Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 02:38 AM EST

PDB ID	:	4W6R
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:

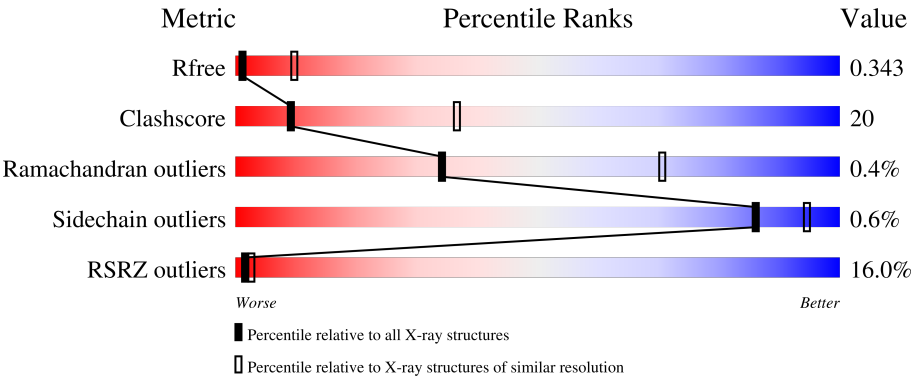
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	13% 59% 31% · 8%
1	B	234	10% 58% 29% · 12%
1	C	234	13% 59% 29% 12%
1	D	234	8% 53% 28% · 17%
1	E	234	9% 66% 23% 11%

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Mol	Chain	Length	Quality of chain
1	F	234	12% 60% 24% 14%
1	G	234	15% 51% 28% 20%
1	H	234	17% 56% 23% 18%
1	I	234	8% 57% 32% 11%
1	J	234	8% 51% 27% 21%
1	K	234	6% 50% 24% 25%
1	L	234	18% 56% 28% 16%
1	M	234	15% 50% 22% 28%
1	N	234	18% 54% 19% 26%
1	O	234	24% 58% 32% 9%
1	P	234	20% 64% 23% 13%

2 Entry composition (i)

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.

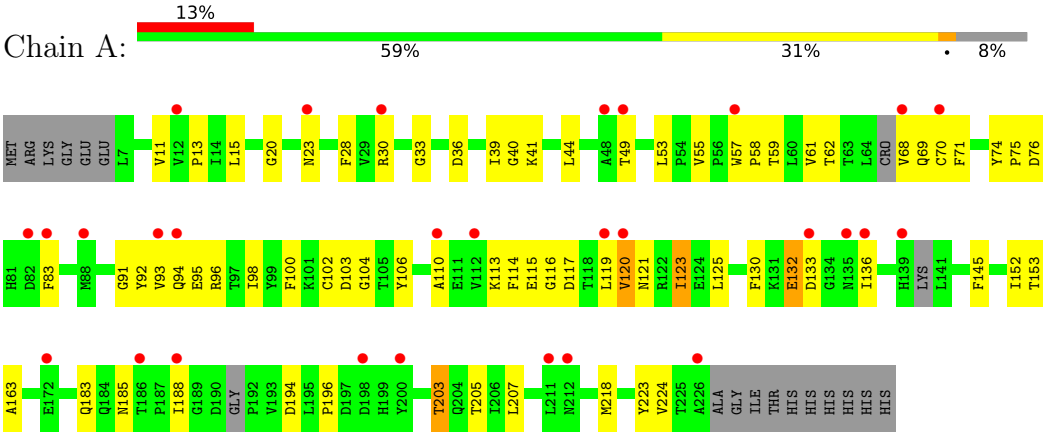
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1721	1098	291	327	5			
1	B	205	Total	C	N	O	S	0	0	0
			1649	1052	280	313	4			
1	C	207	Total	C	N	O	S	0	0	0
			1643	1052	277	309	5			
1	D	194	Total	C	N	O	S	0	0	0
			1552	993	261	293	5			
1	E	208	Total	C	N	O	S	0	0	0
			1661	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.

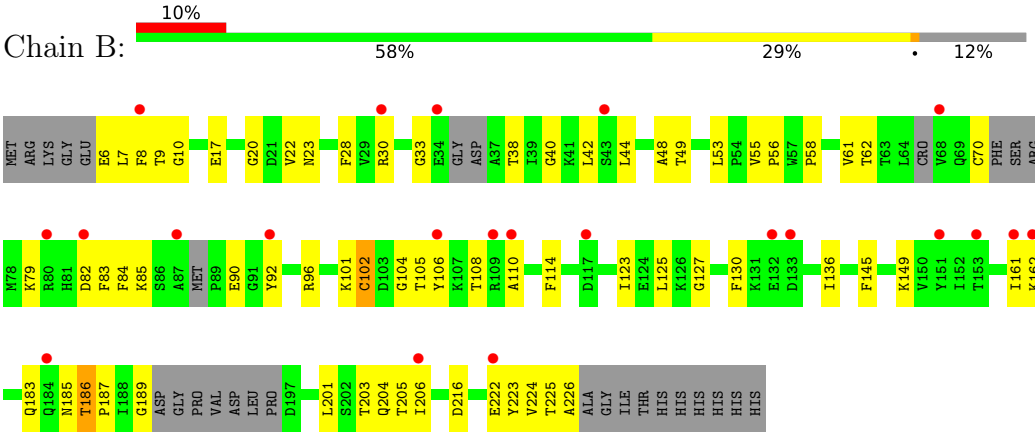
• Molecule 1: fluorescent protein D102C

Chain A:



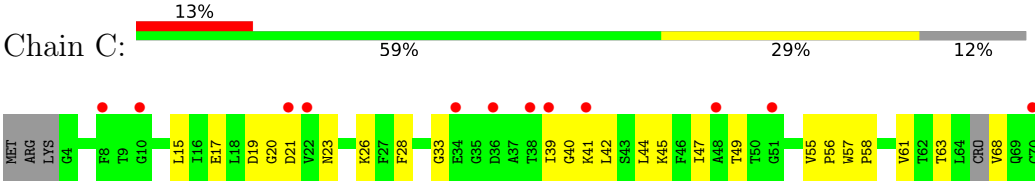
• Molecule 1: fluorescent protein D102C

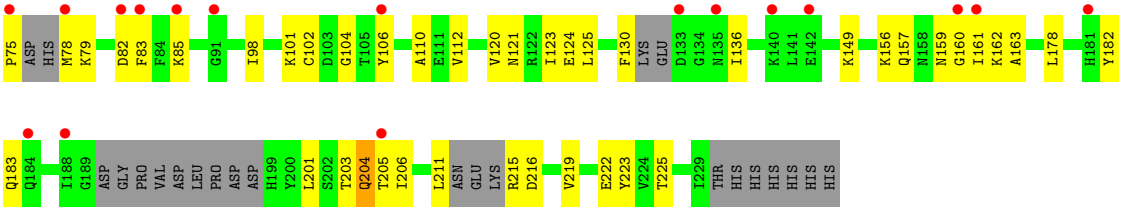
Chain B:



• Molecule 1: fluorescent protein D102C

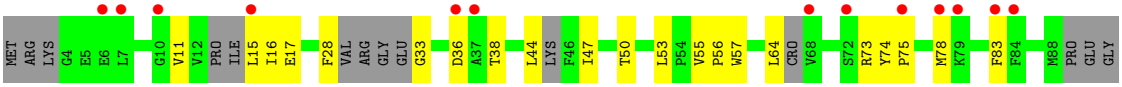
Chain C:

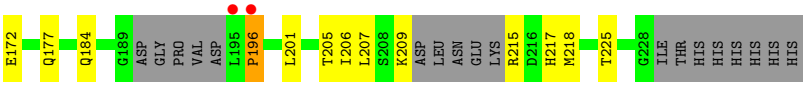




• Molecule 1: fluorescent protein D102C

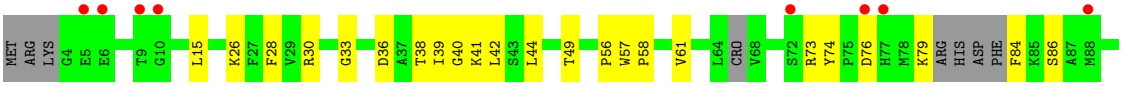
Chain D:

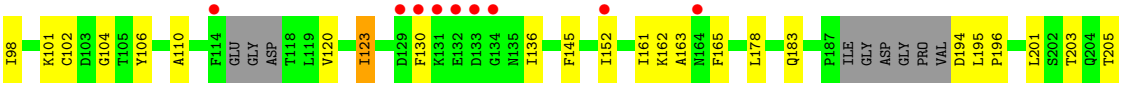




• Molecule 1: fluorescent protein D102C

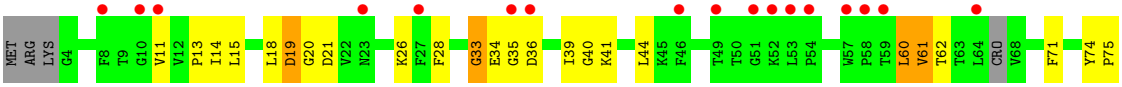
Chain E:

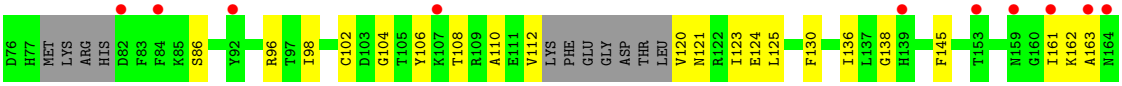


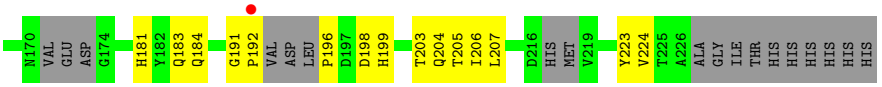


• Molecule 1: fluorescent protein D102C

Chain F:

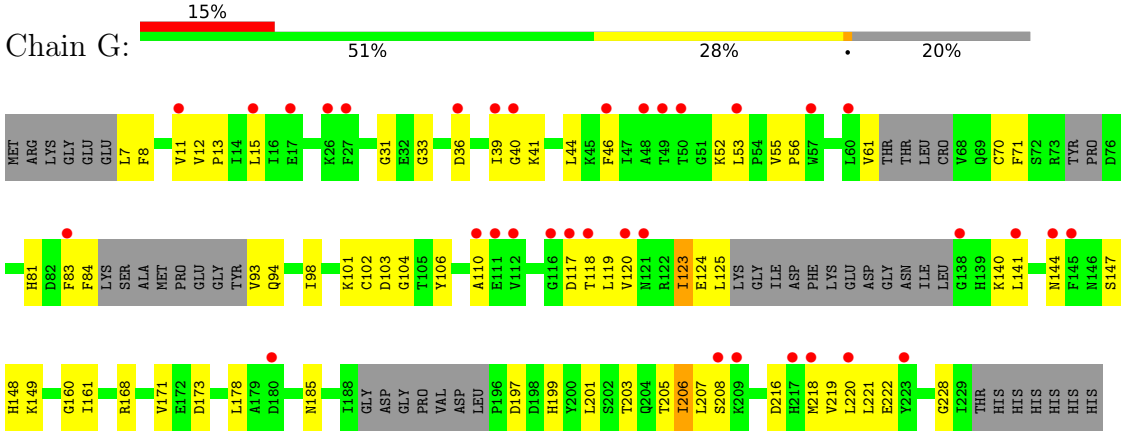






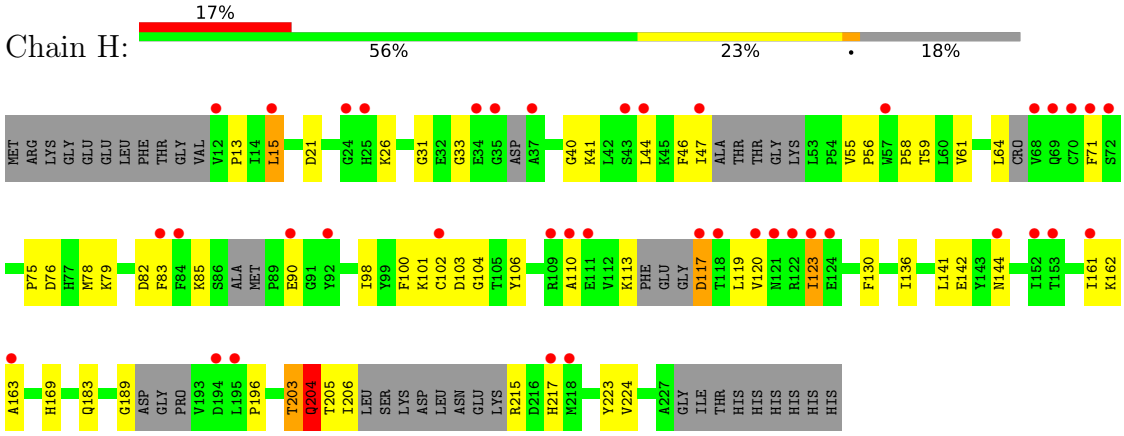
• Molecule 1: fluorescent protein D102C

Chain G:



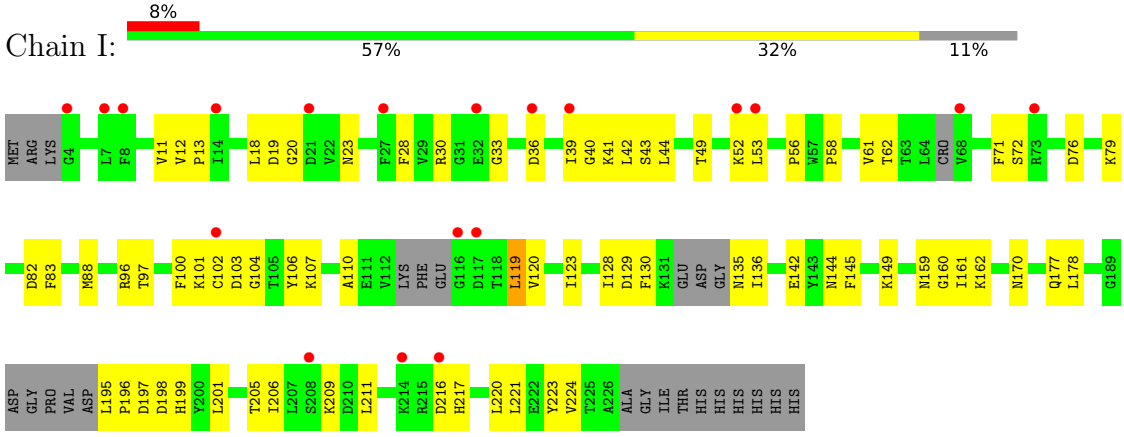
• Molecule 1: fluorescent protein D102C

Chain H:



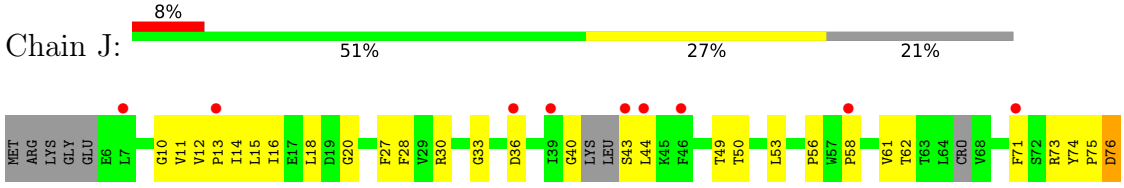
• Molecule 1: fluorescent protein D102C

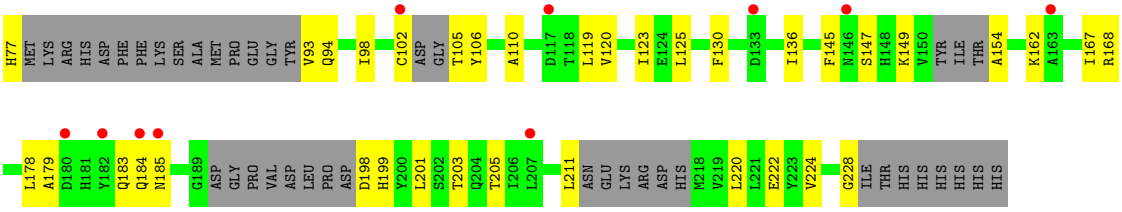
Chain I:



• Molecule 1: fluorescent protein D102C

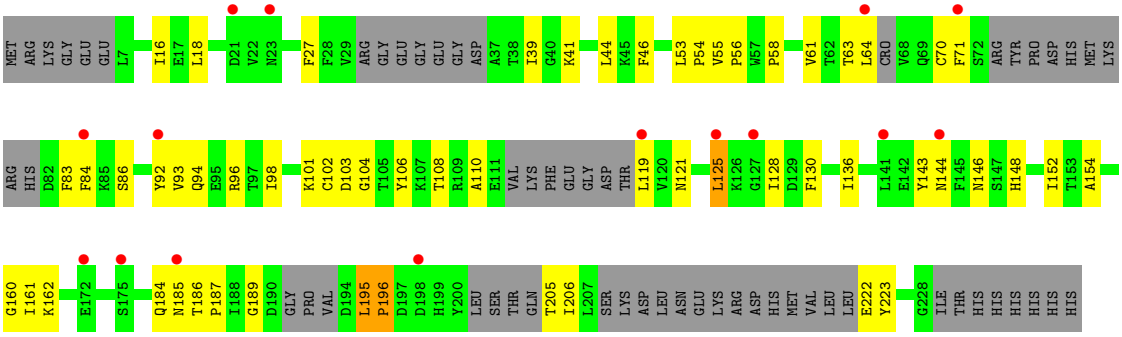
Chain J:





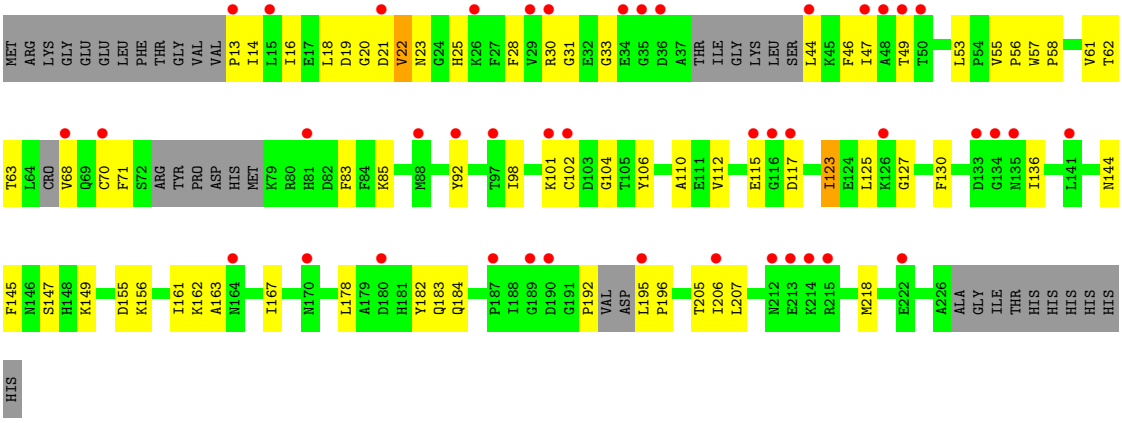
• Molecule 1: fluorescent protein D102C

Chain K:



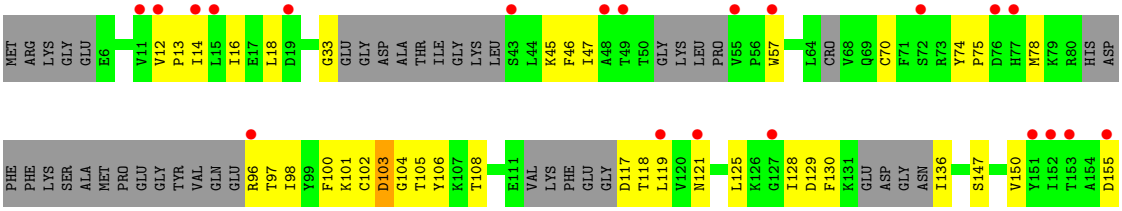
• Molecule 1: fluorescent protein D102C

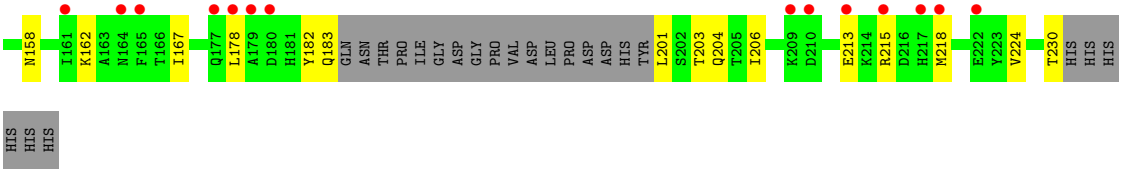
Chain L:



• Molecule 1: fluorescent protein D102C

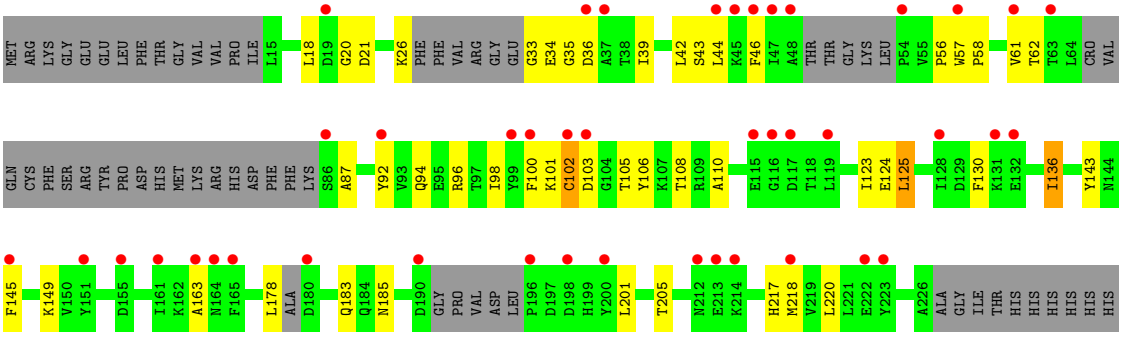
Chain M:





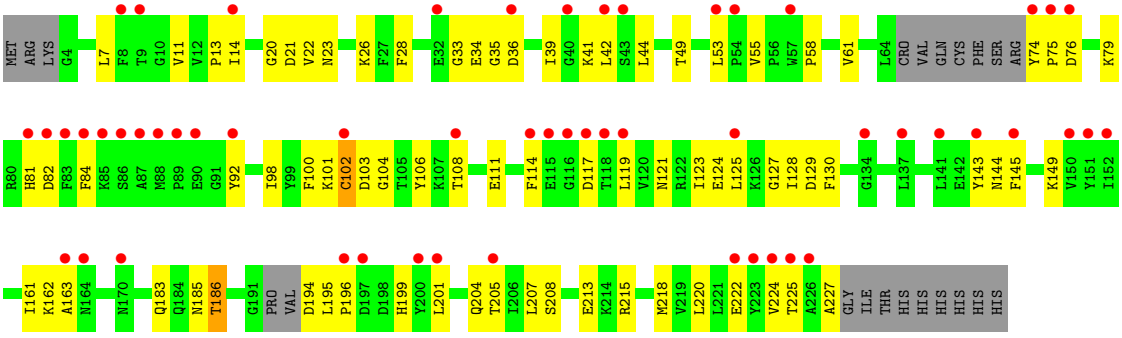
• Molecule 1: fluorescent protein D102C

Chain N:



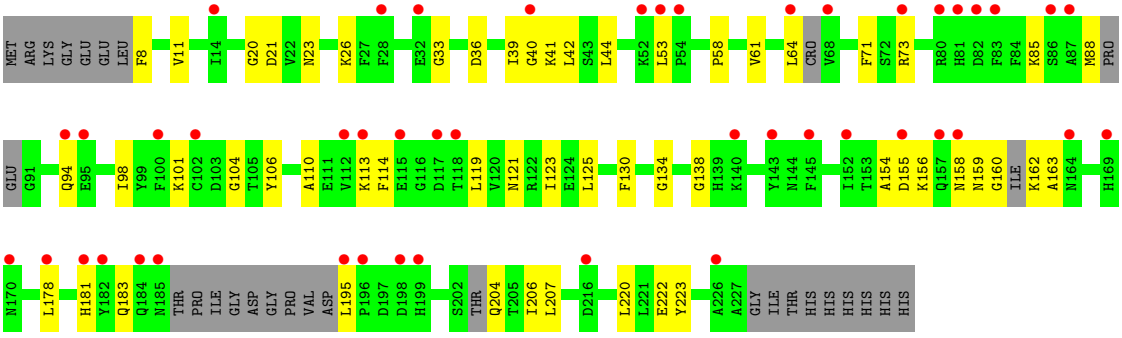
• Molecule 1: fluorescent protein D102C

Chain O:



• Molecule 1: fluorescent protein D102C

Chain P:



4 Data and refinement statistics (i)

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) 86.7 (89.88-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1555)	Depositor
R, R_{free}	0.307 , 0.357 0.326 , 0.343	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 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.38	0/1758	0.82	3/2375 (0.1%)
1	B	0.34	0/1681	0.77	1/2265 (0.0%)
1	C	0.33	0/1675	0.80	1/2258 (0.0%)
1	D	0.38	0/1579	0.89	3/2121 (0.1%)
1	E	0.33	0/1694	0.78	4/2287 (0.2%)
1	F	0.36	0/1631	0.81	2/2199 (0.1%)
1	G	0.35	0/1524	0.82	0/2053
1	H	0.34	0/1567	0.82	4/2112 (0.2%)
1	I	0.35	0/1705	0.84	4/2302 (0.2%)
1	J	0.35	0/1483	0.82	0/1998
1	K	0.41	0/1417	0.81	2/1912 (0.1%)
1	L	0.33	0/1605	0.76	1/2164 (0.0%)
1	M	0.31	0/1373	0.84	0/1847
1	N	0.33	0/1410	0.86	3/1899 (0.2%)
1	O	0.40	0/1712	0.81	1/2314 (0.0%)
1	P	0.33	0/1663	0.79	1/2239 (0.0%)
All	All	0.35	0/25477	0.81	30/34345 (0.1%)

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

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	15	LEU	CA-CB-CG	7.89	133.45	115.30
1	D	125	LEU	CA-CB-CG	7.63	132.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	220	LEU	CA-CB-CG	7.57	132.72	115.30
1	A	203	THR	N-CA-C	7.12	130.21	111.00
1	H	203	THR	N-CA-C	6.86	129.52	111.00
1	K	195	LEU	C-N-CD	-6.75	105.75	120.60
1	N	136	ILE	CG1-CB-CG2	-6.53	97.05	111.40
1	E	26	LYS	N-CA-C	6.47	128.46	111.00
1	N	125	LEU	CA-CB-CG	6.41	130.04	115.30
1	F	33	GLY	N-CA-C	-6.06	97.95	113.10
1	I	195	LEU	C-N-CD	-5.87	107.69	120.60
1	I	20	GLY	N-CA-C	5.83	127.66	113.10
1	L	18	LEU	CA-CB-CG	5.79	128.61	115.30
1	P	162	LYS	N-CA-CB	-5.73	100.29	110.60
1	E	220	LEU	CA-CB-CG	5.66	128.32	115.30
1	H	117	ASP	CB-CA-C	-5.51	99.38	110.40
1	A	69	GLN	O-C-N	5.50	131.51	122.70
1	H	204	GLN	N-CA-C	5.50	125.85	111.00
1	I	120	VAL	CB-CA-C	-5.29	101.34	111.40
1	C	211	LEU	N-CA-C	5.29	125.28	111.00
1	E	195	LEU	C-N-CD	-5.27	109.01	120.60
1	K	125	LEU	CA-CB-CG	5.26	127.40	115.30
1	D	142	GLU	N-CA-C	5.22	125.10	111.00
1	I	82	ASP	CB-CA-C	5.21	120.83	110.40
1	O	194	ASP	N-CA-C	-5.17	97.03	111.00
1	D	133	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	102	CYS	CA-CB-SG	5.17	123.30	114.00
1	A	132	GLU	N-CA-C	-5.14	97.12	111.00
1	F	60	LEU	N-CA-C	-5.10	97.24	111.00
1	E	165	PHE	N-CA-C	-5.00	97.49	111.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1721	0	1680	100	0
1	B	1649	0	1615	84	0
1	C	1643	0	1611	59	1
1	D	1552	0	1511	61	1
1	E	1661	0	1623	38	0
1	F	1600	0	1557	47	1
1	G	1497	0	1460	86	0
1	H	1537	0	1487	56	0
1	I	1671	0	1633	95	0
1	J	1459	0	1431	58	1
1	K	1391	0	1359	51	0
1	L	1573	0	1532	60	0
1	M	1352	0	1339	46	0
1	N	1387	0	1351	40	0
1	O	1677	0	1616	102	0
1	P	1632	0	1586	42	0
All	All	25002	0	24391	986	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 20.

All (986) 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: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
1:B:9:THR:HG23	1:B:10:GLY:H	1.02	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O:74:TYR:CE2	1:O:82:ASP:CG	2.34	0.99
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: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: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:I:135:ASN:C	1:I:136:ILE:HD12	1.87	0.94
1:G:207:LEU:HD13	1:G:218:MET:CE	1.99	0.93
1:N:33:GLY:HA3	1:N:44:LEU:HD23	1.48	0.93
1:H:203:THR:HG22	1:H:224:VAL:CG2	1.99	0.92
1:P:88:MET:HE1	1:P:113:LYS:HA	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:28:PHE:HD2	1:A:49:THR:HG1	1.12	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: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:M:128:ILE:HG22	1:M:129:ASP:CG	1.94	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:O:74:TYR:HE2	1:O:82:ASP:CG	1.78	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: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:P:88:MET:CE	1:P:113:LYS:HA	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:G:207:LEU:HD13	1:G:218:MET:HE2	1.60	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
1:G:44:LEU:O	1:G:219:VAL:CG1	2.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O:104:GLY:C	1:O:130:PHE:CE1	2.55	0.80
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: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: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: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
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:L:33:GLY:HA3	1:L:44:LEU:HD23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:74:TYR:CD2	1:O:82:ASP:CG	2.61	0.73
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:B:185:ASN:O	1:B:186:THR:HB	1.88	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: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:D:128:ILE:HD12	1:D:129:ASP:CG	2.11	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:O:185:ASN:C	1:O:186:THR:HG22	2.04	0.70
1:K:70:CYS:SG	1:K:84:PHE:HB3	2.31	0.70
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:152:ILE:C	1:A:153:THR:HG22	2.11	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LEU:CG	1:G:8:PHE:N	2.31	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:J:222:GLU:OE2	1:J:224:VAL:CG2	2.46	0.64
1:O:104:GLY:CA	1:O:130:PHE:CE1	2.79	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: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:I:135:ASN:C	1:I:136:ILE:CD1	2.65	0.64
1:J:183:GLN:NE2	1:J:185:ASN:HD21	1.95	0.64
1:G:205:THR:CG2	1:G:220:LEU:CD2	2.76	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:PHE:N	1:D:50:THR:OG1	2.26	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: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: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:B:8:PHE:C	1:B:9:THR:HG22	2.22	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
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:8:PHE:O	1:B:9:THR:C	2.39	0.59
1:M:117:ASP:CG	1:M:118:THR:H	2.05	0.59
1:B:185:ASN:O	1:B:186:THR:CB	2.50	0.59
1:C:203:THR:C	1:C:204:GLN:HG3	2.21	0.59
1:K:104:GLY:HA3	1:K:130:PHE:CD1	2.38	0.59
1:A:68:VAL:C	1:A:70:CYS:H	2.04	0.59
1:G:147:SER:CB	1:O:144:ASN:HD22	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:207:LEU:HD13	1:G:218:MET:HE3	1.84	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:68:VAL:C	1:A:70:CYS:N	2.56	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:I:88:MET:CE	1:I:119:LEU:HD12	2.34	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
1:H:104:GLY:HA3	1:H:130:PHE:CD1	2.39	0.57
1:N:100:PHE:O	1:N:101:LYS:C	2.38	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:28:PHE:HD2	1:O:49:THR:HG1	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLY:HA3	1:A:44:LEU:HD23	1.87	0.57
1:A:119:LEU:C	1:A:120:VAL:HG23	2.25	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: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:L:57:TRP:HB3	1:L:218:MET:HE1	1.86	0.56
1:M:14:ILE:H	1:M:33:GLY:C	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:O:224:VAL:HG12	1:O:225:THR:N	2.22	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
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: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: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:C:47:ILE:HD13	1:C:215:ARG:CZ	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:THR:O	1:D:73:ARG:HD3	2.08	0.53
1:P:88:MET:CE	1:P:113:LYS:CA	2.85	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: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:A:207:LEU:HD13	1:A:218:MET:HE2	1.89	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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:88:MET:HE2	1:I:119:LEU:HD12	1.89	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:57:TRP:HE1	1:C:216:ASP:CG	2.14	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: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:M:147:SER:OG	1:M:203:THR:O	2.21	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: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
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:36:ASP:CG	1:E:39:ILE:HG22	2.32	0.50
1:E:73:ARG:HE	1:E:225:THR:HG22	1.77	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:J:162:LYS:HE2	1:J:184:GLN:CD	2.30	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:B:8:PHE:C	1:B:9:THR:CG2	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:O	1:C:216:ASP:C	2.49	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
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: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:L:57:TRP:HB3	1:L:218:MET:CE	2.43	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: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:G:103:ASP:CG	1:G:104:GLY:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:15:LEU:O	1:A:120:VAL:C	2.52	0.48
1:I:41:LYS:C	1:I:42:LEU:HG	2.34	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:L:21:ASP:O	1:L:25:HIS:O	2.32	0.48
1:A:68:VAL:O	1:A:70:CYS:N	2.46	0.47
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
1:J:33:GLY:CA	1:J:44:LEU:HD23	2.42	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:M:100:PHE:O	1:M:101:LYS:C	2.51	0.47
1:N:100:PHE:O	1:N:102:CYS:N	2.47	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: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:P:101:LYS:HD2	1:P:178:LEU:HD12	1.96	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

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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	0.47
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:D:209:LYS:HE3	1:D:218:MET:HE1	1.97	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:207:LEU:HB3	1:O:218:MET:SD	2.55	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
1:L:16:ILE:HG21	1:L:46:PHE:HE1	1.81	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:15:LEU:C	1:A:120:VAL:HA	2.37	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
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:H:100:PHE:O	1:H:101:LYS:C	2.50	0.45
1:M:96:ARG:NE	1:M:183:GLN:OE1	2.46	0.45
1:F:161:ILE:CG2	1:F:162:LYS:N	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TYR:O	1:A:92:TYR:CD1	2.70	0.45
1:B:161:ILE:CG2	1:B:162:LYS:N	2.80	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: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
1:C:205:THR:CG2	1:C:222:GLU:OE1	2.65	0.44
1:I:88:MET:CE	1:I:119:LEU:CD1	2.95	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: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:O:220:LEU:HD21	1:O:222:GLU:CD	2.37	0.44
1:I:53:LEU:HD23	1:I:53:LEU:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:ILE:HD12	1:J:44:LEU:HD13	1.98	0.44
1:E:15:LEU:HB2	1:E:120:VAL:HG22	1.99	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:F:136:ILE:C	1:F:138:GLY:H	2.21	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
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: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: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:G:220:LEU:O	1:G:221:LEU:C	2.57	0.43
1:H:56:PRO:HD3	1:H:136:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:GLY:O	1:L:21:ASP:OD1	2.36	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
1:P:21:ASP:OD1	1:P:26:LYS:HG2	2.19	0.43
1:P:88:MET:HE1	1:P:113:LYS:CA	2.35	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:H:161:ILE:CG2	1:H:162:LYS:N	2.82	0.42
1:I:18:LEU:HD23	1:I:19:ASP:C	2.39	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:B:224:VAL:O	1:B:225:THR:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:CYS:HG	1:K:92:TYR:HE2	1.67	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:O:127:GLY:C	1:O:130:PHE:HE2	2.23	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
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: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:O:121:ASN:CG	1:O:123:ILE:HD11	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:57:TRP:HB3	1:M:218:MET:HE1	2.02	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
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:O:114:PHE:CE1	1:O:119:LEU:HD12	2.55	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:D:162:LYS:HZ3	1:D:184:GLN:CB	2.33	0.41
1:E:58:PRO:HA	1:E:61:VAL:HG23	2.01	0.41
1:F:18:LEU:HD23	1:F:19:ASP:C	2.39	0.41
1:G:83:PHE:CB	1:G:161:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:36:ASP:HB2	1:P:41:LYS:HB2	2.03	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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%)	29	66
1	B	193/234 (82%)	184 (95%)	8 (4%)	1 (0%)	29	66
1	C	195/234 (83%)	188 (96%)	6 (3%)	1 (0%)	29	66
1	D	174/234 (74%)	161 (92%)	12 (7%)	1 (1%)	25	63
1	E	198/234 (85%)	191 (96%)	6 (3%)	1 (0%)	29	66
1	F	187/234 (80%)	180 (96%)	6 (3%)	1 (0%)	29	66
1	G	176/234 (75%)	167 (95%)	8 (4%)	1 (1%)	25	63
1	H	175/234 (75%)	169 (97%)	6 (3%)	0	100	100
1	I	199/234 (85%)	192 (96%)	6 (3%)	1 (0%)	29	66
1	J	168/234 (72%)	163 (97%)	5 (3%)	0	100	100
1	K	159/234 (68%)	154 (97%)	4 (2%)	1 (1%)	25	63
1	L	187/234 (80%)	181 (97%)	5 (3%)	1 (0%)	29	66
1	M	152/234 (65%)	149 (98%)	2 (1%)	1 (1%)	22	60
1	N	162/234 (69%)	159 (98%)	3 (2%)	0	100	100
1	O	207/234 (88%)	198 (96%)	7 (3%)	2 (1%)	15	52
1	P	192/234 (82%)	186 (97%)	6 (3%)	0	100	100
All	All	2931/3744 (78%)	2817 (96%)	101 (3%)	13 (0%)	34	70

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/204 (93%)	188 (100%)	1 (0%)	88	95
1	B	181/204 (89%)	180 (99%)	1 (1%)	86	94
1	C	178/204 (87%)	177 (99%)	1 (1%)	86	94
1	D	170/204 (83%)	170 (100%)	0	100	100
1	E	182/204 (89%)	181 (100%)	1 (0%)	88	95
1	F	175/204 (86%)	174 (99%)	1 (1%)	86	94
1	G	163/204 (80%)	162 (99%)	1 (1%)	86	94
1	H	168/204 (82%)	166 (99%)	2 (1%)	71	87
1	I	183/204 (90%)	181 (99%)	2 (1%)	73	88
1	J	160/204 (78%)	159 (99%)	1 (1%)	86	94
1	K	152/204 (74%)	151 (99%)	1 (1%)	84	93
1	L	171/204 (84%)	170 (99%)	1 (1%)	86	94
1	M	149/204 (73%)	148 (99%)	1 (1%)	84	93
1	N	153/204 (75%)	152 (99%)	1 (1%)	84	93
1	O	179/204 (88%)	178 (99%)	1 (1%)	86	94
1	P	177/204 (87%)	177 (100%)	0	100	100
All	All	2730/3264 (84%)	2714 (99%)	16 (1%)	86	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	B	108	THR
1	C	159	ASN
1	E	123	ILE
1	F	19	ASP
1	G	123	ILE
1	H	123	ILE
1	H	204	GLN

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Mol	Chain	Res	Type
1	I	119	LEU
1	I	159	ASN
1	J	76	ASP
1	K	128	ILE
1	L	123	ILE
1	M	121	ASN
1	N	102	CYS
1	O	102	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	B	94	GLN
1	B	185	ASN
1	C	204	GLN
1	D	121	ASN
1	F	94	GLN
1	H	94	GLN
1	I	135	ASN
1	J	183	GLN
1	K	144	ASN
1	L	23	ASN
1	L	69	GLN
1	L	94	GLN
1	L	184	GLN
1	N	164	ASN
1	O	139	HIS
1	P	94	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.97	30 (13%) 2 4	50, 80, 148, 324	0
1	B	205/234 (87%)	0.74	24 (11%) 4 6	51, 87, 175, 274	0
1	C	207/234 (88%)	0.89	31 (14%) 2 3	55, 91, 164, 338	0
1	D	194/234 (82%)	0.58	18 (9%) 8 10	57, 92, 169, 237	0
1	E	208/234 (88%)	0.67	20 (9%) 8 10	64, 96, 157, 204	0
1	F	201/234 (85%)	0.89	28 (13%) 2 4	69, 106, 174, 357	0
1	G	188/234 (80%)	0.93	35 (18%) 1 2	52, 103, 181, 284	0
1	H	191/234 (81%)	1.08	40 (20%) 1 1	69, 102, 172, 382	0
1	I	209/234 (89%)	0.64	19 (9%) 9 11	64, 98, 165, 249	0
1	J	184/234 (78%)	0.60	19 (10%) 6 8	51, 95, 166, 270	0
1	K	175/234 (74%)	0.64	15 (8%) 10 12	73, 102, 181, 323	0
1	L	197/234 (84%)	1.14	43 (21%) 0 1	67, 114, 206, 293	0
1	M	168/234 (71%)	1.25	35 (20%) 1 1	75, 119, 203, 375	0
1	N	174/234 (74%)	1.22	43 (24%) 0 0	72, 130, 219, 388	0
1	O	213/234 (91%)	1.47	55 (25%) 0 0	54, 126, 205, 302	0
1	P	204/234 (87%)	1.20	46 (22%) 0 0	73, 134, 217, 464	0
All	All	3133/3744 (83%)	0.93	501 (15%) 1 2	50, 104, 188, 464	0

All (501) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	164	ASN	11.3
1	M	164	ASN	9.7
1	O	86	SER	9.2
1	M	76	ASP	8.9
1	O	223	TYR	8.6

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Mol	Chain	Res	Type	RSRZ
1	L	49	THR	7.9
1	H	194	ASP	7.7
1	G	49	THR	7.6
1	O	118	THR	7.5
1	M	152	ILE	7.2
1	N	117	ASP	7.2
1	B	117	ASP	6.8
1	O	224	VAL	6.7
1	P	185	ASN	6.6
1	E	133	ASP	6.6
1	O	222	GLU	6.6
1	O	76	ASP	6.6
1	P	117	ASP	6.2
1	O	196	PRO	6.2
1	H	121	ASN	6.1
1	L	180	ASP	6.1
1	O	8	PHE	6.0
1	H	144	ASN	5.9
1	J	117	ASP	5.9
1	M	153	THR	5.8
1	P	182	TYR	5.8
1	O	85	LYS	5.8
1	L	213	GLU	5.6
1	F	139	HIS	5.6
1	H	110	ALA	5.5
1	D	36	ASP	5.5
1	N	116	GLY	5.4
1	O	87	ALA	5.4
1	O	225	THR	5.4
1	H	122	ARG	5.3
1	P	158	ASN	5.3
1	N	218	MET	5.3
1	C	34	GLU	5.3
1	M	72	SER	5.3
1	K	71	PHE	5.3
1	A	49	THR	5.2
1	I	32	GLU	5.2
1	N	214	LYS	5.2
1	M	12	VAL	5.1
1	L	115	GLU	5.1
1	M	151	TYR	5.1
1	A	133	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	N	213	GLU	5.0
1	O	114	PHE	4.9
1	O	117	ASP	4.9
1	L	212	ASN	4.9
1	D	196	PRO	4.9
1	L	133	ASP	4.8
1	L	117	ASP	4.8
1	P	184	GLN	4.8
1	O	53	LEU	4.8
1	F	49	THR	4.7
1	D	72	SER	4.7
1	P	86	SER	4.6
1	M	48	ALA	4.6
1	B	153	THR	4.6
1	O	197	ASP	4.6
1	O	151	TYR	4.6
1	F	10	GLY	4.4
1	O	150	VAL	4.4
1	L	134	GLY	4.4
1	C	38	THR	4.3
1	C	41	LYS	4.3
1	H	117	ASP	4.3
1	G	217	HIS	4.3
1	G	50	THR	4.3
1	A	112	VAL	4.3
1	M	11	VAL	4.3
1	B	106	TYR	4.3
1	O	75	PRO	4.3
1	O	81	HIS	4.3
1	A	70	CYS	4.2
1	C	51	GLY	4.2
1	L	141	LEU	4.2
1	I	116	GLY	4.2
1	E	6	GLU	4.2
1	F	58	PRO	4.2
1	H	34	GLU	4.2
1	C	188	ILE	4.2
1	G	118	THR	4.1
1	H	195	LEU	4.1
1	L	44	LEU	4.1
1	G	223	TYR	4.1
1	G	57	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	P	82	ASP	4.1
1	O	125	LEU	4.1
1	O	200	TYR	4.1
1	P	216	ASP	4.0
1	J	36	ASP	4.0
1	H	92	TYR	4.0
1	P	157	GLN	4.0
1	A	136	ILE	4.0
1	N	115	GLU	4.0
1	F	51	GLY	4.0
1	K	185	ASN	4.0
1	B	82	ASP	4.0
1	M	178	LEU	4.0
1	G	117	ASP	3.9
1	P	112	VAL	3.9
1	P	181	HIS	3.9
1	O	115	GLU	3.9
1	A	82	ASP	3.9
1	L	190	ASP	3.9
1	F	53	LEU	3.9
1	G	218	MET	3.9
1	P	53	LEU	3.8
1	L	34	GLU	3.8
1	L	26	LYS	3.7
1	B	30	ARG	3.7
1	L	187	PRO	3.7
1	O	74	TYR	3.7
1	H	57	TRP	3.7
1	N	196	PRO	3.7
1	C	21	ASP	3.7
1	I	117	ASP	3.7
1	B	80	ARG	3.7
1	I	4	GLY	3.6
1	A	198	ASP	3.6
1	O	143	TYR	3.6
1	N	86	SER	3.6
1	P	68	VAL	3.6
1	M	217	HIS	3.6
1	I	7	LEU	3.6
1	G	110	ALA	3.6
1	L	47	ILE	3.6
1	F	54	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	O	201	LEU	3.6
1	C	10	GLY	3.6
1	N	131	LYS	3.5
1	B	110	ALA	3.5
1	A	139	HIS	3.5
1	E	76	ASP	3.5
1	O	90	GLU	3.5
1	B	34	GLU	3.5
1	A	30	ARG	3.5
1	H	109	ARG	3.5
1	P	32	GLU	3.5
1	A	186	THR	3.4
1	J	102	CYS	3.4
1	I	52	LYS	3.4
1	P	140	LYS	3.4
1	B	43	SER	3.4
1	H	70	CYS	3.4
1	M	77	HIS	3.4
1	F	23	ASN	3.4
1	A	68	VAL	3.4
1	G	208	SER	3.4
1	M	179	ALA	3.4
1	O	83	PHE	3.4
1	G	111	GLU	3.4
1	P	152	ILE	3.4
1	P	169	HIS	3.4
1	E	227	ALA	3.3
1	L	195	LEU	3.3
1	H	35	GLY	3.3
1	J	180	ASP	3.3
1	P	52	LYS	3.3
1	C	73	ARG	3.3
1	D	7	LEU	3.3
1	H	15	LEU	3.3
1	N	163	ALA	3.3
1	E	134	GLY	3.3
1	A	83	PHE	3.3
1	I	8	PHE	3.3
1	L	21	ASP	3.3
1	F	192	PRO	3.3
1	O	9	THR	3.3
1	G	48	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	84	PHE	3.3
1	P	196	PRO	3.3
1	O	141	LEU	3.3
1	O	170	ASN	3.2
1	F	35	GLY	3.2
1	G	141	LEU	3.2
1	O	88	MET	3.2
1	G	40	GLY	3.2
1	M	155	ASP	3.2
1	B	109	ARG	3.2
1	G	83	PHE	3.2
1	L	222	GLU	3.2
1	E	5	GLU	3.2
1	E	222	GLU	3.2
1	K	92	TYR	3.2
1	K	64	LEU	3.2
1	J	146	ASN	3.2
1	N	103	ASP	3.2
1	O	134	GLY	3.1
1	C	8	PHE	3.1
1	K	119	LEU	3.1
1	D	83	PHE	3.1
1	F	153	THR	3.1
1	H	218	MET	3.1
1	P	81	HIS	3.1
1	O	116	GLY	3.1
1	H	90	GLU	3.1
1	P	95	GLU	3.1
1	H	37	ALA	3.1
1	N	45	LYS	3.1
1	N	119	LEU	3.1
1	F	82	ASP	3.0
1	F	84	PHE	3.0
1	H	161	ILE	3.0
1	L	126	LYS	3.0
1	P	198	ASP	3.0
1	H	120	VAL	3.0
1	H	124	GLU	3.0
1	L	36	ASP	3.0
1	F	46	PHE	3.0
1	I	53	LEU	3.0
1	H	43	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	77	HIS	3.0
1	C	70	CYS	3.0
1	C	160	GLY	3.0
1	I	102	CYS	3.0
1	H	44	LEU	3.0
1	O	89	PRO	3.0
1	C	161	ILE	3.0
1	C	82	ASP	2.9
1	D	116	GLY	2.9
1	M	57	TRP	2.9
1	L	116	GLY	2.9
1	N	36	ASP	2.9
1	P	155	ASP	2.9
1	N	57	TRP	2.9
1	J	133	ASP	2.9
1	F	92	TYR	2.9
1	M	49	THR	2.9
1	B	164	ASN	2.9
1	H	111	GLU	2.9
1	A	110	ALA	2.9
1	I	36	ASP	2.9
1	C	75	PRO	2.9
1	O	54	PRO	2.9
1	A	212	ASN	2.9
1	H	68	VAL	2.8
1	M	218	MET	2.8
1	L	70	CYS	2.8
1	E	131	LYS	2.8
1	O	108	THR	2.8
1	G	26	LYS	2.8
1	P	14	ILE	2.8
1	M	180	ASP	2.8
1	A	48	ALA	2.8
1	O	57	TRP	2.8
1	M	14	ILE	2.8
1	L	102	CYS	2.8
1	L	214	LYS	2.8
1	O	42	LEU	2.8
1	O	92	TYR	2.8
1	G	11	VAL	2.8
1	G	121	ASN	2.8
1	D	195	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	94	GLN	2.8
1	N	161	ILE	2.8
1	H	118	THR	2.8
1	B	151	TYR	2.8
1	P	164	ASN	2.8
1	H	24	GLY	2.8
1	F	57	TRP	2.8
1	O	137	LEU	2.8
1	G	209	LYS	2.8
1	N	223	TYR	2.8
1	M	161	ILE	2.7
1	A	23	ASN	2.7
1	A	93	VAL	2.7
1	N	145	PHE	2.7
1	M	121	ASN	2.7
1	O	14	ILE	2.7
1	O	40	GLY	2.7
1	J	182	TYR	2.7
1	B	161	ILE	2.7
1	F	36	ASP	2.7
1	G	60	LEU	2.7
1	L	68	VAL	2.7
1	L	170	ASN	2.7
1	P	100	PHE	2.7
1	P	143	TYR	2.7
1	C	72	SER	2.7
1	M	177	GLN	2.7
1	H	217	HIS	2.7
1	P	54	PRO	2.7
1	J	185	ASN	2.7
1	P	170	ASN	2.7
1	F	11	VAL	2.7
1	G	112	VAL	2.7
1	L	88	MET	2.7
1	A	188	ILE	2.7
1	N	48	ALA	2.7
1	P	64	LEU	2.7
1	D	78	MET	2.7
1	H	12	VAL	2.7
1	I	68	VAL	2.7
1	I	21	ASP	2.7
1	O	119	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	N	92	TYR	2.7
1	E	129	ASP	2.7
1	D	10	GLY	2.7
1	G	17	GLU	2.7
1	F	64	LEU	2.6
1	H	153	THR	2.6
1	A	226	ALA	2.6
1	L	30	ARG	2.6
1	N	180	ASP	2.6
1	C	91	GLY	2.6
1	O	32	GLU	2.6
1	E	130	PHE	2.6
1	J	184	GLN	2.6
1	L	215	ARG	2.6
1	G	220	LEU	2.6
1	I	39	ILE	2.6
1	L	35	GLY	2.6
1	C	85	LYS	2.6
1	N	200	TYR	2.6
1	N	44	LEU	2.6
1	J	71	PHE	2.6
1	B	162	LYS	2.6
1	O	163	ALA	2.6
1	A	135	ASN	2.6
1	E	10	GLY	2.6
1	G	120	VAL	2.6
1	P	113	LYS	2.6
1	H	163	ALA	2.6
1	L	48	ALA	2.6
1	M	210	ASP	2.6
1	E	88	MET	2.6
1	J	7	LEU	2.6
1	C	78	MET	2.5
1	E	132	GLU	2.5
1	H	71	PHE	2.5
1	N	46	PHE	2.5
1	K	21	ASP	2.5
1	I	214	LYS	2.5
1	N	128	ILE	2.5
1	D	115	GLU	2.5
1	M	213	GLU	2.5
1	G	145	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	222	GLU	2.5
1	L	206	ILE	2.5
1	D	152	ILE	2.5
1	E	164	ASN	2.5
1	G	180	ASP	2.5
1	F	161	ILE	2.5
1	P	102	CYS	2.5
1	C	22	VAL	2.5
1	L	101	LYS	2.5
1	H	102	CYS	2.4
1	L	135	ASN	2.4
1	J	13	PRO	2.4
1	O	102	CYS	2.4
1	G	27	PHE	2.4
1	B	206	ILE	2.4
1	N	102	CYS	2.4
1	J	44	LEU	2.4
1	H	83	PHE	2.4
1	L	189	GLY	2.4
1	N	19	ASP	2.4
1	A	94	GLN	2.4
1	F	27	PHE	2.4
1	C	48	ALA	2.4
1	G	138	GLY	2.4
1	L	15	LEU	2.4
1	F	164	ASN	2.4
1	B	8	PHE	2.4
1	B	222	GLU	2.4
1	B	87	ALA	2.4
1	C	39	ILE	2.4
1	D	15	LEU	2.4
1	K	172	GLU	2.3
1	H	152	ILE	2.3
1	F	159	ASN	2.3
1	L	81	HIS	2.3
1	P	80	ARG	2.3
1	B	133	ASP	2.3
1	P	83	PHE	2.3
1	N	47	ILE	2.3
1	O	152	ILE	2.3
1	E	114	PHE	2.3
1	E	213	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	152	ILE	2.3
1	B	68	VAL	2.3
1	M	215	ARG	2.3
1	K	127	GLY	2.3
1	A	57	TRP	2.3
1	C	140	LYS	2.3
1	D	79	LYS	2.3
1	O	145	PHE	2.3
1	C	142	GLU	2.3
1	H	123	ILE	2.3
1	A	120	VAL	2.3
1	F	163	ALA	2.3
1	I	14	ILE	2.3
1	L	92	TYR	2.3
1	C	133	ASP	2.3
1	E	9	THR	2.3
1	O	205	THR	2.3
1	P	73	ARG	2.3
1	P	178	LEU	2.3
1	N	151	TYR	2.3
1	O	43	SER	2.3
1	D	6	GLU	2.2
1	M	127	GLY	2.2
1	I	208	SER	2.2
1	G	15	LEU	2.2
1	P	195	LEU	2.2
1	L	50	THR	2.2
1	K	175	SER	2.2
1	M	119	LEU	2.2
1	C	135	ASN	2.2
1	G	144	ASN	2.2
1	N	190	ASP	2.2
1	N	212	ASN	2.2
1	L	13	PRO	2.2
1	A	119	LEU	2.2
1	H	84	PHE	2.2
1	I	216	ASP	2.2
1	O	82	ASP	2.2
1	N	63	THR	2.2
1	C	181	HIS	2.2
1	J	39	ILE	2.2
1	J	163	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	106	TYR	2.2
1	D	37	ALA	2.2
1	N	155	ASP	2.2
1	C	205	THR	2.2
1	G	116	GLY	2.2
1	H	72	SER	2.2
1	G	36	ASP	2.2
1	A	77	HIS	2.2
1	H	47	ILE	2.2
1	F	107	LYS	2.2
1	C	184	GLN	2.2
1	N	222	GLU	2.2
1	P	115	GLU	2.2
1	E	77	HIS	2.2
1	M	96	ARG	2.2
1	N	37	ALA	2.2
1	N	54	PRO	2.2
1	A	211	LEU	2.1
1	P	28	PHE	2.1
1	M	209	LYS	2.1
1	B	92	TYR	2.1
1	K	141	LEU	2.1
1	O	226	ALA	2.1
1	K	84	PHE	2.1
1	N	165	PHE	2.1
1	G	39	ILE	2.1
1	K	198	ASP	2.1
1	H	25	HIS	2.1
1	C	83	PHE	2.1
1	D	68	VAL	2.1
1	G	53	LEU	2.1
1	C	36	ASP	2.1
1	I	73	ARG	2.1
1	N	100	PHE	2.1
1	O	36	ASP	2.1
1	P	226	ALA	2.1
1	L	29	VAL	2.1
1	B	184	GLN	2.1
1	A	88	MET	2.1
1	J	207	LEU	2.1
1	G	46	PHE	2.1
1	N	99	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	132	GLU	2.1
1	N	61	VAL	2.1
1	P	199	HIS	2.1
1	H	69	GLN	2.1
1	L	164	ASN	2.1
1	P	145	PHE	2.1
1	N	198	ASP	2.1
1	F	8	PHE	2.1
1	A	200	TYR	2.1
1	J	58	PRO	2.1
1	M	19	ASP	2.1
1	D	84	PHE	2.1
1	M	165	PHE	2.1
1	D	75	PRO	2.1
1	P	40	GLY	2.1
1	K	23	ASN	2.1
1	P	87	ALA	2.1
1	K	125	LEU	2.1
1	O	164	ASN	2.0
1	E	72	SER	2.0
1	J	46	PHE	2.0
1	N	132	GLU	2.0
1	L	97	THR	2.0
1	A	172	GLU	2.0
1	J	43	SER	2.0
1	M	43	SER	2.0
1	F	52	LYS	2.0
1	P	118	THR	2.0
1	M	55	VAL	2.0
1	I	27	PHE	2.0
1	F	59	THR	2.0
1	K	144	ASN	2.0
1	A	12	VAL	2.0
1	M	15	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.