



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 4W6R / pdb_00004w6r
Title : Crystal Structure of Full-Length Split GFP Mutant D102C Disulfide Dimer,
P 1 Space Group
Authors : Leibly, D.J.; Waldo, G.S.; Yeates, T.O.
Deposited on : 2014-08-20
Resolution : 3.47 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

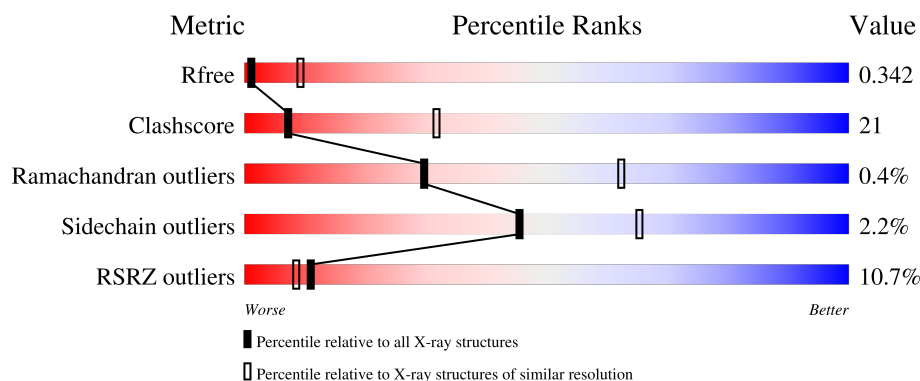
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.47 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	234	9% 55% 31% 6% 8%
1	B	234	7% 56% 29% .. 12%
1	C	234	12% 56% 30% • 12%
1	D	234	7% 53% 24% 5% 17%
1	E	234	15% 65% 24% • 11%

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Mol	Chain	Length	Quality of chain
1	F	234	
1	G	234	
1	H	234	
1	I	234	
1	J	234	
1	K	234	
1	L	234	
1	M	234	
1	N	234	
1	O	234	
1	P	234	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25002 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.

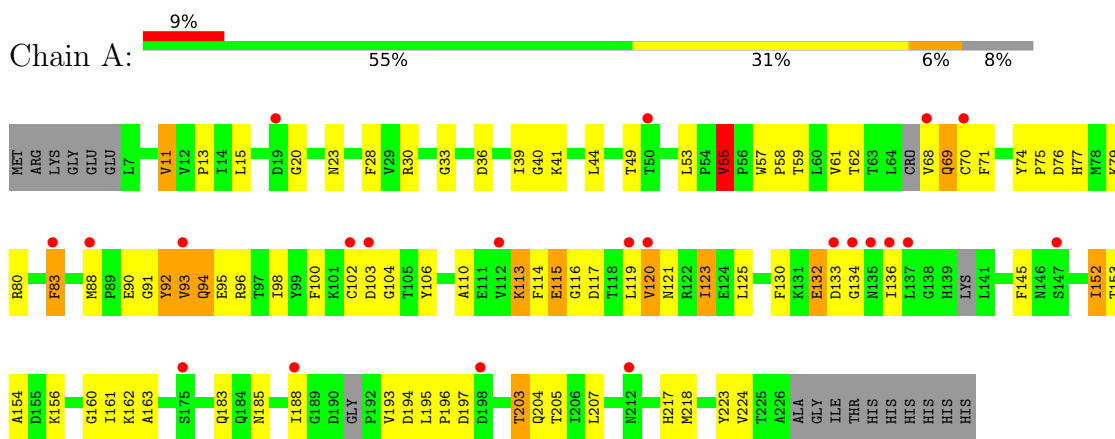
- Molecule 1 is a protein called fluorescent protein D102C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1721	1098	291	327	5			
1	B	205	Total	C	N	O	S	0	0	0
			1649	1052	280	313	4			
1	C	207	Total	C	N	O	S	0	0	0
			1643	1052	277	309	5			
1	D	194	Total	C	N	O	S	0	0	0
			1552	993	261	293	5			
1	E	208	Total	C	N	O	S	0	0	0
			1661	1059	280	317	5			
1	F	201	Total	C	N	O	S	0	0	0
			1600	1020	270	307	3			
1	G	188	Total	C	N	O	S	0	0	0
			1497	949	262	282	4			
1	H	191	Total	C	N	O	S	0	0	0
			1537	980	264	289	4			
1	I	209	Total	C	N	O	S	0	0	0
			1671	1065	285	316	5			
1	J	184	Total	C	N	O	S	0	0	0
			1459	931	247	278	3			
1	K	175	Total	C	N	O	S	0	0	0
			1391	896	229	263	3			
1	L	197	Total	C	N	O	S	0	0	0
			1573	1002	269	298	4			
1	M	168	Total	C	N	O	S	0	0	0
			1352	864	233	251	4			
1	N	174	Total	C	N	O	S	0	0	0
			1387	876	235	273	3			
1	O	213	Total	C	N	O	S	0	0	0
			1677	1065	286	322	4			
1	P	204	Total	C	N	O	S	0	0	0
			1632	1038	281	308	5			

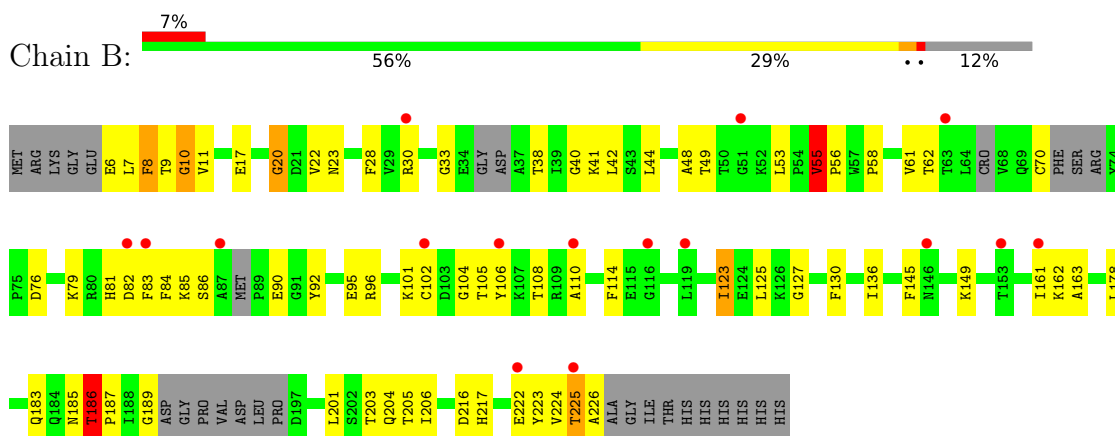
3 Residue-property plots [i](#)

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.

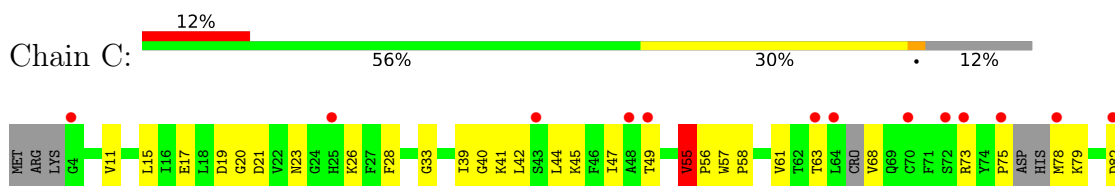
• Molecule 1: fluorescent protein D102C

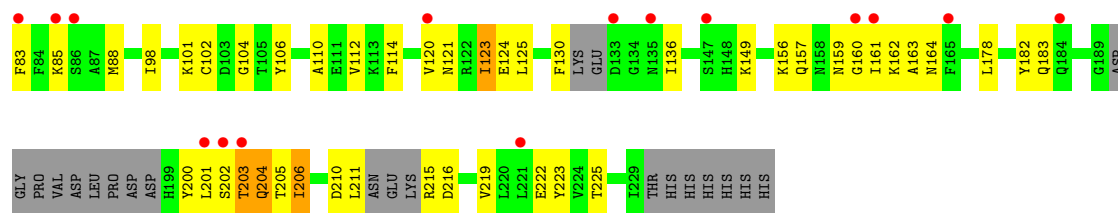


• Molecule 1: fluorescent protein D102C

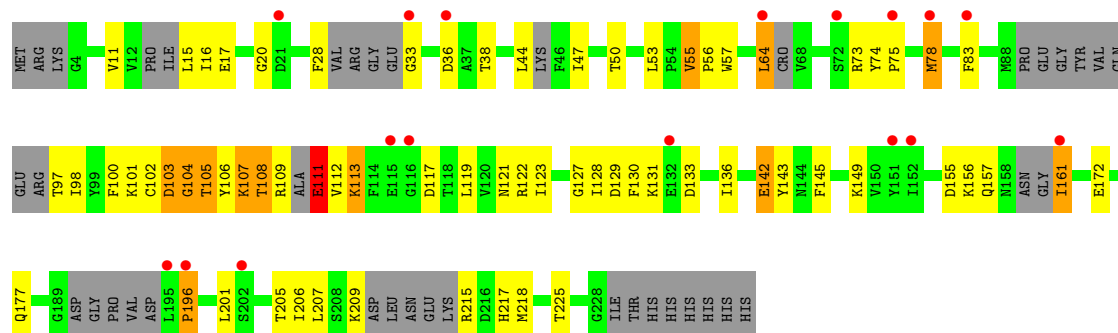


• Molecule 1: fluorescent protein D102C

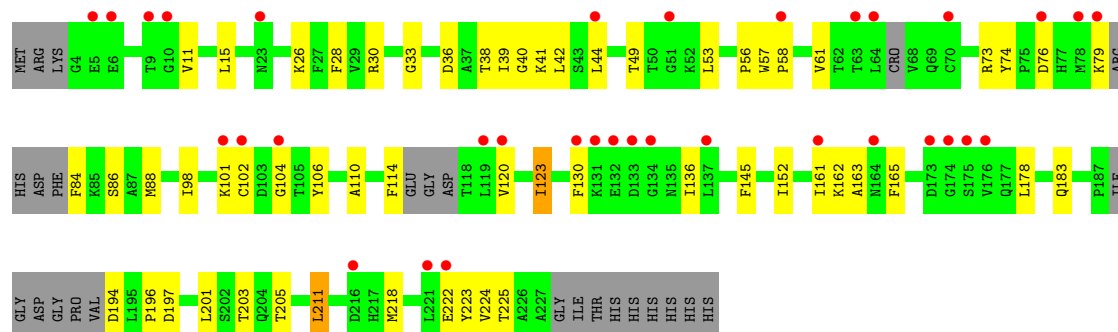




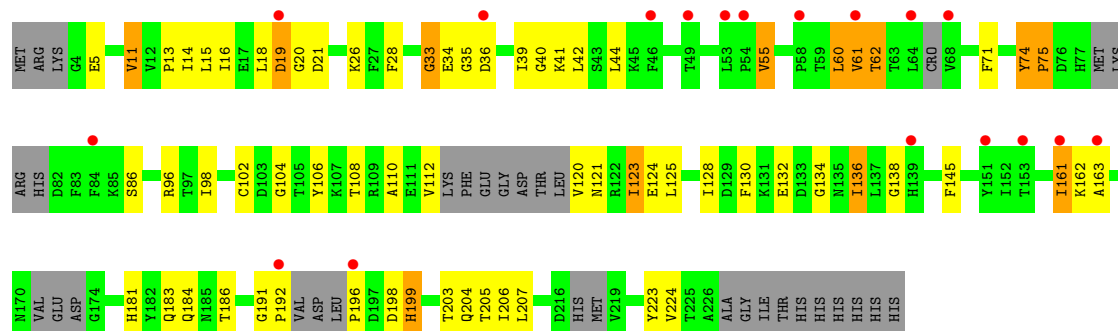
• Molecule 1: fluorescent protein D102C



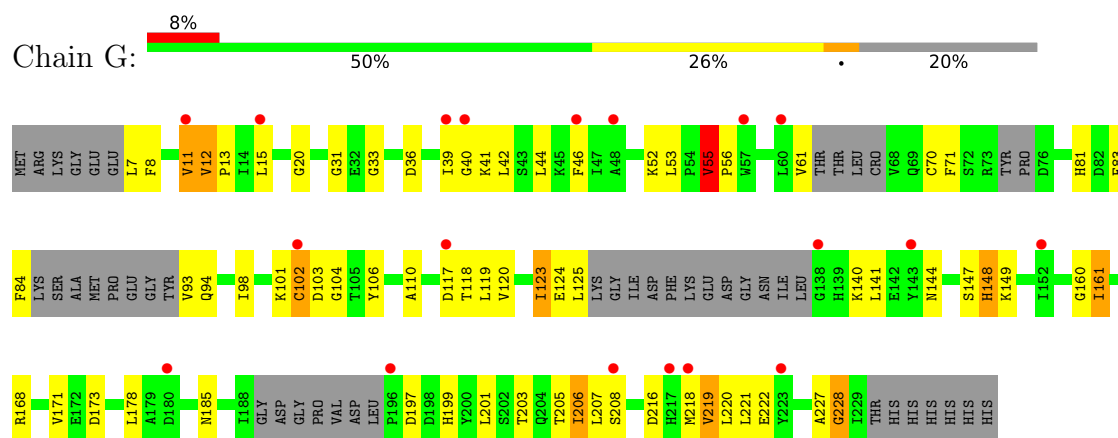
• Molecule 1: fluorescent protein D102C



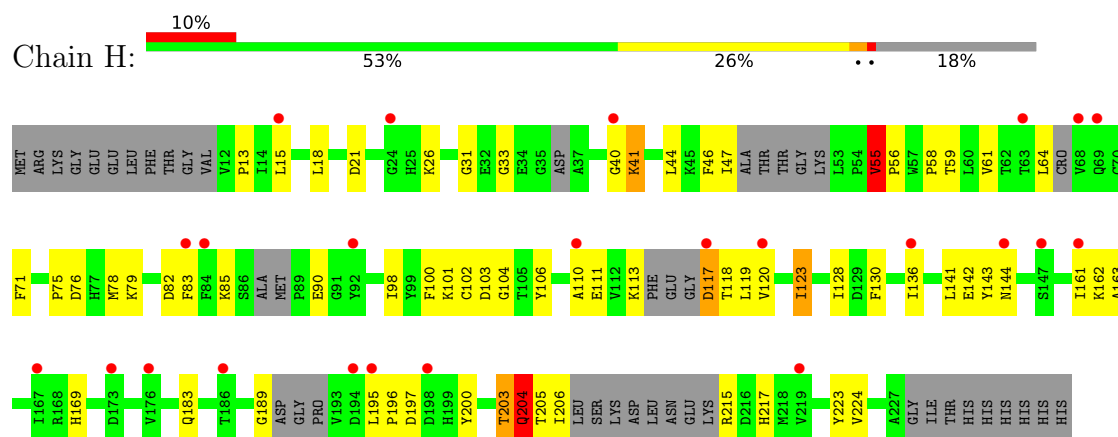
• Molecule 1: fluorescent protein D102C



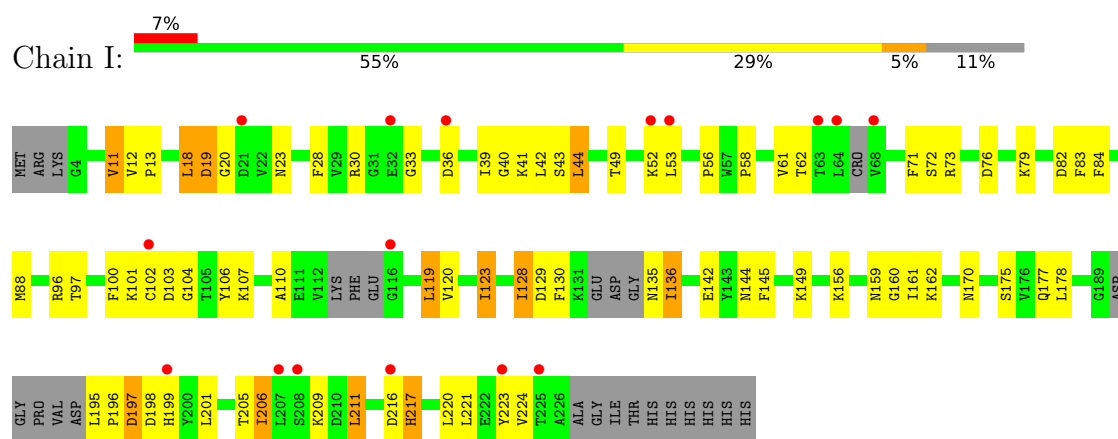
- Molecule 1: fluorescent protein D102C



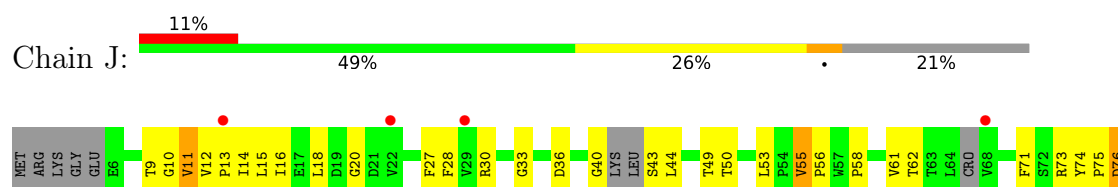
- Molecule 1: fluorescent protein D102C

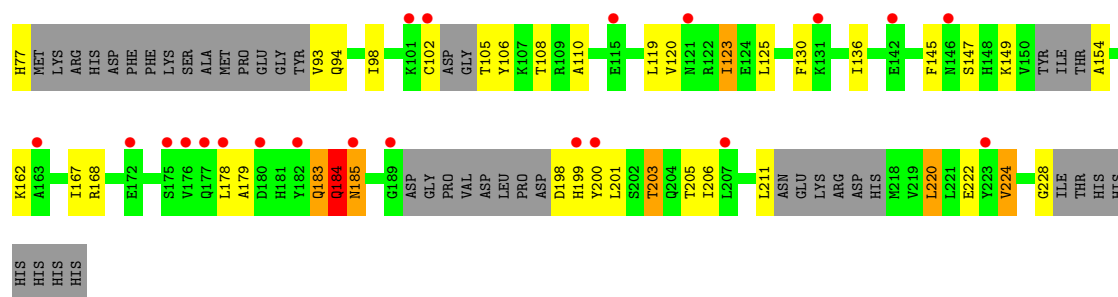


- Molecule 1: fluorescent protein D102C

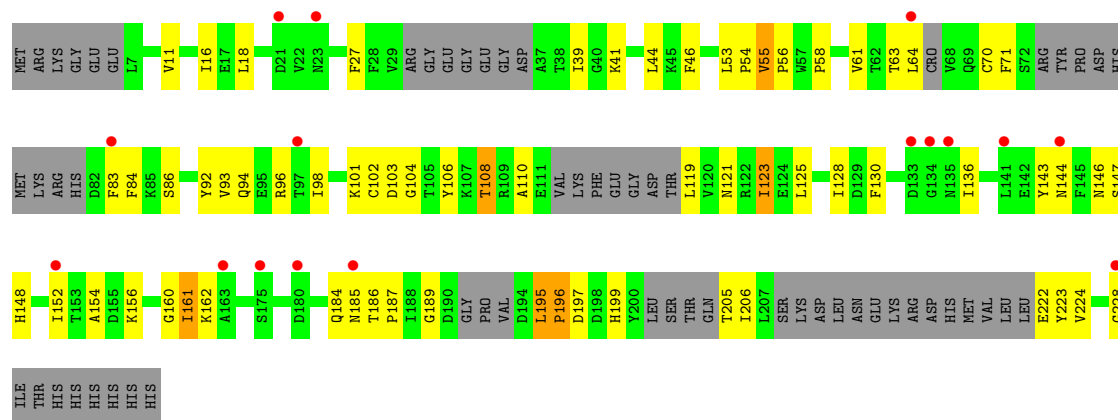


- Molecule 1: fluorescent protein D102C

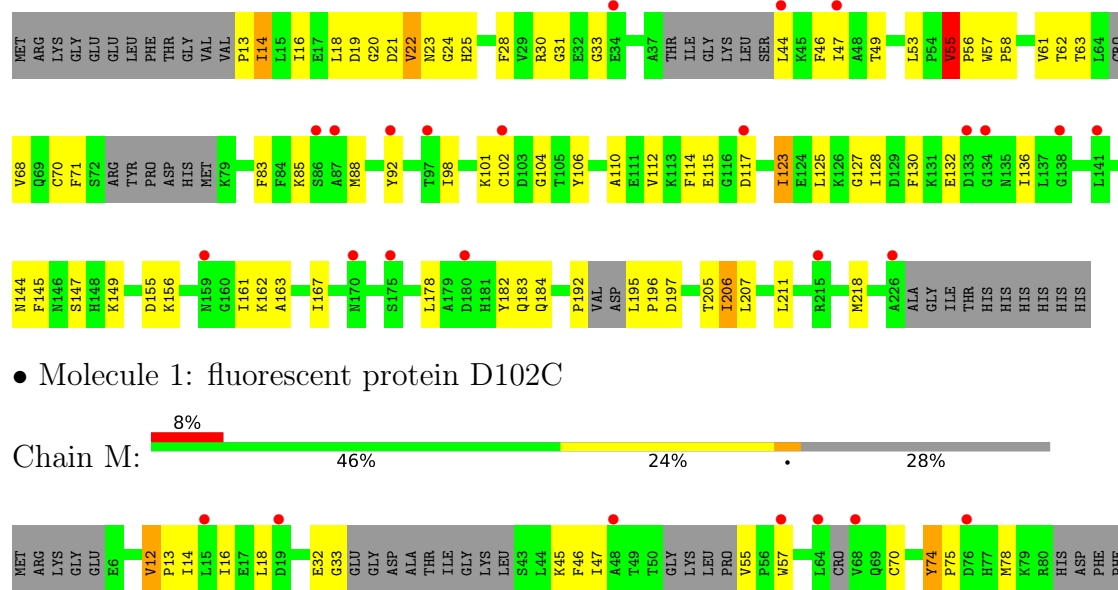




• Molecule 1: fluorescent protein D102C

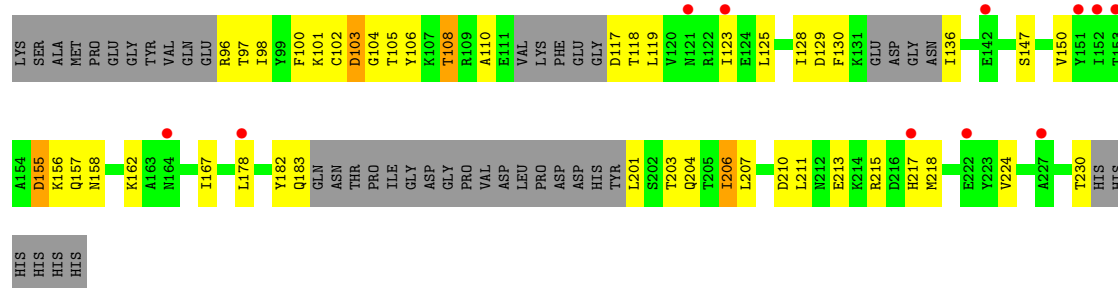


• Molecule 1: fluorescent protein D102C

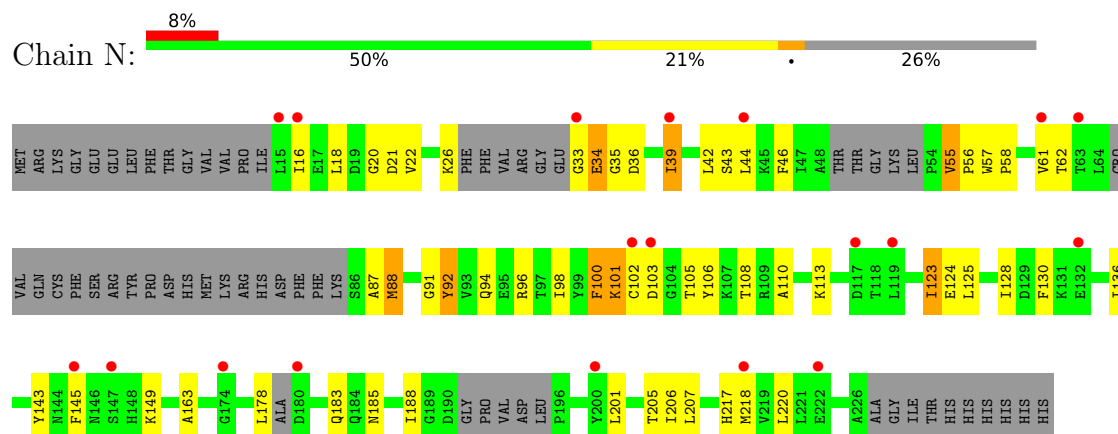


• Molecule 1: fluorescent protein D102C

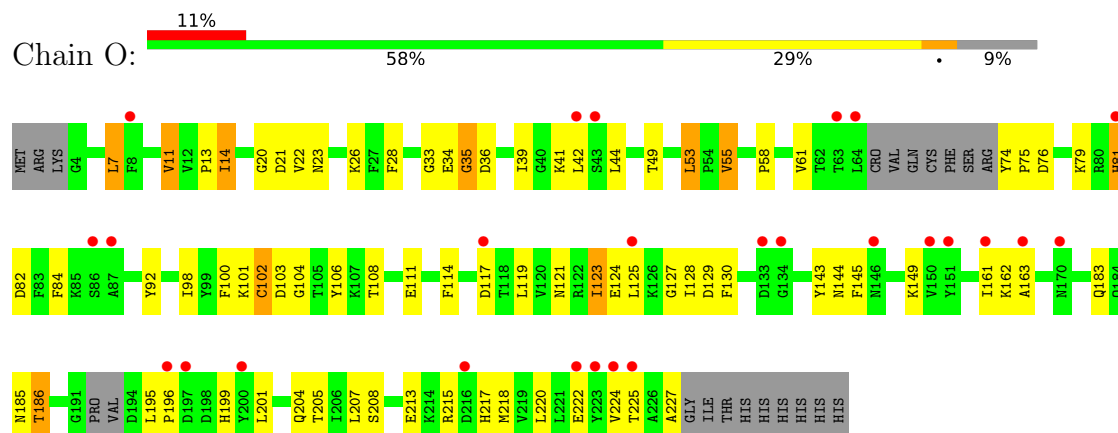




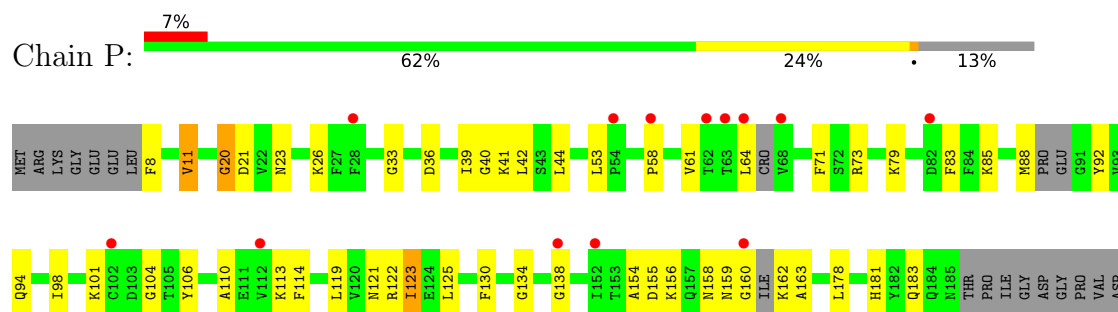
- Molecule 1: fluorescent protein D102C

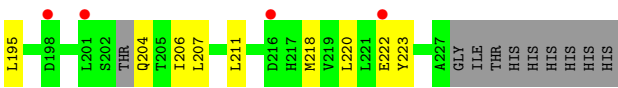


- Molecule 1: fluorescent protein D102C



- Molecule 1: fluorescent protein D102C





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.42Å 92.56Å 124.53Å 94.94° 96.17° 102.25°	Depositor
Resolution (Å)	89.88 – 3.47 89.88 – 3.47	Depositor EDS
% Data completeness (in resolution range)	89.4 (89.88-3.47) 89.4 (89.88-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1555)	Depositor
R, R_{free}	0.307 , 0.357 0.324 , 0.342	Depositor DCC
R_{free} test set	4609 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	101.2	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	25002	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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	0.50	2/1758 (0.1%)	1.24	21/2375 (0.9%)
1	B	0.44	0/1681	1.17	13/2265 (0.6%)
1	C	0.43	0/1675	1.11	10/2258 (0.4%)
1	D	0.50	0/1579	1.25	16/2121 (0.8%)
1	E	0.45	1/1694 (0.1%)	1.09	5/2287 (0.2%)
1	F	0.46	0/1631	1.20	16/2199 (0.7%)
1	G	0.52	1/1524 (0.1%)	1.15	8/2053 (0.4%)
1	H	0.48	1/1567 (0.1%)	1.24	12/2112 (0.6%)
1	I	0.47	0/1705	1.22	19/2302 (0.8%)
1	J	0.50	0/1483	1.22	13/1998 (0.7%)
1	K	0.48	0/1417	1.23	11/1912 (0.6%)
1	L	0.41	0/1605	1.08	4/2164 (0.2%)
1	M	0.41	0/1373	1.27	13/1847 (0.7%)
1	N	0.43	0/1410	1.16	11/1899 (0.6%)
1	O	0.55	0/1712	1.18	10/2314 (0.4%)
1	P	0.44	0/1663	1.11	7/2239 (0.3%)
All	All	0.47	5/25477 (0.0%)	1.18	189/34345 (0.6%)

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	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	203	THR	CA-C	7.16	1.60	1.53
1	G	227	ALA	CA-C	-5.73	1.48	1.53
1	A	203	THR	CA-C	5.47	1.60	1.53
1	A	69	GLN	C-N	-5.34	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	26	LYS	CA-C	5.30	1.58	1.53

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	203	THR	N-CA-C	15.90	129.52	110.91
1	E	26	LYS	N-CA-C	15.00	128.46	110.91
1	A	203	THR	N-CA-C	13.75	130.21	111.24
1	H	204	GLN	N-CA-C	13.62	125.85	111.14
1	I	195	LEU	CA-C-N	12.37	135.31	119.84
1	I	195	LEU	C-N-CA	12.37	135.31	119.84
1	K	195	LEU	CA-C-N	11.71	134.47	119.84
1	K	195	LEU	C-N-CA	11.71	134.47	119.84
1	B	8	PHE	N-CA-C	10.30	122.09	111.07
1	F	74	TYR	CA-C-N	10.10	130.03	120.03
1	F	74	TYR	C-N-CA	10.10	130.03	120.03
1	D	142	GLU	N-CA-C	10.01	125.10	113.19
1	M	157	GLN	N-CA-C	-9.52	100.88	111.07
1	I	119	LEU	N-CA-C	9.43	124.01	111.28
1	C	200	TYR	N-CA-C	9.29	123.27	109.24
1	H	195	LEU	CA-C-N	9.26	129.20	119.85
1	H	195	LEU	C-N-CA	9.26	129.20	119.85
1	A	132	GLU	N-CA-C	-8.89	97.12	110.28
1	G	11	VAL	N-CA-C	8.89	121.07	108.36
1	F	33	GLY	N-CA-C	-8.70	97.95	110.91
1	M	211	LEU	N-CA-C	8.62	122.89	112.38
1	A	115	GLU	N-CA-C	-8.30	100.11	111.56
1	B	11	VAL	N-CA-C	8.25	120.10	109.30
1	H	41	LYS	N-CA-C	8.21	122.82	109.59
1	F	5	GLU	N-CA-C	8.21	120.22	111.28
1	F	60	LEU	N-CA-C	-8.09	97.24	109.94
1	E	165	PHE	N-CA-C	-8.07	97.49	108.38
1	L	55	VAL	N-CA-CB	-7.91	104.94	111.67
1	O	55	VAL	N-CA-CB	-7.85	105.00	111.67
1	K	197	ASP	N-CA-C	-7.72	100.57	110.53
1	P	79	LYS	N-CA-C	7.63	120.27	111.11
1	J	55	VAL	N-CA-CB	-7.46	105.33	111.67
1	O	7	LEU	N-CA-C	7.36	121.52	112.54
1	M	74	TYR	CA-C-N	7.31	127.74	119.92
1	M	74	TYR	C-N-CA	7.31	127.74	119.92
1	N	39	ILE	N-CA-C	-7.21	105.97	112.90
1	B	41	LYS	N-CA-C	7.21	121.20	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	91	GLY	N-CA-C	7.18	123.58	112.45
1	I	156	LYS	N-CA-C	7.15	119.69	111.11
1	D	104	GLY	N-CA-C	7.11	123.61	112.31
1	N	101	LYS	N-CA-C	-7.05	99.45	109.96
1	A	55	VAL	N-CA-CB	-7.03	105.70	111.67
1	B	55	VAL	N-CA-CB	-7.02	105.70	111.67
1	D	111	GLU	CA-C-N	6.98	131.32	121.96
1	D	111	GLU	C-N-CA	6.98	131.32	121.96
1	F	62	THR	N-CA-C	-6.93	104.71	113.72
1	B	81	HIS	N-CA-C	6.87	121.68	113.16
1	H	55	VAL	N-CA-CB	-6.85	105.85	111.67
1	N	22	VAL	N-CA-C	6.84	117.73	107.75
1	C	55	VAL	N-CA-CB	-6.83	105.86	111.67
1	J	108	THR	N-CA-C	6.81	120.26	109.50
1	D	119	LEU	CA-C-N	-6.72	113.78	123.06
1	D	119	LEU	C-N-CA	-6.72	113.78	123.06
1	I	197	ASP	N-CA-C	-6.71	101.88	110.53
1	A	69	GLN	O-C-N	6.71	131.51	122.59
1	A	152	ILE	N-CA-C	6.70	123.28	109.34
1	J	11	VAL	N-CA-C	6.69	117.92	108.36
1	P	211	LEU	N-CA-C	6.65	120.49	112.38
1	F	186	THR	CA-C-N	6.61	126.37	119.76
1	F	186	THR	C-N-CA	6.61	126.37	119.76
1	J	9	THR	N-CA-C	-6.61	100.50	110.28
1	O	123	ILE	N-CA-C	6.58	118.99	108.85
1	B	225	THR	CB-CA-C	-6.56	109.00	116.54
1	A	11	VAL	N-CA-C	6.53	117.69	108.36
1	J	224	VAL	N-CA-CB	6.52	120.68	111.82
1	J	200	TYR	N-CA-C	6.51	119.07	109.24
1	O	81	HIS	N-CA-C	6.49	121.20	113.16
1	C	11	VAL	N-CA-C	6.47	117.62	108.36
1	C	203	THR	CB-CA-C	-6.45	108.46	117.23
1	G	228	GLY	N-CA-C	6.34	120.17	111.54
1	G	55	VAL	N-CA-CB	-6.33	106.28	111.67
1	J	203	THR	N-CA-C	6.31	119.70	107.71
1	I	11	VAL	N-CA-C	6.31	117.38	108.36
1	C	210	ASP	N-CA-C	-6.30	98.27	108.41
1	D	108	THR	N-CA-C	6.30	123.09	113.51
1	J	185	ASN	N-CA-C	6.27	119.01	110.55
1	C	164	ASN	N-CA-C	6.23	120.06	111.71
1	I	175	SER	N-CA-C	6.20	118.91	110.35
1	E	11	VAL	N-CA-C	6.18	117.20	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	83	PHE	N-CA-C	-6.14	104.58	111.28
1	I	120	VAL	CB-CA-C	-6.12	101.34	111.32
1	H	197	ASP	N-CA-C	-6.04	101.83	110.59
1	H	118	THR	N-CA-C	6.03	118.78	109.07
1	A	195	LEU	CA-C-N	6.01	125.92	119.85
1	A	195	LEU	C-N-CA	6.01	125.92	119.85
1	P	162	LYS	N-CA-CB	-6.01	100.29	110.50
1	F	134	GLY	N-CA-C	-5.98	103.45	112.60
1	F	11	VAL	N-CA-C	5.93	116.84	108.36
1	D	20	GLY	N-CA-C	5.89	119.71	111.10
1	A	83	PHE	N-CA-C	-5.88	104.95	111.36
1	I	211	LEU	N-CA-C	5.86	119.53	112.38
1	K	55	VAL	N-CA-CB	-5.86	106.69	111.67
1	N	16	ILE	N-CA-C	5.84	116.53	108.12
1	I	18	LEU	N-CA-C	5.83	123.22	110.80
1	K	147	SER	N-CA-C	-5.83	100.16	109.96
1	B	10	GLY	CA-C-N	-5.81	112.20	120.69
1	B	10	GLY	C-N-CA	-5.81	112.20	120.69
1	P	92	TYR	N-CA-C	5.81	117.90	109.07
1	A	154	ALA	N-CA-C	5.80	119.51	110.17
1	M	157	GLN	N-CA-CB	5.79	118.40	110.01
1	M	32	GLU	N-CA-C	5.78	118.19	109.23
1	J	76	ASP	CB-CA-C	-5.78	109.92	116.63
1	D	107	LYS	N-CA-C	5.75	119.83	112.12
1	O	11	VAL	N-CA-C	5.74	116.57	108.36
1	O	217	HIS	N-CA-C	5.73	116.64	108.74
1	M	155	ASP	CB-CA-C	-5.72	103.91	112.09
1	N	34	GLU	N-CA-C	-5.68	99.67	108.42
1	A	113	LYS	N-CA-C	5.65	116.85	108.60
1	H	117	ASP	CB-CA-C	-5.64	99.38	110.10
1	A	94	GLN	N-CA-C	5.63	117.96	110.53
1	I	120	VAL	N-CA-C	5.63	117.74	109.63
1	M	12	VAL	N-CA-C	5.63	114.31	107.61
1	I	44	LEU	N-CA-C	5.62	118.24	109.52
1	I	82	ASP	CB-CA-C	5.62	120.83	111.83
1	K	161	ILE	N-CA-C	5.62	117.91	108.81
1	A	197	ASP	N-CA-C	-5.61	103.29	110.53
1	N	55	VAL	N-CA-CB	-5.60	106.91	111.67
1	G	12	VAL	CA-C-N	5.59	125.50	119.85
1	G	12	VAL	C-N-CA	5.59	125.50	119.85
1	M	217	HIS	N-CA-C	5.58	116.43	108.74
1	F	5	GLU	CB-CA-C	-5.55	101.58	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	84	PHE	N-CA-C	5.54	120.51	111.37
1	K	224	VAL	N-CA-C	5.54	116.09	108.12
1	A	93	VAL	N-CA-C	5.53	120.84	109.34
1	O	35	GLY	N-CA-C	5.52	120.38	111.38
1	D	55	VAL	N-CA-CB	-5.50	106.99	111.67
1	I	217	HIS	N-CA-C	5.50	116.33	108.74
1	B	20	GLY	N-CA-C	5.50	119.12	111.10
1	B	86	SER	N-CA-C	-5.49	105.68	112.38
1	F	55	VAL	N-CA-CB	-5.49	107.01	111.67
1	I	20	GLY	N-CA-C	5.48	127.66	111.07
1	M	210	ASP	N-CA-C	-5.46	98.87	108.20
1	E	197	ASP	N-CA-C	-5.44	103.72	110.41
1	A	156	LYS	N-CA-C	5.42	117.61	111.11
1	E	211	LEU	N-CA-C	5.41	118.98	112.38
1	C	123	ILE	N-CA-C	5.41	117.17	108.85
1	J	184	GLN	N-CA-C	5.40	119.07	107.67
1	A	90	GLU	N-CA-C	-5.38	103.25	110.24
1	N	92	TYR	N-CA-C	5.37	117.35	109.24
1	D	105	THR	CA-C-N	5.37	131.51	122.87
1	D	105	THR	C-N-CA	5.37	131.51	122.87
1	D	103	ASP	CA-C-N	5.36	129.36	121.96
1	D	103	ASP	C-N-CA	5.36	129.36	121.96
1	K	156	LYS	N-CA-C	5.36	117.55	111.11
1	M	156	LYS	N-CA-C	5.36	117.88	111.71
1	O	14	ILE	N-CA-C	5.36	116.20	108.48
1	N	88	MET	N-CA-C	-5.35	102.37	110.39
1	H	195	LEU	N-CA-C	5.33	118.02	110.24
1	P	20	GLY	N-CA-C	5.30	118.83	111.10
1	G	148	HIS	N-CA-C	5.28	117.01	109.14
1	K	108	THR	N-CA-C	5.28	117.84	109.50
1	K	11	VAL	N-CA-C	5.26	115.88	108.36
1	A	134	GLY	N-CA-C	-5.26	104.56	112.60
1	F	136	ILE	N-CA-C	-5.25	100.82	109.12
1	D	113	LYS	N-CA-C	-5.25	99.28	107.73
1	A	92	TYR	N-CA-C	5.24	118.73	111.71
1	P	11	VAL	N-CA-C	5.22	115.83	108.36
1	F	75	PRO	CA-C-O	-5.20	115.42	122.08
1	B	186	THR	CA-C-N	5.19	126.33	119.84
1	B	186	THR	C-N-CA	5.19	126.33	119.84
1	J	183	GLN	N-CA-C	5.17	117.50	108.76
1	D	117	ASP	N-CA-C	-5.17	106.75	113.16
1	H	200	TYR	CA-C-N	5.16	130.42	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	200	TYR	C-N-CA	5.16	130.42	122.93
1	J	220	LEU	CA-C-N	5.16	130.27	123.00
1	J	220	LEU	C-N-CA	5.16	130.27	123.00
1	I	119	LEU	CA-C-N	5.15	127.40	120.50
1	I	119	LEU	C-N-CA	5.15	127.40	120.50
1	L	197	ASP	N-CA-C	-5.15	103.89	110.53
1	A	193	VAL	N-CA-C	5.14	116.70	108.89
1	N	100	PHE	N-CA-C	-5.14	102.25	109.96
1	F	161	ILE	N-CA-C	5.12	117.40	108.90
1	G	227	ALA	N-CA-C	-5.12	98.32	107.28
1	O	53	LEU	CA-C-N	5.12	125.19	119.87
1	O	53	LEU	C-N-CA	5.12	125.19	119.87
1	A	217	HIS	N-CA-C	5.12	115.80	108.74
1	G	20	GLY	N-CA-C	5.11	118.56	111.10
1	B	217	HIS	N-CA-C	5.11	115.79	108.74
1	C	211	LEU	N-CA-C	5.10	125.28	111.00
1	M	108	THR	N-CA-C	5.10	117.56	109.50
1	M	110	ALA	N-CA-C	5.09	116.93	109.24
1	L	14	ILE	N-CA-C	5.09	116.04	108.46
1	F	16	ILE	N-CA-C	5.07	115.42	108.12
1	N	220	LEU	N-CA-C	5.04	117.65	109.24
1	I	19	ASP	N-CA-C	5.02	115.43	108.00
1	C	203	THR	CA-C-N	5.02	131.13	121.54
1	C	203	THR	C-N-CA	5.02	131.13	121.54
1	L	211	LEU	N-CA-C	5.01	118.49	112.38
1	K	123	ILE	N-CA-C	5.00	117.02	108.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	111	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1721	0	1680	105	0
1	B	1649	0	1615	85	0
1	C	1643	0	1611	62	1
1	D	1552	0	1511	60	1
1	E	1661	0	1623	40	0
1	F	1600	0	1557	50	1
1	G	1497	0	1460	86	0
1	H	1537	0	1487	59	0
1	I	1671	0	1633	99	0
1	J	1459	0	1431	59	1
1	K	1391	0	1359	52	0
1	L	1573	0	1532	67	0
1	M	1352	0	1339	48	0
1	N	1387	0	1351	42	0
1	O	1677	0	1616	103	0
1	P	1632	0	1586	46	0
All	All	25002	0	24391	1023	2

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 21.

All (1023) 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:I:28:PHE:CE2	1:I:30:ARG:HG3	1.44	1.51
1:A:152:ILE:O	1:A:153:THR:HG22	1.19	1.34
1:D:15:LEU:O	1:D:15:LEU:HD12	1.31	1.30
1:B:106:TYR:CE1	1:B:130:PHE:CE1	2.24	1.24
1:G:44:LEU:O	1:G:219:VAL:HG13	1.36	1.24
1:E:28:PHE:CE2	1:E:30:ARG:HG3	1.71	1.24
1:I:42:LEU:HD21	1:I:71:PHE:CB	1.69	1.23
1:O:104:GLY:HA3	1:O:130:PHE:CD1	1.74	1.20
1:P:88:MET:HE1	1:P:113:LYS:HA	1.26	1.17
1:O:185:ASN:O	1:O:186:THR:HG22	1.00	1.16
1:O:74:TYR:CD2	1:O:82:ASP:HB2	1.80	1.16
1:O:185:ASN:O	1:O:186:THR:CG2	1.92	1.16
1:G:7:LEU:CG	1:G:8:PHE:H	1.57	1.15
1:I:42:LEU:HD21	1:I:71:PHE:CG	1.81	1.15
1:A:102:CYS:SG	1:N:102:CYS:HB3	1.88	1.13
1:H:203:THR:CG2	1:H:224:VAL:HG13	1.78	1.13
1:G:7:LEU:HG	1:G:8:PHE:N	1.59	1.12
1:B:106:TYR:CE1	1:B:130:PHE:CZ	2.37	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:THR:HG23	1:B:10:GLY:H	1.02	1.11
1:B:6:GLU:HG3	1:B:7:LEU:H	0.97	1.09
1:I:28:PHE:CE2	1:I:30:ARG:CG	2.36	1.08
1:I:43:SER:HB3	1:I:221:LEU:HD23	1.21	1.08
1:A:203:THR:HG22	1:A:224:VAL:HG13	1.15	1.08
1:E:86:SER:HG	1:E:194:ASP:N	1.51	1.08
1:H:203:THR:HG22	1:H:224:VAL:HG13	1.33	1.06
1:F:33:GLY:HA3	1:F:44:LEU:HD23	1.35	1.06
1:E:28:PHE:HE2	1:E:30:ARG:HG3	1.02	1.06
1:O:74:TYR:CE2	1:O:82:ASP:CG	2.34	1.04
1:H:203:THR:HG22	1:H:224:VAL:CG1	1.88	1.03
1:I:28:PHE:CZ	1:I:30:ARG:HG3	1.93	1.02
1:A:152:ILE:O	1:A:153:THR:CG2	2.08	1.01
1:A:15:LEU:HB2	1:A:120:VAL:HG22	1.40	1.00
1:G:61:VAL:CG1	1:G:220:LEU:HD11	1.91	1.00
1:A:102:CYS:SG	1:N:102:CYS:CB	2.49	1.00
1:A:119:LEU:O	1:A:120:VAL:HG23	1.62	1.00
1:G:7:LEU:HG	1:G:8:PHE:H	0.87	1.00
1:I:43:SER:CB	1:I:221:LEU:HD23	1.91	1.00
1:A:203:THR:CG2	1:A:224:VAL:HG13	1.91	1.00
1:N:103:ASP:OD2	1:N:136:ILE:HD13	1.62	0.99
1:A:203:THR:HG22	1:A:224:VAL:CG1	1.93	0.98
1:I:135:ASN:C	1:I:136:ILE:HD12	1.87	0.98
1:A:93:VAL:HG23	1:A:188:ILE:HG13	1.44	0.98
1:J:43:SER:HB2	1:J:220:LEU:O	1.63	0.98
1:A:94:GLN:HG3	1:A:185:ASN:OD1	1.64	0.97
1:G:61:VAL:HG13	1:G:220:LEU:HD11	1.46	0.97
1:G:207:LEU:HD22	1:G:219:VAL:O	1.64	0.96
1:P:88:MET:HE1	1:P:113:LYS:CA	1.94	0.96
1:O:104:GLY:CA	1:O:130:PHE:CD1	2.47	0.96
1:B:6:GLU:HG3	1:B:7:LEU:N	1.74	0.96
1:G:61:VAL:HG13	1:G:220:LEU:CD1	1.96	0.96
1:H:203:THR:HG22	1:H:224:VAL:HG22	1.49	0.95
1:B:9:THR:HG23	1:B:10:GLY:N	1.80	0.95
1:I:28:PHE:HD2	1:I:49:THR:OG1	1.50	0.95
1:O:104:GLY:HA3	1:O:130:PHE:CG	2.02	0.95
1:I:103:ASP:OD2	1:I:136:ILE:HD13	1.67	0.94
1:B:22:VAL:HG11	1:B:106:TYR:OH	1.67	0.94
1:O:74:TYR:CD2	1:O:82:ASP:CB	2.50	0.94
1:G:207:LEU:HD13	1:G:218:MET:HE3	1.49	0.94
1:G:207:LEU:HD13	1:G:218:MET:CE	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:33:GLY:HA3	1:N:44:LEU:HD23	1.48	0.93
1:M:128:ILE:HG22	1:M:129:ASP:CG	1.94	0.93
1:H:203:THR:HG22	1:H:224:VAL:CG2	1.99	0.92
1:I:33:GLY:HA3	1:I:44:LEU:HD23	1.52	0.91
1:B:106:TYR:HE1	1:B:130:PHE:CE1	1.88	0.91
1:B:9:THR:CG2	1:B:10:GLY:H	1.82	0.90
1:G:61:VAL:HG22	1:G:220:LEU:CD1	2.01	0.90
1:I:28:PHE:HE2	1:I:30:ARG:CG	1.79	0.90
1:G:205:THR:HG23	1:G:220:LEU:HD23	1.50	0.90
1:G:103:ASP:OD1	1:G:104:GLY:N	2.04	0.90
1:D:15:LEU:O	1:D:15:LEU:CD1	2.20	0.89
1:F:33:GLY:CA	1:F:44:LEU:HD23	2.02	0.89
1:O:74:TYR:HE2	1:O:82:ASP:CG	1.78	0.89
1:C:203:THR:O	1:C:204:GLN:HG3	1.73	0.89
1:O:104:GLY:O	1:O:130:PHE:CE1	2.26	0.89
1:A:15:LEU:O	1:A:121:ASN:N	2.05	0.88
1:C:47:ILE:HD13	1:C:215:ARG:NH2	1.88	0.88
1:L:23:ASN:HD21	1:L:130:PHE:N	1.71	0.88
1:K:83:PHE:CE2	1:K:161:ILE:HG13	2.09	0.88
1:A:100:PHE:HB2	1:A:103:ASP:HB3	1.57	0.87
1:D:104:GLY:HA3	1:D:130:PHE:HD1	1.37	0.86
1:H:13:PRO:HD2	1:H:117:ASP:O	1.75	0.86
1:G:199:HIS:HB2	1:G:228:GLY:HA2	1.56	0.86
1:F:20:GLY:HA2	1:F:125:LEU:O	1.76	0.85
1:E:163:ALA:HB3	1:E:183:GLN:HB3	1.56	0.85
1:I:28:PHE:CZ	1:I:30:ARG:CG	2.58	0.85
1:A:15:LEU:O	1:A:120:VAL:HA	1.77	0.85
1:I:42:LEU:HD21	1:I:71:PHE:HB3	1.56	0.85
1:C:110:ALA:HB2	1:C:123:ILE:HG12	1.59	0.85
1:B:106:TYR:CE1	1:B:127:GLY:HA3	2.12	0.84
1:B:22:VAL:CG1	1:B:106:TYR:OH	2.24	0.84
1:D:104:GLY:HA3	1:D:130:PHE:CD1	2.11	0.84
1:O:104:GLY:C	1:O:130:PHE:CE1	2.55	0.84
1:G:205:THR:HG23	1:G:220:LEU:CD2	2.07	0.83
1:A:100:PHE:CB	1:A:103:ASP:HB3	2.08	0.83
1:B:6:GLU:CG	1:B:7:LEU:H	1.85	0.83
1:J:43:SER:CB	1:J:220:LEU:O	2.27	0.83
1:O:185:ASN:C	1:O:186:THR:HG22	2.04	0.83
1:I:135:ASN:HB2	1:I:136:ILE:HD12	1.61	0.82
1:G:61:VAL:HG22	1:G:220:LEU:HD12	1.60	0.82
1:O:127:GLY:CA	1:O:130:PHE:HE2	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:88:MET:CE	1:P:113:LYS:HA	2.08	0.82
1:G:44:LEU:O	1:G:219:VAL:CG1	2.26	0.82
1:I:42:LEU:CD2	1:I:71:PHE:CG	2.62	0.82
1:O:106:TYR:CE1	1:O:130:PHE:CZ	2.68	0.82
1:D:109:ARG:O	1:D:123:ILE:HG23	1.79	0.81
1:I:28:PHE:HE2	1:I:30:ARG:HG3	1.01	0.81
1:I:88:MET:HE2	1:I:119:LEU:CD1	2.11	0.81
1:I:135:ASN:HB2	1:I:136:ILE:CD1	2.11	0.81
1:G:205:THR:HG22	1:G:206:ILE:N	1.96	0.81
1:A:68:VAL:CG2	1:A:71:PHE:CD2	2.65	0.79
1:G:208:SER:HB2	1:G:219:VAL:HB	1.64	0.79
1:O:127:GLY:HA3	1:O:130:PHE:HE2	1.47	0.79
1:F:18:LEU:HD23	1:F:19:ASP:O	1.81	0.79
1:K:162:LYS:HG2	1:K:184:GLN:HG2	1.64	0.79
1:L:57:TRP:HB3	1:L:218:MET:HE3	1.64	0.79
1:E:28:PHE:CE2	1:E:30:ARG:CG	2.62	0.79
1:L:23:ASN:HD21	1:L:130:PHE:H	1.31	0.79
1:O:14:ILE:CD1	1:O:42:LEU:HD22	2.13	0.79
1:A:93:VAL:CG2	1:A:188:ILE:CG1	2.61	0.79
1:B:106:TYR:CD1	1:B:130:PHE:CE1	2.70	0.79
1:O:74:TYR:CD2	1:O:82:ASP:CG	2.61	0.78
1:B:106:TYR:CD1	1:B:130:PHE:CZ	2.70	0.78
1:O:74:TYR:CE2	1:O:82:ASP:CB	2.65	0.78
1:F:14:ILE:HB	1:F:33:GLY:O	1.83	0.78
1:H:203:THR:HG23	1:H:224:VAL:HG13	1.64	0.78
1:A:15:LEU:HD12	1:A:120:VAL:HG22	1.64	0.77
1:E:39:ILE:HG23	1:E:41:LYS:HG3	1.64	0.77
1:G:61:VAL:CG2	1:G:220:LEU:HD11	2.14	0.77
1:L:110:ALA:HB2	1:L:123:ILE:HG23	1.66	0.77
1:C:47:ILE:HD13	1:C:215:ARG:HH21	1.50	0.77
1:L:207:LEU:HD22	1:L:218:MET:HE2	1.66	0.77
1:M:98:ILE:HB	1:M:106:TYR:HB2	1.66	0.77
1:K:108:THR:HG22	1:K:125:LEU:HD23	1.67	0.77
1:A:15:LEU:CB	1:A:120:VAL:HG22	2.15	0.77
1:I:135:ASN:CB	1:I:136:ILE:HD12	2.15	0.77
1:A:102:CYS:HG	1:N:102:CYS:HG	1.32	0.76
1:F:102:CYS:N	1:O:102:CYS:SG	2.51	0.76
1:I:28:PHE:HD2	1:I:49:THR:HG1	0.77	0.76
1:D:83:PHE:CZ	1:D:161:ILE:HG21	2.21	0.75
1:M:104:GLY:HA3	1:M:130:PHE:CD1	2.20	0.75
1:O:106:TYR:CD1	1:O:130:PHE:HZ	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ILE:HD12	1:D:129:ASP:CG	2.11	0.75
1:E:28:PHE:HE2	1:E:30:ARG:CG	1.91	0.75
1:A:68:VAL:HG21	1:A:71:PHE:CE2	2.21	0.75
1:N:110:ALA:HB2	1:N:123:ILE:HG23	1.69	0.75
1:H:141:LEU:HD23	1:H:142:GLU:O	1.86	0.75
1:P:61:VAL:HG22	1:P:218:MET:HE1	1.68	0.75
1:I:88:MET:HE2	1:I:119:LEU:HD12	1.67	0.74
1:L:33:GLY:HA3	1:L:44:LEU:HD23	1.68	0.74
1:A:68:VAL:HG22	1:A:71:PHE:CD2	2.22	0.74
1:G:83:PHE:HB2	1:G:161:ILE:HD12	1.69	0.74
1:H:203:THR:CG2	1:H:224:VAL:CG1	2.56	0.74
1:D:107:LYS:O	1:D:108:THR:OG1	2.06	0.74
1:A:93:VAL:CG2	1:A:188:ILE:HG13	2.18	0.74
1:A:93:VAL:HG23	1:A:188:ILE:CG1	2.15	0.74
1:I:42:LEU:HD21	1:I:71:PHE:HB2	1.69	0.74
1:H:203:THR:HG22	1:H:224:VAL:CB	2.18	0.73
1:F:98:ILE:HB	1:F:106:TYR:HB2	1.70	0.73
1:C:15:LEU:HD12	1:C:120:VAL:HG13	1.69	0.73
1:O:35:GLY:HA2	1:O:42:LEU:HD23	1.71	0.73
1:H:40:GLY:O	1:H:223:TYR:HA	1.88	0.72
1:N:100:PHE:CD2	1:N:130:PHE:HE1	2.07	0.72
1:O:100:PHE:HD2	1:O:104:GLY:O	1.70	0.72
1:P:39:ILE:HG23	1:P:41:LYS:HG3	1.71	0.72
1:H:110:ALA:HB2	1:H:123:ILE:HG23	1.72	0.72
1:A:152:ILE:C	1:A:153:THR:HG22	2.11	0.72
1:M:75:PRO:HD2	1:M:78:MET:HB2	1.72	0.72
1:P:39:ILE:HD13	1:P:41:LYS:HE3	1.72	0.72
1:B:185:ASN:O	1:B:186:THR:HB	1.88	0.72
1:E:28:PHE:HD2	1:E:49:THR:HG1	1.35	0.72
1:I:136:ILE:HD12	1:I:136:ILE:N	2.03	0.71
1:I:18:LEU:HD23	1:I:19:ASP:O	1.90	0.71
1:A:163:ALA:HB3	1:A:183:GLN:HB3	1.73	0.71
1:E:39:ILE:HD13	1:E:41:LYS:HE3	1.71	0.71
1:I:42:LEU:O	1:I:44:LEU:HG	1.90	0.71
1:G:207:LEU:HD21	1:G:220:LEU:HG	1.71	0.71
1:H:203:THR:HA	1:H:223:TYR:O	1.91	0.71
1:A:15:LEU:HB2	1:A:120:VAL:CG2	2.19	0.71
1:A:68:VAL:CG2	1:A:71:PHE:HD2	2.05	0.70
1:I:39:ILE:HG21	1:I:41:LYS:HE3	1.73	0.70
1:I:43:SER:HB3	1:I:221:LEU:CD2	2.11	0.70
1:K:70:CYS:SG	1:K:84:PHE:HB3	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:LEU:HD23	1:G:220:LEU:HA	1.74	0.70
1:I:28:PHE:CD2	1:I:49:THR:OG1	2.34	0.70
1:I:135:ASN:C	1:I:136:ILE:CD1	2.65	0.69
1:H:204:GLN:O	1:H:205:THR:OG1	2.10	0.69
1:A:68:VAL:HG21	1:A:71:PHE:CD2	2.26	0.69
1:E:57:TRP:HB3	1:E:218:MET:SD	2.33	0.69
1:E:110:ALA:HB2	1:E:123:ILE:HG23	1.73	0.69
1:D:128:ILE:HD12	1:D:129:ASP:OD2	1.93	0.69
1:O:14:ILE:HD11	1:O:42:LEU:CD2	2.22	0.69
1:A:93:VAL:CG2	1:A:188:ILE:HG12	2.23	0.68
1:J:93:VAL:O	1:J:185:ASN:HB3	1.93	0.68
1:A:102:CYS:HG	1:N:102:CYS:CB	2.00	0.68
1:J:162:LYS:HE2	1:J:184:GLN:HG3	1.74	0.68
1:E:102:CYS:SG	1:J:102:CYS:N	2.66	0.68
1:F:62:THR:O	1:F:96:ARG:NH1	2.27	0.68
1:A:39:ILE:HG21	1:A:41:LYS:HE3	1.75	0.68
1:G:39:ILE:HG21	1:G:41:LYS:HE3	1.76	0.68
1:N:100:PHE:HD2	1:N:130:PHE:HE1	1.42	0.68
1:B:6:GLU:CG	1:B:7:LEU:N	2.47	0.68
1:J:33:GLY:HA3	1:J:44:LEU:HD23	1.76	0.68
1:A:15:LEU:CD1	1:A:120:VAL:HG22	2.23	0.67
1:E:28:PHE:HD2	1:E:49:THR:OG1	1.76	0.67
1:G:61:VAL:HG13	1:G:220:LEU:HD13	1.76	0.67
1:K:98:ILE:HB	1:K:106:TYR:HB2	1.76	0.67
1:H:203:THR:CG2	1:H:224:VAL:HG22	2.21	0.67
1:G:61:VAL:CG2	1:G:220:LEU:CD1	2.72	0.67
1:G:83:PHE:O	1:G:84:PHE:CB	2.43	0.67
1:N:100:PHE:HD2	1:N:130:PHE:CE1	2.12	0.67
1:B:7:LEU:O	1:B:9:THR:HG22	1.93	0.66
1:B:106:TYR:CZ	1:B:130:PHE:CZ	2.83	0.66
1:J:110:ALA:HB2	1:J:123:ILE:HG23	1.77	0.66
1:D:111:GLU:O	1:D:112:VAL:HG13	1.95	0.66
1:I:43:SER:CB	1:I:221:LEU:CD2	2.70	0.66
1:A:15:LEU:HD12	1:A:120:VAL:CG2	2.25	0.66
1:C:215:ARG:O	1:C:215:ARG:HG3	1.94	0.66
1:D:209:LYS:HE3	1:D:218:MET:HE1	1.78	0.66
1:I:33:GLY:HA3	1:I:44:LEU:CD2	2.24	0.66
1:C:73:ARG:HD3	1:C:225:THR:HG22	1.78	0.66
1:H:206:ILE:HG13	1:L:206:ILE:HG13	1.78	0.66
1:H:102:CYS:N	1:M:102:CYS:SG	2.69	0.65
1:O:106:TYR:CD1	1:O:130:PHE:CZ	2.84	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:LEU:CD2	1:I:19:ASP:O	2.44	0.65
1:G:7:LEU:CD1	1:G:8:PHE:H	2.09	0.65
1:I:83:PHE:HB3	1:I:161:ILE:HD11	1.78	0.65
1:I:135:ASN:CA	1:I:136:ILE:HD12	2.25	0.65
1:M:100:PHE:CG	1:M:136:ILE:HD11	2.32	0.65
1:P:207:LEU:HD22	1:P:218:MET:HE3	1.79	0.65
1:C:149:LYS:HE3	1:I:142:GLU:OE2	1.96	0.65
1:J:145:PHE:HB3	1:J:205:THR:OG1	1.97	0.65
1:G:205:THR:HG22	1:G:206:ILE:H	1.60	0.65
1:A:15:LEU:O	1:A:120:VAL:CA	2.45	0.64
1:B:8:PHE:C	1:B:9:THR:HG22	2.22	0.64
1:J:222:GLU:OE2	1:J:224:VAL:CG2	2.46	0.64
1:A:13:PRO:HD2	1:A:117:ASP:O	1.98	0.64
1:G:13:PRO:HB2	1:G:118:THR:HG22	1.78	0.64
1:B:8:PHE:O	1:B:9:THR:C	2.39	0.64
1:F:206:ILE:HG13	1:P:206:ILE:HG13	1.80	0.64
1:H:141:LEU:HD11	1:H:169:HIS:HB3	1.80	0.64
1:J:183:GLN:NE2	1:J:185:ASN:HD21	1.95	0.64
1:M:117:ASP:CG	1:M:118:THR:H	2.05	0.64
1:C:203:THR:C	1:C:204:GLN:HG3	2.21	0.64
1:G:205:THR:CG2	1:G:220:LEU:CD2	2.76	0.64
1:O:104:GLY:CA	1:O:130:PHE:CE1	2.79	0.64
1:A:15:LEU:HB2	1:A:120:VAL:HA	1.80	0.64
1:N:62:THR:O	1:N:96:ARG:NH1	2.30	0.64
1:P:159:ASN:O	1:P:195:LEU:HD21	1.97	0.63
1:A:68:VAL:C	1:A:70:CYS:H	2.04	0.63
1:A:68:VAL:C	1:A:70:CYS:N	2.56	0.63
1:D:73:ARG:NH1	1:D:74:TYR:O	2.30	0.63
1:O:14:ILE:HD11	1:O:42:LEU:HD22	1.81	0.63
1:O:145:PHE:HB3	1:O:205:THR:OG1	1.97	0.63
1:F:110:ALA:HB2	1:F:123:ILE:HG23	1.80	0.63
1:I:72:SER:HA	1:I:224:VAL:HG13	1.79	0.63
1:K:83:PHE:CZ	1:K:161:ILE:HG13	2.34	0.63
1:I:56:PRO:HD3	1:I:136:ILE:O	1.99	0.62
1:P:88:MET:SD	1:P:114:PHE:N	2.72	0.62
1:I:110:ALA:HB2	1:I:123:ILE:HG23	1.80	0.62
1:C:39:ILE:HG21	1:C:41:LYS:HE3	1.81	0.62
1:M:104:GLY:HA3	1:M:130:PHE:HD1	1.62	0.62
1:B:186:THR:HG22	1:B:187:PRO:N	2.15	0.62
1:J:16:ILE:CD1	1:J:44:LEU:HD13	2.30	0.62
1:N:100:PHE:O	1:N:101:LYS:C	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:100:PHE:CD2	1:N:130:PHE:CE1	2.87	0.62
1:A:119:LEU:O	1:A:120:VAL:CG2	2.44	0.62
1:A:132:GLU:HG2	1:P:156:LYS:HD3	1.82	0.62
1:J:11:VAL:HG22	1:J:36:ASP:OD1	2.00	0.62
1:M:167:ILE:O	1:M:178:LEU:HD23	1.99	0.62
1:H:76:ASP:HA	1:H:79:LYS:HE3	1.82	0.62
1:I:119:LEU:HD23	1:I:119:LEU:O	2.00	0.62
1:O:22:VAL:HG13	1:O:130:PHE:CD2	2.35	0.62
1:C:68:VAL:HG23	1:C:68:VAL:O	2.00	0.62
1:A:119:LEU:C	1:A:120:VAL:HG23	2.25	0.61
1:I:83:PHE:CZ	1:I:160:GLY:HA2	2.36	0.61
1:K:160:GLY:O	1:K:161:ILE:HD13	2.00	0.61
1:N:35:GLY:HA3	1:N:42:LEU:HD23	1.81	0.61
1:C:47:ILE:CD1	1:C:215:ARG:HH21	2.14	0.61
1:D:28:PHE:N	1:D:50:THR:OG1	2.26	0.61
1:I:88:MET:HE2	1:I:119:LEU:HD11	1.81	0.61
1:I:135:ASN:CB	1:I:136:ILE:CD1	2.78	0.61
1:P:58:PRO:HA	1:P:61:VAL:HG23	1.81	0.61
1:P:110:ALA:HB2	1:P:123:ILE:HG23	1.81	0.61
1:O:127:GLY:HA3	1:O:130:PHE:CE2	2.32	0.61
1:M:150:VAL:O	1:M:201:LEU:N	2.34	0.61
1:P:98:ILE:HB	1:P:106:TYR:HB2	1.82	0.61
1:A:57:TRP:HB3	1:A:218:MET:HE3	1.83	0.60
1:B:70:CYS:HB3	1:B:84:PHE:HB2	1.82	0.60
1:G:148:HIS:CE1	1:G:168:ARG:H	2.19	0.60
1:D:73:ARG:HB3	1:D:225:THR:HA	1.83	0.60
1:N:36:ASP:OD2	1:N:39:ILE:HG22	2.01	0.60
1:O:14:ILE:HD12	1:O:42:LEU:HD22	1.83	0.60
1:B:76:ASP:HA	1:B:79:LYS:HE3	1.82	0.60
1:H:205:THR:O	1:H:206:ILE:HG13	2.01	0.60
1:M:14:ILE:H	1:M:33:GLY:C	2.09	0.60
1:C:102:CYS:SG	1:D:102:CYS:N	2.74	0.60
1:F:18:LEU:CD2	1:F:19:ASP:O	2.49	0.60
1:G:199:HIS:CB	1:G:228:GLY:HA2	2.28	0.60
1:C:182:TYR:OH	1:L:156:LYS:HD2	2.01	0.60
1:J:76:ASP:O	1:J:77:HIS:HB3	2.01	0.60
1:J:168:ARG:HG2	1:J:178:LEU:HD23	1.83	0.60
1:F:198:ASP:O	1:F:199:HIS:ND1	2.34	0.60
1:C:110:ALA:CB	1:C:123:ILE:HG12	2.32	0.60
1:D:105:THR:O	1:D:127:GLY:HA2	2.01	0.60
1:E:73:ARG:HH21	1:E:225:THR:HG21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:HA	1:A:79:LYS:HE3	1.84	0.59
1:A:100:PHE:HB3	1:A:103:ASP:HB3	1.84	0.59
1:D:17:GLU:HB2	1:D:122:ARG:HA	1.83	0.59
1:K:41:LYS:HG2	1:K:223:TYR:CE2	2.36	0.59
1:A:98:ILE:HB	1:A:106:TYR:HB2	1.84	0.59
1:E:76:ASP:HA	1:E:79:LYS:HE3	1.84	0.59
1:H:215:ARG:HB2	1:H:217:HIS:NE2	2.16	0.59
1:I:43:SER:CB	1:I:221:LEU:HA	2.32	0.59
1:L:98:ILE:HB	1:L:106:TYR:HB2	1.85	0.59
1:B:185:ASN:O	1:B:186:THR:CB	2.50	0.59
1:L:207:LEU:CD2	1:L:218:MET:HE2	2.31	0.59
1:K:104:GLY:HA3	1:K:130:PHE:CD1	2.38	0.59
1:G:147:SER:CB	1:O:144:ASN:HD22	2.14	0.59
1:N:143:TYR:HD1	1:N:143:TYR:O	1.86	0.59
1:O:104:GLY:HA3	1:O:130:PHE:CE1	2.34	0.59
1:O:74:TYR:CD2	1:O:82:ASP:OD2	2.56	0.59
1:B:92:TYR:HB2	1:B:186:THR:O	2.03	0.58
1:B:201:LEU:HA	1:B:226:ALA:HB2	1.84	0.58
1:B:106:TYR:CD1	1:B:127:GLY:CA	2.87	0.58
1:O:33:GLY:HA3	1:O:44:LEU:HD23	1.85	0.58
1:O:76:ASP:HA	1:O:79:LYS:HE3	1.85	0.58
1:O:92:TYR:HB2	1:O:186:THR:O	2.04	0.58
1:A:83:PHE:CZ	1:A:160:GLY:HA2	2.39	0.58
1:M:108:THR:HG22	1:M:125:LEU:HD23	1.83	0.58
1:C:104:GLY:HA3	1:C:130:PHE:CD1	2.38	0.58
1:D:108:THR:O	1:D:123:ILE:CG2	2.51	0.58
1:M:70:CYS:SG	1:M:119:LEU:HD11	2.43	0.58
1:C:20:GLY:HA2	1:C:125:LEU:O	2.03	0.58
1:J:12:VAL:HG13	1:J:71:PHE:HE1	1.69	0.58
1:L:104:GLY:HA3	1:L:130:PHE:CD1	2.39	0.58
1:B:83:PHE:CD2	1:B:161:ILE:HD11	2.38	0.58
1:C:163:ALA:HB3	1:C:183:GLN:HB3	1.85	0.58
1:I:43:SER:HB3	1:I:221:LEU:HA	1.85	0.58
1:B:110:ALA:HB2	1:B:123:ILE:HG23	1.86	0.58
1:J:94:GLN:HA	1:J:185:ASN:OD1	2.02	0.58
1:D:111:GLU:OE1	1:D:111:GLU:HA	2.04	0.57
1:O:205:THR:HG22	1:O:222:GLU:HG2	1.86	0.57
1:A:110:ALA:HB2	1:A:123:ILE:HG23	1.86	0.57
1:A:145:PHE:HB3	1:A:205:THR:OG1	2.04	0.57
1:B:33:GLY:HA3	1:B:44:LEU:HD23	1.85	0.57
1:B:203:THR:HG22	1:B:224:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:GLY:HA3	1:H:130:PHE:CD1	2.39	0.57
1:M:147:SER:OG	1:M:203:THR:O	2.21	0.57
1:A:88:MET:HE3	1:A:114:PHE:CD2	2.39	0.57
1:D:98:ILE:HB	1:D:106:TYR:HB2	1.85	0.57
1:J:149:LYS:HA	1:J:201:LEU:O	2.05	0.57
1:L:28:PHE:HE2	1:L:30:ARG:HG3	1.69	0.57
1:O:81:HIS:O	1:O:196:PRO:HB3	2.04	0.57
1:L:28:PHE:CE2	1:L:30:ARG:HG3	2.40	0.57
1:P:104:GLY:HA3	1:P:130:PHE:CD1	2.39	0.57
1:F:39:ILE:HG21	1:F:41:LYS:HE3	1.84	0.57
1:A:33:GLY:HA3	1:A:44:LEU:HD23	1.87	0.57
1:F:60:LEU:O	1:F:61:VAL:HB	2.05	0.57
1:J:36:ASP:O	1:J:40:GLY:N	2.37	0.57
1:D:121:ASN:HD21	1:D:123:ILE:HD11	1.70	0.57
1:M:150:VAL:HB	1:M:201:LEU:HB2	1.87	0.57
1:D:106:TYR:CE1	1:D:130:PHE:HZ	2.23	0.57
1:D:121:ASN:ND2	1:D:123:ILE:HD11	2.20	0.57
1:G:103:ASP:CG	1:G:104:GLY:H	2.09	0.57
1:J:27:PHE:HA	1:J:50:THR:HG21	1.87	0.57
1:C:79:LYS:NZ	1:M:230:THR:OG1	2.23	0.56
1:F:36:ASP:HB2	1:F:41:LYS:HB2	1.86	0.56
1:J:73:ARG:HG2	1:J:75:PRO:HD3	1.86	0.56
1:B:105:THR:HG23	1:B:105:THR:O	2.04	0.56
1:B:8:PHE:O	1:B:10:GLY:N	2.37	0.56
1:J:43:SER:CA	1:J:220:LEU:O	2.52	0.56
1:B:48:ALA:HB3	1:B:216:ASP:HB3	1.88	0.56
1:I:76:ASP:HA	1:I:79:LYS:HE3	1.88	0.56
1:K:83:PHE:HA	1:K:86:SER:HB2	1.87	0.56
1:E:33:GLY:HA3	1:E:44:LEU:HD23	1.87	0.56
1:K:94:GLN:HB3	1:K:110:ALA:HB3	1.87	0.56
1:E:145:PHE:HB3	1:E:205:THR:OG1	2.05	0.56
1:H:90:GLU:OE2	1:H:189:GLY:HA2	2.06	0.56
1:D:108:THR:O	1:D:109:ARG:O	2.23	0.56
1:H:31:GLY:HA3	1:H:46:PHE:CD1	2.41	0.56
1:K:83:PHE:CD2	1:K:161:ILE:HG13	2.40	0.56
1:B:101:LYS:HD2	1:B:178:LEU:HD12	1.86	0.56
1:D:155:ASP:O	1:D:156:LYS:HB2	2.06	0.56
1:H:144:ASN:HD22	1:L:147:SER:CB	2.18	0.56
1:I:83:PHE:CB	1:I:161:ILE:HD11	2.35	0.56
1:C:203:THR:O	1:C:204:GLN:CG	2.52	0.55
1:B:186:THR:HG23	1:B:187:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:TRP:HE1	1:C:216:ASP:CG	2.14	0.55
1:L:58:PRO:HA	1:L:61:VAL:HG23	1.88	0.55
1:L:163:ALA:HB3	1:L:183:GLN:HB3	1.87	0.55
1:P:11:VAL:HG22	1:P:36:ASP:OD1	2.05	0.55
1:D:55:VAL:HG21	1:D:106:TYR:OH	2.07	0.55
1:K:71:PHE:HE2	1:K:119:LEU:HD22	1.72	0.55
1:A:104:GLY:HA3	1:A:130:PHE:CD1	2.42	0.55
1:B:82:ASP:OD2	1:B:85:LYS:HD2	2.06	0.55
1:M:155:ASP:HB2	1:M:162:LYS:HG3	1.88	0.55
1:O:163:ALA:HB3	1:O:183:GLN:HB3	1.88	0.55
1:H:141:LEU:CD1	1:H:169:HIS:HB3	2.35	0.55
1:J:130:PHE:HE2	1:J:136:ILE:HG12	1.71	0.55
1:N:18:LEU:HD12	1:N:123:ILE:HD13	1.88	0.55
1:N:143:TYR:O	1:N:143:TYR:CD1	2.60	0.55
1:E:36:ASP:CG	1:E:39:ILE:HG22	2.32	0.55
1:I:41:LYS:O	1:I:42:LEU:HG	2.06	0.55
1:B:28:PHE:CE2	1:B:30:ARG:HG3	2.41	0.55
1:G:207:LEU:CD2	1:G:220:LEU:HG	2.36	0.55
1:C:206:ILE:HG13	1:I:206:ILE:HG13	1.89	0.55
1:I:88:MET:CE	1:I:119:LEU:HD12	2.34	0.55
1:J:162:LYS:HE2	1:J:184:GLN:CD	2.30	0.55
1:N:145:PHE:HB3	1:N:205:THR:OG1	2.06	0.54
1:F:98:ILE:HG12	1:F:181:HIS:CD2	2.42	0.54
1:J:56:PRO:HD3	1:J:136:ILE:O	2.07	0.54
1:L:23:ASN:ND2	1:L:130:PHE:H	2.01	0.54
1:E:145:PHE:HB3	1:E:205:THR:HG1	1.72	0.54
1:H:58:PRO:HA	1:H:61:VAL:HG23	1.89	0.54
1:L:22:VAL:HG12	1:L:23:ASN:N	2.22	0.54
1:B:104:GLY:HA3	1:B:130:PHE:CD1	2.43	0.54
1:H:161:ILE:HD11	1:H:196:PRO:HG3	1.88	0.54
1:I:145:PHE:HB3	1:I:205:THR:OG1	2.06	0.54
1:J:162:LYS:HE2	1:J:184:GLN:CG	2.36	0.54
1:K:18:LEU:HD21	1:K:125:LEU:HD12	1.89	0.54
1:B:8:PHE:C	1:B:9:THR:CG2	2.80	0.54
1:B:106:TYR:CD1	1:B:127:GLY:HA2	2.43	0.54
1:G:171:VAL:HG12	1:G:173:ASP:H	1.72	0.54
1:J:16:ILE:HD11	1:J:44:LEU:HD13	1.89	0.54
1:J:28:PHE:CE2	1:J:30:ARG:HG3	2.41	0.54
1:B:42:LEU:HB2	1:B:222:GLU:HB3	1.89	0.54
1:D:128:ILE:CD1	1:D:129:ASP:OD2	2.55	0.54
1:K:102:CYS:N	1:L:102:CYS:SG	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:94:GLN:HG3	1:N:185:ASN:OD1	2.08	0.54
1:A:68:VAL:CG2	1:A:70:CYS:SG	2.96	0.54
1:I:145:PHE:HB3	1:I:205:THR:HG1	1.72	0.54
1:C:101:LYS:HD2	1:C:178:LEU:HD12	1.90	0.54
1:D:33:GLY:HA3	1:D:44:LEU:HD23	1.90	0.54
1:H:33:GLY:HA3	1:H:44:LEU:HD23	1.89	0.54
1:I:101:LYS:HD2	1:I:178:LEU:HD12	1.88	0.54
1:B:106:TYR:CD1	1:B:127:GLY:HA3	2.42	0.54
1:H:98:ILE:HB	1:H:106:TYR:HB2	1.88	0.54
1:O:224:VAL:HG12	1:O:225:THR:N	2.22	0.54
1:G:98:ILE:HB	1:G:106:TYR:HB2	1.90	0.53
1:H:41:LYS:HE2	1:H:223:TYR:OH	2.08	0.53
1:K:70:CYS:SG	1:K:92:TYR:HE2	2.31	0.53
1:N:163:ALA:HB3	1:N:183:GLN:HE21	1.73	0.53
1:A:28:PHE:HD2	1:A:49:THR:OG1	1.91	0.53
1:C:47:ILE:HD13	1:C:215:ARG:CZ	2.38	0.53
1:D:38:THR:O	1:D:73:ARG:HD3	2.08	0.53
1:I:11:VAL:HG22	1:I:36:ASP:OD1	2.08	0.53
1:J:14:ILE:HB	1:J:44:LEU:HD21	1.89	0.53
1:B:186:THR:CG2	1:B:187:PRO:N	2.72	0.53
1:C:47:ILE:CD1	1:C:215:ARG:NH2	2.65	0.53
1:E:39:ILE:HA	1:E:73:ARG:HD3	1.91	0.53
1:F:112:VAL:HG22	1:F:121:ASN:OD1	2.09	0.53
1:O:104:GLY:O	1:O:130:PHE:HE1	1.82	0.53
1:B:90:GLU:HG2	1:B:189:GLY:HA3	1.90	0.53
1:G:103:ASP:CG	1:G:104:GLY:N	2.66	0.53
1:G:208:SER:HB2	1:G:219:VAL:CB	2.37	0.53
1:H:82:ASP:OD2	1:H:85:LYS:HD2	2.09	0.53
1:J:74:TYR:CD1	1:J:74:TYR:O	2.61	0.53
1:K:187:PRO:HB2	1:K:189:GLY:O	2.08	0.53
1:E:40:GLY:N	1:E:73:ARG:HB2	2.24	0.53
1:E:101:LYS:HD2	1:E:178:LEU:HD12	1.90	0.53
1:F:11:VAL:HG22	1:F:36:ASP:OD1	2.08	0.53
1:G:7:LEU:O	1:G:8:PHE:HB2	2.07	0.53
1:J:183:GLN:HE21	1:J:185:ASN:ND2	2.05	0.53
1:A:59:THR:HG21	1:A:136:ILE:HD12	1.90	0.53
1:A:207:LEU:HD13	1:A:218:MET:HE2	1.91	0.53
1:B:58:PRO:HA	1:B:61:VAL:HG23	1.91	0.53
1:A:93:VAL:HG12	1:A:93:VAL:O	2.09	0.53
1:D:130:PHE:CE2	1:D:136:ILE:HG21	2.44	0.53
1:F:207:LEU:O	1:P:204:GLN:NE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:THR:CG2	1:G:220:LEU:HD21	2.39	0.53
1:P:33:GLY:HA3	1:P:44:LEU:HD23	1.91	0.53
1:A:15:LEU:O	1:A:120:VAL:C	2.52	0.53
1:G:70:CYS:SG	1:G:119:LEU:HD11	2.49	0.53
1:J:71:PHE:CE2	1:J:119:LEU:HD23	2.44	0.53
1:M:104:GLY:HA3	1:M:130:PHE:CE1	2.43	0.53
1:N:100:PHE:HB3	1:N:103:ASP:HB3	1.91	0.53
1:O:11:VAL:HG22	1:O:36:ASP:OD1	2.09	0.53
1:O:58:PRO:HA	1:O:61:VAL:HG23	1.90	0.53
1:P:114:PHE:HE1	1:P:119:LEU:HD12	1.74	0.53
1:I:41:LYS:C	1:I:42:LEU:HG	2.34	0.52
1:L:28:PHE:HD2	1:L:49:THR:HG1	1.57	0.52
1:A:132:GLU:O	1:A:133:ASP:HB3	2.08	0.52
1:C:157:GLN:HE22	1:L:184:GLN:NE2	2.07	0.52
1:C:215:ARG:O	1:C:216:ASP:C	2.49	0.52
1:F:145:PHE:HB3	1:F:205:THR:OG1	2.09	0.52
1:F:163:ALA:HB3	1:F:183:GLN:HB3	1.91	0.52
1:I:42:LEU:CD2	1:I:71:PHE:CD2	2.93	0.52
1:O:127:GLY:CA	1:O:130:PHE:CE2	2.84	0.52
1:A:92:TYR:HD1	1:A:92:TYR:O	1.92	0.52
1:A:115:GLU:O	1:A:115:GLU:HG2	2.09	0.52
1:K:16:ILE:HD13	1:K:64:LEU:O	2.09	0.52
1:N:21:ASP:HB3	1:N:26:LYS:HG2	1.92	0.52
1:O:74:TYR:HE2	1:O:82:ASP:OD1	1.92	0.52
1:G:144:ASN:OD1	1:O:204:GLN:NE2	2.42	0.52
1:K:161:ILE:HG22	1:K:162:LYS:N	2.25	0.52
1:L:70:CYS:O	1:L:85:LYS:NZ	2.39	0.52
1:M:100:PHE:O	1:M:101:LYS:C	2.51	0.52
1:O:35:GLY:CA	1:O:42:LEU:HD23	2.38	0.52
1:D:142:GLU:HG2	1:D:172:GLU:OE2	2.10	0.52
1:G:220:LEU:O	1:G:222:GLU:HG3	2.10	0.52
1:A:68:VAL:HG22	1:A:71:PHE:HD2	1.65	0.52
1:B:106:TYR:HD1	1:B:127:GLY:HA2	1.75	0.52
1:G:33:GLY:HA3	1:G:44:LEU:HD23	1.91	0.52
1:I:198:ASP:O	1:I:199:HIS:ND1	2.43	0.52
1:K:18:LEU:HD11	1:K:125:LEU:HD11	1.91	0.52
1:O:101:LYS:O	1:O:102:CYS:HB2	2.10	0.52
1:O:100:PHE:CD2	1:O:104:GLY:O	2.59	0.52
1:P:64:LEU:O	1:P:121:ASN:ND2	2.42	0.52
1:M:100:PHE:CD2	1:M:136:ILE:HD11	2.44	0.52
1:K:161:ILE:HD11	1:K:196:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:128:ILE:HG22	1:O:129:ASP:CG	2.35	0.52
1:K:143:TYR:O	1:K:144:ASN:ND2	2.43	0.51
1:L:56:PRO:HD3	1:L:136:ILE:O	2.11	0.51
1:O:199:HIS:ND1	1:O:227:ALA:O	2.42	0.51
1:P:36:ASP:HB3	1:P:39:ILE:HG22	1.91	0.51
1:P:41:LYS:HE2	1:P:223:TYR:OH	2.10	0.51
1:H:21:ASP:OD1	1:H:26:LYS:HG2	2.11	0.51
1:J:62:THR:HG21	1:J:167:ILE:HG13	1.93	0.51
1:A:68:VAL:HG13	1:A:68:VAL:O	2.09	0.51
1:D:16:ILE:HG21	1:D:64:LEU:HD23	1.92	0.51
1:E:104:GLY:HA3	1:E:130:PHE:CD1	2.45	0.51
1:D:145:PHE:HB3	1:D:205:THR:HB	1.90	0.51
1:G:147:SER:HB2	1:O:144:ASN:HD22	1.75	0.51
1:I:83:PHE:HB3	1:I:161:ILE:CD1	2.40	0.51
1:C:63:THR:O	1:C:123:ILE:HD11	2.11	0.51
1:B:145:PHE:HB3	1:B:205:THR:OG1	2.10	0.51
1:D:149:LYS:HA	1:D:201:LEU:O	2.10	0.51
1:E:38:THR:O	1:E:73:ARG:HG3	2.11	0.51
1:L:101:LYS:HD2	1:L:178:LEU:HD12	1.93	0.51
1:O:74:TYR:CE2	1:O:82:ASP:OD2	2.64	0.51
1:B:8:PHE:O	1:B:9:THR:CG2	2.59	0.51
1:K:83:PHE:CZ	1:K:84:PHE:CE1	2.99	0.51
1:K:93:VAL:N	1:K:186:THR:O	2.35	0.51
1:B:183:GLN:HE21	1:B:185:ASN:HD21	1.58	0.51
1:H:15:LEU:CD1	1:H:120:VAL:HG22	2.41	0.51
1:J:28:PHE:HD2	1:J:49:THR:OG1	1.94	0.51
1:N:207:LEU:HB3	1:N:218:MET:HE3	1.92	0.51
1:P:155:ASP:O	1:P:160:GLY:N	2.44	0.51
1:D:11:VAL:HG22	1:D:36:ASP:OD1	2.11	0.51
1:G:123:ILE:HG22	1:G:124:GLU:O	2.11	0.51
1:K:146:ASN:HB2	1:K:148:HIS:CE1	2.45	0.51
1:D:17:GLU:O	1:D:123:ILE:HG13	2.11	0.50
1:D:97:THR:HA	1:D:106:TYR:O	2.11	0.50
1:M:128:ILE:HG22	1:M:129:ASP:OD2	2.11	0.50
1:B:106:TYR:CE1	1:B:127:GLY:CA	2.91	0.50
1:G:11:VAL:HG22	1:G:36:ASP:OD1	2.11	0.50
1:L:22:VAL:HA	1:L:127:GLY:O	2.11	0.50
1:A:15:LEU:C	1:A:120:VAL:HA	2.37	0.50
1:H:144:ASN:HD22	1:L:147:SER:HB2	1.77	0.50
1:K:144:ASN:HD22	1:M:204:GLN:NE2	2.08	0.50
1:L:30:ARG:O	1:L:47:ILE:N	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:34:GLU:O	1:N:43:SER:O	2.29	0.50
1:O:100:PHE:CB	1:O:103:ASP:CB	2.90	0.50
1:E:73:ARG:HE	1:E:225:THR:HG22	1.77	0.50
1:H:100:PHE:O	1:H:101:LYS:C	2.50	0.50
1:L:22:VAL:HG12	1:L:23:ASN:H	1.77	0.50
1:B:9:THR:CG2	1:B:10:GLY:N	2.52	0.50
1:C:73:ARG:HH21	1:I:211:LEU:HD21	1.76	0.50
1:C:203:THR:O	1:C:223:TYR:O	2.29	0.50
1:A:68:VAL:HG22	1:A:70:CYS:SG	2.52	0.50
1:A:161:ILE:HD11	1:A:196:PRO:HG3	1.93	0.50
1:F:21:ASP:HB3	1:F:26:LYS:HG2	1.93	0.50
1:I:36:ASP:HB2	1:I:41:LYS:HB2	1.94	0.50
1:L:22:VAL:HA	1:L:127:GLY:CA	2.42	0.50
1:L:145:PHE:HB3	1:L:205:THR:OG1	2.11	0.49
1:G:93:VAL:HG13	1:G:110:ALA:O	2.13	0.49
1:J:183:GLN:HE21	1:J:185:ASN:HD21	1.60	0.49
1:H:83:PHE:HB2	1:H:196:PRO:HD3	1.93	0.49
1:K:63:THR:HG21	1:K:125:LEU:HD21	1.94	0.49
1:E:98:ILE:HB	1:E:106:TYR:HB2	1.93	0.49
1:E:152:ILE:HG23	1:E:161:ILE:HG23	1.94	0.49
1:H:215:ARG:HB2	1:H:217:HIS:CE1	2.48	0.49
1:I:62:THR:HB	1:I:96:ARG:HH12	1.78	0.49
1:M:128:ILE:CG2	1:M:129:ASP:N	2.76	0.49
1:D:75:PRO:HD2	1:D:78:MET:HB2	1.94	0.49
1:B:104:GLY:HA3	1:B:130:PHE:CE1	2.48	0.49
1:F:19:ASP:N	1:F:19:ASP:OD1	2.44	0.49
1:G:101:LYS:HG2	1:G:102:CYS:SG	2.52	0.49
1:L:83:PHE:CD1	1:L:196:PRO:HD3	2.47	0.49
1:A:11:VAL:HG22	1:A:36:ASP:OD1	2.13	0.49
1:F:21:ASP:HB3	1:F:26:LYS:HA	1.95	0.49
1:G:205:THR:CG2	1:G:220:LEU:HD23	2.32	0.49
1:L:23:ASN:ND2	1:L:130:PHE:O	2.46	0.49
1:N:46:PHE:O	1:N:217:HIS:HB2	2.12	0.49
1:O:100:PHE:HB2	1:O:103:ASP:CB	2.42	0.49
1:F:20:GLY:CA	1:F:125:LEU:O	2.55	0.49
1:O:23:ASN:ND2	1:O:130:PHE:O	2.45	0.49
1:A:83:PHE:HB2	1:A:196:PRO:HD3	1.95	0.49
1:F:98:ILE:HG12	1:F:181:HIS:HD2	1.78	0.49
1:C:123:ILE:CG2	1:C:124:GLU:N	2.76	0.49
1:B:6:GLU:OE1	1:B:6:GLU:HA	2.13	0.48
1:F:35:GLY:HA3	1:F:71:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:SER:CB	1:G:219:VAL:HB	2.40	0.48
1:H:141:LEU:HD11	1:H:169:HIS:CG	2.48	0.48
1:O:220:LEU:HD21	1:O:222:GLU:CD	2.37	0.48
1:G:140:LYS:O	1:G:171:VAL:HG13	2.13	0.48
1:G:219:VAL:HG12	1:G:220:LEU:H	1.78	0.48
1:M:18:LEU:HD11	1:M:125:LEU:HD11	1.93	0.48
1:O:162:LYS:HA	1:O:183:GLN:O	2.13	0.48
1:B:145:PHE:HB3	1:B:205:THR:HG1	1.78	0.48
1:H:47:ILE:HG12	1:H:217:HIS:ND1	2.28	0.48
1:L:19:ASP:O	1:L:125:LEU:N	2.41	0.48
1:P:98:ILE:HG23	1:P:181:HIS:CD2	2.48	0.48
1:A:62:THR:O	1:A:96:ARG:NH1	2.46	0.48
1:C:79:LYS:HZ2	1:M:230:THR:HG1	1.57	0.48
1:F:19:ASP:HA	1:F:28:PHE:HD1	1.78	0.48
1:G:13:PRO:HD2	1:G:117:ASP:O	2.14	0.48
1:M:128:ILE:HG22	1:M:129:ASP:N	2.28	0.48
1:A:153:THR:O	1:A:161:ILE:HG12	2.13	0.48
1:G:205:THR:HG23	1:G:220:LEU:HD21	1.92	0.48
1:J:15:LEU:HD22	1:J:120:VAL:HG23	1.96	0.48
1:K:58:PRO:HA	1:K:61:VAL:HG23	1.94	0.48
1:O:74:TYR:HD2	1:O:82:ASP:OD2	1.97	0.48
1:G:55:VAL:HG11	1:G:106:TYR:OH	2.13	0.48
1:I:42:LEU:HD21	1:I:71:PHE:CD2	2.43	0.48
1:P:20:GLY:HA2	1:P:125:LEU:O	2.13	0.48
1:B:102:CYS:SG	1:I:102:CYS:N	2.86	0.48
1:D:102:CYS:O	1:D:131:LYS:HE3	2.13	0.48
1:G:205:THR:CG2	1:G:206:ILE:H	2.22	0.48
1:I:41:LYS:HG2	1:I:223:TYR:CE1	2.48	0.48
1:K:130:PHE:CE2	1:K:136:ILE:HG21	2.49	0.48
1:F:136:ILE:C	1:F:138:GLY:H	2.21	0.48
1:F:145:PHE:HB3	1:F:205:THR:HG1	1.79	0.48
1:A:68:VAL:HG21	1:A:71:PHE:HE2	1.73	0.48
1:D:17:GLU:N	1:D:121:ASN:O	2.38	0.48
1:D:56:PRO:HD3	1:D:136:ILE:O	2.14	0.48
1:D:100:PHE:HE1	1:D:106:TYR:CD1	2.32	0.48
1:G:220:LEU:O	1:G:221:LEU:C	2.57	0.48
1:L:21:ASP:O	1:L:25:HIS:O	2.32	0.48
1:A:94:GLN:HG2	1:A:95:GLU:N	2.29	0.47
1:I:58:PRO:HA	1:I:61:VAL:HG23	1.95	0.47
1:N:20:GLY:HA3	1:N:125:LEU:HG	1.96	0.47
1:A:80:ARG:O	1:A:194:ASP:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:33:GLY:CA	1:J:44:LEU:HD23	2.42	0.47
1:L:145:PHE:HB3	1:L:205:THR:HG1	1.78	0.47
1:D:16:ILE:CG2	1:D:64:LEU:HD23	2.44	0.47
1:G:61:VAL:CB	1:G:220:LEU:HD11	2.42	0.47
1:M:45:LYS:NZ	1:M:213:GLU:OE2	2.40	0.47
1:N:100:PHE:O	1:N:102:CYS:N	2.47	0.47
1:A:68:VAL:O	1:A:70:CYS:N	2.46	0.47
1:C:102:CYS:SG	1:D:101:LYS:HG2	2.54	0.47
1:M:167:ILE:O	1:M:178:LEU:CD2	2.62	0.47
1:I:18:LEU:HD23	1:I:19:ASP:C	2.39	0.47
1:I:28:PHE:HE2	1:I:30:ARG:CD	2.26	0.47
1:O:21:ASP:OD1	1:O:26:LYS:HG2	2.14	0.47
1:B:106:TYR:CD1	1:B:130:PHE:HZ	2.31	0.47
1:O:127:GLY:C	1:O:130:PHE:HE2	2.23	0.47
1:P:101:LYS:HD2	1:P:178:LEU:HD12	1.96	0.47
1:B:224:VAL:O	1:B:225:THR:C	2.57	0.47
1:G:207:LEU:CD2	1:G:219:VAL:O	2.48	0.47
1:J:18:LEU:HB2	1:J:123:ILE:HD12	1.96	0.47
1:L:55:VAL:HG22	1:L:136:ILE:HG22	1.97	0.47
1:L:144:ASN:CA	1:L:207:LEU:HD12	2.44	0.47
1:N:87:ALA:HB3	1:N:92:TYR:CZ	2.49	0.47
1:C:21:ASP:OD1	1:C:26:LYS:HG2	2.15	0.47
1:H:71:PHE:HE2	1:H:119:LEU:HD23	1.79	0.47
1:K:154:ALA:HB1	1:K:195:LEU:HD23	1.96	0.47
1:G:205:THR:O	1:G:206:ILE:CB	2.63	0.47
1:I:161:ILE:CG2	1:I:162:LYS:N	2.77	0.47
1:B:225:THR:O	1:B:226:ALA:HB3	2.15	0.47
1:C:58:PRO:HA	1:C:61:VAL:HG23	1.97	0.47
1:K:206:ILE:HG13	1:M:206:ILE:HG13	1.97	0.47
1:L:155:ASP:OD2	1:L:162:LYS:HE2	2.15	0.47
1:M:100:PHE:CD2	1:M:136:ILE:CD1	2.98	0.47
1:O:7:LEU:HD13	1:O:114:PHE:CE2	2.50	0.47
1:O:121:ASN:CG	1:O:123:ILE:HD11	2.40	0.47
1:O:207:LEU:HB3	1:O:218:MET:SD	2.55	0.47
1:P:88:MET:HE1	1:P:113:LYS:C	2.39	0.47
1:A:152:ILE:HG22	1:A:153:THR:N	2.29	0.46
1:B:40:GLY:O	1:B:223:TYR:HA	2.15	0.46
1:C:75:PRO:HD2	1:C:78:MET:HB2	1.96	0.46
1:E:56:PRO:HD3	1:E:136:ILE:O	2.15	0.46
1:F:104:GLY:HA3	1:F:130:PHE:CD1	2.50	0.46
1:G:207:LEU:CD2	1:G:220:LEU:HA	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:16:ILE:HG21	1:L:46:PHE:HE1	1.81	0.46
1:L:88:MET:HE3	1:L:114:PHE:CD2	2.51	0.46
1:B:106:TYR:CD1	1:B:130:PHE:HE1	2.30	0.46
1:C:157:GLN:HE22	1:L:184:GLN:HE22	1.62	0.46
1:G:31:GLY:HA3	1:G:46:PHE:CD1	2.51	0.46
1:J:167:ILE:HB	1:J:179:ALA:HB3	1.97	0.46
1:D:161:ILE:HD13	1:D:196:PRO:HG3	1.98	0.46
1:F:74:TYR:HA	1:F:75:PRO:HD2	1.76	0.46
1:I:44:LEU:N	1:I:220:LEU:O	2.49	0.46
1:I:135:ASN:HD22	1:I:177:GLN:NE2	2.13	0.46
1:P:220:LEU:HD21	1:P:222:GLU:HB2	1.98	0.46
1:B:28:PHE:HD2	1:B:49:THR:OG1	1.98	0.46
1:E:28:PHE:CZ	1:E:30:ARG:HG3	2.37	0.46
1:E:74:TYR:OH	1:E:84:PHE:HD2	1.99	0.46
1:A:58:PRO:HA	1:A:61:VAL:HG23	1.98	0.46
1:F:15:LEU:HD22	1:F:120:VAL:HG13	1.98	0.46
1:G:7:LEU:CG	1:G:8:PHE:N	2.31	0.46
1:M:100:PHE:CD1	1:M:136:ILE:HD11	2.50	0.46
1:A:15:LEU:HB2	1:A:120:VAL:CA	2.45	0.46
1:E:42:LEU:HB2	1:E:222:GLU:HB3	1.97	0.46
1:I:28:PHE:CE2	1:I:30:ARG:CD	2.98	0.46
1:P:40:GLY:HA2	1:P:71:PHE:O	2.15	0.46
1:A:68:VAL:HG22	1:A:68:VAL:O	2.16	0.46
1:A:68:VAL:HG23	1:A:70:CYS:SG	2.54	0.46
1:B:204:GLN:NE2	1:D:207:LEU:O	2.48	0.46
1:B:206:ILE:HG13	1:D:206:ILE:HG13	1.98	0.46
1:F:18:LEU:HD23	1:F:19:ASP:C	2.39	0.46
1:H:15:LEU:HD11	1:H:120:VAL:HG22	1.98	0.46
1:J:222:GLU:OE2	1:J:224:VAL:HG21	2.16	0.46
1:O:224:VAL:O	1:O:225:THR:CG2	2.64	0.46
1:B:22:VAL:HG13	1:B:106:TYR:OH	2.14	0.46
1:L:55:VAL:HG13	1:L:56:PRO:HD2	1.98	0.46
1:G:147:SER:HB2	1:G:203:THR:O	2.16	0.46
1:I:76:ASP:O	1:I:79:LYS:HG3	2.16	0.46
1:N:108:THR:HA	1:N:124:GLU:O	2.17	0.46
1:O:14:ILE:HD11	1:O:42:LEU:HD21	1.95	0.46
1:O:20:GLY:HA2	1:O:125:LEU:O	2.15	0.46
1:C:33:GLY:HA3	1:C:44:LEU:HD23	1.97	0.45
1:O:36:ASP:HB3	1:O:39:ILE:HG22	1.98	0.45
1:B:20:GLY:HA2	1:B:125:LEU:O	2.16	0.45
1:C:82:ASP:OD2	1:C:85:LYS:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:75:PRO:HD2	1:H:78:MET:HB2	1.98	0.45
1:I:104:GLY:HA3	1:I:130:PHE:CD1	2.51	0.45
1:A:55:VAL:HG11	1:A:106:TYR:OH	2.17	0.45
1:A:57:TRP:HB3	1:A:218:MET:CE	2.46	0.45
1:C:40:GLY:HA3	1:C:73:ARG:HB2	1.97	0.45
1:C:149:LYS:HA	1:C:201:LEU:O	2.16	0.45
1:M:96:ARG:NE	1:M:183:GLN:OE1	2.46	0.45
1:N:88:MET:HE1	1:N:113:LYS:HA	1.98	0.45
1:F:161:ILE:CG2	1:F:162:LYS:N	2.80	0.45
1:M:128:ILE:CG2	1:M:129:ASP:CG	2.80	0.45
1:C:63:THR:O	1:C:123:ILE:CD1	2.65	0.45
1:I:100:PHE:HE2	1:I:106:TYR:CE2	2.35	0.45
1:P:218:MET:HE2	1:P:220:LEU:HD12	1.97	0.45
1:F:203:THR:HG22	1:F:224:VAL:HG13	1.97	0.45
1:J:58:PRO:HA	1:J:61:VAL:HG23	1.99	0.45
1:K:55:VAL:HG13	1:K:56:PRO:HD2	1.99	0.45
1:O:224:VAL:O	1:O:225:THR:HG23	2.16	0.45
1:A:20:GLY:HA2	1:A:125:LEU:O	2.16	0.45
1:A:113:LYS:O	1:A:119:LEU:HA	2.17	0.45
1:B:70:CYS:HB3	1:B:84:PHE:CB	2.47	0.45
1:L:23:ASN:HD21	1:L:130:PHE:CA	2.28	0.45
1:A:88:MET:HE1	1:A:113:LYS:HA	1.98	0.45
1:B:149:LYS:HA	1:B:201:LEU:O	2.17	0.45
1:B:163:ALA:HB3	1:B:183:GLN:HB3	1.99	0.45
1:K:16:ILE:HG12	1:K:121:ASN:HB3	1.99	0.45
1:L:62:THR:HG21	1:L:167:ILE:HG13	1.99	0.45
1:A:92:TYR:O	1:A:92:TYR:CD1	2.70	0.45
1:H:15:LEU:HD12	1:H:120:VAL:HG13	1.98	0.45
1:J:20:GLY:HA2	1:J:125:LEU:O	2.17	0.45
1:M:18:LEU:HD21	1:M:125:LEU:HD12	1.99	0.45
1:O:100:PHE:HB3	1:O:103:ASP:CB	2.47	0.45
1:O:224:VAL:CG1	1:O:225:THR:N	2.80	0.45
1:B:161:ILE:CG2	1:B:162:LYS:N	2.80	0.44
1:I:23:ASN:OD1	1:I:130:PHE:HB2	2.17	0.44
1:K:93:VAL:O	1:K:185:ASN:HA	2.18	0.44
1:K:161:ILE:CG2	1:K:162:LYS:N	2.80	0.44
1:M:98:ILE:O	1:M:105:THR:HA	2.17	0.44
1:O:28:PHE:HD2	1:O:49:THR:OG1	2.00	0.44
1:A:36:ASP:HB2	1:A:41:LYS:HB2	2.00	0.44
1:H:163:ALA:HB3	1:H:183:GLN:HB3	1.98	0.44
1:L:92:TYR:CZ	1:L:112:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:THR:CG2	1:C:222:GLU:OE1	2.65	0.44
1:J:98:ILE:O	1:J:105:THR:HA	2.18	0.44
1:J:162:LYS:HE2	1:J:184:GLN:NE2	2.32	0.44
1:P:8:PHE:CE1	1:P:85:LYS:HB3	2.53	0.44
1:P:94:GLN:HE21	1:P:183:GLN:NE2	2.16	0.44
1:A:83:PHE:CD2	1:A:161:ILE:HD12	2.53	0.44
1:C:19:ASP:O	1:C:125:LEU:N	2.45	0.44
1:I:142:GLU:OE1	1:I:170:ASN:HB3	2.17	0.44
1:J:12:VAL:HG13	1:J:71:PHE:CE1	2.51	0.44
1:K:93:VAL:HB	1:K:186:THR:OG1	2.18	0.44
1:N:101:LYS:HB2	1:N:178:LEU:HB2	1.99	0.44
1:O:22:VAL:HG13	1:O:130:PHE:CE2	2.52	0.44
1:A:68:VAL:CG2	1:A:71:PHE:CE2	2.91	0.44
1:F:86:SER:HB2	1:F:192:PRO:O	2.17	0.44
1:H:113:LYS:O	1:H:119:LEU:HD12	2.18	0.44
1:I:28:PHE:HZ	1:I:30:ARG:CG	2.24	0.44
1:I:43:SER:HA	1:I:220:LEU:O	2.17	0.44
1:K:199:HIS:HD2	1:K:228:GLY:C	2.25	0.44
1:L:57:TRP:HB3	1:L:218:MET:CE	2.43	0.44
1:M:97:THR:OG1	1:M:182:TYR:HB2	2.17	0.44
1:O:14:ILE:HG21	1:O:44:LEU:HD21	2.00	0.44
1:D:133:ASP:OD2	1:L:192:PRO:HA	2.17	0.44
1:M:101:LYS:N	1:M:178:LEU:O	2.23	0.44
1:M:155:ASP:OD2	1:M:158:ASN:ND2	2.51	0.44
1:O:55:VAL:HG21	1:O:106:TYR:OH	2.18	0.44
1:I:53:LEU:HD23	1:I:53:LEU:HA	1.79	0.44
1:J:16:ILE:HD12	1:J:44:LEU:HD13	1.98	0.44
1:A:69:GLN:C	1:A:71:PHE:N	2.75	0.44
1:E:15:LEU:HB2	1:E:120:VAL:HG22	1.99	0.44
1:M:57:TRP:HB3	1:M:218:MET:HE3	2.00	0.44
1:N:56:PRO:HD2	1:N:136:ILE:HG23	1.99	0.44
1:C:42:LEU:HB2	1:C:222:GLU:HB3	2.00	0.43
1:D:100:PHE:CD2	1:D:136:ILE:HD11	2.53	0.43
1:L:63:THR:HG21	1:L:125:LEU:HD12	2.00	0.43
1:N:98:ILE:HB	1:N:106:TYR:HB2	1.99	0.43
1:P:40:GLY:N	1:P:73:ARG:HB3	2.33	0.43
1:F:204:GLN:NE2	1:P:207:LEU:O	2.49	0.43
1:G:53:LEU:HD23	1:G:53:LEU:HA	1.81	0.43
1:G:83:PHE:CZ	1:G:160:GLY:HA2	2.53	0.43
1:H:100:PHE:HB2	1:H:103:ASP:HB3	2.00	0.43
1:H:141:LEU:HD11	1:H:169:HIS:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:130:PHE:HE2	1:K:136:ILE:HG21	1.83	0.43
1:E:41:LYS:HE2	1:E:223:TYR:OH	2.19	0.43
1:M:12:VAL:HA	1:M:13:PRO:HD3	1.90	0.43
1:O:104:GLY:N	1:O:130:PHE:CD1	2.86	0.43
1:A:94:GLN:CG	1:A:185:ASN:OD1	2.52	0.43
1:G:205:THR:CG2	1:G:206:ILE:N	2.65	0.43
1:I:197:ASP:OD1	1:I:198:ASP:N	2.52	0.43
1:I:209:LYS:HG3	1:I:217:HIS:CE1	2.54	0.43
1:K:18:LEU:C	1:K:18:LEU:HD23	2.44	0.43
1:K:27:PHE:CD2	1:K:54:PRO:HD3	2.53	0.43
1:M:47:ILE:HD13	1:M:215:ARG:NH2	2.34	0.43
1:A:23:ASN:ND2	1:A:130:PHE:O	2.51	0.43
1:D:103:ASP:OD2	1:D:177:GLN:NE2	2.49	0.43
1:L:144:ASN:HA	1:L:207:LEU:HD12	1.99	0.43
1:P:134:GLY:O	1:P:138:GLY:HA3	2.18	0.43
1:F:14:ILE:N	1:F:33:GLY:O	2.50	0.43
1:L:155:ASP:CG	1:L:162:LYS:HE2	2.42	0.43
1:L:161:ILE:HD11	1:L:196:PRO:HG3	2.00	0.43
1:O:108:THR:HA	1:O:124:GLU:O	2.19	0.43
1:O:161:ILE:CG2	1:O:162:LYS:N	2.81	0.43
1:P:154:ALA:HB1	1:P:195:LEU:HD13	2.00	0.43
1:A:91:GLY:HA3	1:A:188:ILE:HD12	2.00	0.43
1:C:204:GLN:O	1:C:222:GLU:HG3	2.18	0.43
1:C:204:GLN:HE21	1:I:144:ASN:HB3	1.84	0.43
1:D:53:LEU:HD12	1:D:57:TRP:CE2	2.53	0.43
1:F:13:PRO:HA	1:F:34:GLU:HG3	2.01	0.43
1:G:36:ASP:HB2	1:G:41:LYS:HB2	2.01	0.43
1:H:56:PRO:HD3	1:H:136:ILE:O	2.19	0.43
1:L:20:GLY:O	1:L:21:ASP:OD1	2.36	0.43
1:M:207:LEU:HD22	1:M:218:MET:HE2	2.01	0.43
1:O:163:ALA:N	1:O:183:GLN:O	2.44	0.43
1:P:71:PHE:CE2	1:P:119:LEU:HD13	2.54	0.43
1:P:114:PHE:CE1	1:P:119:LEU:HD12	2.53	0.43
1:A:203:THR:HG22	1:A:224:VAL:HG22	2.01	0.43
1:N:98:ILE:O	1:N:105:THR:HA	2.18	0.43
1:O:14:ILE:HG13	1:O:34:GLU:HA	2.01	0.43
1:O:213:GLU:OE2	1:O:215:ARG:HD3	2.17	0.43
1:E:203:THR:HG22	1:E:224:VAL:HG13	2.00	0.43
1:J:147:SER:HA	1:J:203:THR:O	2.18	0.43
1:L:53:LEU:HD23	1:L:53:LEU:HA	1.84	0.43
1:O:23:ASN:OD1	1:O:130:PHE:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:21:ASP:OD1	1:P:26:LYS:HG2	2.19	0.43
1:D:57:TRP:CE2	1:D:218:MET:HG2	2.54	0.43
1:F:191:GLY:HA2	1:F:192:PRO:HD3	1.86	0.43
1:H:59:THR:HG21	1:H:136:ILE:HD12	2.01	0.43
1:D:143:TYR:OH	1:D:218:MET:SD	2.72	0.42
1:J:199:HIS:CE1	1:J:228:GLY:HA2	2.53	0.42
1:O:84:PHE:HE1	1:O:185:ASN:ND2	2.17	0.42
1:O:143:TYR:C	1:O:144:ASN:OD1	2.61	0.42
1:H:161:ILE:CG2	1:H:162:LYS:N	2.82	0.42
1:H:204:GLN:C	1:H:205:THR:HG1	2.21	0.42
1:J:14:ILE:HG12	1:J:71:PHE:CZ	2.54	0.42
1:J:40:GLY:HA3	1:J:73:ARG:HB2	2.01	0.42
1:J:154:ALA:N	1:J:198:ASP:OD1	2.53	0.42
1:K:103:ASP:OD2	1:K:136:ILE:HD13	2.19	0.42
1:K:205:THR:HA	1:K:222:GLU:HA	2.01	0.42
1:M:178:LEU:HD23	1:M:178:LEU:HA	1.80	0.42
1:O:111:GLU:O	1:O:121:ASN:HA	2.19	0.42
1:B:22:VAL:CG2	1:B:106:TYR:CZ	3.02	0.42
1:F:14:ILE:CB	1:F:33:GLY:O	2.60	0.42
1:I:42:LEU:CD2	1:I:71:PHE:CB	2.64	0.42
1:J:12:VAL:CG1	1:J:71:PHE:HE1	2.32	0.42
1:K:56:PRO:HD3	1:K:136:ILE:O	2.20	0.42
1:L:55:VAL:HG11	1:L:106:TYR:OH	2.19	0.42
1:P:158:ASN:O	1:P:159:ASN:CB	2.68	0.42
1:G:12:VAL:HA	1:G:13:PRO:HD3	1.84	0.42
1:G:61:VAL:HG11	1:G:220:LEU:HD11	1.92	0.42
1:I:43:SER:HB2	1:I:220:LEU:O	2.18	0.42
1:I:97:THR:HG22	1:I:107:LYS:HG2	2.00	0.42
1:N:149:LYS:HA	1:N:201:LEU:O	2.19	0.42
1:O:7:LEU:HD13	1:O:114:PHE:HE2	1.83	0.42
1:A:152:ILE:O	1:A:162:LYS:O	2.37	0.42
1:B:9:THR:O	1:B:38:THR:HG23	2.19	0.42
1:B:62:THR:O	1:B:96:ARG:NH1	2.51	0.42
1:D:103:ASP:HB3	1:D:104:GLY:H	1.64	0.42
1:L:22:VAL:CG1	1:L:23:ASN:N	2.81	0.42
1:O:74:TYR:CE2	1:O:82:ASP:HA	2.54	0.42
1:D:215:ARG:O	1:D:217:HIS:N	2.52	0.42
1:G:71:PHE:CE2	1:G:119:LEU:HD13	2.54	0.42
1:J:198:ASP:HB3	1:J:199:HIS:H	1.71	0.42
1:M:16:ILE:HD13	1:M:46:PHE:HE1	1.85	0.42
1:O:98:ILE:HB	1:O:106:TYR:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:163:ALA:HB3	1:P:183:GLN:HB3	2.02	0.42
1:F:40:GLY:HA2	1:F:71:PHE:O	2.19	0.42
1:G:124:GLU:HG2	1:G:125:LEU:H	1.85	0.42
1:G:168:ARG:HG2	1:G:178:LEU:HD23	2.02	0.42
1:H:46:PHE:CD2	1:H:64:LEU:HD13	2.54	0.42
1:I:36:ASP:O	1:I:40:GLY:N	2.53	0.42
1:K:83:PHE:CZ	1:K:161:ILE:CG1	3.02	0.42
1:L:14:ILE:HD13	1:L:68:VAL:HG21	2.01	0.42
1:N:39:ILE:HD12	1:N:39:ILE:HA	1.87	0.42
1:A:203:THR:HA	1:A:223:TYR:O	2.18	0.42
1:B:55:VAL:HG13	1:B:56:PRO:HD2	2.01	0.42
1:B:56:PRO:HD3	1:B:136:ILE:O	2.19	0.42
1:C:23:ASN:OD1	1:C:130:PHE:HB2	2.20	0.42
1:H:143:TYR:C	1:H:144:ASN:OD1	2.63	0.42
1:I:12:VAL:HA	1:I:13:PRO:HD3	1.92	0.42
1:I:52:LYS:HD2	1:I:216:ASP:OD2	2.18	0.42
1:I:161:ILE:HG22	1:I:162:LYS:N	2.34	0.42
1:K:101:LYS:HG3	1:L:102:CYS:SG	2.60	0.42
1:M:103:ASP:HB3	1:M:104:GLY:H	1.57	0.42
1:A:36:ASP:O	1:A:40:GLY:N	2.53	0.42
1:A:161:ILE:CG2	1:A:162:LYS:N	2.83	0.42
1:C:156:LYS:HD2	1:L:182:TYR:OH	2.18	0.42
1:C:161:ILE:CG2	1:C:162:LYS:N	2.83	0.42
1:H:55:VAL:HG13	1:H:56:PRO:HD2	2.02	0.42
1:H:203:THR:CB	1:H:224:VAL:HG22	2.50	0.42
1:I:28:PHE:HZ	1:I:30:ARG:HE	1.68	0.42
1:C:55:VAL:HG13	1:C:56:PRO:HD2	2.02	0.42
1:C:98:ILE:HB	1:C:106:TYR:HB2	2.02	0.42
1:N:18:LEU:HB2	1:N:123:ILE:HD12	2.00	0.42
1:A:15:LEU:HD22	1:A:30:ARG:NH2	2.35	0.41
1:C:40:GLY:CA	1:C:73:ARG:HB2	2.51	0.41
1:E:28:PHE:CZ	1:E:30:ARG:CG	3.01	0.41
1:F:136:ILE:O	1:F:138:GLY:N	2.53	0.41
1:G:52:LYS:HG2	1:G:216:ASP:OD2	2.20	0.41
1:G:141:LEU:HD23	1:G:141:LEU:HA	1.85	0.41
1:B:7:LEU:HD22	1:B:114:PHE:CD2	2.55	0.41
1:B:106:TYR:HE1	1:B:127:GLY:HA3	1.74	0.41
1:F:33:GLY:N	1:F:44:LEU:HD23	2.34	0.41
1:I:211:LEU:HD23	1:I:211:LEU:HA	1.76	0.41
1:J:211:LEU:HD23	1:J:211:LEU:HA	1.90	0.41
1:K:96:ARG:HB2	1:K:108:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:143:TYR:OH	1:O:208:SER:O	2.37	0.41
1:O:149:LYS:HA	1:O:201:LEU:O	2.20	0.41
1:A:114:PHE:CD1	1:A:116:GLY:O	2.73	0.41
1:C:112:VAL:HG22	1:C:121:ASN:OD1	2.21	0.41
1:H:142:GLU:OE2	1:L:149:LYS:HE3	2.21	0.41
1:I:28:PHE:CZ	1:I:30:ARG:HG2	2.50	0.41
1:I:149:LYS:HA	1:I:201:LEU:O	2.21	0.41
1:L:22:VAL:C	1:L:24:GLY:H	2.28	0.41
1:O:114:PHE:CE1	1:O:119:LEU:HD12	2.55	0.41
1:F:41:LYS:C	1:F:42:LEU:HD12	2.45	0.41
1:L:31:GLY:HA2	1:L:46:PHE:HA	2.02	0.41
1:N:100:PHE:CB	1:N:103:ASP:HB3	2.50	0.41
1:O:205:THR:CG2	1:O:222:GLU:HG2	2.50	0.41
1:G:36:ASP:O	1:G:40:GLY:N	2.54	0.41
1:G:149:LYS:HA	1:G:201:LEU:O	2.21	0.41
1:K:53:LEU:HD23	1:K:53:LEU:HA	1.88	0.41
1:K:195:LEU:HA	1:K:196:PRO:HD2	1.77	0.41
1:P:42:LEU:HB2	1:P:222:GLU:HB3	2.02	0.41
1:B:23:ASN:OD1	1:B:130:PHE:HB2	2.20	0.41
1:D:143:TYR:CZ	1:D:218:MET:SD	3.14	0.41
1:E:58:PRO:HA	1:E:61:VAL:HG23	2.01	0.41
1:G:83:PHE:CB	1:G:161:ILE:HD12	2.46	0.41
1:I:39:ILE:C	1:I:73:ARG:HD2	2.46	0.41
1:I:161:ILE:HG21	1:I:161:ILE:HD13	1.90	0.41
1:L:13:PRO:HD2	1:L:117:ASP:O	2.21	0.41
1:L:23:ASN:ND2	1:L:130:PHE:HB2	2.36	0.41
1:O:123:ILE:CG2	1:O:124:GLU:N	2.83	0.41
1:O:195:LEU:HA	1:O:196:PRO:HD2	1.92	0.41
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.87	0.41
1:C:45:LYS:HD3	1:C:219:VAL:HG22	2.01	0.41
1:C:56:PRO:HD3	1:C:136:ILE:O	2.21	0.41
1:C:83:PHE:CZ	1:C:160:GLY:HA2	2.55	0.41
1:D:47:ILE:HD11	1:D:215:ARG:HG3	2.03	0.41
1:E:152:ILE:CD1	1:E:201:LEU:HD11	2.51	0.41
1:N:57:TRP:CG	1:N:218:MET:HG2	2.55	0.41
1:N:58:PRO:HA	1:N:61:VAL:HG23	2.02	0.41
1:D:108:THR:O	1:D:123:ILE:HG23	2.21	0.41
1:D:112:VAL:O	1:D:113:LYS:HB3	2.21	0.41
1:H:15:LEU:HG	1:H:120:VAL:HG22	2.02	0.41
1:J:12:VAL:HA	1:J:13:PRO:HD3	1.95	0.41
1:M:203:THR:HG22	1:M:224:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:36:ASP:HB2	1:P:41:LYS:HB2	2.03	0.41
1:A:69:GLN:C	1:A:71:PHE:H	2.28	0.41
1:B:17:GLU:OE2	1:B:30:ARG:NH2	2.54	0.41
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.87	0.41
1:C:202:SER:C	1:C:203:THR:HG1	2.22	0.41
1:D:47:ILE:HD11	1:D:215:ARG:CB	2.51	0.41
1:F:41:LYS:HE2	1:F:223:TYR:OH	2.21	0.41
1:F:108:THR:HA	1:F:124:GLU:O	2.21	0.41
1:G:205:THR:HG22	1:G:206:ILE:O	2.21	0.41
1:I:43:SER:CA	1:I:220:LEU:O	2.69	0.41
1:I:128:ILE:HD12	1:I:129:ASP:OD2	2.20	0.41
1:J:10:GLY:HA3	1:L:115:GLU:C	2.44	0.41
1:K:71:PHE:CE2	1:K:119:LEU:HD22	2.54	0.41
1:O:13:PRO:HD2	1:O:117:ASP:O	2.20	0.41
1:O:35:GLY:CA	1:O:42:LEU:CD2	2.99	0.41
1:P:53:LEU:HA	1:P:53:LEU:HD23	1.80	0.41
1:B:28:PHE:HE2	1:B:30:ARG:HG3	1.86	0.41
1:B:33:GLY:CA	1:B:44:LEU:HD23	2.51	0.41
1:C:203:THR:C	1:C:223:TYR:O	2.64	0.41
1:E:161:ILE:CG2	1:E:162:LYS:N	2.84	0.41
1:G:55:VAL:HG13	1:G:56:PRO:HD2	2.03	0.41
1:G:94:GLN:HB2	1:G:185:ASN:ND2	2.35	0.41
1:J:76:ASP:HB3	1:J:77:HIS:H	1.51	0.41
1:K:152:ILE:HG23	1:K:161:ILE:CG2	2.51	0.41
1:N:102:CYS:O	1:N:102:CYS:SG	2.79	0.41
1:A:77:HIS:O	1:A:77:HIS:ND1	2.54	0.40
1:C:88:MET:HE3	1:C:114:PHE:CD2	2.56	0.40
1:E:88:MET:HE3	1:E:114:PHE:CD2	2.56	0.40
1:F:161:ILE:HD11	1:F:196:PRO:HG3	2.03	0.40
1:M:74:TYR:HA	1:M:75:PRO:HD3	1.87	0.40
1:O:114:PHE:HE1	1:O:119:LEU:HD12	1.86	0.40
1:P:23:ASN:OD1	1:P:130:PHE:HB2	2.21	0.40
1:A:55:VAL:HG22	1:A:136:ILE:HG22	2.04	0.40
1:I:104:GLY:HA3	1:I:130:PHE:CG	2.57	0.40
1:K:39:ILE:HG22	1:K:39:ILE:O	2.21	0.40
1:K:44:LEU:HD13	1:K:46:PHE:CZ	2.56	0.40
1:L:156:LYS:HG2	1:L:195:LEU:HD12	2.04	0.40
1:M:101:LYS:CB	1:M:178:LEU:HB2	2.52	0.40
1:B:22:VAL:HG22	1:B:106:TYR:CZ	2.55	0.40
1:G:81:HIS:CE1	1:G:197:ASP:HB2	2.55	0.40
1:I:18:LEU:HD23	1:I:18:LEU:C	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14:ILE:HD11	1:L:71:PHE:CE2	2.57	0.40
1:O:39:ILE:HG23	1:O:41:LYS:HB2	2.03	0.40
1:O:224:VAL:C	1:O:225:THR:HG23	2.47	0.40
1:P:122:ARG:C	1:P:123:ILE:HG13	2.45	0.40
1:A:74:TYR:HA	1:A:75:PRO:HD3	1.95	0.40
1:B:9:THR:O	1:B:38:THR:CG2	2.69	0.40
1:B:23:ASN:ND2	1:B:130:PHE:O	2.55	0.40
1:C:123:ILE:HG22	1:C:124:GLU:N	2.35	0.40
1:E:211:LEU:HD23	1:E:211:LEU:HA	1.83	0.40
1:G:15:LEU:HB2	1:G:120:VAL:HG22	2.03	0.40
1:H:18:LEU:C	1:H:18:LEU:HD23	2.46	0.40
1:J:10:GLY:HA3	1:L:115:GLU:O	2.21	0.40
1:J:53:LEU:HD23	1:J:53:LEU:HA	1.87	0.40
1:J:98:ILE:HB	1:J:106:TYR:HB2	2.04	0.40
1:A:40:GLY:HA2	1:A:71:PHE:O	2.21	0.40
1:C:28:PHE:HD2	1:C:49:THR:CG2	2.34	0.40
1:F:136:ILE:C	1:F:138:GLY:N	2.80	0.40
1:O:53:LEU:HA	1:O:53:LEU:HD23	1.80	0.40
1:O:76:ASP:O	1:O:79:LYS:HG3	2.22	0.40
1:O:128:ILE:HG22	1:O:129:ASP:N	2.36	0.40
1:O:205:THR:CB	1:O:222:GLU:HG2	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLN:OE1	1:F:184:GLN:NE2[1_445]	2.14	0.06
1:C:17:GLU:OE2	1:J:50:THR:OG1[1_455]	2.17	0.03

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	207/234 (88%)	195 (94%)	11 (5%)	1 (0%)	24	58
1	B	193/234 (82%)	184 (95%)	8 (4%)	1 (0%)	24	58
1	C	195/234 (83%)	188 (96%)	6 (3%)	1 (0%)	24	58
1	D	174/234 (74%)	161 (92%)	12 (7%)	1 (1%)	21	53
1	E	198/234 (85%)	191 (96%)	6 (3%)	1 (0%)	24	58
1	F	187/234 (80%)	180 (96%)	6 (3%)	1 (0%)	24	58
1	G	176/234 (75%)	167 (95%)	8 (4%)	1 (1%)	21	53
1	H	175/234 (75%)	169 (97%)	6 (3%)	0	100	100
1	I	199/234 (85%)	192 (96%)	6 (3%)	1 (0%)	24	58
1	J	168/234 (72%)	163 (97%)	5 (3%)	0	100	100
1	K	159/234 (68%)	154 (97%)	4 (2%)	1 (1%)	21	53
1	L	187/234 (80%)	181 (97%)	5 (3%)	1 (0%)	24	58
1	M	152/234 (65%)	149 (98%)	2 (1%)	1 (1%)	18	51
1	N	162/234 (69%)	159 (98%)	3 (2%)	0	100	100
1	O	207/234 (88%)	198 (96%)	7 (3%)	2 (1%)	12	44
1	P	192/234 (82%)	186 (97%)	6 (3%)	0	100	100
All	All	2931/3744 (78%)	2817 (96%)	101 (3%)	13 (0%)	30	62

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	VAL
1	F	61	VAL
1	G	206	ILE
1	D	196	PRO
1	C	204	GLN
1	E	196	PRO
1	L	22	VAL
1	K	196	PRO
1	M	103	ASP
1	O	75	PRO
1	B	186	THR
1	I	196	PRO
1	O	186	THR

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	189/204 (93%)	186 (98%)	3 (2%)	55	70
1	B	181/204 (89%)	177 (98%)	4 (2%)	45	65
1	C	178/204 (87%)	175 (98%)	3 (2%)	53	69
1	D	170/204 (83%)	167 (98%)	3 (2%)	51	69
1	E	182/204 (89%)	180 (99%)	2 (1%)	65	74
1	F	175/204 (86%)	169 (97%)	6 (3%)	32	58
1	G	163/204 (80%)	157 (96%)	6 (4%)	30	56
1	H	168/204 (82%)	163 (97%)	5 (3%)	36	60
1	I	183/204 (90%)	178 (97%)	5 (3%)	39	62
1	J	160/204 (78%)	156 (98%)	4 (2%)	42	63
1	K	152/204 (74%)	150 (99%)	2 (1%)	61	72
1	L	171/204 (84%)	165 (96%)	6 (4%)	32	57
1	M	149/204 (73%)	146 (98%)	3 (2%)	48	66
1	N	153/204 (75%)	148 (97%)	5 (3%)	33	58
1	O	179/204 (88%)	178 (99%)	1 (1%)	78	79
1	P	177/204 (87%)	176 (99%)	1 (1%)	78	79
All	All	2730/3264 (84%)	2671 (98%)	59 (2%)	45	65

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

Mol	Chain	Res	Type
1	A	55	VAL
1	A	123	ILE
1	A	204	GLN
1	B	55	VAL
1	B	95	GLU
1	B	108	THR
1	B	123	ILE
1	C	55	VAL

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Mol	Chain	Res	Type
1	C	159	ASN
1	C	206	ILE
1	D	64	LEU
1	D	78	MET
1	D	161	ILE
1	E	53	LEU
1	E	123	ILE
1	F	19	ASP
1	F	55	VAL
1	F	123	ILE
1	F	128	ILE
1	F	132	GLU
1	F	199	HIS
1	G	42	LEU
1	G	55	VAL
1	G	102	CYS
1	G	123	ILE
1	G	161	ILE
1	G	219	VAL
1	H	55	VAL
1	H	111	GLU
1	H	123	ILE
1	H	128	ILE
1	H	204	GLN
1	I	123	ILE
1	I	128	ILE
1	I	136	ILE
1	I	159	ASN
1	I	206	ILE
1	J	55	VAL
1	J	123	ILE
1	J	184	GLN
1	J	206	ILE
1	K	123	ILE
1	K	128	ILE
1	L	18	LEU
1	L	55	VAL
1	L	123	ILE
1	L	128	ILE
1	L	132	GLU
1	L	206	ILE
1	M	55	VAL

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Mol	Chain	Res	Type
1	M	123	ILE
1	M	206	ILE
1	N	55	VAL
1	N	123	ILE
1	N	128	ILE
1	N	188	ILE
1	N	206	ILE
1	O	102	CYS
1	P	123	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	B	94	GLN
1	B	121	ASN
1	B	164	ASN
1	B	185	ASN
1	C	204	GLN
1	D	146	ASN
1	E	121	ASN
1	F	94	GLN
1	F	139	HIS
1	F	164	ASN
1	F	181	HIS
1	G	164	ASN
1	H	94	GLN
1	H	121	ASN
1	H	146	ASN
1	H	204	GLN
1	I	121	ASN
1	I	135	ASN
1	I	146	ASN
1	I	170	ASN
1	J	139	HIS
1	J	183	GLN
1	K	121	ASN
1	K	144	ASN
1	K	159	ASN
1	L	23	ASN
1	L	164	ASN
1	L	184	GLN

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Mol	Chain	Res	Type
1	M	158	ASN
1	N	121	ASN
1	N	146	ASN
1	N	170	ASN
1	N	183	GLN
1	O	81	HIS
1	O	139	HIS
1	O	185	ASN
1	P	94	GLN
1	P	121	ASN
1	P	139	HIS
1	P	181	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/234 (91%)	0.87	22 (10%) 12 9	50, 80, 148, 324	0
1	B	205/234 (87%)	0.70	16 (7%) 19 13	51, 87, 175, 274	0
1	C	207/234 (88%)	0.91	28 (13%) 7 6	55, 91, 164, 338	0
1	D	194/234 (82%)	0.86	17 (8%) 15 11	57, 92, 169, 237	0
1	E	208/234 (88%)	0.99	34 (16%) 4 4	64, 96, 157, 204	0
1	F	201/234 (85%)	0.69	18 (8%) 15 10	69, 106, 174, 357	0
1	G	188/234 (80%)	0.72	19 (10%) 12 9	52, 103, 181, 284	0
1	H	191/234 (81%)	0.99	24 (12%) 8 6	69, 102, 172, 382	0
1	I	209/234 (89%)	0.73	16 (7%) 19 13	64, 98, 165, 249	0
1	J	184/234 (78%)	0.90	25 (13%) 7 6	51, 95, 166, 270	0
1	K	175/234 (74%)	0.89	16 (9%) 15 10	73, 102, 181, 323	0
1	L	197/234 (84%)	0.77	19 (9%) 13 9	67, 114, 206, 293	0
1	M	168/234 (71%)	0.74	18 (10%) 11 8	75, 119, 203, 375	0
1	N	174/234 (74%)	0.83	19 (10%) 10 8	72, 130, 219, 388	0
1	O	213/234 (91%)	1.03	26 (12%) 8 7	54, 126, 205, 302	0
1	P	204/234 (87%)	0.84	17 (8%) 17 12	73, 134, 217, 464	0
All	All	3133/3744 (83%)	0.84	334 (10%) 11 8	50, 104, 188, 464	0

All (334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	102	CYS	7.6
1	D	196	PRO	6.9
1	M	164	ASN	6.6
1	E	133	ASP	6.6
1	O	224	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
1	H	92	TYR	6.1
1	J	178	LEU	5.9
1	H	195	LEU	5.5
1	A	70	CYS	5.3
1	M	152	ILE	5.2
1	E	134	GLY	5.2
1	O	196	PRO	5.2
1	D	72	SER	5.0
1	H	24	GLY	5.0
1	J	146	ASN	4.8
1	P	64	LEU	4.7
1	J	163	ALA	4.6
1	H	194	ASP	4.6
1	B	106	TYR	4.4
1	O	150	VAL	4.4
1	K	185	ASN	4.4
1	G	217	HIS	4.2
1	A	212	ASN	4.2
1	M	178	LEU	4.2
1	O	86	SER	4.1
1	D	83	PHE	4.0
1	I	32	GLU	3.9
1	G	218	MET	3.9
1	H	83	PHE	3.9
1	F	49	THR	3.8
1	J	176	VAL	3.8
1	P	68	VAL	3.8
1	N	102	CYS	3.8
1	L	180	ASP	3.8
1	O	223	TYR	3.8
1	A	68	VAL	3.7
1	C	147	SER	3.7
1	A	133	ASP	3.7
1	P	28	PHE	3.6
1	O	163	ALA	3.6
1	I	52	LYS	3.6
1	L	215	ARG	3.6
1	C	75	PRO	3.6
1	M	151	TYR	3.6
1	J	101	LYS	3.5
1	B	119	LEU	3.5
1	H	144	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	36	ASP	3.5
1	K	134	GLY	3.5
1	C	72	SER	3.5
1	K	21	ASP	3.5
1	K	175	SER	3.4
1	E	64	LEU	3.4
1	N	119	LEU	3.4
1	P	63	THR	3.4
1	B	153	THR	3.4
1	I	116	GLY	3.3
1	E	164	ASN	3.3
1	C	73	ARG	3.3
1	G	11	VAL	3.3
1	E	222	GLU	3.3
1	F	161	ILE	3.3
1	E	10	GLY	3.3
1	H	110	ALA	3.3
1	G	15	LEU	3.2
1	I	102	CYS	3.2
1	D	115	GLU	3.2
1	A	103	ASP	3.2
1	B	102	CYS	3.2
1	O	63	THR	3.2
1	E	131	LYS	3.2
1	A	188	ILE	3.2
1	C	135	ASN	3.2
1	L	226	ALA	3.2
1	H	117	ASP	3.1
1	G	60	LEU	3.1
1	N	147	SER	3.1
1	G	40	GLY	3.1
1	O	197	ASP	3.1
1	L	34	GLU	3.1
1	O	225	THR	3.1
1	E	176	VAL	3.1
1	F	58	PRO	3.1
1	F	61	VAL	3.1
1	J	180	ASP	3.1
1	K	83	PHE	3.1
1	O	222	GLU	3.1
1	E	102	CYS	3.1
1	H	84	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	133	ASP	3.1
1	I	53	LEU	3.0
1	O	42	LEU	3.0
1	E	175	SER	3.0
1	G	46	PHE	3.0
1	H	167	ILE	3.0
1	A	112	VAL	3.0
1	B	63	THR	3.0
1	G	208	SER	3.0
1	A	93	VAL	3.0
1	H	68	VAL	3.0
1	E	23	ASN	3.0
1	D	116	GLY	2.9
1	I	64	LEU	2.9
1	L	102	CYS	2.9
1	N	44	LEU	2.9
1	B	51	GLY	2.9
1	B	83	PHE	2.9
1	K	64	LEU	2.9
1	H	63	THR	2.9
1	D	33	GLY	2.9
1	O	81	HIS	2.9
1	N	15	LEU	2.9
1	K	97	THR	2.9
1	K	144	ASN	2.9
1	L	175	SER	2.9
1	F	192	PRO	2.9
1	M	153	THR	2.9
1	B	87	ALA	2.8
1	M	48	ALA	2.8
1	O	87	ALA	2.8
1	A	198	ASP	2.8
1	C	133	ASP	2.8
1	E	76	ASP	2.8
1	O	170	ASN	2.8
1	E	137	LEU	2.8
1	E	70	CYS	2.8
1	N	222	GLU	2.8
1	P	216	ASP	2.8
1	C	70	CYS	2.8
1	N	63	THR	2.8
1	D	152	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	133	ASP	2.8
1	P	152	ILE	2.8
1	I	199	HIS	2.8
1	C	201	LEU	2.8
1	E	221	LEU	2.8
1	H	69	GLN	2.7
1	C	64	LEU	2.7
1	F	196	PRO	2.7
1	K	152	ILE	2.7
1	P	198	ASP	2.7
1	G	102	CYS	2.7
1	L	134	GLY	2.7
1	C	48	ALA	2.7
1	F	19	ASP	2.7
1	N	180	ASP	2.7
1	A	136	ILE	2.7
1	F	54	PRO	2.7
1	P	222	GLU	2.7
1	C	203	THR	2.7
1	H	120	VAL	2.7
1	K	141	LEU	2.7
1	K	228	GLY	2.6
1	L	138	GLY	2.6
1	A	119	LEU	2.6
1	H	15	LEU	2.6
1	O	43	SER	2.6
1	G	223	TYR	2.6
1	H	219	VAL	2.6
1	L	92	TYR	2.6
1	C	161	ILE	2.6
1	E	130	PHE	2.6
1	A	120	VAL	2.6
1	O	151	TYR	2.6
1	A	88	MET	2.6
1	B	82	ASP	2.6
1	H	40	GLY	2.6
1	G	196	PRO	2.6
1	C	82	ASP	2.6
1	L	170	ASN	2.6
1	C	160	GLY	2.5
1	E	174	GLY	2.5
1	O	134	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	117	ASP	2.5
1	I	225	THR	2.5
1	C	4	GLY	2.5
1	A	19	ASP	2.5
1	G	180	ASP	2.5
1	F	84	PHE	2.5
1	A	137	LEU	2.5
1	J	177	GLN	2.5
1	B	110	ALA	2.5
1	H	161	ILE	2.5
1	I	216	ASP	2.5
1	L	117	ASP	2.5
1	M	19	ASP	2.5
1	N	103	ASP	2.5
1	A	83	PHE	2.5
1	E	9	THR	2.5
1	C	85	LYS	2.5
1	B	222	GLU	2.4
1	K	180	ASP	2.4
1	D	78	MET	2.4
1	N	218	MET	2.4
1	J	115	GLU	2.4
1	C	221	LEU	2.4
1	L	44	LEU	2.4
1	J	121	ASN	2.4
1	P	58	PRO	2.4
1	J	199	HIS	2.4
1	E	79	LYS	2.4
1	E	101	LYS	2.4
1	M	68	VAL	2.4
1	L	159	ASN	2.4
1	C	25	HIS	2.4
1	D	36	ASP	2.4
1	J	200	TYR	2.4
1	E	78	MET	2.4
1	I	207	LEU	2.4
1	O	125	LEU	2.4
1	A	175	SER	2.4
1	J	22	VAL	2.4
1	A	134	GLY	2.3
1	L	97	THR	2.3
1	J	185	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	173	ASP	2.3
1	J	223	TYR	2.3
1	N	200	TYR	2.3
1	D	64	LEU	2.3
1	E	44	LEU	2.3
1	I	63	THR	2.3
1	C	78	MET	2.3
1	D	21	ASP	2.3
1	O	216	ASP	2.3
1	N	145	PHE	2.3
1	I	68	VAL	2.3
1	J	13	PRO	2.3
1	B	116	GLY	2.3
1	K	163	ALA	2.3
1	O	133	ASP	2.3
1	D	75	PRO	2.3
1	E	51	GLY	2.3
1	E	161	ILE	2.3
1	G	138	GLY	2.3
1	F	153	THR	2.3
1	H	186	THR	2.3
1	I	223	TYR	2.3
1	I	21	ASP	2.3
1	L	87	ALA	2.3
1	H	147	SER	2.3
1	G	143	TYR	2.3
1	H	173	ASP	2.3
1	E	6	GLU	2.2
1	N	132	GLU	2.2
1	E	119	LEU	2.2
1	D	151	TYR	2.2
1	O	200	TYR	2.2
1	E	5	GLU	2.2
1	G	117	ASP	2.2
1	M	222	GLU	2.2
1	E	63	THR	2.2
1	C	86	SER	2.2
1	K	23	ASN	2.2
1	D	195	LEU	2.2
1	G	48	ALA	2.2
1	N	174	GLY	2.2
1	P	201	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	62	THR	2.2
1	F	151	TYR	2.2
1	C	120	VAL	2.2
1	C	202	SER	2.2
1	J	175	SER	2.2
1	A	135	ASN	2.2
1	M	121	ASN	2.2
1	O	146	ASN	2.2
1	M	15	LEU	2.2
1	E	58	PRO	2.2
1	F	36	ASP	2.2
1	J	131	LYS	2.2
1	P	82	ASP	2.2
1	M	57	TRP	2.2
1	J	68	VAL	2.2
1	A	102	CYS	2.2
1	O	8	PHE	2.2
1	O	117	ASP	2.2
1	C	63	THR	2.1
1	P	112	VAL	2.1
1	N	39	ILE	2.1
1	A	147	SER	2.1
1	A	50	THR	2.1
1	G	39	ILE	2.1
1	H	136	ILE	2.1
1	B	30	ARG	2.1
1	E	132	GLU	2.1
1	J	189	GLY	2.1
1	M	76	ASP	2.1
1	M	217	HIS	2.1
1	N	16	ILE	2.1
1	O	64	LEU	2.1
1	J	142	GLU	2.1
1	N	33	GLY	2.1
1	I	208	SER	2.1
1	L	86	SER	2.1
1	B	146	ASN	2.1
1	B	161	ILE	2.1
1	D	161	ILE	2.1
1	E	216	ASP	2.1
1	F	64	LEU	2.1
1	G	152	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	207	LEU	2.1
1	M	64	LEU	2.1
1	C	184	GLN	2.1
1	D	132	GLU	2.1
1	H	176	VAL	2.1
1	G	57	TRP	2.1
1	M	123	ILE	2.1
1	O	161	ILE	2.1
1	F	163	ALA	2.1
1	F	68	VAL	2.0
1	J	29	VAL	2.0
1	N	61	VAL	2.0
1	C	43	SER	2.0
1	D	202	SER	2.0
1	K	135	ASN	2.0
1	F	139	HIS	2.0
1	H	198	ASP	2.0
1	M	227	ALA	2.0
1	P	102	CYS	2.0
1	C	83	PHE	2.0
1	E	104	GLY	2.0
1	P	138	GLY	2.0
1	P	160	GLY	2.0
1	J	172	GLU	2.0
1	M	142	GLU	2.0
1	E	120	VAL	2.0
1	F	53	LEU	2.0
1	L	47	ILE	2.0
1	B	225	THR	2.0
1	C	49	THR	2.0
1	J	182	TYR	2.0
1	C	165	PHE	2.0
1	F	46	PHE	2.0
1	P	54	PRO	2.0
1	L	141	LEU	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 [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.