



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:44 AM UTC

PDB ID : 4RHC / pdb_00004rhc
Title : Crystal structure of 3-Dehydroquinate dehydratase from *Acinetobacter baumannii* at 2.68 Å resolution
Authors : Iqbal, N.; Singh, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2014-10-01
Resolution : 2.68 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:

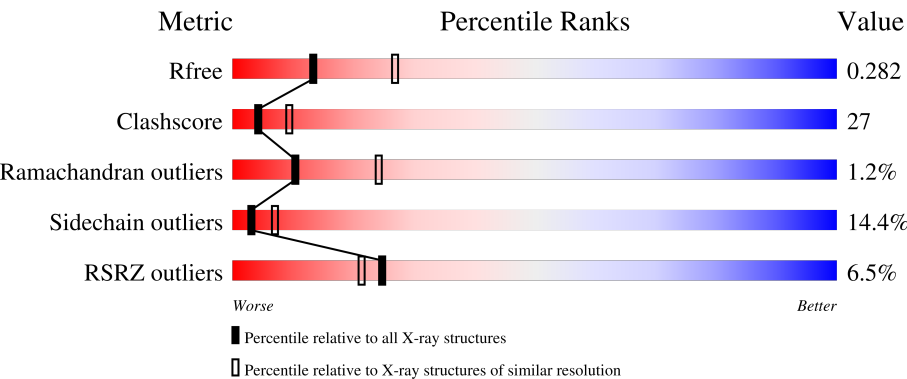
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	150	
1	B	150	
1	C	150	
1	D	150	
1	E	150	

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Mol	Chain	Length	Quality of chain
1	F	150	3% 45% 38% 12%
1	G	150	3% 47% 35% 13%
1	H	150	5% 38% 47% 11%
1	I	150	9% 38% 47% 11%
1	J	150	7% 41% 43% 11%
1	K	150	7% 47% 37% 10%
1	L	150	7% 43% 35% 14% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13972 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 3-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1157	734	206	216	1			
1	B	150	Total	C	N	O	S	0	0	0
			1157	734	206	216	1			
1	C	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	D	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	E	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	F	144	Total	C	N	O	S	0	0	0
			1114	710	198	205	1			
1	G	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	H	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	I	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	J	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	K	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	L	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	49	Total	O	0	0
			49	49		

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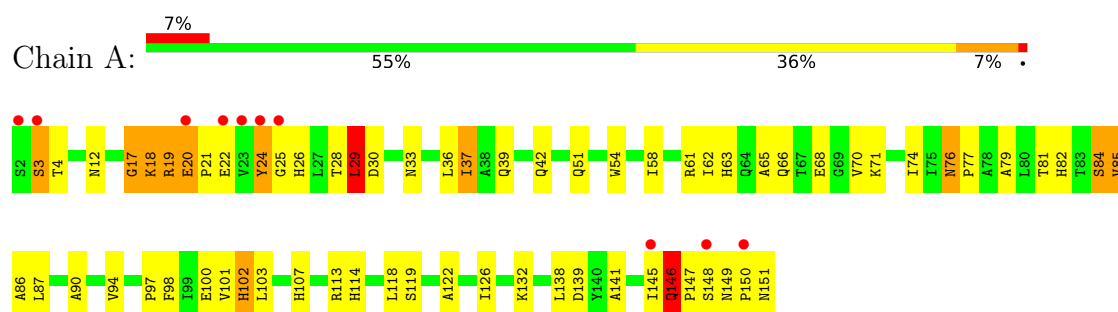
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	43	Total 43	O 43	0	0
2	D	32	Total 32	O 32	0	0
2	E	39	Total 39	O 39	0	0
2	F	41	Total 41	O 41	0	0
2	G	44	Total 44	O 44	0	0
2	H	33	Total 33	O 33	0	0
2	I	30	Total 30	O 30	0	0
2	J	35	Total 35	O 35	0	0
2	K	32	Total 32	O 32	0	0
2	L	28	Total 28	O 28	0	0

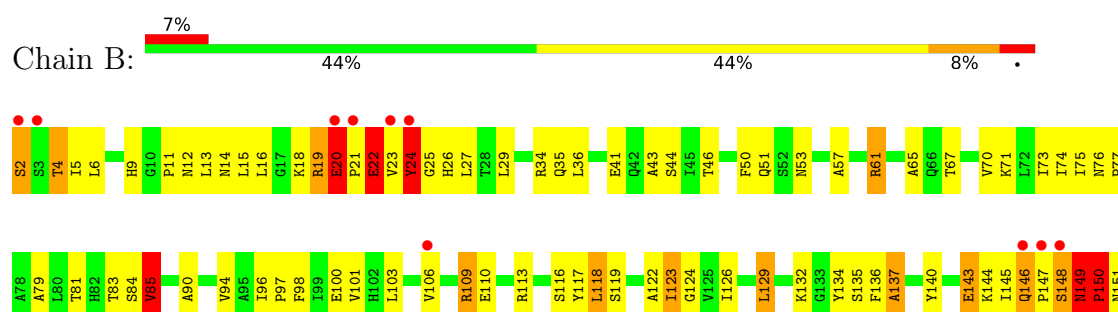
3 Residue-property plots [i](#)

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.

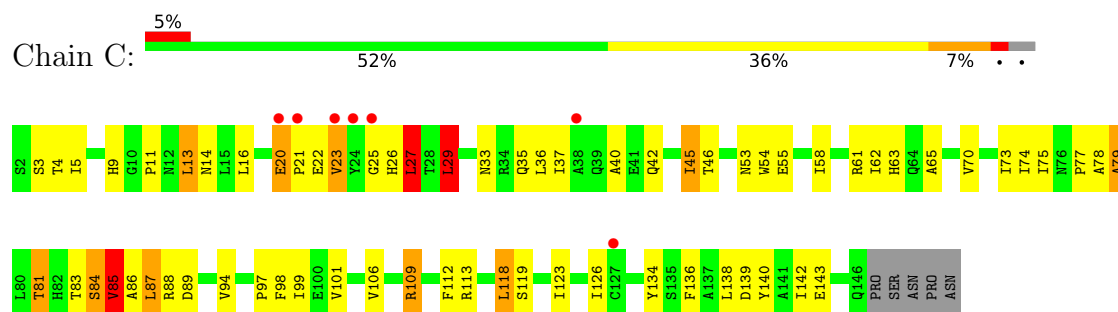
• Molecule 1: 3-dehydroquinase dehydratase



• Molecule 1: 3-dehydroquinase dehydratase

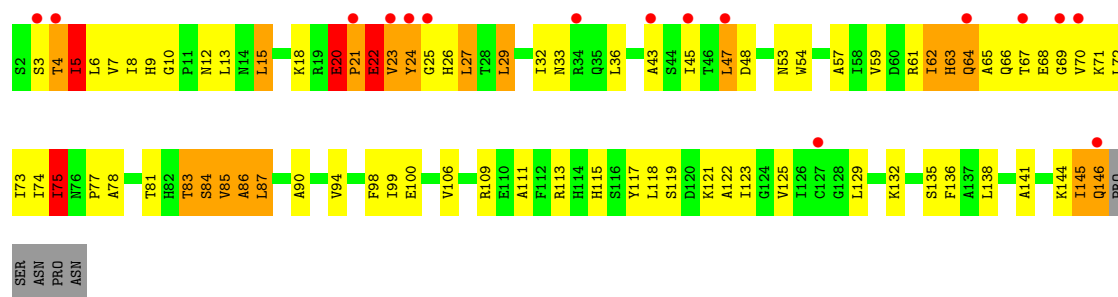


• Molecule 1: 3-dehydroquinase dehydratase

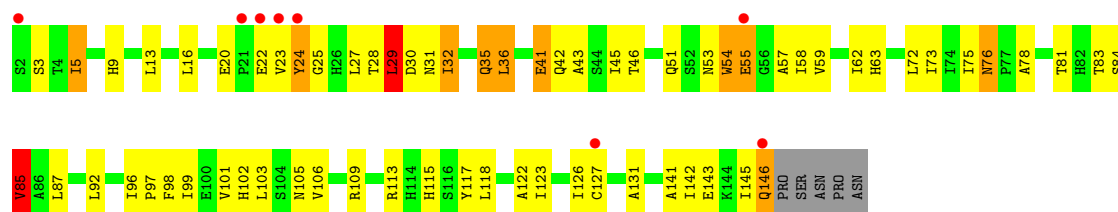


• Molecule 1: 3-dehydroquinase dehydratase

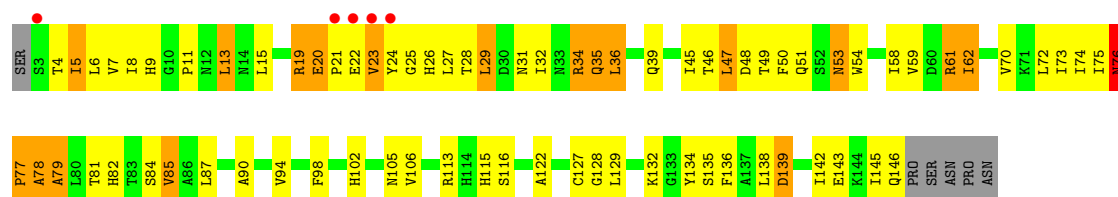
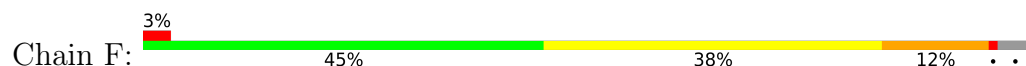




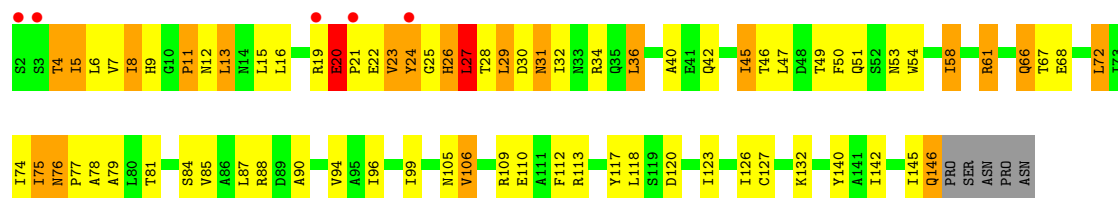
• Molecule 1: 3-dehydroquinatase dehydratase



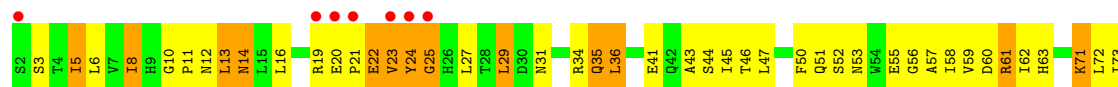
• Molecule 1: 3-dehydroquinatase dehydratase

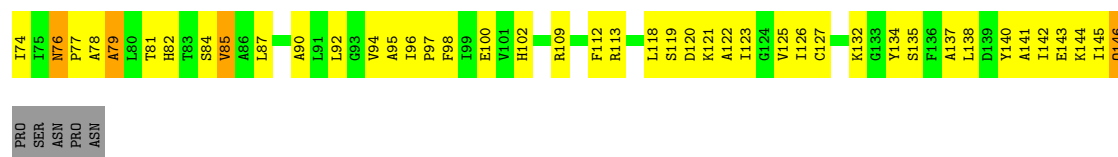


• Molecule 1: 3-dehydroquinatase dehydratase

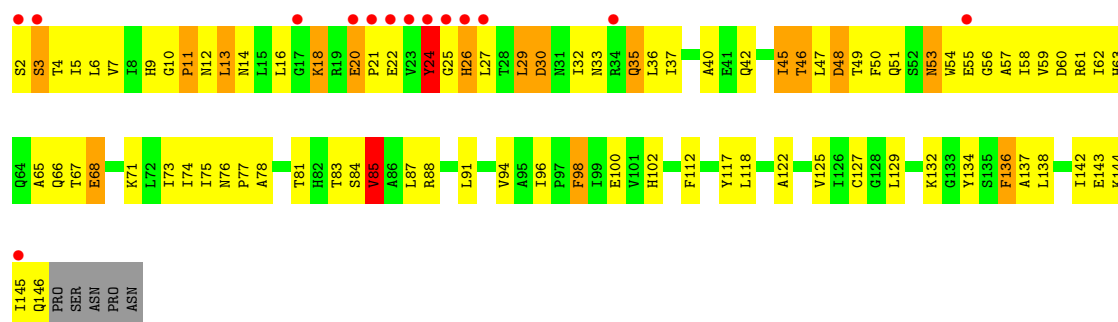


• Molecule 1: 3-dehydroquinatase dehydratase

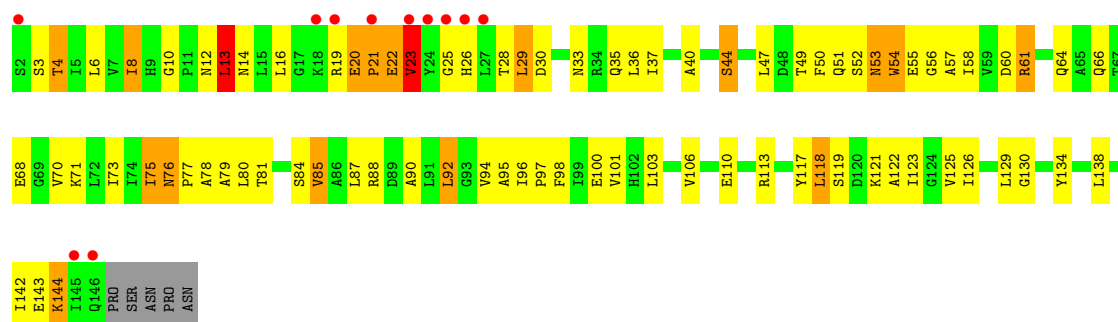
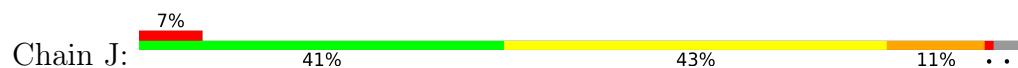




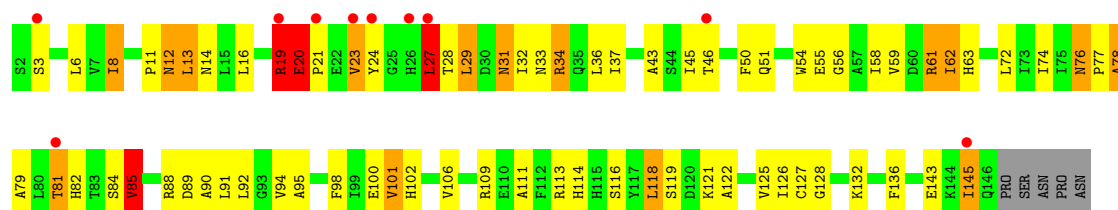
• Molecule 1: 3-dehydroquinate dehydratase



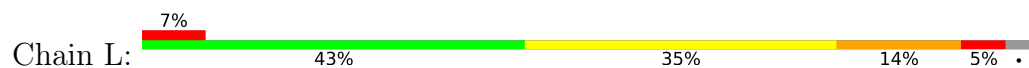
• Molecule 1: 3-dehydroquinate dehydratase

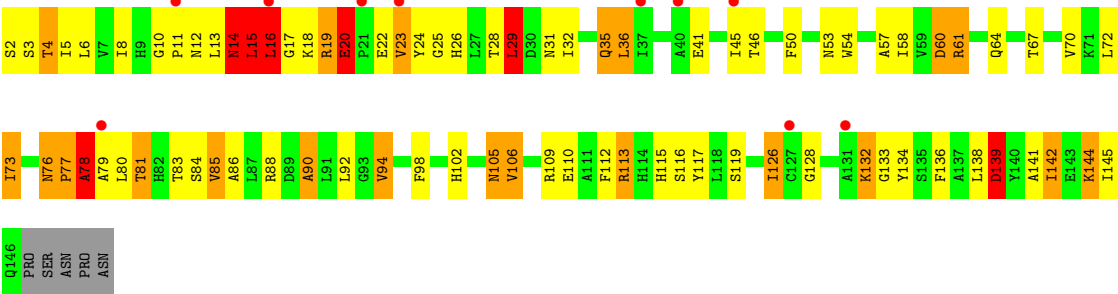


• Molecule 1: 3-dehydroquinate dehydratase



• Molecule 1: 3-dehydroquinate dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.83Å 133.24Å 136.85Å 90.00° 97.99° 90.00°	Depositor
Resolution (Å)	38.38 – 2.68 38.38 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.38-2.68) 99.1 (38.38-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032, CNS 0.9	Depositor
R, R_{free}	0.227 , 0.287 0.225 , 0.282	Depositor DCC
R_{free} test set	2561 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13972	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	9/1180 (0.8%)	1.26	14/1605 (0.9%)
1	B	0.92	3/1180 (0.3%)	1.20	14/1605 (0.9%)
1	C	1.00	5/1141 (0.4%)	1.25	14/1551 (0.9%)
1	D	0.80	2/1141 (0.2%)	1.32	16/1551 (1.0%)
1	E	0.83	3/1141 (0.3%)	1.25	13/1551 (0.8%)
1	F	0.86	4/1135 (0.4%)	1.22	16/1543 (1.0%)
1	G	0.80	6/1141 (0.5%)	1.21	14/1551 (0.9%)
1	H	0.67	3/1141 (0.3%)	1.26	17/1551 (1.1%)
1	I	0.64	1/1141 (0.1%)	1.21	17/1551 (1.1%)
1	J	0.80	1/1141 (0.1%)	1.22	15/1551 (1.0%)
1	K	0.60	1/1141 (0.1%)	1.28	12/1551 (0.8%)
1	L	0.86	1/1141 (0.1%)	1.43	26/1551 (1.7%)
All	All	0.84	39/13764 (0.3%)	1.26	188/18712 (1.0%)

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	D	0	1
1	K	0	1
1	L	0	3
All	All	0	6

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	77	PRO	N-CD	-12.17	1.30	1.47
1	A	146	GLN	C-N	9.26	1.45	1.33
1	A	28	THR	C-N	-8.96	1.22	1.33
1	C	74	ILE	C-O	-8.26	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	GLU	C-O	-7.20	1.17	1.24
1	J	126	ILE	C-O	-7.17	1.16	1.24
1	A	17	GLY	C-N	7.11	1.44	1.33
1	A	37	ILE	C-O	-6.88	1.16	1.24
1	E	126	ILE	C-O	-6.73	1.16	1.24
1	L	15	LEU	CA-C	-6.61	1.45	1.53
1	C	5	ILE	C-O	-6.19	1.17	1.24
1	A	74	ILE	C-O	-6.18	1.17	1.24
1	K	101	VAL	C-O	-6.11	1.17	1.24
1	C	89	ASP	C-O	-6.05	1.16	1.24
1	C	126	ILE	C-O	-6.01	1.18	1.24
1	H	126	ILE	C-O	-5.86	1.17	1.24
1	D	20	GLU	C-O	-5.83	1.16	1.24
1	H	8	ILE	C-O	-5.80	1.18	1.24
1	A	102	HIS	C-O	-5.78	1.17	1.24
1	G	126	ILE	C-O	-5.66	1.17	1.24
1	E	55	GLU	C-O	-5.60	1.17	1.24
1	F	5	ILE	CA-C	-5.60	1.46	1.52
1	A	58	ILE	C-O	-5.58	1.17	1.24
1	B	126	ILE	C-O	-5.51	1.18	1.24
1	I	37	ILE	C-N	5.45	1.40	1.33
1	B	5	ILE	C-O	-5.43	1.18	1.24
1	E	99	ILE	C-O	-5.39	1.18	1.24
1	F	8	ILE	C-O	-5.37	1.18	1.24
1	G	58	ILE	C-O	-5.34	1.18	1.24
1	G	99	ILE	C-O	-5.33	1.18	1.24
1	C	35	GLN	C-O	-5.31	1.18	1.24
1	F	145	ILE	C-O	-5.31	1.18	1.24
1	H	5	ILE	C-O	-5.24	1.18	1.24
1	G	8	ILE	C-O	-5.17	1.18	1.24
1	A	62	ILE	C-O	-5.14	1.18	1.24
1	G	75	ILE	C-O	-5.06	1.18	1.24
1	G	110	GLU	C-O	-5.05	1.17	1.23
1	D	75	ILE	C-O	-5.05	1.19	1.24
1	A	100	GLU	C-O	-5.03	1.18	1.24

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	23	VAL	N-CA-C	-11.72	97.01	113.07
1	D	119	SER	N-CA-C	11.21	123.07	111.07
1	E	96	ILE	O-C-N	10.94	128.26	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	94	VAL	N-CA-C	-10.79	102.57	113.47
1	A	85	VAL	N-CA-C	-10.38	98.08	112.50
1	C	20	GLU	N-CA-C	10.16	126.57	112.75
1	L	84	SER	N-CA-C	9.90	125.38	109.24
1	D	123	ILE	N-CA-C	-9.88	100.23	111.00
1	L	15	LEU	CA-C-O	9.34	132.69	122.13
1	G	4	THR	N-CA-C	9.28	123.97	110.42
1	L	83	THR	N-CA-C	9.25	124.68	113.12
1	L	78	ALA	CA-C-N	8.83	135.97	122.37
1	L	78	ALA	C-N-CA	8.83	135.97	122.37
1	D	84	SER	N-CA-C	8.72	122.83	108.96
1	A	146	GLN	CA-C-N	8.62	128.48	120.21
1	A	146	GLN	C-N-CA	8.62	128.48	120.21
1	I	20	GLU	N-CA-C	8.51	123.75	112.35
1	L	53	ASN	N-CA-C	-8.48	102.64	113.16
1	K	145	ILE	N-CA-C	8.44	119.22	110.36
1	A	18	LYS	N-CA-C	8.42	125.56	113.02
1	F	53	ASN	N-CA-C	-8.27	102.75	112.92
1	B	24	TYR	N-CA-C	-8.14	97.40	108.38
1	K	74	ILE	N-CA-C	-8.13	96.11	107.99
1	K	84	SER	N-CA-C	8.09	122.15	108.23
1	E	106	VAL	N-CA-C	8.00	118.80	110.72
1	L	132	LYS	N-CA-C	-7.92	102.25	112.23
1	G	5	ILE	N-CA-C	-7.88	96.77	108.12
1	E	29	LEU	N-CA-C	-7.84	102.35	112.23
1	L	105	ASN	N-CA-C	-7.79	98.14	109.59
1	G	84	SER	N-CA-C	7.72	122.82	107.62
1	D	86	ALA	N-CA-C	-7.62	102.91	111.14
1	E	96	ILE	CA-C-O	-7.60	113.48	119.25
1	K	31	ASN	N-CA-C	-7.55	103.05	111.28
1	J	22	GLU	N-CA-C	7.55	121.31	107.73
1	K	19	ARG	N-CA-C	-7.44	95.92	108.26
1	D	75	ILE	N-CA-C	7.41	118.99	108.17
1	E	85	VAL	N-CA-C	-7.38	104.31	112.80
1	F	23	VAL	N-CA-C	-7.36	97.13	107.80
1	J	84	SER	N-CA-C	7.20	121.15	107.75
1	G	19	ARG	N-CA-C	-7.13	95.76	109.24
1	I	10	GLY	CA-C-N	7.01	128.60	119.84
1	I	10	GLY	C-N-CA	7.01	128.60	119.84
1	C	23	VAL	N-CA-C	-7.00	98.72	106.21
1	E	41	GLU	N-CA-C	-6.98	102.88	111.40
1	F	84	SER	N-CA-C	6.95	120.68	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	75	ILE	N-CA-C	6.94	119.05	108.71
1	C	27	LEU	N-CA-C	6.90	119.08	109.15
1	K	145	ILE	O-C-N	6.87	128.81	121.94
1	E	32	ILE	N-CA-C	-6.83	103.65	110.62
1	K	20	GLU	N-CA-C	6.81	124.87	109.81
1	C	87	LEU	N-CA-C	-6.81	103.94	111.36
1	H	22	GLU	N-CA-C	6.79	125.27	110.80
1	G	22	GLU	N-CA-C	6.77	121.40	112.13
1	I	84	SER	N-CA-C	6.68	119.62	108.20
1	D	85	VAL	N-CA-C	-6.67	106.23	112.83
1	H	96	ILE	CA-C-O	-6.67	115.22	119.15
1	B	22	GLU	N-CA-C	6.64	120.08	108.52
1	H	3	SER	N-CA-C	6.56	119.21	108.52
1	B	84	SER	N-CA-C	6.52	120.24	107.98
1	L	15	LEU	N-CA-CB	6.51	120.07	110.49
1	L	41	GLU	N-CA-C	-6.51	104.26	111.36
1	F	20	GLU	N-CA-C	6.50	124.16	109.81
1	J	4	THR	N-CA-C	6.49	120.46	110.20
1	D	64	GLN	N-CA-C	-6.47	104.64	112.54
1	C	84	SER	N-CA-C	6.45	118.79	108.41
1	I	53	ASN	N-CA-C	-6.44	103.86	112.94
1	K	8	ILE	N-CA-C	6.41	117.09	107.80
1	A	33	ASN	N-CA-C	6.40	118.26	111.28
1	J	53	ASN	N-CA-C	-6.37	105.08	112.92
1	D	43	ALA	N-CA-C	-6.36	103.15	113.19
1	K	145	ILE	CA-C-O	-6.33	114.68	121.27
1	F	26	HIS	N-CA-C	6.32	120.25	112.54
1	A	119	SER	N-CA-C	6.31	121.78	111.37
1	F	79	ALA	N-CA-C	6.25	124.12	110.80
1	H	85	VAL	N-CA-C	-6.25	104.50	113.07
1	G	20	GLU	N-CA-C	6.25	123.62	109.81
1	J	20	GLU	N-CA-C	-6.25	100.95	110.01
1	B	75	ILE	N-CA-C	6.24	117.75	108.46
1	I	26	HIS	N-CA-C	6.20	120.11	111.74
1	I	136	PHE	N-CA-C	-6.17	104.66	111.82
1	I	68	GLU	N-CA-C	6.14	117.98	111.28
1	A	58	ILE	N-CA-C	6.12	116.28	110.53
1	I	83	THR	N-CA-C	6.08	123.75	110.80
1	K	85	VAL	N-CA-C	-6.07	104.81	113.07
1	G	123	ILE	N-CA-C	-6.06	104.59	110.72
1	I	5	ILE	N-CA-C	-6.06	99.69	108.89
1	J	30	ASP	CA-C-O	-6.05	114.07	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	LEU	N-CA-C	6.05	120.46	112.72
1	H	25	GLY	N-CA-C	6.03	127.46	113.18
1	F	5	ILE	N-CA-C	-6.01	101.09	109.45
1	E	5	ILE	N-CA-C	-5.99	99.85	108.53
1	H	96	ILE	O-C-N	5.97	126.76	121.57
1	C	119	SER	N-CA-C	5.96	118.54	111.33
1	B	129	LEU	N-CA-C	5.96	120.24	113.15
1	E	24	TYR	CB-CA-C	-5.96	109.69	116.54
1	G	31	ASN	N-CA-C	-5.95	104.72	111.14
1	G	96	ILE	N-CA-C	-5.94	101.76	107.76
1	C	75	ILE	N-CA-C	5.94	116.67	108.12
1	A	76	ASN	N-CA-C	-5.92	95.87	108.66
1	K	63	HIS	N-CA-C	-5.92	104.91	111.36
1	J	13	LEU	N-CA-C	-5.92	105.16	112.38
1	E	20	GLU	N-CA-C	5.89	122.84	109.81
1	L	90	ALA	N-CA-C	-5.89	104.21	111.40
1	B	150	PRO	CA-N-CD	-5.87	103.28	111.50
1	E	143	GLU	N-CA-C	-5.87	104.88	111.28
1	F	27	LEU	N-CA-C	5.84	118.81	110.10
1	I	24	TYR	N-CA-C	5.81	117.69	111.36
1	H	74	ILE	N-CA-C	-5.80	99.39	107.80
1	I	45	ILE	CB-CA-C	-5.80	102.80	110.98
1	D	20	GLU	O-C-N	5.79	127.98	121.32
1	E	84	SER	N-CA-C	5.78	118.16	107.99
1	C	85	VAL	N-CA-C	-5.73	104.97	113.39
1	D	53	ASN	N-CA-C	-5.72	106.07	113.16
1	B	41	GLU	N-CA-C	5.70	117.58	111.36
1	G	74	ILE	N-CA-C	-5.69	98.94	107.37
1	G	90	ALA	N-CA-C	-5.69	104.99	111.14
1	I	98	PHE	N-CA-C	5.68	116.05	108.38
1	F	76	ASN	N-CA-C	-5.68	96.47	108.39
1	L	86	ALA	N-CA-C	-5.68	105.09	111.28
1	H	84	SER	N-CA-C	5.67	117.90	108.20
1	J	44	SER	N-CA-C	5.66	119.06	111.24
1	C	79	ALA	N-CA-C	5.66	120.70	111.37
1	L	113	ARG	N-CA-C	-5.66	106.42	113.38
1	A	20	GLU	N-CA-C	5.63	121.16	113.16
1	L	139	ASP	N-CA-C	-5.62	104.85	110.97
1	B	85	VAL	N-CA-C	-5.57	105.50	113.07
1	B	149	ASN	C-N-CD	5.57	132.85	120.60
1	D	121	LYS	N-CA-C	-5.54	107.52	114.56
1	J	30	ASP	O-C-N	5.54	128.88	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	101	VAL	N-CA-C	5.51	116.68	108.46
1	J	10	GLY	CA-C-N	5.51	125.51	119.89
1	J	10	GLY	C-N-CA	5.51	125.51	119.89
1	A	29	LEU	N-CA-C	-5.50	105.29	111.28
1	J	85	VAL	N-CA-C	-5.49	105.60	113.07
1	B	83	THR	N-CA-C	5.45	120.80	114.04
1	E	87	LEU	N-CA-C	-5.45	105.24	111.07
1	H	95	ALA	CA-C-N	-5.42	118.69	122.59
1	H	95	ALA	C-N-CA	-5.42	118.69	122.59
1	C	29	LEU	N-CA-C	-5.40	105.55	111.82
1	L	144	LYS	N-CA-C	-5.40	106.67	113.20
1	L	15	LEU	O-C-N	-5.39	116.45	122.55
1	L	64	GLN	N-CA-C	-5.39	105.30	111.07
1	D	23	VAL	N-CA-C	5.39	120.55	109.34
1	J	92	LEU	O-C-N	5.37	129.54	122.30
1	H	79	ALA	N-CA-C	5.36	117.88	111.71
1	L	92	LEU	N-CA-C	-5.36	106.80	113.55
1	A	24	TYR	CB-CA-C	-5.35	110.43	116.63
1	B	35	GLN	N-CA-C	-5.34	105.12	111.69
1	A	3	SER	N-CA-C	5.32	117.67	111.02
1	F	94	VAL	N-CA-C	-5.31	105.79	113.07
1	G	27	LEU	N-CA-C	-5.30	98.39	107.61
1	G	78	ALA	CB-CA-C	-5.30	110.48	116.63
1	I	71	LYS	N-CA-C	5.30	119.80	113.23
1	I	67	THR	N-CA-C	-5.30	105.42	111.14
1	F	74	ILE	N-CA-C	-5.30	99.62	107.51
1	H	23	VAL	CA-C-O	5.30	125.61	119.36
1	K	106	VAL	CB-CA-C	-5.28	102.64	111.29
1	I	75	ILE	N-CA-C	5.25	116.22	108.45
1	C	16	LEU	N-CA-C	5.24	118.16	110.30
1	F	115	HIS	N-CA-C	5.24	118.16	109.46
1	L	29	LEU	N-CA-C	-5.22	105.50	111.14
1	B	123	ILE	CB-CA-C	-5.20	105.21	112.02
1	C	83	THR	N-CA-C	5.20	121.16	114.56
1	F	78	ALA	CB-CA-C	-5.19	110.57	116.54
1	F	19	ARG	N-CA-C	-5.18	99.44	109.24
1	H	95	ALA	N-CA-C	5.17	118.86	112.24
1	J	129	LEU	N-CA-C	-5.16	106.66	113.17
1	I	85	VAL	N-CA-C	-5.16	105.07	112.35
1	D	63	HIS	N-CA-C	-5.14	105.75	112.23
1	F	25	GLY	N-CA-C	-5.14	103.69	110.74
1	C	4	THR	N-CA-C	5.13	116.56	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14	ASN	CA-C-N	-5.13	115.18	122.41
1	L	14	ASN	C-N-CA	-5.13	115.18	122.41
1	A	90	ALA	N-CA-C	-5.11	105.62	111.14
1	H	119	SER	N-CA-C	5.10	117.50	111.33
1	L	60	ASP	N-CA-C	-5.10	105.72	111.28
1	L	20	GLU	N-CA-C	5.08	119.66	112.75
1	H	24	TYR	N-CA-C	-5.07	100.00	110.80
1	G	11	PRO	N-CA-C	5.06	119.18	111.34
1	D	5	ILE	N-CA-C	5.06	115.73	107.24
1	D	20	GLU	CA-C-O	-5.04	113.26	120.16
1	F	139	ASP	N-CA-C	-5.03	105.88	111.36
1	A	84	SER	N-CA-C	5.01	116.86	108.23
1	B	137	ALA	N-CA-C	-5.01	105.71	111.07
1	H	137	ALA	N-CA-C	-5.01	105.71	111.07
1	D	145	ILE	CB-CA-C	-5.01	105.55	111.81
1	L	15	LEU	CA-C-N	5.01	131.10	121.54
1	L	15	LEU	C-N-CA	5.01	131.10	121.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	22	GLU	Peptide
1	D	22	GLU	Peptide
1	K	20	GLU	Peptide
1	L	15	LEU	Peptide
1	L	77	PRO	Peptide
1	L	78	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1157	0	1162	50	0
1	B	1157	0	1162	78	0
1	C	1120	0	1131	36	0
1	D	1120	0	1131	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1120	0	1131	48	0
1	F	1114	0	1126	55	0
1	G	1120	0	1131	61	0
1	H	1120	0	1131	59	0
1	I	1120	0	1131	88	0
1	J	1120	0	1131	77	0
1	K	1120	0	1131	67	0
1	L	1120	0	1131	94	0
2	A	58	0	0	3	0
2	B	49	0	0	0	0
2	C	43	0	0	0	0
2	D	32	0	0	1	0
2	E	39	0	0	0	0
2	F	41	0	0	0	0
2	G	44	0	0	2	0
2	H	33	0	0	0	0
2	I	30	0	0	1	0
2	J	35	0	0	1	0
2	K	32	0	0	1	0
2	L	28	0	0	1	0
All	All	13972	0	13629	736	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 27.

All (736) 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:L:78:ALA:HA	1:L:81:THR:HG22	1.18	1.15
1:L:18:LYS:HE2	1:L:18:LYS:HA	1.31	1.12
1:L:16:LEU:HD12	1:L:17:GLY:H	1.07	1.08
1:I:45:ILE:CD1	1:I:142:ILE:HG12	1.85	1.07
1:D:20:GLU:HB2	1:D:21:PRO:CD	1.84	1.06
1:A:79:ALA:HB1	1:B:85:VAL:HG22	1.39	1.05
1:D:86:ALA:HA	1:L:79:ALA:HB1	1.33	1.05
1:I:45:ILE:HD12	1:I:142:ILE:HG12	1.39	1.05
1:L:4:THR:CG2	1:L:70:VAL:HG22	1.85	1.05
1:B:149:ASN:HB3	1:B:150:PRO:HA	1.41	1.01
1:G:45:ILE:HD12	1:G:142:ILE:HG12	1.47	0.96
1:H:79:ALA:HB1	1:L:85:VAL:HG23	1.49	0.95
1:H:97:PRO:HB2	1:H:123:ILE:HD11	1.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ILE:HD11	1:E:145:ILE:HD11	1.53	0.91
1:B:20:GLU:HB2	1:B:21:PRO:HD3	1.51	0.91
1:L:6:LEU:HB3	1:L:73:ILE:HD12	1.52	0.91
1:D:86:ALA:CA	1:L:79:ALA:HB1	2.01	0.91
1:D:86:ALA:HA	1:L:79:ALA:CB	2.01	0.89
1:E:63:HIS:NE2	1:G:15:LEU:HD11	1.88	0.89
1:I:77:PRO:HG2	1:I:81:THR:HB	1.54	0.88
1:I:9:HIS:HB2	1:I:51:GLN:HG2	1.55	0.88
1:L:16:LEU:HD12	1:L:17:GLY:N	1.90	0.86
1:L:16:LEU:HG	1:L:18:LYS:HG2	1.56	0.85
1:L:78:ALA:CA	1:L:81:THR:HG22	2.04	0.85
1:J:78:ALA:O	1:J:81:THR:HG22	1.76	0.85
1:L:14:ASN:HD22	1:L:14:ASN:H	1.24	0.84
1:D:22:GLU:HB3	1:D:25:GLY:N	1.93	0.84
1:D:4:THR:HG23	1:D:70:VAL:HA	1.61	0.83
1:D:10:GLY:HA3	1:D:77:PRO:O	1.79	0.83
1:J:13:LEU:HD12	1:J:16:LEU:HD11	1.60	0.83
1:E:97:PRO:HB3	1:E:123:ILE:HD11	1.60	0.83
1:F:106:VAL:HG13	1:F:113:ARG:HB3	1.60	0.83
1:F:77:PRO:HG2	1:F:81:THR:OG1	1.80	0.82
1:F:79:ALA:HB1	1:G:85:VAL:HG23	1.59	0.82
1:I:98:PHE:CE2	1:I:122:ALA:HB2	2.15	0.82
1:D:20:GLU:HB2	1:D:21:PRO:HD2	1.63	0.81
1:K:20:GLU:CB	1:K:21:PRO:HD3	2.11	0.80
1:B:20:GLU:CB	1:B:21:PRO:HD3	2.10	0.80
1:I:129:LEU:CD1	1:L:126:ILE:HD11	2.12	0.80
1:L:18:LYS:HA	1:L:18:LYS:CE	2.01	0.80
1:D:8:ILE:HB	1:D:75:ILE:HG13	1.63	0.80
1:L:19:ARG:O	1:L:23:VAL:HB	1.81	0.80
1:I:18:LYS:HD2	1:I:18:LYS:O	1.82	0.79
1:L:78:ALA:HB2	1:L:102:HIS:CE1	2.18	0.79
1:B:149:ASN:HB3	1:B:150:PRO:CA	2.11	0.79
1:F:4:THR:HG23	1:F:70:VAL:HA	1.63	0.79
1:D:4:THR:HG21	1:D:69:GLY:HA3	1.64	0.78
1:F:62:ILE:CD1	1:F:90:ALA:HB1	2.14	0.78
1:G:20:GLU:HG3	1:G:21:PRO:HD3	1.65	0.78
1:D:5:ILE:HG22	1:D:47:LEU:HB2	1.66	0.78
1:L:138:LEU:O	1:L:142:ILE:HG12	1.83	0.78
1:D:4:THR:HG23	1:D:70:VAL:HG23	1.65	0.78
1:D:22:GLU:HB3	1:D:25:GLY:H	1.49	0.77
1:B:19:ARG:HD2	1:B:19:ARG:C	2.09	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:VAL:HG13	1:D:113:ARG:O	1.84	0.77
1:B:19:ARG:HD2	1:B:19:ARG:O	1.85	0.77
1:A:20:GLU:HG2	1:A:21:PRO:HD3	1.67	0.77
1:B:94:VAL:HG23	1:B:96:ILE:HG13	1.67	0.77
1:A:149:ASN:H	1:A:150:PRO:HA	1.49	0.76
1:E:85:VAL:HG22	1:G:79:ALA:HB1	1.65	0.76
1:A:20:GLU:HB2	1:A:26:HIS:NE2	2.00	0.76
1:K:20:GLU:HB3	1:K:21:PRO:HD3	1.67	0.76
1:J:20:GLU:HB2	1:J:25:GLY:CA	2.16	0.76
1:G:12:ASN:H	1:G:53:ASN:ND2	1.84	0.76
1:D:29:LEU:HD13	1:D:33:ASN:HD21	1.50	0.75
1:I:129:LEU:HD11	1:L:126:ILE:CD1	2.17	0.75
1:D:5:ILE:HG22	1:D:47:LEU:HD12	1.68	0.75
1:I:16:LEU:HB3	1:I:27:LEU:O	1.86	0.75
1:B:20:GLU:CD	1:B:21:PRO:HD3	2.12	0.75
1:L:78:ALA:CB	1:L:81:THR:HG21	2.17	0.75
1:L:78:ALA:HA	1:L:81:THR:CG2	2.09	0.75
1:A:149:ASN:N	1:A:150:PRO:HA	2.02	0.75
1:J:3:SER:HB2	1:J:71:LYS:HG3	1.69	0.74
1:F:45:ILE:HG13	1:F:142:ILE:HD12	1.69	0.74
1:L:4:THR:HG23	1:L:70:VAL:HG22	1.70	0.74
1:E:142:ILE:HA	1:E:145:ILE:HD12	1.70	0.74
1:L:145:ILE:O	1:L:145:ILE:HG22	1.88	0.73
1:L:77:PRO:HG2	1:L:81:THR:HB	1.70	0.73
1:F:139:ASP:O	1:F:143:GLU:HG2	1.89	0.73
1:I:85:VAL:HG22	1:K:79:ALA:HB1	1.71	0.73
1:K:98:PHE:CE2	1:K:122:ALA:HB2	2.23	0.73
1:K:55:GLU:O	1:K:59:VAL:HG23	1.89	0.72
1:A:79:ALA:HB1	1:B:85:VAL:CG2	2.19	0.72
1:D:20:GLU:CB	1:D:21:PRO:CD	2.66	0.72
1:K:58:ILE:O	1:K:62:ILE:HG23	1.88	0.72
1:G:23:VAL:C	1:G:25:GLY:H	1.95	0.72
1:I:62:ILE:HD13	1:I:91:LEU:CD2	2.19	0.72
1:B:77:PRO:HG2	1:B:81:THR:HG23	1.71	0.72
1:D:3:SER:HB3	1:D:71:LYS:HG3	1.72	0.72
1:C:77:PRO:HG2	1:C:81:THR:HB	1.72	0.71
1:I:24:TYR:HD1	1:I:25:GLY:N	1.86	0.71
1:E:63:HIS:CD2	1:G:15:LEU:HD11	2.25	0.71
1:D:20:GLU:HB2	1:D:21:PRO:HD3	1.73	0.71
1:B:79:ALA:HB1	1:C:85:VAL:HG22	1.73	0.71
1:H:138:LEU:O	1:H:142:ILE:HG13	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:PRO:CG	1:B:81:THR:HG23	2.21	0.70
1:F:35:GLN:HE21	1:F:36:LEU:HD13	1.55	0.69
1:K:76:ASN:C	1:K:76:ASN:HD22	1.98	0.69
1:D:5:ILE:CG2	1:D:47:LEU:HD12	2.23	0.69
1:E:78:ALA:O	1:E:81:THR:HG22	1.93	0.69
1:A:20:GLU:HG3	1:A:26:HIS:CE1	2.28	0.69
1:F:7:VAL:HB	1:F:49:THR:HG22	1.73	0.69
1:G:72:LEU:C	1:G:72:LEU:HD23	2.17	0.69
1:L:78:ALA:CB	1:L:81:THR:CG2	2.71	0.69
1:I:129:LEU:HD12	1:L:126:ILE:HD11	1.75	0.69
1:L:6:LEU:HB3	1:L:73:ILE:CD1	2.22	0.68
1:G:76:ASN:C	1:G:76:ASN:HD22	2.01	0.68
1:J:94:VAL:HG23	1:J:96:ILE:HG13	1.75	0.68
1:I:62:ILE:HD13	1:I:91:LEU:HD21	1.73	0.68
1:L:78:ALA:HB1	1:L:81:THR:HG21	1.76	0.68
1:E:45:ILE:HD13	1:E:145:ILE:HD13	1.75	0.68
1:G:6:LEU:HD21	1:G:8:ILE:HD11	1.74	0.68
1:I:117:TYR:C	1:I:118:LEU:HD12	2.18	0.68
1:L:16:LEU:CD1	1:L:17:GLY:H	1.96	0.68
1:I:47:LEU:HD23	1:I:48:ASP:N	2.10	0.67
1:B:9:HIS:HB2	1:B:51:GLN:CG	2.25	0.67
1:I:6:LEU:HD21	1:I:61:ARG:HD3	1.74	0.67
1:H:109:ARG:HB2	1:H:113:ARG:HD2	1.76	0.67
1:I:24:TYR:HE1	1:I:26:HIS:H	1.39	0.67
1:D:3:SER:HB3	1:D:71:LYS:CG	2.26	0.66
1:C:20:GLU:O	1:C:22:GLU:N	2.25	0.66
1:J:20:GLU:CB	1:J:25:GLY:HA3	2.26	0.66
1:A:20:GLU:HB2	1:A:26:HIS:CE1	2.29	0.66
1:D:62:ILE:O	1:D:65:ALA:HB3	1.96	0.66
1:I:58:ILE:CG2	1:I:87:LEU:HD11	2.25	0.66
1:L:28:THR:O	1:L:32:ILE:HG13	1.95	0.66
1:K:11:PRO:C	1:K:12:ASN:HD22	2.04	0.65
1:B:143:GLU:O	1:B:147:PRO:HD2	1.96	0.65
1:J:64:GLN:O	1:J:68:GLU:HG3	1.97	0.65
1:B:149:ASN:CB	1:B:150:PRO:CA	2.73	0.65
1:H:79:ALA:HB1	1:L:85:VAL:CG2	2.26	0.65
1:L:76:ASN:C	1:L:76:ASN:HD22	2.04	0.65
1:B:19:ARG:HH21	1:B:23:VAL:HG13	1.61	0.65
1:J:119:SER:HB3	1:J:125:VAL:HG21	1.77	0.65
1:K:20:GLU:CB	1:K:21:PRO:CD	2.75	0.65
1:A:19:ARG:O	1:A:19:ARG:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:PRO:HG3	1:I:53:ASN:HA	1.79	0.64
1:K:23:VAL:O	1:K:24:TYR:HB2	1.96	0.64
1:I:50:PHE:CD2	1:I:61:ARG:HG3	2.31	0.64
1:J:20:GLU:CG	1:J:21:PRO:HA	2.27	0.64
1:C:87:LEU:HD23	1:C:118:LEU:HD21	1.78	0.64
1:F:4:THR:HA	1:F:46:THR:O	1.98	0.64
1:C:13:LEU:CD2	1:C:78:ALA:HB2	2.28	0.64
1:B:9:HIS:HB2	1:B:51:GLN:HG2	1.80	0.64
1:H:31:ASN:O	1:H:35:GLN:HG2	1.97	0.63
1:J:138:LEU:O	1:J:142:ILE:HG13	1.97	0.63
1:L:70:VAL:HG11	1:L:73:ILE:HD11	1.78	0.63
1:D:62:ILE:HD11	1:D:90:ALA:C	2.24	0.63
1:B:109:ARG:HG3	1:B:113:ARG:HD2	1.81	0.63
1:F:9:HIS:HB3	1:F:13:LEU:HD23	1.79	0.63
1:I:9:HIS:HB2	1:I:51:GLN:CG	2.27	0.63
1:F:23:VAL:O	1:F:24:TYR:HB2	1.98	0.63
1:I:6:LEU:O	1:I:73:ILE:HG23	1.99	0.63
1:I:45:ILE:HD11	1:I:142:ILE:HG23	1.81	0.63
1:I:45:ILE:HD11	1:I:142:ILE:HG12	1.77	0.63
1:B:4:THR:HA	1:B:46:THR:O	1.98	0.63
1:I:47:LEU:HD23	1:I:48:ASP:H	1.64	0.63
1:A:76:ASN:HA	1:A:101:VAL:O	1.99	0.62
1:J:55:GLU:OE2	1:J:80:LEU:HD22	2.00	0.62
1:D:6:LEU:HD12	1:D:48:ASP:O	2.00	0.62
1:I:145:ILE:HD12	1:I:146:GLN:N	2.14	0.62
1:H:14:ASN:HA	1:H:29:LEU:HD12	1.81	0.62
1:H:78:ALA:O	1:H:81:THR:HG22	1.98	0.62
1:A:20:GLU:HG2	1:A:21:PRO:CD	2.30	0.62
1:G:27:LEU:O	1:G:27:LEU:HG	2.00	0.62
1:J:76:ASN:C	1:J:76:ASN:HD22	2.06	0.62
1:L:3:SER:O	1:L:45:ILE:HG23	1.99	0.62
1:A:20:GLU:N	1:A:21:PRO:HD2	2.15	0.62
1:B:20:GLU:HB2	1:B:21:PRO:CD	2.29	0.62
1:D:4:THR:CG2	1:D:69:GLY:HA3	2.29	0.62
1:C:40:ALA:HB1	1:C:45:ILE:HG22	1.82	0.61
1:L:19:ARG:HB3	1:L:23:VAL:HG21	1.82	0.61
1:F:6:LEU:HD12	1:F:48:ASP:O	2.01	0.61
1:A:24:TYR:OH	1:A:103:LEU:HD13	2.00	0.61
1:C:11:PRO:HA	1:C:53:ASN:OD1	2.00	0.61
1:I:3:SER:O	1:I:46:THR:HG23	2.00	0.61
1:I:129:LEU:HD11	1:L:126:ILE:HD11	1.76	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:ILE:HD11	1:F:90:ALA:HB1	1.80	0.61
1:G:29:LEU:HD11	1:G:51:GLN:HG3	1.81	0.61
1:A:4:THR:HG23	1:A:70:VAL:HA	1.82	0.61
1:D:27:LEU:HD11	1:D:32:ILE:HG13	1.81	0.61
1:B:149:ASN:CB	1:B:150:PRO:HA	2.12	0.61
1:B:20:GLU:CB	1:B:21:PRO:CD	2.79	0.61
1:D:109:ARG:HB2	1:D:113:ARG:HD2	1.82	0.61
1:J:20:GLU:HG3	1:J:21:PRO:HA	1.82	0.60
1:L:90:ALA:O	1:L:94:VAL:HG22	2.01	0.60
1:F:9:HIS:HB2	1:F:51:GLN:HG2	1.81	0.60
1:J:20:GLU:CD	1:J:26:HIS:HB2	2.26	0.60
1:D:63:HIS:CE1	1:L:15:LEU:HD21	2.36	0.60
1:I:7:VAL:HA	1:I:74:ILE:O	2.02	0.60
1:L:10:GLY:HA3	1:L:77:PRO:O	2.02	0.60
1:E:16:LEU:HD11	1:E:103:LEU:HD11	1.84	0.60
1:H:41:GLU:C	1:H:43:ALA:H	2.09	0.60
1:H:146:GLN:HE21	1:H:146:GLN:CA	2.13	0.60
1:J:54:TRP:CD2	1:K:56:GLY:HA3	2.36	0.60
1:L:78:ALA:HB2	1:L:102:HIS:HE1	1.67	0.60
1:E:85:VAL:CG2	1:G:79:ALA:HB1	2.32	0.60
1:I:85:VAL:O	1:I:88:ARG:HB3	2.01	0.60
1:D:22:GLU:HB2	1:D:24:TYR:N	2.17	0.60
1:E:146:GLN:HE21	1:E:146:GLN:HA	1.66	0.60
1:D:115:HIS:HE1	1:D:117:TYR:CE1	2.19	0.59
1:A:145:ILE:HG22	1:A:145:ILE:O	2.01	0.59
1:F:106:VAL:CG1	1:F:113:ARG:HB3	2.32	0.59
1:K:13:LEU:O	1:K:16:LEU:HG	2.03	0.59
1:F:45:ILE:HG13	1:F:142:ILE:CD1	2.31	0.59
1:H:53:ASN:ND2	1:L:60:ASP:OD1	2.36	0.59
1:H:57:ALA:O	1:H:61:ARG:HB2	2.02	0.59
1:I:53:ASN:ND2	1:J:60:ASP:OD1	2.36	0.59
1:C:55:GLU:OE1	1:C:86:ALA:HB3	2.02	0.59
1:H:102:HIS:O	1:H:127:CYS:HA	2.02	0.59
1:E:29:LEU:HD11	1:E:51:GLN:HG3	1.85	0.59
1:G:20:GLU:CG	1:G:21:PRO:HD3	2.32	0.59
1:L:16:LEU:CD1	1:L:28:THR:HG22	2.32	0.59
1:E:27:LEU:HD12	1:E:31:ASN:HD22	1.68	0.58
1:G:6:LEU:CD2	1:G:8:ILE:HD11	2.32	0.58
1:K:43:ALA:O	1:K:45:ILE:HG12	2.04	0.58
1:G:11:PRO:HB3	1:G:53:ASN:HA	1.84	0.58
1:K:100:GLU:HB3	1:K:125:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:VAL:O	1:K:95:ALA:HB3	2.04	0.58
1:H:112:PHE:CE1	1:L:85:VAL:HG11	2.38	0.58
1:E:115:HIS:HE1	1:E:117:TYR:CZ	2.22	0.57
1:A:20:GLU:CB	1:A:26:HIS:CE1	2.87	0.57
1:B:94:VAL:CG2	1:B:96:ILE:HG13	2.34	0.57
1:I:58:ILE:HG21	1:I:87:LEU:HD11	1.85	0.57
1:A:22:GLU:O	1:A:22:GLU:HG3	2.03	0.57
1:F:32:ILE:HG22	1:F:36:LEU:HD22	1.87	0.57
1:J:53:ASN:HB3	1:K:59:VAL:HG11	1.85	0.57
1:L:77:PRO:CG	1:L:81:THR:HB	2.34	0.57
1:G:47:LEU:O	1:G:47:LEU:HD23	2.04	0.57
1:B:73:ILE:O	1:B:98:PHE:HA	2.05	0.56
1:E:58:ILE:O	1:E:62:ILE:HG13	2.04	0.56
1:I:30:ASP:HA	1:I:33:ASN:HB2	1.87	0.56
1:J:118:LEU:HD12	1:J:118:LEU:N	2.19	0.56
1:D:59:VAL:HG22	1:D:87:LEU:HD12	1.86	0.56
1:F:34:ARG:HA	1:F:34:ARG:CZ	2.35	0.56
1:F:81:THR:HG22	1:F:116:SER:HA	1.87	0.56
1:G:106:VAL:HG12	1:G:113:ARG:O	2.05	0.56
1:L:70:VAL:HG11	1:L:73:ILE:CD1	2.35	0.56
1:A:20:GLU:HB2	1:A:26:HIS:CD2	2.41	0.56
1:A:146:GLN:N	1:A:147:PRO:CD	2.69	0.56
1:D:20:GLU:CB	1:D:21:PRO:HD3	2.34	0.56
1:J:100:GLU:HB3	1:J:125:VAL:HG13	1.87	0.56
1:I:7:VAL:O	1:I:49:THR:HA	2.05	0.56
1:K:81:THR:HG23	1:K:116:SER:OG	2.06	0.56
1:A:77:PRO:HD2	1:A:102:HIS:CE1	2.41	0.56
1:D:109:ARG:CB	1:D:113:ARG:HD2	2.35	0.56
1:E:54:TRP:N	1:E:54:TRP:CD1	2.73	0.56
1:J:14:ASN:HD21	1:J:53:ASN:HD21	1.52	0.56
1:K:8:ILE:HD13	1:K:62:ILE:HG22	1.88	0.56
1:K:14:ASN:HA	1:K:29:LEU:HD12	1.87	0.56
1:L:4:THR:HG22	1:L:70:VAL:HA	1.87	0.56
1:D:9:HIS:ND1	1:D:29:LEU:HD21	2.21	0.55
1:A:149:ASN:H	1:A:150:PRO:CA	2.19	0.55
1:G:12:ASN:H	1:G:53:ASN:HD22	1.54	0.55
1:C:139:ASP:O	1:C:143:GLU:HG2	2.06	0.55
1:J:20:GLU:HA	1:J:25:GLY:HA3	1.89	0.55
1:L:4:THR:HG21	1:L:70:VAL:HG22	1.82	0.55
1:E:109:ARG:HB2	1:E:113:ARG:HD2	1.87	0.55
1:E:32:ILE:O	1:E:36:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:THR:HG22	1:L:70:VAL:HG22	1.83	0.55
1:L:141:ALA:O	1:L:144:LYS:HB3	2.06	0.55
1:D:5:ILE:HG22	1:D:47:LEU:CD1	2.35	0.55
1:L:29:LEU:HA	1:L:32:ILE:HD12	1.89	0.55
1:L:116:SER:HB3	1:L:119:SER:OG	2.06	0.55
1:A:113:ARG:HD3	2:A:202:HOH:O	2.07	0.55
1:D:77:PRO:O	1:D:78:ALA:HB3	2.04	0.55
1:B:65:ALA:HB1	1:B:70:VAL:HB	1.89	0.55
1:D:27:LEU:CD1	1:D:32:ILE:HG13	2.36	0.55
1:D:25:GLY:C	1:D:26:HIS:CD2	2.85	0.55
1:F:39:GLN:HB3	1:F:138:LEU:CD2	2.37	0.55
1:J:19:ARG:O	1:J:19:ARG:HG3	2.07	0.55
1:K:19:ARG:HB2	2:K:215:HOH:O	2.06	0.55
1:B:11:PRO:HA	1:B:53:ASN:OD1	2.07	0.54
1:B:143:GLU:O	1:B:146:GLN:N	2.34	0.54
1:D:4:THR:HG23	1:D:70:VAL:CG2	2.36	0.54
1:E:5:ILE:CD1	1:E:145:ILE:HD11	2.33	0.54
1:B:29:LEU:CD2	1:B:51:GLN:HG3	2.36	0.54
1:E:45:ILE:HD12	1:E:142:ILE:HG12	1.89	0.54
1:F:62:ILE:HD12	1:F:90:ALA:HB1	1.87	0.54
1:J:20:GLU:CB	1:J:25:GLY:CA	2.84	0.54
1:B:98:PHE:CE2	1:B:122:ALA:HB2	2.41	0.54
1:H:51:GLN:CD	1:H:52:SER:N	2.66	0.54
1:J:143:GLU:HA	1:J:143:GLU:OE1	2.06	0.54
1:J:77:PRO:CG	1:J:81:THR:HB	2.37	0.54
1:G:7:VAL:HB	1:G:49:THR:HG22	1.90	0.54
1:I:29:LEU:HD11	1:I:51:GLN:HG3	1.90	0.54
1:G:23:VAL:C	1:G:25:GLY:N	2.64	0.54
1:G:26:HIS:H	1:G:26:HIS:CD2	2.25	0.54
1:G:34:ARG:HB2	2:G:209:HOH:O	2.08	0.54
1:H:19:ARG:O	1:H:23:VAL:HG22	2.08	0.54
1:H:72:LEU:HD23	1:H:73:ILE:N	2.23	0.54
1:L:78:ALA:CB	1:L:102:HIS:CE1	2.91	0.54
1:L:105:ASN:N	1:L:128:GLY:HA2	2.23	0.54
1:I:2:SER:HB3	2:I:224:HOH:O	2.08	0.54
1:G:20:GLU:O	1:G:25:GLY:HA2	2.08	0.54
1:G:40:ALA:HB2	1:G:47:LEU:HD13	1.90	0.54
1:A:20:GLU:HG3	1:A:26:HIS:NE2	2.22	0.53
1:I:102:HIS:O	1:I:127:CYS:HA	2.08	0.53
1:K:76:ASN:C	1:K:76:ASN:ND2	2.66	0.53
1:L:78:ALA:HB1	1:L:81:THR:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:VAL:O	1:F:23:VAL:HG23	2.08	0.53
1:F:45:ILE:HD11	1:F:146:GLN:NE2	2.24	0.53
1:G:66:GLN:HB2	1:G:94:VAL:HB	1.90	0.53
1:H:76:ASN:C	1:H:76:ASN:HD22	2.16	0.53
1:K:82:HIS:CE1	1:K:113:ARG:HA	2.43	0.53
1:G:50:PHE:CG	1:G:61:ARG:HG3	2.43	0.53
1:I:24:TYR:HE1	1:I:26:HIS:N	2.06	0.53
1:I:129:LEU:HD11	1:L:126:ILE:HD12	1.90	0.53
1:I:24:TYR:HE1	1:I:26:HIS:HA	1.74	0.53
1:B:20:GLU:N	1:B:21:PRO:CD	2.72	0.53
1:D:64:GLN:O	1:D:68:GLU:HG2	2.09	0.53
1:D:145:ILE:HB	1:D:146:GLN:NE2	2.24	0.53
1:H:13:LEU:HD12	1:H:16:LEU:HD11	1.90	0.53
1:I:21:PRO:HB3	1:I:22:GLU:HG2	1.91	0.53
1:I:24:TYR:CE1	1:I:26:HIS:N	2.73	0.53
1:D:57:ALA:HB2	1:L:54:TRP:CH2	2.43	0.53
1:A:149:ASN:N	1:A:150:PRO:CA	2.71	0.52
1:F:102:HIS:O	1:F:127:CYS:HA	2.09	0.52
1:G:76:ASN:C	1:G:76:ASN:ND2	2.67	0.52
1:H:14:ASN:HD22	1:H:14:ASN:H	1.57	0.52
1:H:58:ILE:O	1:H:62:ILE:HG13	2.09	0.52
1:A:98:PHE:CE2	1:A:122:ALA:HB2	2.45	0.52
1:C:85:VAL:O	1:C:88:ARG:HB3	2.10	0.52
1:J:54:TRP:N	1:J:54:TRP:CD1	2.77	0.52
1:K:116:SER:HB3	1:K:119:SER:HB2	1.90	0.52
1:J:66:GLN:HB2	1:J:94:VAL:HB	1.92	0.52
1:D:4:THR:C	1:D:70:VAL:HG23	2.35	0.52
1:H:47:LEU:HD23	1:H:47:LEU:O	2.10	0.52
1:B:12:ASN:HA	1:C:63:HIS:HE1	1.73	0.52
1:D:129:LEU:HD13	1:D:136:PHE:HE2	1.76	0.52
1:J:92:LEU:O	1:J:95:ALA:N	2.43	0.52
1:L:76:ASN:C	1:L:76:ASN:ND2	2.65	0.52
1:B:15:LEU:HD22	1:B:18:LYS:HD2	1.92	0.51
1:J:22:GLU:O	1:J:23:VAL:HG13	2.10	0.51
1:A:71:LYS:O	1:A:97:PRO:HD2	2.10	0.51
1:C:13:LEU:HD21	1:C:78:ALA:HB2	1.91	0.51
1:L:36:LEU:HD21	1:L:134:TYR:HB3	1.93	0.51
1:B:22:GLU:HA	1:B:24:TYR:O	2.11	0.51
1:C:97:PRO:HB2	1:C:123:ILE:HD11	1.92	0.51
1:H:45:ILE:HG22	1:H:46:THR:O	2.11	0.51
1:K:62:ILE:CD1	1:K:91:LEU:HG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASN:HA	1:B:101:VAL:O	2.11	0.51
1:E:23:VAL:HG23	1:E:23:VAL:O	2.10	0.51
1:I:100:GLU:O	1:I:125:VAL:HA	2.11	0.51
1:L:16:LEU:HD13	1:L:28:THR:HG22	1.92	0.51
1:A:20:GLU:CG	1:A:26:HIS:CE1	2.94	0.51
1:E:98:PHE:CE2	1:E:122:ALA:HB2	2.46	0.51
1:H:10:GLY:N	1:H:76:ASN:O	2.44	0.51
1:K:88:ARG:O	1:K:92:LEU:HB2	2.10	0.51
1:B:147:PRO:O	1:B:148:SER:HB2	2.11	0.51
1:H:81:THR:HG23	1:H:82:HIS:CE1	2.46	0.51
1:J:29:LEU:CD1	1:J:51:GLN:HG3	2.41	0.51
1:A:63:HIS:CE1	1:C:14:ASN:HD21	2.29	0.51
1:A:54:TRP:CH2	1:B:57:ALA:HB2	2.46	0.50
1:G:145:ILE:O	1:G:145:ILE:HG22	2.11	0.50
1:H:55:GLU:O	1:H:59:VAL:HG23	2.11	0.50
1:J:8:ILE:HB	1:J:75:ILE:HG13	1.92	0.50
1:L:10:GLY:N	1:L:76:ASN:O	2.43	0.50
1:B:81:THR:HG21	1:B:100:GLU:OE2	2.10	0.50
1:B:143:GLU:O	1:B:145:ILE:N	2.44	0.50
1:K:62:ILE:HD13	1:K:91:LEU:HG	1.94	0.50
1:A:82:HIS:CE1	1:A:113:ARG:HA	2.47	0.50
1:I:94:VAL:HG21	1:I:96:ILE:HD12	1.93	0.50
1:L:6:LEU:HD13	1:L:61:ARG:NH1	2.27	0.50
1:A:107:HIS:CD2	1:A:107:HIS:H	2.29	0.50
1:E:41:GLU:C	1:E:43:ALA:H	2.20	0.50
1:H:146:GLN:HE21	1:H:146:GLN:HA	1.77	0.50
1:I:7:VAL:HB	1:I:49:THR:HG22	1.92	0.50
1:K:8:ILE:HG21	1:K:58:ILE:HG23	1.94	0.50
1:L:133:GLY:HA2	1:L:136:PHE:CD2	2.47	0.50
1:G:28:THR:O	1:G:31:ASN:HB2	2.12	0.50
1:H:41:GLU:C	1:H:43:ALA:N	2.70	0.50
1:J:25:GLY:O	1:J:26:HIS:HB3	2.12	0.50
1:L:78:ALA:CB	1:L:102:HIS:ND1	2.75	0.50
1:F:72:LEU:HD23	1:F:73:ILE:N	2.26	0.49
1:J:144:LYS:C	1:J:144:LYS:CD	2.85	0.49
1:A:39:GLN:CD	1:A:138:LEU:HD23	2.36	0.49
1:I:62:ILE:CD1	1:I:91:LEU:HD21	2.41	0.49
1:J:20:GLU:HG2	1:J:21:PRO:HA	1.93	0.49
1:J:50:PHE:CG	1:J:61:ARG:HG3	2.48	0.49
1:L:23:VAL:O	1:L:23:VAL:CG1	2.57	0.49
1:C:99:ILE:HD11	1:C:140:TYR:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:LYS:HZ1	1:J:143:GLU:HG3	1.76	0.49
1:I:94:VAL:HG23	1:I:96:ILE:HG13	1.94	0.49
1:K:20:GLU:HB2	1:K:21:PRO:HD3	1.91	0.49
1:H:73:ILE:O	1:H:98:PHE:HA	2.12	0.49
1:E:45:ILE:CD1	1:E:145:ILE:HD13	2.42	0.49
1:E:55:GLU:O	1:E:59:VAL:HG23	2.13	0.49
1:D:74:ILE:HD11	1:D:138:LEU:HA	1.94	0.49
1:B:136:PHE:HB3	1:K:136:PHE:CG	2.47	0.49
1:E:72:LEU:HD23	1:E:72:LEU:C	2.38	0.49
1:K:27:LEU:HD12	1:K:31:ASN:HB2	1.94	0.49
1:B:6:LEU:HD22	1:B:61:ARG:NH1	2.28	0.49
1:G:45:ILE:HD11	1:G:142:ILE:HG23	1.94	0.49
1:J:14:ASN:HB3	1:J:51:GLN:NE2	2.28	0.49
1:L:72:LEU:C	1:L:72:LEU:HD23	2.37	0.49
1:C:106:VAL:HG13	1:C:113:ARG:HB3	1.93	0.49
1:D:64:GLN:HA	1:D:67:THR:OG1	2.13	0.49
1:E:28:THR:H	1:E:31:ASN:ND2	2.11	0.49
1:K:28:THR:H	1:K:31:ASN:HD22	1.61	0.48
1:K:33:ASN:O	1:K:37:ILE:HG13	2.13	0.48
1:B:81:THR:HG22	1:B:118:LEU:HB2	1.95	0.48
1:D:141:ALA:O	1:D:144:LYS:HB3	2.14	0.48
1:I:47:LEU:HD12	1:I:138:LEU:HD11	1.95	0.48
1:D:4:THR:CG2	1:D:70:VAL:HA	2.37	0.48
1:F:35:GLN:HE21	1:F:36:LEU:CD1	2.23	0.48
1:H:92:LEU:HD21	1:H:121:LYS:HB3	1.96	0.48
1:I:134:TYR:O	1:I:137:ALA:HB3	2.13	0.48
1:G:16:LEU:HB3	1:G:27:LEU:O	2.13	0.48
1:B:100:GLU:OE1	1:B:119:SER:HA	2.13	0.48
1:C:140:TYR:CD2	1:F:129:LEU:HD22	2.48	0.48
1:F:47:LEU:C	1:F:47:LEU:HD23	2.38	0.48
1:G:5:ILE:O	1:G:47:LEU:HA	2.14	0.48
1:H:11:PRO:O	1:H:12:ASN:HB2	2.13	0.48
1:D:12:ASN:ND2	1:H:90:ALA:HA	2.29	0.48
1:I:4:THR:HA	1:I:46:THR:O	2.13	0.48
1:L:20:GLU:OE1	1:L:26:HIS:HA	2.14	0.48
1:I:54:TRP:CH2	1:J:57:ALA:HB2	2.49	0.48
1:J:66:GLN:HG3	2:J:225:HOH:O	2.13	0.48
1:K:19:ARG:HE	1:K:23:VAL:HG21	1.79	0.48
1:L:139:ASP:C	1:L:139:ASP:OD1	2.56	0.48
1:G:140:TYR:CD1	1:G:140:TYR:C	2.92	0.48
1:I:20:GLU:HG2	1:I:26:HIS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:142:ILE:O	1:I:144:LYS:N	2.47	0.48
1:G:9:HIS:HB3	1:G:13:LEU:HD23	1.96	0.48
1:I:58:ILE:HG22	1:I:87:LEU:HD11	1.96	0.48
1:K:3:SER:HB3	1:K:145:ILE:HD13	1.96	0.48
1:K:50:PHE:CD1	1:K:51:GLN:N	2.82	0.48
1:E:27:LEU:HD21	1:E:131:ALA:CB	2.44	0.48
1:G:77:PRO:HG2	1:G:81:THR:HB	1.95	0.48
1:I:57:ALA:HB2	1:K:54:TRP:CH2	2.49	0.48
1:L:106:VAL:HG22	1:L:113:ARG:HB3	1.95	0.48
1:A:141:ALA:O	1:A:145:ILE:HG13	2.13	0.47
1:D:12:ASN:O	1:D:15:LEU:HB2	2.13	0.47
1:F:98:PHE:CE2	1:F:122:ALA:HB2	2.49	0.47
1:I:24:TYR:HD1	1:I:24:TYR:C	2.22	0.47
1:J:20:GLU:OE1	1:J:26:HIS:HB2	2.13	0.47
1:J:103:LEU:HD23	1:J:130:GLY:C	2.39	0.47
1:K:111:ALA:HA	1:K:114:HIS:CE1	2.49	0.47
1:B:16:LEU:HD11	1:B:103:LEU:HD11	1.96	0.47
1:A:101:VAL:HA	1:A:126:ILE:O	2.14	0.47
1:L:14:ASN:HD22	1:L:14:ASN:N	1.99	0.47
1:D:98:PHE:CE2	1:D:122:ALA:HB2	2.49	0.47
1:B:29:LEU:HD21	1:B:51:GLN:HG3	1.96	0.47
1:L:28:THR:H	1:L:31:ASN:HD22	1.61	0.47
1:C:62:ILE:O	1:C:65:ALA:HB3	2.14	0.47
1:D:5:ILE:O	1:D:47:LEU:HB2	2.14	0.47
1:B:140:TYR:CD1	1:B:140:TYR:C	2.93	0.47
1:C:13:LEU:HD22	1:C:78:ALA:HB2	1.95	0.47
1:H:35:GLN:HE21	1:H:35:GLN:CA	2.28	0.47
1:I:87:LEU:HD23	1:I:118:LEU:HD21	1.97	0.47
1:I:145:ILE:HD12	1:I:145:ILE:C	2.39	0.47
1:J:20:GLU:HB2	1:J:26:HIS:N	2.30	0.47
1:C:3:SER:O	1:C:70:VAL:HG22	2.14	0.47
1:I:142:ILE:C	1:I:144:LYS:N	2.72	0.47
1:J:20:GLU:CA	1:J:25:GLY:HA3	2.45	0.47
1:A:54:TRP:CD1	1:A:54:TRP:N	2.83	0.47
1:J:76:ASN:C	1:J:76:ASN:ND2	2.73	0.47
1:L:50:PHE:CG	1:L:61:ARG:HG3	2.50	0.47
1:C:25:GLY:C	1:C:27:LEU:H	2.23	0.46
1:F:39:GLN:HB3	1:F:138:LEU:HD23	1.96	0.46
1:G:105:ASN:ND2	1:J:122:ALA:O	2.47	0.46
1:J:52:SER:HG	1:J:54:TRP:CD1	2.33	0.46
1:A:77:PRO:HG2	1:A:81:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ILE:O	1:D:75:ILE:HG23	2.14	0.46
1:I:142:ILE:C	1:I:144:LYS:H	2.23	0.46
1:J:57:ALA:O	1:J:60:ASP:HB2	2.15	0.46
1:L:11:PRO:O	1:L:12:ASN:HB2	2.15	0.46
1:C:136:PHE:CD2	1:F:136:PHE:HB3	2.49	0.46
1:D:111:ALA:HB2	2:D:207:HOH:O	2.15	0.46
1:L:73:ILE:O	1:L:98:PHE:HA	2.15	0.46
1:L:76:ASN:ND2	1:L:78:ALA:H	2.14	0.46
1:B:6:LEU:HD21	1:B:61:ARG:HD3	1.98	0.46
1:D:4:THR:HG23	1:D:70:VAL:CA	2.40	0.46
1:F:28:THR:O	1:F:31:ASN:HB2	2.15	0.46
1:L:57:ALA:O	1:L:61:ARG:HB2	2.15	0.46
1:D:72:LEU:HD22	1:D:141:ALA:HB2	1.98	0.46
1:F:5:ILE:HG22	1:F:6:LEU:N	2.30	0.46
1:A:29:LEU:HD11	1:A:51:GLN:HG3	1.97	0.46
1:E:53:ASN:HB3	1:F:59:VAL:HG11	1.96	0.46
1:G:112:PHE:CD1	1:G:113:ARG:HG3	2.51	0.46
1:H:20:GLU:N	1:H:21:PRO:CD	2.79	0.46
1:J:12:ASN:C	1:J:14:ASN:N	2.72	0.46
1:B:19:ARG:HE	1:B:23:VAL:HG22	1.81	0.46
1:I:73:ILE:O	1:I:98:PHE:HA	2.14	0.46
1:J:6:LEU:HB3	1:J:70:VAL:HG11	1.98	0.46
1:E:115:HIS:HE1	1:E:117:TYR:CE2	2.34	0.46
1:K:16:LEU:N	1:K:16:LEU:HD23	2.30	0.46
1:L:18:LYS:CE	1:L:18:LYS:CA	2.85	0.46
1:E:76:ASN:C	1:E:76:ASN:HD22	2.23	0.46
1:G:23:VAL:O	1:G:25:GLY:N	2.49	0.46
1:L:17:GLY:HA3	1:L:25:GLY:O	2.16	0.46
1:B:19:ARG:C	1:B:19:ARG:CD	2.85	0.45
1:D:4:THR:CG2	1:D:70:VAL:HG23	2.40	0.45
1:G:88:ARG:NH1	1:G:117:TYR:O	2.39	0.45
1:H:142:ILE:O	1:H:146:GLN:N	2.30	0.45
1:I:32:ILE:HA	1:I:35:GLN:HB3	1.97	0.45
1:B:34:ARG:HH21	1:B:34:ARG:HG3	1.81	0.45
1:J:40:ALA:HB2	1:J:138:LEU:HD21	1.97	0.45
1:A:84:SER:HB3	1:A:87:LEU:H	1.82	0.45
1:H:72:LEU:HD23	1:H:72:LEU:C	2.41	0.45
1:I:24:TYR:C	1:I:24:TYR:CD1	2.95	0.45
1:J:106:VAL:HG22	1:J:113:ARG:O	2.16	0.45
1:D:3:SER:C	1:D:4:THR:HG22	2.40	0.45
1:F:19:ARG:O	1:F:23:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:ASN:OD1	1:I:14:ASN:N	2.50	0.45
1:A:107:HIS:HA	1:A:114:HIS:CD2	2.51	0.45
1:D:90:ALA:O	1:D:94:VAL:HG22	2.16	0.45
1:F:4:THR:CG2	1:F:70:VAL:HA	2.42	0.45
1:H:50:PHE:CG	1:H:61:ARG:HG3	2.51	0.45
1:J:36:LEU:HD21	1:J:134:TYR:HB3	1.98	0.45
1:H:22:GLU:OE2	1:H:22:GLU:N	2.49	0.45
1:I:132:LYS:O	1:I:136:PHE:CD2	2.69	0.45
1:I:14:ASN:HA	1:I:29:LEU:HB2	1.99	0.45
1:K:125:VAL:HG12	1:K:126:ILE:N	2.32	0.45
1:B:13:LEU:HD11	1:B:76:ASN:CG	2.42	0.45
1:J:75:ILE:HG23	1:J:77:PRO:HD3	1.99	0.45
1:K:76:ASN:HA	1:K:101:VAL:O	2.17	0.45
1:B:106:VAL:HG13	1:B:113:ARG:HG2	1.98	0.45
1:D:77:PRO:HB2	1:D:81:THR:OG1	2.17	0.45
1:H:98:PHE:CE2	1:H:122:ALA:HB2	2.52	0.45
1:I:47:LEU:CD2	1:I:49:THR:HG23	2.47	0.45
1:K:6:LEU:HD22	1:K:61:ARG:NH1	2.32	0.45
1:L:145:ILE:O	1:L:145:ILE:CG2	2.60	0.45
1:B:81:THR:O	1:B:116:SER:HA	2.17	0.45
1:G:112:PHE:CE1	1:G:113:ARG:HG3	2.52	0.45
1:E:35:GLN:HG3	1:E:36:LEU:N	2.32	0.44
1:F:73:ILE:O	1:F:98:PHE:HA	2.17	0.44
1:I:76:ASN:C	1:I:76:ASN:HD22	2.24	0.44
1:K:19:ARG:NE	1:K:23:VAL:HG21	2.32	0.44
1:B:97:PRO:CB	1:B:123:ILE:HD11	2.47	0.44
1:C:36:LEU:HD11	1:C:134:TYR:HB3	1.99	0.44
1:G:54:TRP:N	1:G:54:TRP:CD1	2.84	0.44
1:H:81:THR:HG23	1:H:82:HIS:ND1	2.32	0.44
1:B:124:GLY:HA2	1:K:128:GLY:HA3	1.98	0.44
1:G:109:ARG:HB2	1:G:113:ARG:HD2	1.99	0.44
1:H:141:ALA:O	1:H:145:ILE:HD12	2.17	0.44
1:I:13:LEU:HD12	1:I:13:LEU:HA	1.73	0.44
1:I:55:GLU:O	1:I:59:VAL:HG23	2.18	0.44
1:K:77:PRO:O	1:K:78:ALA:HB3	2.16	0.44
1:B:50:PHE:CD2	1:B:61:ARG:HG3	2.52	0.44
1:E:145:ILE:O	1:E:145:ILE:HG22	2.17	0.44
1:J:47:LEU:HD23	1:J:47:LEU:C	2.43	0.44
1:D:83:THR:CG2	1:D:84:SER:N	2.79	0.44
1:E:102:HIS:O	1:E:127:CYS:HA	2.18	0.44
1:G:29:LEU:CD1	1:G:51:GLN:HG3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:88:ARG:NH1	1:L:117:TYR:O	2.50	0.44
1:I:20:GLU:HG2	1:I:26:HIS:CB	2.48	0.44
1:J:90:ALA:O	1:J:94:VAL:HG13	2.17	0.44
1:D:3:SER:HB3	1:D:71:LYS:HG2	2.00	0.44
1:E:32:ILE:HD11	1:E:131:ALA:HB2	2.00	0.44
1:E:57:ALA:HB2	1:G:54:TRP:CH2	2.53	0.44
1:F:75:ILE:HD11	1:F:87:LEU:HD21	1.99	0.44
1:I:25:GLY:O	1:I:26:HIS:CG	2.70	0.44
1:D:25:GLY:O	1:D:26:HIS:CD2	2.70	0.44
1:E:45:ILE:HG22	1:E:46:THR:O	2.18	0.44
1:E:75:ILE:CG1	1:E:76:ASN:N	2.80	0.44
1:H:81:THR:CG2	1:H:82:HIS:CE1	3.01	0.44
1:I:142:ILE:O	1:I:145:ILE:HG13	2.18	0.44
1:J:3:SER:HB2	1:J:71:LYS:CG	2.43	0.44
1:J:26:HIS:O	1:J:26:HIS:CG	2.71	0.44
1:J:28:THR:HG22	1:J:29:LEU:N	2.33	0.44
1:J:110:GLU:O	1:J:113:ARG:HB2	2.18	0.44
1:K:20:GLU:HB3	1:K:21:PRO:CD	2.40	0.44
1:D:54:TRP:CD2	1:H:56:GLY:HA3	2.53	0.44
1:E:141:ALA:O	1:E:145:ILE:HG13	2.17	0.44
1:F:75:ILE:HG12	1:F:77:PRO:HD3	2.00	0.44
1:G:45:ILE:HD12	1:G:142:ILE:CG1	2.33	0.44
1:J:88:ARG:CD	1:J:117:TYR:O	2.66	0.44
1:K:13:LEU:HD21	1:K:76:ASN:CG	2.43	0.44
1:B:14:ASN:OD1	1:B:14:ASN:N	2.46	0.43
1:B:20:GLU:CG	1:B:21:PRO:HD3	2.48	0.43
1:D:7:VAL:HG11	1:D:36:LEU:HD23	1.99	0.43
1:E:105:ASN:OD1	1:E:105:ASN:C	2.61	0.43
1:F:75:ILE:CD1	1:F:87:LEU:HD21	2.48	0.43
1:K:16:LEU:O	1:K:28:THR:HA	2.17	0.43
1:K:101:VAL:HA	1:K:126:ILE:O	2.17	0.43
1:E:73:ILE:O	1:E:98:PHE:HA	2.18	0.43
1:I:63:HIS:O	1:I:66:GLN:HG2	2.17	0.43
1:I:78:ALA:O	1:I:81:THR:HG22	2.18	0.43
1:L:23:VAL:O	1:L:23:VAL:HG13	2.18	0.43
1:B:149:ASN:N	1:B:149:ASN:ND2	2.63	0.43
1:J:50:PHE:CG	1:J:51:GLN:N	2.85	0.43
1:B:12:ASN:HA	1:C:63:HIS:CE1	2.53	0.43
1:G:32:ILE:HG22	1:G:36:LEU:HD22	1.99	0.43
1:J:26:HIS:O	1:J:26:HIS:CD2	2.70	0.43
1:A:4:THR:HG22	2:A:227:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:PRO:O	1:B:151:ASN:HB3	2.19	0.43
1:G:25:GLY:HA3	2:G:219:HOH:O	2.18	0.43
1:I:24:TYR:CD1	1:I:25:GLY:N	2.77	0.43
1:L:81:THR:HA	2:L:203:HOH:O	2.18	0.43
1:A:18:LYS:N	2:A:231:HOH:O	2.51	0.43
1:B:136:PHE:CG	1:K:136:PHE:HB3	2.53	0.43
1:F:72:LEU:HD23	1:F:72:LEU:C	2.43	0.43
1:C:109:ARG:HB2	1:C:113:ARG:HD2	2.00	0.43
1:E:9:HIS:HB2	1:E:51:GLN:HG2	2.00	0.43
1:L:45:ILE:HD12	1:L:142:ILE:HD12	2.00	0.43
1:L:115:HIS:CG	1:L:116:SER:N	2.87	0.43
1:B:74:ILE:HG12	1:B:137:ALA:HB1	2.00	0.43
1:C:9:HIS:CG	1:C:29:LEU:HD21	2.53	0.43
1:C:33:ASN:O	1:C:37:ILE:HG13	2.19	0.43
1:F:54:TRP:O	1:F:58:ILE:HG13	2.19	0.43
1:G:106:VAL:HG23	1:G:127:CYS:HB2	2.01	0.43
1:I:40:ALA:CB	1:I:47:LEU:HB2	2.49	0.43
1:F:11:PRO:HA	1:F:53:ASN:OD1	2.19	0.43
1:J:29:LEU:HD11	1:J:51:GLN:HG3	2.01	0.43
1:J:79:ALA:HB1	1:K:85:VAL:HG22	1.99	0.43
1:B:149:ASN:N	1:B:149:ASN:HD22	2.17	0.43
1:D:100:GLU:HB3	1:D:125:VAL:HG13	2.01	0.43
1:F:105:ASN:N	1:F:128:GLY:HA2	2.34	0.43
1:H:140:TYR:CE2	1:H:144:LYS:HG3	2.53	0.43
1:J:73:ILE:O	1:J:98:PHE:HA	2.18	0.43
1:K:11:PRO:C	1:K:12:ASN:ND2	2.75	0.43
1:B:43:ALA:O	1:B:44:SER:HB2	2.19	0.42
1:G:142:ILE:O	1:G:146:GLN:HG2	2.19	0.42
1:I:13:LEU:HD21	1:I:76:ASN:CG	2.44	0.42
1:K:36:LEU:N	1:K:36:LEU:CD1	2.82	0.42
1:L:45:ILE:HD12	1:L:142:ILE:CD1	2.49	0.42
1:B:2:SER:O	1:B:71:LYS:HG2	2.20	0.42
1:F:20:GLU:O	1:F:22:GLU:N	2.50	0.42
1:I:112:PHE:CD1	1:I:112:PHE:C	2.98	0.42
1:J:12:ASN:ND2	1:K:89:ASP:HB2	2.34	0.42
1:L:8:ILE:HG21	1:L:58:ILE:HG23	2.01	0.42
1:L:18:LYS:O	1:L:19:ARG:HB2	2.18	0.42
1:C:20:GLU:OE1	1:C:26:HIS:ND1	2.53	0.42
1:C:58:ILE:HG21	1:C:87:LEU:HD11	2.01	0.42
1:D:3:SER:O	1:D:4:THR:HG22	2.18	0.42
1:D:132:LYS:O	1:D:135:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:36:LEU:HD21	1:H:134:TYR:HB3	2.01	0.42
1:J:8:ILE:HG21	1:J:58:ILE:HG23	2.01	0.42
1:H:50:PHE:CD1	1:H:61:ARG:HG3	2.53	0.42
1:I:56:GLY:HA3	1:K:54:TRP:CD2	2.54	0.42
1:I:65:ALA:HA	1:I:68:GLU:HB2	2.01	0.42
1:A:86:ALA:HA	1:C:79:ALA:CB	2.49	0.42
1:G:26:HIS:CD2	1:G:26:HIS:N	2.88	0.42
1:A:17:GLY:HA2	1:A:25:GLY:O	2.19	0.42
1:B:19:ARG:NH2	1:B:23:VAL:HG13	2.32	0.42
1:C:54:TRP:CD1	1:C:54:TRP:N	2.87	0.42
1:D:62:ILE:HD11	1:D:90:ALA:O	2.20	0.42
1:F:9:HIS:CD2	1:F:29:LEU:HD21	2.55	0.42
1:H:6:LEU:HD21	1:H:61:ARG:NE	2.34	0.42
1:H:60:ASP:O	1:H:63:HIS:HB2	2.19	0.42
1:J:144:LYS:C	1:J:144:LYS:HD2	2.44	0.42
1:L:54:TRP:CD1	1:L:54:TRP:N	2.87	0.42
1:B:109:ARG:HB2	1:B:110:GLU:OE1	2.20	0.42
1:E:42:GLN:CG	1:E:42:GLN:O	2.67	0.42
1:G:9:HIS:CG	1:G:29:LEU:HD21	2.55	0.42
1:G:88:ARG:HH22	1:G:120:ASP:CG	2.27	0.42
1:I:54:TRP:CG	1:J:56:GLY:HA3	2.54	0.42
1:K:92:LEU:HD21	1:K:121:LYS:HD2	2.00	0.42
1:L:14:ASN:N	1:L:14:ASN:ND2	2.66	0.42
1:B:77:PRO:HG3	1:B:81:THR:HG23	2.00	0.42
1:D:72:LEU:HD21	1:D:99:ILE:HD12	2.01	0.42
1:F:13:LEU:HD12	1:F:13:LEU:HA	1.74	0.42
1:J:33:ASN:OD1	1:J:49:THR:HG21	2.20	0.42
1:J:94:VAL:CG2	1:J:96:ILE:HG13	2.47	0.42
1:J:110:GLU:HB2	1:J:113:ARG:HG3	2.01	0.42
1:A:3:SER:HB3	1:A:145:ILE:HD13	2.02	0.42
1:C:62:ILE:O	1:C:94:VAL:HG11	2.19	0.42
1:D:54:TRP:CD1	1:D:54:TRP:N	2.88	0.42
1:F:82:HIS:CE1	1:F:113:ARG:O	2.73	0.42
1:G:45:ILE:CD1	1:G:142:ILE:HG23	2.49	0.42
1:L:6:LEU:HD13	1:L:61:ARG:HH11	1.84	0.42
1:B:20:GLU:N	1:B:21:PRO:HD2	2.34	0.42
1:C:112:PHE:CD1	1:C:112:PHE:C	2.98	0.42
1:C:138:LEU:HG	1:C:142:ILE:CD1	2.50	0.42
1:E:24:TYR:HB3	1:E:25:GLY:H	1.50	0.42
1:F:39:GLN:HB3	1:F:138:LEU:HD21	2.01	0.42
1:F:76:ASN:HD22	1:F:78:ALA:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:19:ARG:CD	1:K:23:VAL:HG21	2.50	0.42
1:L:78:ALA:HB2	1:L:81:THR:HG21	1.98	0.42
1:F:50:PHE:CG	1:F:61:ARG:HG3	2.55	0.41
1:I:58:ILE:O	1:I:62:ILE:HG13	2.20	0.41
1:B:147:PRO:O	1:B:148:SER:CB	2.68	0.41
1:H:87:LEU:HD23	1:H:118:LEU:HD21	2.00	0.41
1:H:100:GLU:O	1:H:125:VAL:HA	2.20	0.41
1:J:96:ILE:HG22	1:J:97:PRO:O	2.20	0.41
1:L:15:LEU:HA	1:L:16:LEU:HB2	2.01	0.41
1:F:13:LEU:C	1:F:15:LEU:H	2.28	0.41
1:K:13:LEU:HD12	1:K:13:LEU:HA	1.90	0.41
1:F:36:LEU:HD21	1:F:134:TYR:HB3	2.02	0.41
1:K:32:ILE:O	1:K:36:LEU:HD13	2.21	0.41
1:L:112:PHE:CD1	1:L:112:PHE:C	2.99	0.41
1:A:12:ASN:HD21	1:B:90:ALA:HB2	1.86	0.41
1:A:79:ALA:CB	1:B:85:VAL:CG2	2.96	0.41
1:G:72:LEU:C	1:G:72:LEU:CD2	2.88	0.41
1:I:9:HIS:CE1	1:I:134:TYR:HH	2.35	0.41
1:B:81:THR:O	1:B:117:TYR:N	2.42	0.41
1:C:13:LEU:HD13	1:C:13:LEU:HA	1.89	0.41
1:E:63:HIS:CE1	1:G:15:LEU:HD11	2.52	0.41
1:K:94:VAL:O	1:K:95:ALA:CB	2.68	0.41
1:A:65:ALA:HA	1:A:68:GLU:OE1	2.21	0.41
1:D:4:THR:HG23	1:D:70:VAL:CB	2.49	0.41
1:H:71:LYS:HG2	1:H:145:ILE:HG23	2.02	0.41
1:H:77:PRO:O	1:H:78:ALA:HB3	2.20	0.41
1:I:21:PRO:HA	1:I:22:GLU:HA	1.56	0.41
1:I:60:ASP:OD1	1:I:60:ASP:N	2.54	0.41
1:J:76:ASN:HA	1:J:101:VAL:O	2.20	0.41
1:B:19:ARG:NE	1:B:21:PRO:O	2.54	0.41
1:B:134:TYR:O	1:B:137:ALA:HB3	2.20	0.41
1:C:73:ILE:O	1:C:98:PHE:HA	2.20	0.41
1:H:109:ARG:CB	1:H:113:ARG:HD2	2.47	0.41
1:H:146:GLN:HE21	1:H:146:GLN:C	2.29	0.41
1:K:34:ARG:HA	1:K:37:ILE:HD12	2.02	0.41
1:K:72:LEU:HD23	1:K:72:LEU:C	2.46	0.41
1:B:29:LEU:HD12	1:B:29:LEU:HA	1.83	0.41
1:G:61:ARG:NH1	1:G:68:GLU:OE1	2.54	0.41
1:I:27:LEU:C	1:I:27:LEU:HD12	2.46	0.41
1:K:81:THR:HG23	1:K:116:SER:CB	2.51	0.41
1:A:84:SER:CB	1:A:87:LEU:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.91	0.41
1:H:120:ASP:OD1	1:H:120:ASP:N	2.54	0.41
1:J:87:LEU:HD12	1:J:87:LEU:HA	1.88	0.41
1:D:54:TRP:NE1	1:H:60:ASP:OD2	2.47	0.40
1:D:77:PRO:O	1:D:78:ALA:CB	2.69	0.40
1:E:83:THR:CG2	1:F:85:VAL:HG12	2.51	0.40
1:K:62:ILE:HD11	1:K:90:ALA:C	2.46	0.40
1:H:35:GLN:HE21	1:H:35:GLN:N	2.20	0.40
1:H:87:LEU:CD2	1:H:118:LEU:HD21	2.51	0.40
1:L:35:GLN:HG3	1:L:36:LEU:N	2.34	0.40
1:B:129:LEU:HD11	1:K:126:ILE:HD11	2.03	0.40
1:D:141:ALA:O	1:D:144:LYS:N	2.54	0.40
1:K:28:THR:H	1:K:31:ASN:ND2	2.19	0.40
1:K:77:PRO:HG3	1:K:118:LEU:CD1	2.51	0.40
1:L:5:ILE:HD13	1:L:5:ILE:HG21	1.87	0.40
1:A:20:GLU:N	1:A:21:PRO:CD	2.83	0.40
1:A:66:GLN:NE2	1:A:94:VAL:HA	2.37	0.40
1:H:146:GLN:CA	1:H:146:GLN:NE2	2.83	0.40
1:K:102:HIS:HB2	1:K:127:CYS:HB2	2.02	0.40
1:D:25:GLY:O	1:D:26:HIS:CB	2.70	0.40
1:D:83:THR:HG22	1:D:84:SER:N	2.36	0.40
1:E:101:VAL:HG12	1:E:102:HIS:N	2.36	0.40
1:G:6:LEU:HD13	1:G:61:ARG:NH2	2.36	0.40
1:G:75:ILE:HG12	1:G:77:PRO:HD3	2.03	0.40
1:J:16:LEU:O	1:J:28:THR:HG23	2.21	0.40
1:J:33:ASN:O	1:J:37:ILE:HG13	2.21	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	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	18	37
1	B	148/150 (99%)	135 (91%)	9 (6%)	4 (3%)	4	9
1	C	143/150 (95%)	130 (91%)	11 (8%)	2 (1%)	9	21
1	D	143/150 (95%)	112 (78%)	29 (20%)	2 (1%)	9	21
1	E	143/150 (95%)	133 (93%)	10 (7%)	0	100	100
1	F	142/150 (95%)	127 (89%)	14 (10%)	1 (1%)	18	37
1	G	143/150 (95%)	130 (91%)	12 (8%)	1 (1%)	18	37
1	H	143/150 (95%)	127 (89%)	14 (10%)	2 (1%)	9	21
1	I	143/150 (95%)	126 (88%)	14 (10%)	3 (2%)	5	13
1	J	143/150 (95%)	131 (92%)	10 (7%)	2 (1%)	9	21
1	K	143/150 (95%)	125 (87%)	16 (11%)	2 (1%)	9	21
1	L	143/150 (95%)	132 (92%)	10 (7%)	1 (1%)	18	37
All	All	1725/1800 (96%)	1542 (89%)	162 (9%)	21 (1%)	10	24

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	SER
1	C	21	PRO
1	D	20	GLU
1	J	21	PRO
1	B	144	LYS
1	D	4	THR
1	J	23	VAL
1	I	11	PRO
1	I	143	GLU
1	B	150	PRO
1	H	24	TYR
1	I	12	ASN
1	C	109	ARG
1	G	24	TYR
1	H	25	GLY
1	K	78	ALA
1	L	16	LEU
1	F	21	PRO
1	K	27	LEU
1	A	146	GLN
1	B	25	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/124 (100%)	110 (89%)	14 (11%)	5	13
1	B	124/124 (100%)	106 (86%)	18 (14%)	3	7
1	C	119/124 (96%)	107 (90%)	12 (10%)	7	16
1	D	119/124 (96%)	96 (81%)	23 (19%)	1	3
1	E	119/124 (96%)	107 (90%)	12 (10%)	7	16
1	F	118/124 (95%)	106 (90%)	12 (10%)	7	16
1	G	119/124 (96%)	96 (81%)	23 (19%)	1	3
1	H	119/124 (96%)	100 (84%)	19 (16%)	2	5
1	I	119/124 (96%)	107 (90%)	12 (10%)	7	16
1	J	119/124 (96%)	104 (87%)	15 (13%)	4	10
1	K	119/124 (96%)	101 (85%)	18 (15%)	3	6
1	L	119/124 (96%)	90 (76%)	29 (24%)	1	2
All	All	1437/1488 (97%)	1230 (86%)	207 (14%)	3	7

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	29	LEU
1	A	30	ASP
1	A	36	LEU
1	A	37	ILE
1	A	42	GLN
1	A	61	ARG
1	A	85	VAL
1	A	118	LEU
1	A	132	LYS
1	A	139	ASP
1	A	146	GLN
1	A	148	SER
1	A	151	ASN

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Mol	Chain	Res	Type
1	B	2	SER
1	B	4	THR
1	B	19	ARG
1	B	20	GLU
1	B	24	TYR
1	B	26	HIS
1	B	27	LEU
1	B	36	LEU
1	B	61	ARG
1	B	67	THR
1	B	85	VAL
1	B	109	ARG
1	B	132	LYS
1	B	135	SER
1	B	143	GLU
1	B	146	GLN
1	B	149	ASN
1	B	150	PRO
1	C	13	LEU
1	C	23	VAL
1	C	27	LEU
1	C	29	LEU
1	C	42	GLN
1	C	45	ILE
1	C	46	THR
1	C	61	ARG
1	C	81	THR
1	C	84	SER
1	C	85	VAL
1	C	118	LEU
1	D	5	ILE
1	D	13	LEU
1	D	15	LEU
1	D	18	LYS
1	D	20	GLU
1	D	21	PRO
1	D	22	GLU
1	D	23	VAL
1	D	24	TYR
1	D	27	LEU
1	D	29	LEU
1	D	45	ILE

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Mol	Chain	Res	Type
1	D	47	LEU
1	D	61	ARG
1	D	62	ILE
1	D	66	GLN
1	D	73	ILE
1	D	75	ILE
1	D	83	THR
1	D	85	VAL
1	D	87	LEU
1	D	118	LEU
1	D	146	GLN
1	E	3	SER
1	E	13	LEU
1	E	22	GLU
1	E	29	LEU
1	E	30	ASP
1	E	35	GLN
1	E	36	LEU
1	E	54	TRP
1	E	76	ASN
1	E	85	VAL
1	E	118	LEU
1	E	146	GLN
1	F	13	LEU
1	F	29	LEU
1	F	34	ARG
1	F	35	GLN
1	F	36	LEU
1	F	47	LEU
1	F	61	ARG
1	F	62	ILE
1	F	76	ASN
1	F	85	VAL
1	F	132	LYS
1	F	135	SER
1	G	4	THR
1	G	13	LEU
1	G	20	GLU
1	G	23	VAL
1	G	24	TYR
1	G	26	HIS
1	G	27	LEU

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Mol	Chain	Res	Type
1	G	29	LEU
1	G	30	ASP
1	G	36	LEU
1	G	42	GLN
1	G	45	ILE
1	G	46	THR
1	G	58	ILE
1	G	61	ARG
1	G	66	GLN
1	G	67	THR
1	G	72	LEU
1	G	76	ASN
1	G	87	LEU
1	G	106	VAL
1	G	118	LEU
1	G	146	GLN
1	H	5	ILE
1	H	8	ILE
1	H	13	LEU
1	H	14	ASN
1	H	27	LEU
1	H	29	LEU
1	H	34	ARG
1	H	35	GLN
1	H	36	LEU
1	H	44	SER
1	H	61	ARG
1	H	71	LYS
1	H	76	ASN
1	H	85	VAL
1	H	94	VAL
1	H	132	LYS
1	H	135	SER
1	H	143	GLU
1	H	146	GLN
1	I	3	SER
1	I	13	LEU
1	I	18	LYS
1	I	24	TYR
1	I	29	LEU
1	I	30	ASP
1	I	35	GLN

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Mol	Chain	Res	Type
1	I	36	LEU
1	I	42	GLN
1	I	46	THR
1	I	48	ASP
1	I	85	VAL
1	J	4	THR
1	J	8	ILE
1	J	13	LEU
1	J	23	VAL
1	J	29	LEU
1	J	35	GLN
1	J	44	SER
1	J	54	TRP
1	J	61	ARG
1	J	76	ASN
1	J	85	VAL
1	J	118	LEU
1	J	121	LYS
1	J	123	ILE
1	J	144	LYS
1	K	12	ASN
1	K	13	LEU
1	K	19	ARG
1	K	20	GLU
1	K	23	VAL
1	K	27	LEU
1	K	29	LEU
1	K	34	ARG
1	K	46	THR
1	K	61	ARG
1	K	62	ILE
1	K	76	ASN
1	K	81	THR
1	K	85	VAL
1	K	109	ARG
1	K	118	LEU
1	K	132	LYS
1	K	143	GLU
1	L	2	SER
1	L	4	THR
1	L	13	LEU
1	L	14	ASN

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Mol	Chain	Res	Type
1	L	15	LEU
1	L	16	LEU
1	L	19	ARG
1	L	20	GLU
1	L	22	GLU
1	L	23	VAL
1	L	24	TYR
1	L	29	LEU
1	L	35	GLN
1	L	36	LEU
1	L	46	THR
1	L	61	ARG
1	L	67	THR
1	L	73	ILE
1	L	76	ASN
1	L	80	LEU
1	L	81	THR
1	L	85	VAL
1	L	106	VAL
1	L	109	ARG
1	L	110	GLU
1	L	126	ILE
1	L	132	LYS
1	L	139	ASP
1	L	142	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	35	GLN
1	A	64	GLN
1	A	66	GLN
1	A	107	HIS
1	A	146	GLN
1	A	151	ASN
1	B	31	ASN
1	B	35	GLN
1	B	107	HIS
1	B	114	HIS
1	B	146	GLN
1	B	149	ASN

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Mol	Chain	Res	Type
1	B	151	ASN
1	C	14	ASN
1	C	31	ASN
1	C	42	GLN
1	C	115	HIS
1	D	12	ASN
1	D	26	HIS
1	D	33	ASN
1	D	76	ASN
1	D	114	HIS
1	D	115	HIS
1	D	146	GLN
1	E	31	ASN
1	E	76	ASN
1	E	107	HIS
1	E	115	HIS
1	E	146	GLN
1	F	35	GLN
1	F	76	ASN
1	F	146	GLN
1	G	26	HIS
1	G	35	GLN
1	G	42	GLN
1	G	53	ASN
1	G	64	GLN
1	G	66	GLN
1	G	76	ASN
1	G	114	HIS
1	G	146	GLN
1	H	14	ASN
1	H	26	HIS
1	H	33	ASN
1	H	35	GLN
1	H	53	ASN
1	H	63	HIS
1	H	76	ASN
1	H	146	GLN
1	I	35	GLN
1	I	64	GLN
1	I	76	ASN
1	I	114	HIS
1	J	12	ASN

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Mol	Chain	Res	Type
1	J	14	ASN
1	J	26	HIS
1	J	76	ASN
1	J	107	HIS
1	J	114	HIS
1	K	12	ASN
1	K	63	HIS
1	K	76	ASN
1	K	114	HIS
1	L	9	HIS
1	L	14	ASN
1	L	31	ASN
1	L	35	GLN
1	L	42	GLN
1	L	76	ASN
1	L	107	HIS
1	L	146	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	150/150 (100%)	0.05	10 (6%)	24 20	11, 24, 73, 100	1 (0%)
1	B	150/150 (100%)	0.06	10 (6%)	24 20	12, 27, 82, 99	1 (0%)
1	C	145/150 (96%)	-0.14	7 (4%)	35 31	10, 24, 52, 85	1 (0%)
1	D	145/150 (96%)	0.68	16 (11%)	10 8	16, 43, 85, 94	1 (0%)
1	E	145/150 (96%)	0.09	8 (5%)	30 26	15, 29, 69, 96	1 (0%)
1	F	144/150 (96%)	-0.06	5 (3%)	47 42	11, 24, 56, 93	1 (0%)
1	G	145/150 (96%)	0.13	5 (3%)	48 43	16, 32, 70, 92	1 (0%)
1	H	145/150 (96%)	0.40	7 (4%)	35 31	19, 40, 78, 99	1 (0%)
1	I	145/150 (96%)	0.87	14 (9%)	13 11	28, 51, 88, 99	1 (0%)
1	J	145/150 (96%)	0.51	11 (7%)	20 17	20, 42, 83, 99	1 (0%)
1	K	145/150 (96%)	0.55	10 (6%)	23 19	20, 39, 72, 99	1 (0%)
1	L	145/150 (96%)	0.89	10 (6%)	23 19	29, 51, 84, 99	1 (0%)
All	All	1749/1800 (97%)	0.33	113 (6%)	25 21	10, 36, 80, 100	12 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	79	ALA	7.2
1	A	24	TYR	5.2
1	K	23	VAL	5.1
1	B	147	PRO	5.1
1	F	24	TYR	4.7
1	H	23	VAL	4.5
1	J	27	LEU	4.4
1	K	24	TYR	4.4
1	A	23	VAL	4.1
1	E	23	VAL	4.0
1	G	2	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	150	PRO	3.8
1	K	21	PRO	3.8
1	I	23	VAL	3.8
1	F	23	VAL	3.7
1	J	26	HIS	3.5
1	I	25	GLY	3.5
1	L	23	VAL	3.5
1	D	24	TYR	3.5
1	A	22	GLU	3.5
1	I	24	TYR	3.4
1	G	24	TYR	3.4
1	D	23	VAL	3.4
1	H	24	TYR	3.3
1	L	16	LEU	3.3
1	C	24	TYR	3.2
1	I	145	ILE	3.2
1	A	25	GLY	3.2
1	B	2	SER	3.2
1	B	3	SER	3.2
1	K	3	SER	3.2
1	G	3	SER	3.1
1	D	67	THR	3.1
1	J	146	GLN	3.1
1	I	17	GLY	3.1
1	B	146	GLN	3.1
1	B	23	VAL	3.1
1	F	21	PRO	3.0
1	J	2	SER	3.0
1	D	21	PRO	3.0
1	H	20	GLU	3.0
1	E	24	TYR	3.0
1	B	148	SER	2.9
1	J	21	PRO	2.9
1	D	45	ILE	2.9
1	H	19	ARG	2.9
1	I	27	LEU	2.9
1	H	21	PRO	2.9
1	C	23	VAL	2.9
1	J	24	TYR	2.8
1	L	40	ALA	2.8
1	L	131	ALA	2.8
1	L	21	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	21	PRO	2.8
1	I	22	GLU	2.8
1	C	21	PRO	2.7
1	D	64	GLN	2.7
1	C	127	CYS	2.7
1	A	148	SER	2.7
1	I	3	SER	2.7
1	E	21	PRO	2.7
1	E	22	GLU	2.6
1	C	25	GLY	2.5
1	L	127	CYS	2.5
1	F	22	GLU	2.5
1	F	3	SER	2.5
1	K	46	THR	2.4
1	I	34	ARG	2.4
1	L	37	ILE	2.4
1	E	2	SER	2.4
1	I	20	GLU	2.4
1	B	106	VAL	2.4
1	J	145	ILE	2.4
1	B	20	GLU	2.4
1	A	20	GLU	2.4
1	H	25	GLY	2.4
1	J	25	GLY	2.4
1	D	34	ARG	2.4
1	C	20	GLU	2.3
1	I	55	GLU	2.3
1	G	19	ARG	2.3
1	J	19	ARG	2.3
1	K	27	LEU	2.3
1	K	145	ILE	2.3
1	D	47	LEU	2.3
1	E	127	CYS	2.3
1	L	45	ILE	2.3
1	D	3	SER	2.3
1	D	43	ALA	2.2
1	K	26	HIS	2.2
1	E	146	GLN	2.2
1	D	25	GLY	2.2
1	J	23	VAL	2.2
1	D	4	THR	2.2
1	D	69	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	26	HIS	2.2
1	J	18	LYS	2.2
1	A	3	SER	2.2
1	K	81	THR	2.1
1	B	21	PRO	2.1
1	K	19	ARG	2.1
1	L	11	PRO	2.1
1	D	127	CYS	2.1
1	A	145	ILE	2.1
1	D	70	VAL	2.1
1	A	2	SER	2.1
1	H	2	SER	2.1
1	G	21	PRO	2.1
1	D	146	GLN	2.1
1	B	24	TYR	2.1
1	C	38	ALA	2.0
1	E	55	GLU	2.0
1	I	2	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.