1:D:222:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:CD	1:C:279:ARG:HD3	2.34	0.52
1:A:455:LEU:HB3	1:A:457:PHE:H	1.74	0.52
1:C:325:PRO:HB3	1:C:684:ARG:HH21	1.72	0.52
1:A:271:LYS:HG3	1:A:272:LYS:N	2.24	0.52
1:B:435:VAL:O	1:B:439:MET:HG3	2.10	0.52
1:D:426:GLU:HB3	1:D:427:PRO:HD3	1.91	0.52
1:B:362:GLY:HA3	1:B:364:ALA:N	2.24	0.52
1:A:435:VAL:O	1:A:439:MET:HG3	2.10	0.52
1:B:162:ILE:HG13	1:B:163:GLU:N	2.25	0.52
1:B:415:LEU:HD21	1:B:419:ARG:HH21	1.75	0.52
1:D:252:ILE:O	1:D:255:LYS:HB3	2.10	0.52
1:C:93:PHE:HB3	1:C:95:HIS:HD2	1.75	0.51
1:C:488:ALA:HA	1:C:491:LEU:HD13	1.92	0.51
1:C:630:LEU:HD21	1:C:634:LYS:HE3	1.91	0.51
1:C:421:ILE:HD13	1:C:629:PHE:CD2	2.44	0.51
1:D:347:THR:O	1:D:363:GLY:N	2.43	0.51
1:A:387:LEU:HD12	1:A:391:ASP:HB2	1.93	0.51
1:A:217:LEU:HB2	1:A:245:VAL:CG1	2.40	0.51
1:A:489:ILE:CD1	1:B:482:MET:HE2	2.40	0.51
1:C:88:GLU:HG2	1:C:89:GLU:HG3	1.93	0.51
1:A:62:PRO:HB3	1:A:147:LEU:HD23	1.93	0.51
1:A:435:VAL:HG21	1:A:644:VAL:HG11	1.92	0.51
1:B:438:GLU:O	1:B:442:ILE:HG13	2.10	0.51
1:C:93:PHE:HB2	1:C:96:THR:HB	1.92	0.51
1:C:129:PRO:HG2	1:C:131:HIS:CE1	2.45	0.51
1:B:161:ASP:OD1	1:B:162:ILE:N	2.43	0.51
1:D:365:ARG:HG2	1:D:438:GLU:CD	2.36	0.51
1:C:360:LEU:HB2	1:C:365:ARG:HD3	1.92	0.51
1:C:482:MET:HE2	1:D:489:ILE:HD11	1.93	0.51
1:B:318:LEU:HG	1:B:322:TYR:CE2	2.45	0.51
1:C:645:MET:HG3	1:D:493:TYR:CD1	2.46	0.51
1:C:661:VAL:O	1:C:665:TYR:HB2	2.11	0.51
1:A:4:LEU:HD11	1:A:298:ARG:HB3	1.92	0.51
1:A:348:ILE:HG13	1:A:349:GLU:N	2.26	0.51
1:B:365:ARG:CZ	1:B:369:ILE:HD11	2.41	0.51
1:D:88:GLU:HG2	1:D:89:GLU:HG3	1.93	0.51
1:B:5:ILE:HD11	1:B:294:MET:HE2	1.93	0.51
1:D:476:LEU:O	1:D:480:ASN:ND2	2.44	0.51
1:C:657:GLN:HA	1:C:657:GLN:NE2	2.25	0.50
1:B:228:ASP:HB2	1:B:233:ARG:O	2.10	0.50
1:D:42:LEU:HA	1:D:45:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:689:ASP:HA	1:D:692:LYS:HE3	1.93	0.50
1:D:160:LYS:HG2	1:D:162:ILE:HG22	1.94	0.50
1:D:242:ILE:HG21	1:D:285:LEU:HB2	1.93	0.50
1:B:217:LEU:HB2	1:B:245:VAL:HG13	1.94	0.50
1:A:460:LEU:HD12	1:A:673:LEU:HB3	1.93	0.50
1:B:150:MET:HE1	1:B:196:ALA:HA	1.93	0.50
1:C:346:ASN:O	1:C:350:GLY:N	2.43	0.50
1:D:456:ARG:HB2	1:D:680:MET:HE1	1.94	0.50
1:A:671:ASP:OD1	1:A:672:ASP:N	2.45	0.50
1:B:457:PHE:HB2	1:B:460:LEU:HB3	1.93	0.50
1:C:392:ILE:HG23	1:C:621:ILE:HD11	1.94	0.50
1:C:49:ASP:O	1:C:108:ARG:NH1	2.45	0.50
1:C:53:ARG:HH11	1:C:53:ARG:HG3	1.76	0.50
1:C:127:PRO:HB3	1:C:172:ARG:NH2	2.27	0.50
1:C:645:MET:O	1:C:650:ASN:HB2	2.11	0.50
1:B:57:ILE:HG22	1:B:58:VAL:H	1.76	0.49
1:A:490:GLU:HA	1:B:642:LYS:HZ2	1.76	0.49
1:B:234:VAL:HG22	1:B:235:ILE:H	1.77	0.49
1:D:367:CYS:O	1:D:371:HIS:N	2.36	0.49
1:A:5:ILE:N	1:A:6:PRO:HD2	2.27	0.49
1:B:59:THR:HA	1:B:115:THR:HG21	1.94	0.49
1:B:176:ASN:HB3	1:B:179:SER:HB3	1.93	0.49
1:C:271:LYS:HG3	1:C:272:LYS:H	1.76	0.49
1:D:413:PHE:CE2	1:D:494:ILE:HD11	2.47	0.49
1:A:482:MET:HE2	1:B:489:ILE:HG21	1.94	0.49
1:B:284:TYR:O	1:B:287:ARG:HG2	2.13	0.49
1:D:493:TYR:CE2	1:D:495:ASN:HB3	2.47	0.49
1:A:432:VAL:HG22	1:A:644:VAL:HG22	1.95	0.49
1:B:185:THR:HG21	1:B:191:MET:HG2	1.95	0.49
1:C:417:VAL:HG22	1:C:625:ILE:HG23	1.94	0.49
1:D:345:CYS:O	1:D:349:GLU:HG2	2.13	0.49
1:D:391:ASP:O	1:D:394:THR:HG22	2.12	0.49
1:D:417:VAL:HG22	1:D:421:ILE:HG13	1.93	0.49
1:A:362:GLY:HA2	1:A:442:ILE:HD11	1.93	0.49
1:C:345:CYS:O	1:C:349:GLU:HG2	2.12	0.49
1:C:439:MET:O	1:C:442:ILE:HG22	2.12	0.49
1:C:493:TYR:CD1	1:D:645:MET:HG3	2.47	0.49
1:C:621:ILE:HG13	1:C:622:GLU:H	1.78	0.49
1:D:62:PRO:HB3	1:D:147:LEU:HD23	1.94	0.49
1:D:230:LEU:HD22	1:D:276:LEU:HD13	1.92	0.49
1:C:324:GLU:OE1	1:C:324:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:ILE:HD13	1:C:629:PHE:HD2	1.78	0.49
1:A:48:ARG:NH1	1:A:89:GLU:OE1	2.41	0.49
1:A:426:GLU:HB3	1:A:427:PRO:HD3	1.94	0.49
1:C:276:LEU:HD23	1:C:279:ARG:NH2	2.28	0.49
1:D:337:ILE:HD11	1:D:661:VAL:HG22	1.95	0.49
1:A:230:LEU:HA	1:A:241:ILE:HG21	1.94	0.48
1:A:438:GLU:O	1:A:442:ILE:HG13	2.13	0.48
1:B:72:GLN:NE2	1:B:73:GLU:OE2	2.44	0.48
1:B:365:ARG:CZ	1:C:386:GLY:H	2.26	0.48
1:C:435:VAL:O	1:C:439:MET:HG3	2.13	0.48
1:A:408:VAL:O	1:A:411:VAL:HG12	2.12	0.48
1:B:300:CYS:O	1:B:303:GLU:HG2	2.12	0.48
1:D:460:LEU:HD23	1:D:673:LEU:HB3	1.95	0.48
1:A:442:ILE:O	1:A:445:HIS:HB3	2.13	0.48
1:B:702:ALA:O	1:B:703:GLU:HG2	2.13	0.48
1:C:101:TYR:HD2	1:C:106:GLU:HG3	1.78	0.48
1:D:372:GLU:OE2	1:D:376:ARG:NH2	2.40	0.48
1:A:436:HIS:CE1	1:A:476:LEU:HD11	2.48	0.48
1:C:198:LYS:O	1:C:201:ARG:HG2	2.13	0.48
1:D:15:PHE:O	1:D:20:ALA:HB2	2.14	0.48
1:D:126:SER:OG	1:D:128:GLU:OE1	2.30	0.48
1:D:150:MET:HE1	1:D:199:ILE:HG21	1.95	0.48
1:A:4:LEU:CD1	1:A:298:ARG:HB3	2.43	0.48
1:C:161:ASP:OD1	1:C:162:ILE:HG22	2.14	0.48
1:D:48:ARG:NE	1:D:89:GLU:OE1	2.36	0.48
1:A:333:LEU:O	1:A:337:ILE:HB	2.13	0.48
1:D:333:LEU:O	1:D:337:ILE:HG12	2.13	0.48
1:A:307:ARG:O	1:A:311:LEU:HD13	2.14	0.48
1:B:297:ILE:HA	1:B:300:CYS:SG	2.54	0.48
1:B:329:LYS:O	1:B:332:THR:HG22	2.14	0.48
1:B:426:GLU:HB3	1:B:427:PRO:HD3	1.95	0.48
1:C:170:ILE:O	1:C:174:ILE:HG22	2.14	0.48
1:D:336:LEU:HD21	1:D:455:LEU:HG	1.96	0.48
1:B:323:GLY:HA2	1:B:324:GLU:HB3	1.95	0.48
1:B:378:LEU:HD23	1:B:637:GLN:HB2	1.96	0.48
1:B:417:VAL:HG22	1:B:625:ILE:HG23	1.95	0.48
1:C:348:ILE:HG13	1:C:349:GLU:N	2.29	0.48
1:D:217:LEU:HD21	1:D:273:TYR:CE1	2.49	0.48
1:D:438:GLU:O	1:D:442:ILE:HG13	2.14	0.48
1:C:61:ARG:CD	1:C:126:SER:HB3	2.42	0.47
1:C:98:ASN:O	1:C:100:LEU:HD12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:TYR:CE2	1:A:495:ASN:HB3	2.49	0.47
1:D:381:VAL:HG11	1:D:629:PHE:HZ	1.78	0.47
1:A:21:ASP:OD1	1:A:21:ASP:N	2.48	0.47
1:B:493:TYR:CE2	1:B:495:ASN:HB3	2.49	0.47
1:C:421:ILE:HD12	1:C:632:VAL:HG11	1.96	0.47
1:D:222:ALA:HB3	1:D:224:THR:HG23	1.95	0.47
1:D:615:GLN:OE1	1:D:615:GLN:HA	2.14	0.47
1:D:659:GLU:O	1:D:659:GLU:HG2	2.13	0.47
1:C:368:TYR:O	1:C:372:GLU:N	2.38	0.47
1:C:472:LEU:HD23	1:C:652:VAL:HG21	1.97	0.47
1:D:475:ARG:HD3	1:D:651:HIS:CE1	2.50	0.47
1:A:657:GLN:HA	1:A:657:GLN:NE2	2.30	0.47
1:B:226:ALA:HB1	1:B:229:VAL:CG1	2.44	0.47
1:C:455:LEU:HG	1:C:456:ARG:H	1.79	0.47
1:D:49:ASP:HB3	1:D:247:ARG:NH2	2.29	0.47
1:D:384:LEU:HB2	1:D:385:GLY:HA2	1.96	0.47
1:B:340:PHE:CD2	1:B:464:ILE:HG21	2.49	0.47
1:D:333:LEU:HG	1:D:674:LEU:HD21	1.97	0.47
1:D:348:ILE:HD11	1:D:653:LYS:HG3	1.97	0.47
1:D:392:ILE:HG21	1:D:618:CYS:HB2	1.97	0.47
1:B:421:ILE:HD12	1:B:632:VAL:HG11	1.96	0.47
1:C:482:MET:HE2	1:D:489:ILE:CD1	2.45	0.47
1:D:417:VAL:HA	1:D:420:GLN:HB2	1.97	0.47
1:C:305:LYS:HD3	1:C:701:ILE:HG21	1.97	0.47
1:C:430:ARG:HG3	1:C:430:ARG:HH11	1.80	0.47
1:D:2:GLU:O	1:D:6:PRO:HD2	2.15	0.47
1:D:260:ASP:CG	1:D:263:ARG:HH21	2.22	0.47
1:B:421:ILE:HD13	1:B:629:PHE:HD1	1.80	0.47
1:C:16:ASN:HB3	1:C:131:HIS:CE1	2.50	0.47
1:C:26:PRO:HB3	1:C:300:CYS:SG	2.55	0.47
1:C:158:GLN:N	1:C:159:PRO:HD3	2.30	0.47
1:C:493:TYR:CE2	1:C:495:ASN:HB3	2.50	0.47
1:C:475:ARG:O	1:C:479:THR:HG22	2.15	0.46
1:A:93:PHE:CE2	1:A:132:LEU:HD13	2.50	0.46
1:B:463:ALA:O	1:B:467:VAL:HG23	2.15	0.46
1:B:330:SER:HA	1:B:670:LEU:HD21	1.97	0.46
1:A:227:MET:HE2	1:A:227:MET:HB2	1.73	0.46
1:A:333:LEU:CD2	1:A:460:LEU:HD11	2.46	0.46
1:B:334:LEU:HA	1:B:334:LEU:HD12	1.33	0.46
1:C:171:LEU:HA	1:C:174:ILE:HG22	1.95	0.46
1:C:235:ILE:CD1	1:C:241:ILE:HG12	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:HB	1:D:6:PRO:HD3	1.97	0.46
1:A:374:PHE:CE2	1:A:637:GLN:HA	2.50	0.46
1:B:151:THR:O	1:B:151:THR:HG22	2.16	0.46
1:B:225:ASP:CB	1:B:226:ALA:HA	2.42	0.46
1:B:193:THR:O	1:B:198:LYS:NZ	2.48	0.46
1:B:416:LEU:HD23	1:B:416:LEU:HA	1.76	0.46
1:C:340:PHE:CD2	1:C:464:ILE:HG21	2.51	0.46
1:C:697:ALA:HA	1:C:700:ILE:HD12	1.96	0.46
1:D:475:ARG:O	1:D:479:THR:HG22	2.15	0.46
1:A:493:TYR:CD1	1:B:645:MET:HG3	2.50	0.46
1:A:679:ASP:OD1	1:A:680:MET:N	2.49	0.46
1:C:438:GLU:HA	1:C:441:ARG:HD2	1.98	0.46
1:D:408:VAL:H	1:D:409:PRO:HD2	1.81	0.46
1:D:701:ILE:O	1:D:704:ILE:HG22	2.16	0.46
1:D:617:ASP:O	1:D:620:VAL:HG12	2.15	0.46
1:C:374:PHE:CE1	1:C:428:SER:HA	2.51	0.46
1:D:235:ILE:HG23	1:D:237:VAL:HG22	1.97	0.46
1:B:348:ILE:O	1:B:363:GLY:HA2	2.16	0.46
1:A:94:LEU:HB2	1:A:131:HIS:HB2	1.98	0.45
1:C:231:MET:HE3	1:C:233:ARG:HH21	1.80	0.45
1:C:340:PHE:HA	1:C:343:GLU:CD	2.40	0.45
1:C:474:LYS:O	1:C:477:PRO:HD2	2.15	0.45
1:B:250:LEU:HD23	1:B:253:ASN:ND2	2.32	0.45
1:B:616:ARG:NH1	1:B:617:ASP:OD1	2.41	0.45
1:A:490:GLU:HA	1:B:642:LYS:NZ	2.30	0.45
1:C:242:ILE:HD12	1:C:284:TYR:HE2	1.82	0.45
1:D:464:ILE:O	1:D:468:VAL:HG23	2.17	0.45
1:A:418:LYS:O	1:A:422:LYS:HG3	2.16	0.45
1:B:28:ILE:HG12	1:B:180:ILE:HB	1.98	0.45
1:B:361:CYS:SG	1:B:362:GLY:N	2.89	0.45
1:C:435:VAL:HG21	1:C:644:VAL:HG11	1.97	0.45
1:D:220:MET:HE1	1:D:226:ALA:HB3	1.98	0.45
1:B:88:GLU:H	1:B:88:GLU:CD	2.25	0.45
1:D:651:HIS:CE1	1:D:655:THR:HG21	2.52	0.45
1:A:225:ASP:O	1:A:229:VAL:HG23	2.17	0.45
1:A:333:LEU:HD22	1:A:333:LEU:HA	1.61	0.45
1:A:378:LEU:O	1:A:633:ARG:HD2	2.17	0.45
1:C:460:LEU:HD12	1:C:673:LEU:HB3	1.99	0.45
1:D:348:ILE:HG13	1:D:349:GLU:N	2.31	0.45
1:A:370:PHE:CD2	1:A:641:PRO:HB3	2.51	0.45
1:C:50:LEU:C	1:C:108:ARG:HG2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:TYR:CD2	1:C:106:GLU:HG3	2.51	0.45
1:C:316:GLN:N	1:C:691:LEU:HD21	2.32	0.45
1:C:333:LEU:HA	1:C:333:LEU:HD22	1.59	0.45
1:B:95:HIS:NE2	1:B:110:GLU:OE2	2.46	0.45
1:B:377:THR:CG2	1:C:380:SER:HB2	2.47	0.45
1:D:24:GLN:HA	1:D:176:ASN:HD21	1.82	0.45
1:C:413:PHE:CZ	1:C:417:VAL:HG21	2.52	0.44
1:A:46:VAL:HG11	1:A:50:LEU:HD21	1.98	0.44
1:A:493:TYR:HB3	1:B:642:LYS:HG2	1.98	0.44
1:B:8:ILE:HG13	1:B:297:ILE:HG21	1.98	0.44
1:B:342:THR:C	1:B:344:TYR:H	2.23	0.44
1:B:8:ILE:HD13	1:B:11:LEU:HD12	1.99	0.44
1:B:620:VAL:O	1:B:624:LEU:HG	2.17	0.44
1:C:64:ILE:HD12	1:C:131:HIS:NE2	2.31	0.44
1:C:126:SER:HA	1:C:127:PRO:HD3	1.78	0.44
1:A:100:LEU:HD13	1:C:291:ARG:NH2	2.33	0.44
1:B:5:ILE:HB	1:B:6:PRO:HD3	1.99	0.44
1:B:25:LEU:HA	1:B:26:PRO:HD3	1.78	0.44
1:D:194:SER:HB3	1:D:197:LEU:HD13	1.98	0.44
1:D:225:ASP:OD1	1:D:226:ALA:N	2.51	0.44
1:A:15:PHE:O	1:A:20:ALA:HB2	2.18	0.44
1:C:233:ARG:HA	1:C:234:VAL:HA	1.57	0.44
1:D:190:ASP:HB3	1:D:193:THR:HG22	1.98	0.44
1:A:231:MET:HA	1:A:279:ARG:HH22	1.83	0.44
1:B:62:PRO:HB3	1:B:147:LEU:HD23	2.00	0.44
1:B:340:PHE:HA	1:B:343:GLU:HG2	2.00	0.44
1:B:645:MET:O	1:B:650:ASN:HB2	2.17	0.44
1:C:162:ILE:HG23	1:C:163:GLU:N	2.33	0.44
1:A:104:PHE:CD2	1:A:107:ILE:HD12	2.53	0.44
1:A:463:ALA:O	1:A:467:VAL:HG23	2.18	0.44
1:B:168:GLU:O	1:B:172:ARG:HG3	2.17	0.44
1:B:209:ARG:HA	1:B:239:LEU:HD11	1.98	0.44
1:C:365:ARG:HG3	1:C:438:GLU:HG3	1.98	0.44
1:C:443:ILE:HD12	1:C:468:VAL:HB	2.00	0.44
1:D:235:ILE:CG2	1:D:237:VAL:HG22	2.47	0.44
1:A:148:PRO:HB2	1:A:166:ILE:HG23	1.99	0.44
1:B:226:ALA:O	1:B:229:VAL:HG12	2.18	0.44
1:C:374:PHE:CD1	1:C:431:CYS:HB2	2.53	0.44
1:D:256:LYS:HE3	1:D:256:LYS:HB2	1.83	0.44
1:A:242:ILE:HD12	1:A:284:TYR:HE2	1.82	0.43
1:A:365:ARG:HA	1:A:365:ARG:HD2	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:HG22	1:A:625:ILE:HG23	1.99	0.43
1:A:640:VAL:HB	1:A:641:PRO:HD3	1.99	0.43
1:B:418:LYS:HZ2	1:B:491:LEU:C	2.26	0.43
1:C:486:LEU:O	1:C:489:ILE:HG12	2.17	0.43
1:B:10:LYS:HG3	1:B:700:ILE:HD13	2.00	0.43
1:C:301:LEU:N	1:C:302:PRO:HD2	2.33	0.43
1:D:109:GLN:NE2	1:D:113:ASN:OD1	2.48	0.43
1:D:657:GLN:OE1	1:D:657:GLN:HA	2.17	0.43
1:A:454:LEU:C	1:A:455:LEU:HD12	2.44	0.43
1:C:52:PRO:HD3	1:C:111:ILE:HG21	1.99	0.43
1:C:374:PHE:CZ	1:C:378:LEU:HD11	2.54	0.43
1:D:191:MET:HE1	1:D:214:ILE:HG23	2.00	0.43
1:A:297:ILE:HA	1:A:300:CYS:SG	2.59	0.43
1:B:305:LYS:O	1:B:308:ILE:HG13	2.19	0.43
1:B:322:TYR:HB3	1:B:684:ARG:HG2	2.00	0.43
1:A:336:LEU:HD21	1:A:455:LEU:HD11	2.00	0.43
1:A:381:VAL:HG22	1:A:423:ARG:NH2	2.34	0.43
1:B:152:LYS:HG2	1:B:195:GLU:HG3	1.99	0.43
1:D:316:GLN:NE2	1:D:691:LEU:HD21	2.32	0.43
1:B:71:SER:HA	1:B:72:GLN:HA	1.52	0.43
1:B:390:ILE:HG13	1:B:391:ASP:N	2.33	0.43
1:C:342:THR:C	1:C:344:TYR:H	2.25	0.43
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.76	0.43
1:D:365:ARG:O	1:D:369:ILE:HG13	2.19	0.43
1:A:106:GLU:OE1	1:C:279:ARG:HD3	2.18	0.43
1:B:303:GLU:O	1:B:306:THR:OG1	2.30	0.43
1:C:8:ILE:HD11	1:C:26:PRO:HD2	2.01	0.43
1:C:221:ASP:O	1:C:224:THR:HG22	2.19	0.43
1:C:390:ILE:HD12	1:C:390:ILE:H	1.84	0.43
1:C:62:PRO:HG3	1:C:169:LEU:HD21	2.00	0.43
1:C:188:ASN:OD1	1:C:219:LEU:HB2	2.18	0.43
1:D:413:PHE:HE1	1:D:625:ILE:N	2.16	0.43
1:A:114:GLU:HA	1:A:117:ARG:NH1	2.33	0.43
1:A:636:ILE:HG23	1:A:640:VAL:CG2	2.49	0.43
1:A:475:ARG:HD3	1:A:651:HIS:CE1	2.54	0.43
1:B:628:TYR:O	1:B:631:ILE:HG13	2.19	0.43
1:C:93:PHE:CZ	1:C:132:LEU:HD13	2.54	0.43
1:C:220:MET:HE2	1:C:225:ASP:C	2.44	0.43
1:C:417:VAL:O	1:C:420:GLN:N	2.52	0.43
1:D:348:ILE:HD11	1:D:653:LYS:HE2	2.00	0.43
1:A:185:THR:O	1:A:214:ILE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:THR:C	1:B:344:TYR:N	2.77	0.42
1:C:163:GLU:O	1:C:167:ARG:HG2	2.19	0.42
1:C:371:HIS:NE2	1:D:497:LYS:HB2	2.34	0.42
1:D:474:LYS:O	1:D:477:PRO:HD2	2.19	0.42
1:A:305:LYS:HD3	1:A:701:ILE:CG2	2.49	0.42
1:B:181:ILE:HD12	1:B:210:THR:OG1	2.19	0.42
1:C:164:LEU:HD23	1:C:167:ARG:HG3	2.00	0.42
1:A:11:LEU:HA	1:A:11:LEU:HD23	1.84	0.42
1:A:341:ALA:O	1:A:344:TYR:HB3	2.20	0.42
1:B:60:ARG:H	1:B:115:THR:HG23	1.84	0.42
1:D:348:ILE:HD11	1:D:653:LYS:CG	2.49	0.42
1:A:8:ILE:HD13	1:A:11:LEU:HD12	2.01	0.42
1:A:176:ASN:HB3	1:A:179:SER:CB	2.46	0.42
1:A:327:ASP:OD1	1:A:327:ASP:N	2.53	0.42
1:A:439:MET:HB3	1:A:439:MET:HE2	1.74	0.42
1:B:225:ASP:HB2	1:B:228:ASP:OD1	2.18	0.42
1:D:344:TYR:CZ	1:D:348:ILE:HG21	2.55	0.42
1:A:71:SER:HB2	1:A:137:PRO:HB3	2.02	0.42
1:A:242:ILE:HD12	1:A:284:TYR:CE2	2.55	0.42
1:A:377:THR:OG1	1:A:378:LEU:N	2.52	0.42
1:A:505:CYS:C	1:A:507:LEU:H	2.27	0.42
1:B:475:ARG:O	1:B:479:THR:HG22	2.19	0.42
1:C:652:VAL:HA	1:C:655:THR:OG1	2.20	0.42
1:D:152:LYS:HG3	1:D:153:VAL:HB	2.01	0.42
1:C:271:LYS:HG3	1:C:272:LYS:N	2.34	0.42
1:D:221:ASP:O	1:D:223:GLY:N	2.53	0.42
1:D:329:LYS:NZ	1:D:671:ASP:OD1	2.52	0.42
1:D:378:LEU:HD21	1:D:636:ILE:HG22	2.02	0.42
1:D:416:LEU:HD23	1:D:416:LEU:HA	1.81	0.42
1:D:495:ASN:OD1	1:D:498:HIS:HB2	2.20	0.42
1:A:241:ILE:O	1:A:242:ILE:HD13	2.20	0.42
1:A:349:GLU:OE1	1:A:653:LYS:NZ	2.31	0.42
1:A:438:GLU:OE1	1:A:441:ARG:NH1	2.53	0.42
1:A:449:TYR:C	1:A:454:LEU:HD11	2.45	0.42
1:D:226:ALA:HB1	1:D:229:VAL:HG12	2.02	0.42
1:D:456:ARG:HH12	1:D:684:ARG:HH22	1.66	0.42
1:B:392:ILE:HG21	1:B:618:CYS:SG	2.59	0.42
1:B:640:VAL:HB	1:B:641:PRO:HD3	2.00	0.42
1:D:342:THR:C	1:D:344:TYR:H	2.28	0.42
1:D:382:ASP:HB2	1:D:383:PRO:C	2.45	0.42
1:D:442:ILE:O	1:D:445:HIS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LYS:HE2	1:B:272:LYS:HB3	1.91	0.42
1:D:64:ILE:HD12	1:D:131:HIS:NE2	2.35	0.42
1:D:334:LEU:O	1:D:338:THR:OG1	2.28	0.42
1:B:191:MET:HB2	1:B:226:ALA:HB2	2.01	0.42
1:C:489:ILE:HG21	1:D:482:MET:HE2	2.02	0.42
1:A:64:ILE:HG12	1:A:145:VAL:HG22	2.02	0.41
1:A:417:VAL:O	1:A:421:ILE:HG12	2.20	0.41
1:D:376:ARG:O	1:D:380:SER:HB3	2.19	0.41
1:A:4:LEU:HD21	1:A:301:LEU:HD22	2.02	0.41
1:A:620:VAL:HG23	1:A:621:ILE:N	2.35	0.41
1:C:150:MET:HE1	1:C:199:ILE:HG21	2.01	0.41
1:D:176:ASN:HB3	1:D:179:SER:OG	2.19	0.41
1:D:454:LEU:C	1:D:455:LEU:HD12	2.45	0.41
1:D:645:MET:O	1:D:650:ASN:HB2	2.20	0.41
1:B:181:ILE:HB	1:B:210:THR:HA	2.01	0.41
1:C:229:VAL:HA	1:C:233:ARG:O	2.20	0.41
1:D:640:VAL:HB	1:D:641:PRO:HD3	2.01	0.41
1:B:616:ARG:N	1:B:619:GLU:OE1	2.53	0.41
1:C:5:ILE:N	1:C:6:PRO:HD2	2.36	0.41
1:C:60:ARG:HD3	1:C:125:VAL:HG12	2.02	0.41
1:C:128:GLU:H	1:C:128:GLU:HG2	1.60	0.41
1:C:242:ILE:HD12	1:C:284:TYR:CE2	2.56	0.41
1:D:187:ALA:HA	1:D:191:MET:HE2	2.02	0.41
1:C:220:MET:HE3	1:C:224:THR:HG23	2.03	0.41
1:C:338:THR:O	1:C:341:ALA:HB3	2.19	0.41
1:D:455:LEU:C	1:D:457:PHE:H	2.28	0.41
1:A:180:ILE:HD13	1:A:292:LEU:HD23	2.02	0.41
1:A:475:ARG:O	1:A:479:THR:HG22	2.20	0.41
1:A:701:ILE:C	1:A:703:GLU:H	2.29	0.41
1:B:60:ARG:H	1:B:115:THR:CG2	2.33	0.41
1:B:226:ALA:HB1	1:B:229:VAL:HG12	2.02	0.41
1:C:90:TRP:HZ3	1:C:92:LYS:HE3	1.86	0.41
1:C:124:GLY:HA3	1:C:162:ILE:CD1	2.51	0.41
1:C:185:THR:CG2	1:C:191:MET:HG2	2.50	0.41
1:D:46:VAL:HG21	1:D:50:LEU:HD21	2.03	0.41
1:D:413:PHE:HE2	1:D:494:ILE:HD11	1.84	0.41
1:D:417:VAL:HG13	1:D:418:LYS:N	2.35	0.41
1:D:652:VAL:HA	1:D:655:THR:OG1	2.20	0.41
1:D:656:LEU:O	1:D:660:LEU:HB3	2.21	0.41
1:C:61:ARG:HA	1:C:62:PRO:HD3	1.93	0.41
1:C:218:ASP:OD1	1:C:218:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ASP:OD1	1:D:273:TYR:OH	2.25	0.41
1:A:333:LEU:HD21	1:A:460:LEU:HD11	2.03	0.41
1:A:455:LEU:HA	1:A:456:ARG:HB2	2.02	0.41
1:B:322:TYR:O	1:B:324:GLU:HB2	2.21	0.41
1:B:333:LEU:O	1:B:337:ILE:HG12	2.21	0.41
1:B:365:ARG:NE	1:C:386:GLY:H	2.19	0.41
1:C:660:LEU:O	1:C:664:LEU:HB2	2.20	0.41
1:D:459:LYS:HD2	1:D:459:LYS:HA	1.75	0.41
1:D:669:LEU:H	1:D:669:LEU:HD23	1.86	0.41
1:A:340:PHE:HZ	1:A:443:ILE:HG23	1.85	0.41
1:B:4:LEU:HB3	1:B:297:ILE:CD1	2.51	0.41
1:B:365:ARG:NH2	1:C:386:GLY:H	2.18	0.41
1:B:444:GLN:HA	1:B:447:SER:HB2	2.02	0.41
1:C:374:PHE:HE1	1:C:428:SER:HA	1.86	0.41
1:C:640:VAL:HB	1:C:641:PRO:HD3	2.01	0.41
1:A:300:CYS:O	1:A:303:GLU:HG2	2.21	0.41
1:A:457:PHE:N	1:A:458:PRO:HD3	2.36	0.41
1:B:417:VAL:HG11	1:B:628:TYR:HD2	1.86	0.41
1:B:680:MET:HE3	1:B:683:ARG:NH1	2.35	0.41
1:C:416:LEU:HA	1:C:416:LEU:HD23	1.77	0.41
1:B:233:ARG:HA	1:B:234:VAL:HA	1.92	0.40
1:B:273:TYR:N	1:B:274:PRO:HD3	2.37	0.40
1:B:376:ARG:O	1:B:379:GLU:HG2	2.22	0.40
1:B:425:GLU:HA	1:B:487:VAL:HG21	2.02	0.40
1:B:491:LEU:H	1:B:491:LEU:HD12	1.86	0.40
1:C:194:SER:HB3	1:C:197:LEU:HD13	2.03	0.40
1:C:333:LEU:O	1:C:337:ILE:HG12	2.21	0.40
1:C:370:PHE:CD2	1:C:641:PRO:HB3	2.56	0.40
1:D:104:PHE:CD2	1:D:107:ILE:HD12	2.56	0.40
1:D:383:PRO:HB3	1:D:629:PHE:CD1	2.56	0.40
1:D:397:ARG:HB2	1:D:397:ARG:NH1	2.36	0.40
1:D:425:GLU:HA	1:D:487:VAL:HG21	2.03	0.40
1:A:129:PRO:HG2	1:A:131:HIS:HE1	1.87	0.40
1:C:341:ALA:O	1:C:344:TYR:HB3	2.20	0.40
1:C:620:VAL:O	1:C:621:ILE:C	2.64	0.40
1:C:623:ARG:HD2	1:C:623:ARG:HA	1.80	0.40
1:A:471:LEU:HD11	1:A:655:THR:HG22	2.02	0.40
1:A:230:LEU:O	1:A:230:LEU:HD23	2.22	0.40
1:B:377:THR:OG1	1:B:378:LEU:N	2.53	0.40
1:C:410:GLU:HA	1:C:413:PHE:HB3	2.02	0.40
1:D:21:ASP:OD1	1:D:21:ASP:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLU:HA	1:A:487:VAL:HG21	2.03	0.40
1:B:374:PHE:CD1	1:B:431:CYS:HB2	2.56	0.40
1:C:25:LEU:HA	1:C:26:PRO:HD3	1.81	0.40
1:C:30:VAL:HG22	1:C:182:LEU:HD23	2.03	0.40
1:D:11:LEU:HD23	1:D:11:LEU:HA	1.90	0.40
1:D:160:LYS:CG	1:D:162:ILE:HG22	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/617 (84%)	487 (94%)	28 (5%)	3 (1%)	21	53
1	B	529/617 (86%)	497 (94%)	31 (6%)	1 (0%)	43	74
1	C	512/617 (83%)	479 (94%)	30 (6%)	3 (1%)	21	53
1	D	520/617 (84%)	498 (96%)	20 (4%)	2 (0%)	30	62
All	All	2079/2468 (84%)	1961 (94%)	109 (5%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	222	ALA
1	A	323	GLY
1	B	665	TYR
1	A	387	LEU
1	C	19	GLY
1	C	665	TYR
1	C	162	ILE
1	A	236	PRO
1	D	408	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/546 (89%)	460 (95%)	24 (5%)	22	48
1	B	488/546 (89%)	461 (94%)	27 (6%)	19	46
1	C	480/546 (88%)	455 (95%)	25 (5%)	21	48
1	D	487/546 (89%)	461 (95%)	26 (5%)	20	47
All	All	1939/2184 (89%)	1837 (95%)	102 (5%)	20	47

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	63	LEU
1	A	85	VAL
1	A	117	ARG
1	A	130	ILE
1	A	152	LYS
1	A	162	ILE
1	A	163	GLU
1	A	164	LEU
1	A	235	ILE
1	A	306	THR
1	A	333	LEU
1	A	378	LEU
1	A	390	ILE
1	A	393	LEU
1	A	420	GLN
1	A	432	VAL
1	A	456	ARG
1	A	505	CYS
1	A	631	ILE
1	A	638	ASP
1	A	657	GLN
1	A	661	VAL
1	A	668	SER

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Mol	Chain	Res	Type
1	B	14	VAL
1	B	23	ILE
1	B	29	VAL
1	B	57	ILE
1	B	63	LEU
1	B	70	VAL
1	B	72	GLN
1	B	73	GLU
1	B	86	GLU
1	B	88	GLU
1	B	163	GLU
1	B	164	LEU
1	B	235	ILE
1	B	249	GLN
1	B	250	LEU
1	B	251	ASP
1	B	252	ILE
1	B	310	VAL
1	B	324	GLU
1	B	378	LEU
1	B	422	LYS
1	B	432	VAL
1	B	631	ILE
1	B	638	ASP
1	B	661	VAL
1	B	674	LEU
1	B	691	LEU
1	C	8	ILE
1	C	14	VAL
1	C	29	VAL
1	C	58	VAL
1	C	63	LEU
1	C	96	THR
1	C	125	VAL
1	C	128	GLU
1	C	163	GLU
1	C	219	LEU
1	C	326	VAL
1	C	333	LEU
1	C	342	THR
1	C	412	SER
1	C	426	GLU

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Mol	Chain	Res	Type
1	C	432	VAL
1	C	438	GLU
1	C	623	ARG
1	C	624	LEU
1	C	638	ASP
1	C	648	LEU
1	C	657	GLN
1	C	661	VAL
1	C	669	LEU
1	C	675	THR
1	D	6	PRO
1	D	14	VAL
1	D	29	VAL
1	D	42	LEU
1	D	63	LEU
1	D	151	THR
1	D	153	VAL
1	D	164	LEU
1	D	234	VAL
1	D	235	ILE
1	D	269	LEU
1	D	299	ASP
1	D	333	LEU
1	D	390	ILE
1	D	400	THR
1	D	406	LEU
1	D	410	GLU
1	D	411	VAL
1	D	420	GLN
1	D	422	LYS
1	D	432	VAL
1	D	464	ILE
1	D	631	ILE
1	D	657	GLN
1	D	661	VAL
1	D	690	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	69	HIS

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Mol	Chain	Res	Type
1	A	290	ASN
1	B	246	ASN
1	B	253	ASN
1	B	290	ASN
1	B	651	HIS
1	C	95	HIS
1	C	109	GLN
1	C	113	ASN
1	C	131	HIS
1	C	290	ASN
1	C	295	HIS
1	C	335	GLN
1	D	16	ASN
1	D	34	GLN
1	D	141	ASN
1	D	290	ASN
1	D	420	GLN
1	D	484	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	540/617 (87%)	0.10	8 (1%) 72 48	4, 48, 90, 140	0
1	B	547/617 (88%)	0.24	14 (2%) 57 34	8, 58, 105, 141	0
1	C	534/617 (86%)	0.22	16 (2%) 52 31	8, 59, 104, 128	0
1	D	540/617 (87%)	0.15	13 (2%) 59 36	9, 54, 97, 126	0
All	All	2161/2468 (87%)	0.18	51 (2%) 59 36	4, 54, 102, 141	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	344	TYR	6.8
1	C	344	TYR	5.8
1	A	344	TYR	5.6
1	B	344	TYR	5.3
1	C	53	ARG	3.3
1	D	502	ALA	3.2
1	C	408	VAL	3.1
1	D	259	THR	3.0
1	C	191	MET	3.0
1	B	315	TYR	2.9
1	B	444	GLN	2.9
1	C	501	PHE	2.9
1	C	447	SER	2.8
1	D	454	LEU	2.8
1	B	343	GLU	2.8
1	A	85	VAL	2.7
1	A	433	GLU	2.6
1	B	22	ILE	2.5
1	D	383	PRO	2.5
1	B	504	ALA	2.5
1	A	191	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	118	ILE	2.5
1	D	49	ASP	2.5
1	A	90	TRP	2.5
1	D	671	ASP	2.4
1	D	260	ASP	2.4
1	C	387	LEU	2.4
1	C	326	VAL	2.4
1	D	420	GLN	2.4
1	C	15	PHE	2.3
1	D	449	TYR	2.3
1	C	382	ASP	2.3
1	C	249	GLN	2.3
1	B	622	GLU	2.3
1	B	329	LYS	2.3
1	B	365	ARG	2.3
1	B	191	MET	2.3
1	B	12	GLN	2.3
1	A	679	ASP	2.2
1	C	363	GLY	2.2
1	C	617	ASP	2.2
1	D	369	ILE	2.1
1	B	456	ARG	2.1
1	B	337	ILE	2.1
1	D	426	GLU	2.1
1	C	44	SER	2.1
1	D	153	VAL	2.1
1	C	54	GLY	2.1
1	B	57	ILE	2.0
1	A	49	ASP	2.0
1	C	689	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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.