



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:44 AM UTC

PDB ID : 6S3U / pdb_00006s3u
Title : Adhesin P140 from Mycoplasma Genitalium
Authors : Fita, I.; Aparicio, D.
Deposited on : 2019-06-26
Resolution : 3.24 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

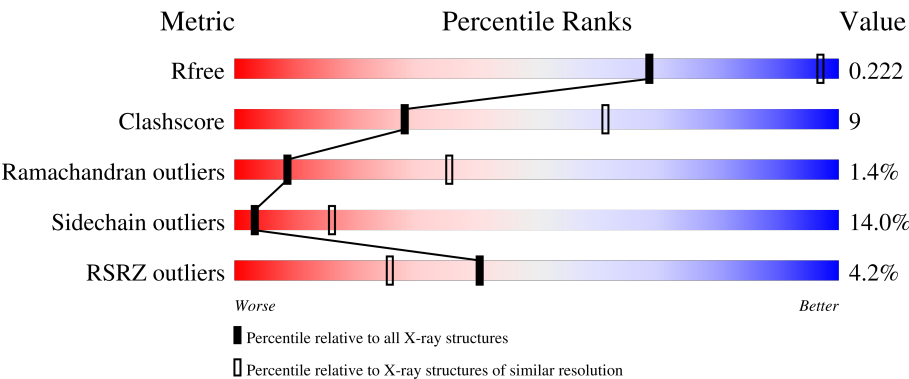
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	1304	% 66% 27% 5% . .
1	B	1304	2% 65% 27% 5% .
1	C	1304	% 66% 26% 5% .
1	D	1304	% 66% 27% 5% . .
1	E	1304	10% 67% 25% 5% .

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Mol	Chain	Length	Quality of chain
1	F	1304	9% 67% 25%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 59767 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 Adhesin P1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1278	Total	C	N	O	S	0	0	0
			10016	6351	1692	1960	13			
1	B	1275	Total	C	N	O	S	0	0	0
			9999	6340	1689	1957	13			
1	C	1274	Total	C	N	O	S	0	0	0
			9993	6339	1688	1953	13			
1	D	1271	Total	C	N	O	S	0	0	0
			9976	6328	1685	1950	13			
1	E	1262	Total	C	N	O	S	0	0	0
			9886	6272	1666	1935	13			
1	F	1262	Total	C	N	O	S	0	0	0
			9897	6281	1668	1935	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1352	HIS	-	expression tag	UNP P20796
A	1353	HIS	-	expression tag	UNP P20796
A	1354	HIS	-	expression tag	UNP P20796
A	1355	HIS	-	expression tag	UNP P20796
A	1356	HIS	-	expression tag	UNP P20796
A	1357	HIS	-	expression tag	UNP P20796
B	1352	HIS	-	expression tag	UNP P20796
B	1353	HIS	-	expression tag	UNP P20796
B	1354	HIS	-	expression tag	UNP P20796
B	1355	HIS	-	expression tag	UNP P20796
B	1356	HIS	-	expression tag	UNP P20796
B	1357	HIS	-	expression tag	UNP P20796
C	1352	HIS	-	expression tag	UNP P20796
C	1353	HIS	-	expression tag	UNP P20796
C	1354	HIS	-	expression tag	UNP P20796
C	1355	HIS	-	expression tag	UNP P20796
C	1356	HIS	-	expression tag	UNP P20796

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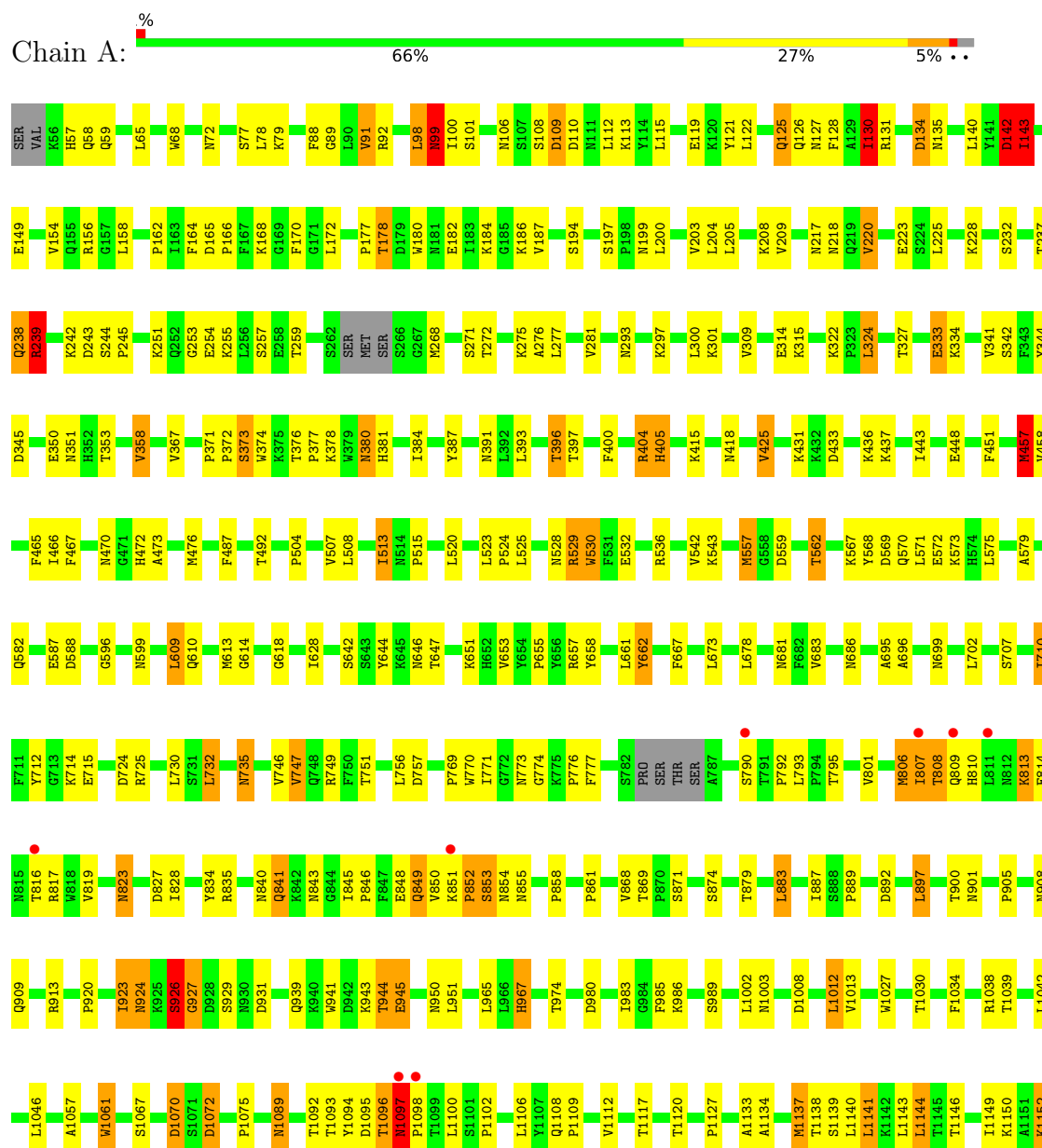
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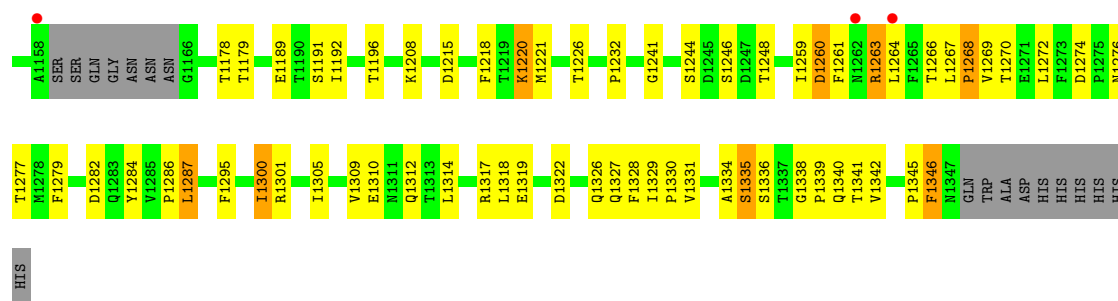
Chain	Residue	Modelled	Actual	Comment	Reference
C	1357	HIS	-	expression tag	UNP P20796
D	1352	HIS	-	expression tag	UNP P20796
D	1353	HIS	-	expression tag	UNP P20796
D	1354	HIS	-	expression tag	UNP P20796
D	1355	HIS	-	expression tag	UNP P20796
D	1356	HIS	-	expression tag	UNP P20796
D	1357	HIS	-	expression tag	UNP P20796
E	1352	HIS	-	expression tag	UNP P20796
E	1353	HIS	-	expression tag	UNP P20796
E	1354	HIS	-	expression tag	UNP P20796
E	1355	HIS	-	expression tag	UNP P20796
E	1356	HIS	-	expression tag	UNP P20796
E	1357	HIS	-	expression tag	UNP P20796
F	1352	HIS	-	expression tag	UNP P20796
F	1353	HIS	-	expression tag	UNP P20796
F	1354	HIS	-	expression tag	UNP P20796
F	1355	HIS	-	expression tag	UNP P20796
F	1356	HIS	-	expression tag	UNP P20796
F	1357	HIS	-	expression tag	UNP P20796

3 Residue-property plots

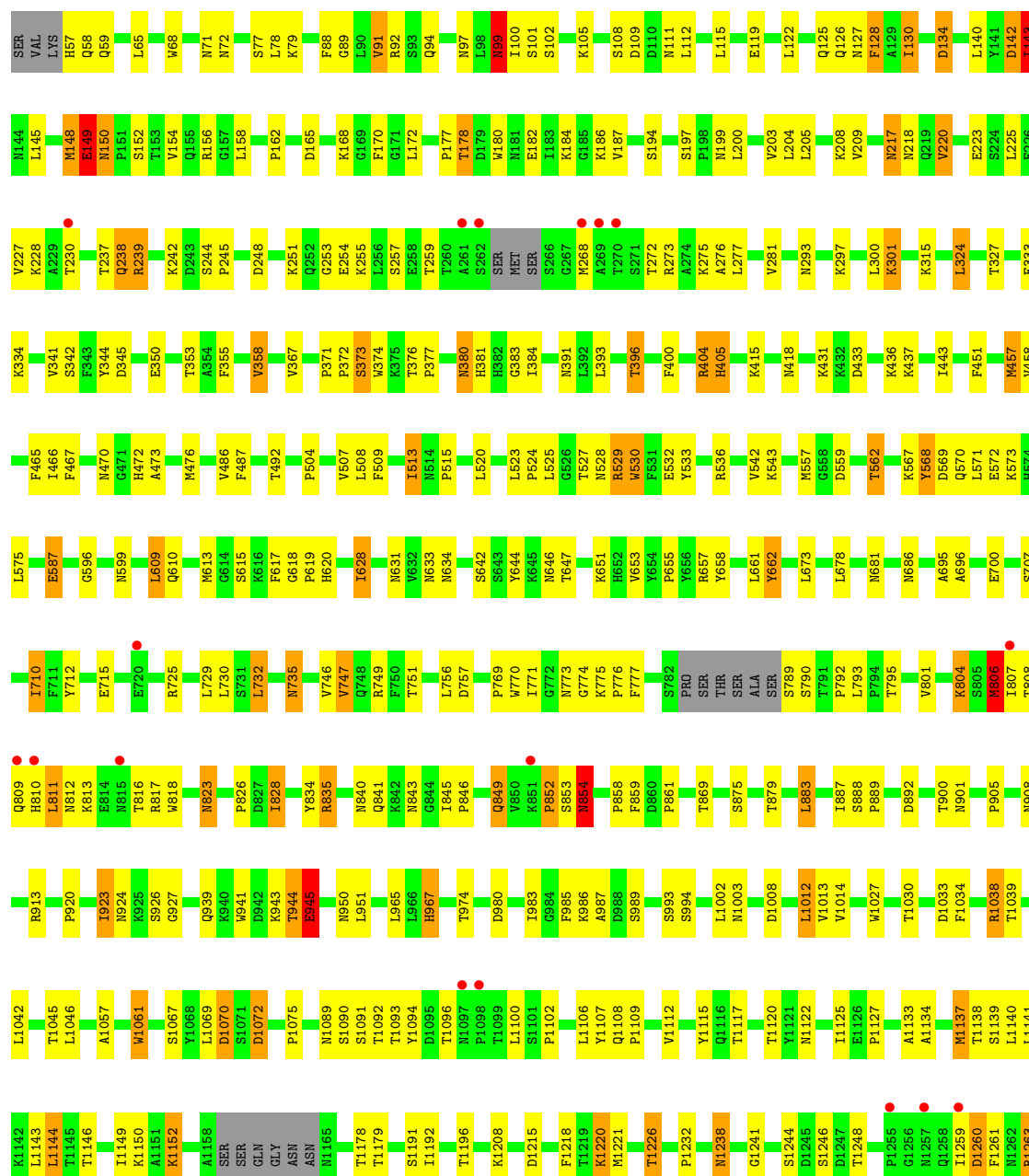
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

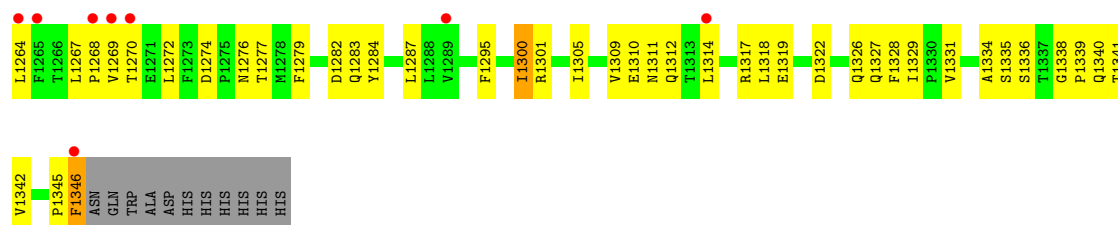
• Molecule 1: Adhesin P1



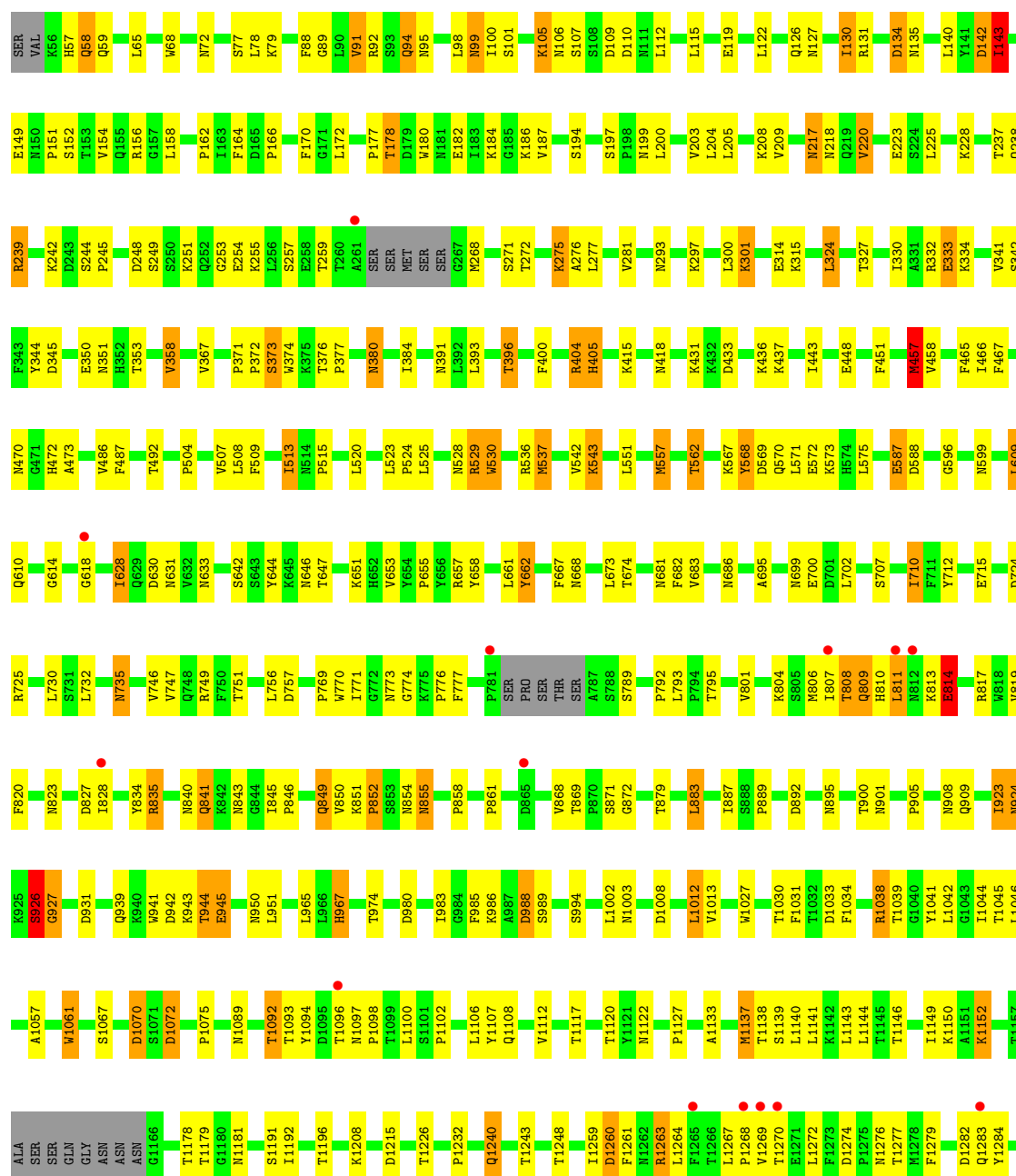


• Molecule 1: Adhesin P1

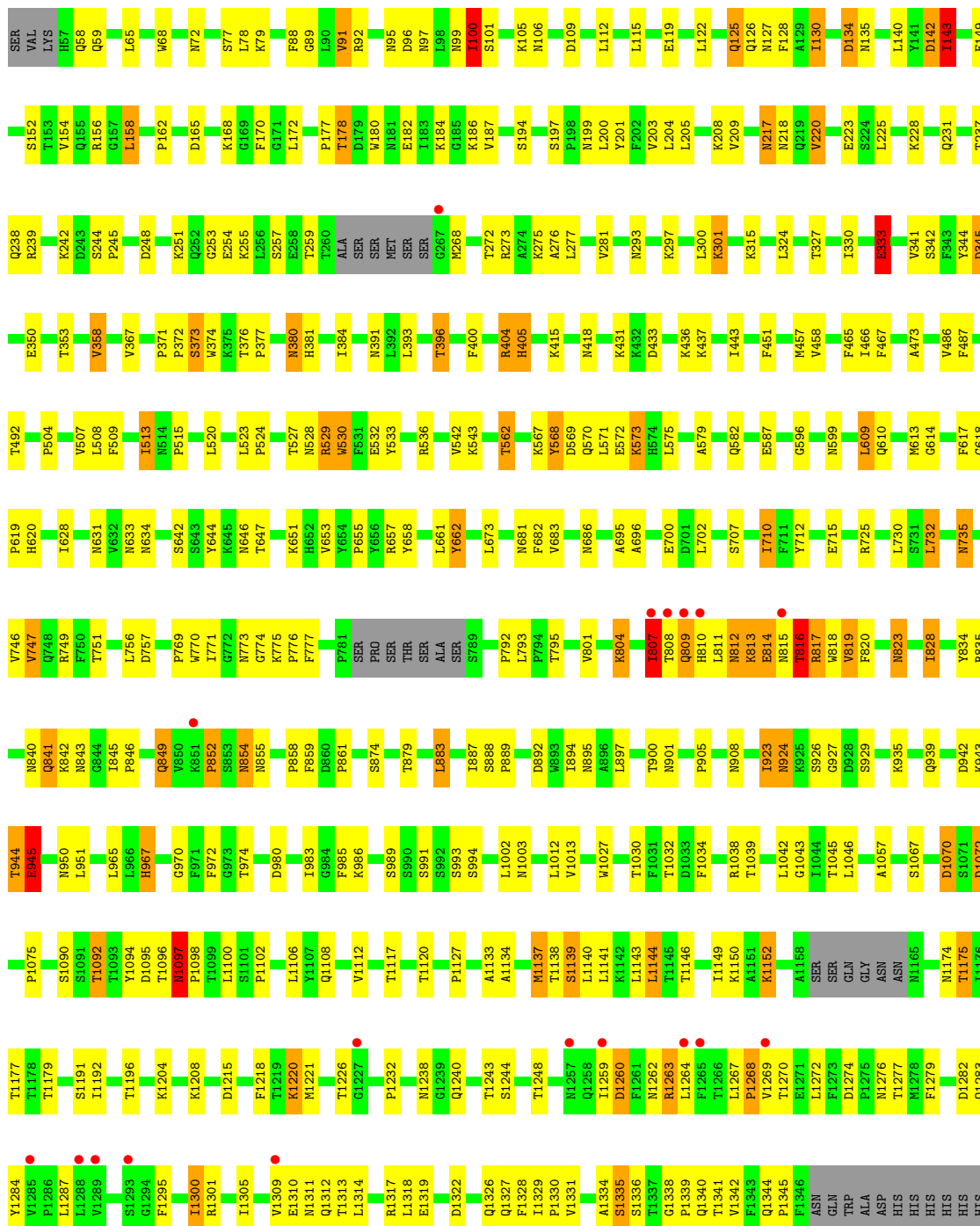




• Molecule 1: Adhesin P1



- Molecule 1: Adhesin P1

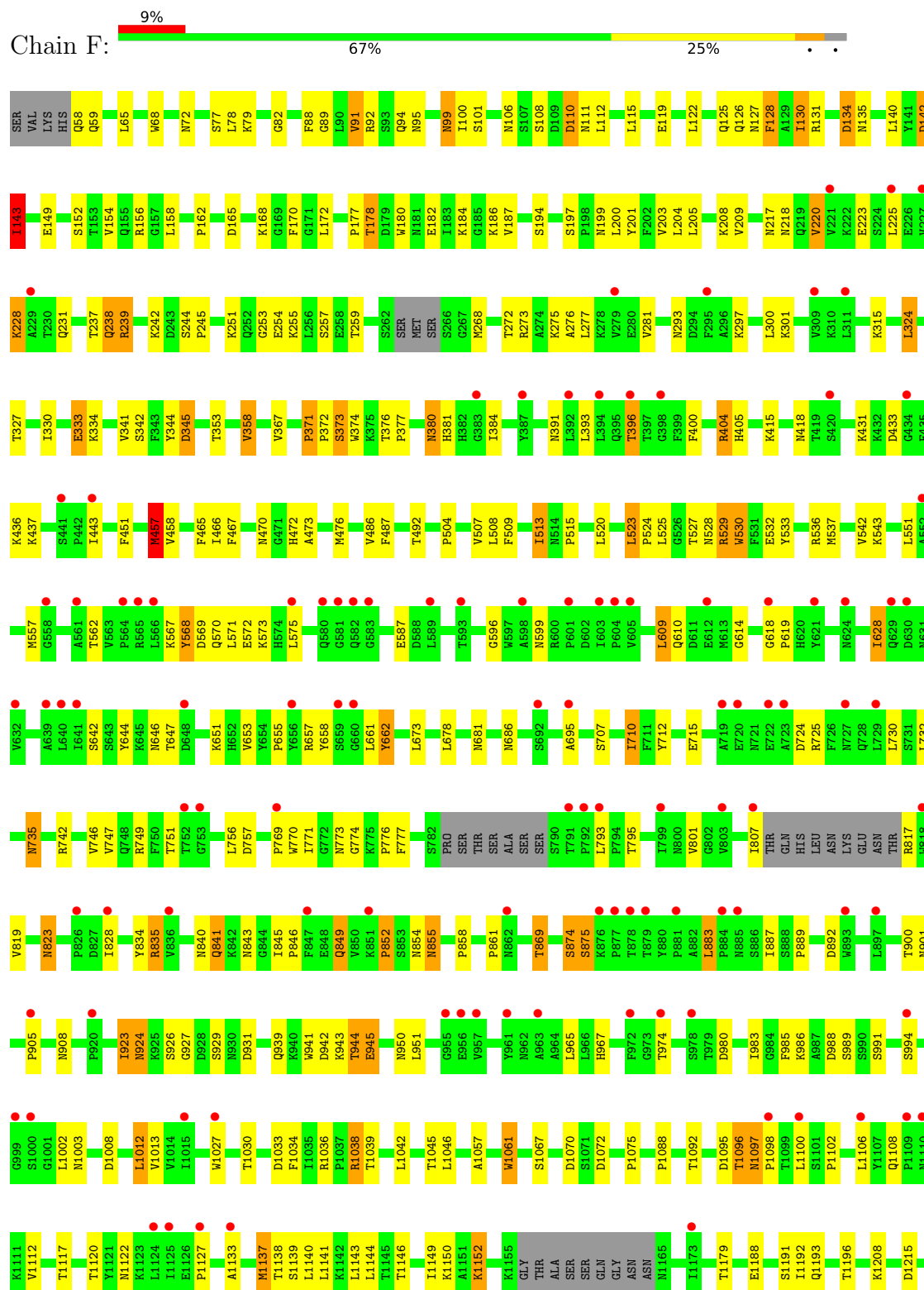


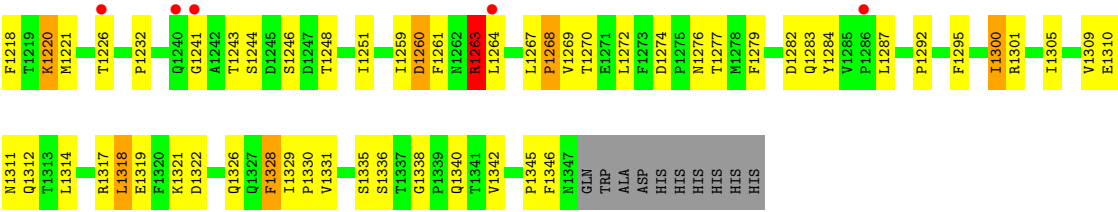
- Molecule 1: Adhesin P1





- Molecule 1: Adhesin P1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	459.19Å 116.66Å 285.64Å 90.00° 124.20° 90.00°	Depositor
Resolution (Å)	37.36 – 3.24 37.36 – 3.24	Depositor EDS
% Data completeness (in resolution range)	61.7 (37.36-3.24) 61.9 (37.36-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.184 , 0.205 (Not available) , 0.222	Depositor DCC
R_{free} test set	6155 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 99.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	59767	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	0.87	8/10269 (0.1%)	1.39	82/13978 (0.6%)
1	B	0.83	5/10252 (0.0%)	1.37	81/13956 (0.6%)
1	C	0.83	6/10246 (0.1%)	1.36	86/13947 (0.6%)
1	D	0.83	4/10229 (0.0%)	1.37	89/13925 (0.6%)
1	E	0.78	4/10135 (0.0%)	1.34	77/13795 (0.6%)
1	F	0.77	6/10147 (0.1%)	1.34	72/13812 (0.5%)
All	All	0.82	33/61278 (0.1%)	1.36	487/83413 (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	A	0	1
1	C	0	1
All	All	0	2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	557	MET	SD-CE	-10.72	1.52	1.79
1	A	1137	MET	SD-CE	-10.60	1.53	1.79
1	A	1097	ASN	CA-C	7.49	1.62	1.52
1	B	1137	MET	SD-CE	-7.12	1.61	1.79
1	F	143	ILE	CA-C	6.99	1.61	1.52
1	C	143	ILE	CA-C	6.86	1.61	1.52
1	C	457	MET	SD-CE	-6.65	1.62	1.79
1	B	143	ILE	CA-C	6.61	1.61	1.52
1	C	557	MET	SD-CE	-6.59	1.63	1.79
1	D	143	ILE	CA-C	6.59	1.61	1.52
1	E	143	ILE	CA-C	6.41	1.60	1.52
1	E	476	MET	SD-CE	-6.36	1.63	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1137	MET	SD-CE	-6.25	1.64	1.79
1	D	100	ILE	CG1-CD1	6.21	1.75	1.51
1	A	807	ILE	CA-CB	5.96	1.61	1.53
1	C	1137	MET	SD-CE	-5.82	1.65	1.79
1	A	476	MET	SD-CE	-5.81	1.65	1.79
1	B	476	MET	SD-CE	-5.70	1.65	1.79
1	D	268	MET	CA-C	5.68	1.60	1.52
1	F	457	MET	SD-CE	-5.52	1.65	1.79
1	F	1328	PHE	CA-C	-5.50	1.46	1.52
1	B	148	MET	SD-CE	-5.50	1.65	1.79
1	A	557	MET	SD-CE	-5.46	1.66	1.79
1	F	1137	MET	SD-CE	-5.31	1.66	1.79
1	C	537	MET	SD-CE	-5.29	1.66	1.79
1	C	1092	THR	CA-C	5.26	1.57	1.53
1	B	150	ASN	CA-C	5.19	1.57	1.53
1	A	322	LYS	CA-C	5.18	1.57	1.52
1	E	1137	MET	SD-CE	-5.14	1.66	1.79
1	A	99	ASN	CA-C	5.09	1.59	1.52
1	A	457	MET	SD-CE	-5.09	1.66	1.79
1	F	476	MET	SD-CE	-5.07	1.66	1.79
1	F	371	PRO	CA-C	5.04	1.54	1.51

All (487) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	SER	N-CA-C	10.76	124.15	111.02
1	A	806	MET	CA-C-N	10.63	137.12	121.18
1	A	806	MET	C-N-CA	10.63	137.12	121.18
1	E	861	PRO	N-CA-C	-10.52	94.65	111.38
1	F	861	PRO	N-CA-C	-10.42	94.81	111.38
1	C	988	ASP	CA-CB-CG	10.40	123.00	112.60
1	D	849	GLN	CA-C-N	9.83	136.00	122.34
1	D	849	GLN	C-N-CA	9.83	136.00	122.34
1	C	849	GLN	CA-C-N	9.57	135.65	122.34
1	C	849	GLN	C-N-CA	9.57	135.65	122.34
1	A	849	GLN	CA-C-N	9.48	135.51	122.34
1	A	849	GLN	C-N-CA	9.48	135.51	122.34
1	B	149	GLU	N-CA-C	-8.93	96.58	110.42
1	A	142	ASP	N-CA-C	-8.86	97.12	110.14
1	D	134	ASP	CA-CB-CG	8.63	121.23	112.60
1	B	134	ASP	CA-CB-CG	8.59	121.19	112.60
1	F	849	GLN	CA-C-N	8.49	134.14	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	849	GLN	C-N-CA	8.49	134.14	122.34
1	E	849	GLN	CA-C-N	8.39	134.01	122.34
1	E	849	GLN	C-N-CA	8.39	134.01	122.34
1	C	134	ASP	CA-CB-CG	8.36	120.96	112.60
1	E	134	ASP	CA-CB-CG	8.34	120.94	112.60
1	F	134	ASP	CA-CB-CG	8.32	120.92	112.60
1	B	849	GLN	CA-C-N	8.30	136.00	122.64
1	B	849	GLN	C-N-CA	8.30	136.00	122.64
1	A	109	ASP	CA-C-N	8.10	137.21	121.66
1	A	109	ASP	C-N-CA	8.10	137.21	121.66
1	B	208	LYS	CA-C-N	8.04	130.69	120.56
1	B	208	LYS	C-N-CA	8.04	130.69	120.56
1	A	134	ASP	CA-CB-CG	7.93	120.53	112.60
1	E	1262	ASN	CA-CB-CG	7.66	120.26	112.60
1	F	208	LYS	CA-C-N	7.66	130.21	120.56
1	F	208	LYS	C-N-CA	7.66	130.21	120.56
1	E	208	LYS	CA-C-N	7.57	130.09	120.56
1	E	208	LYS	C-N-CA	7.57	130.09	120.56
1	D	208	LYS	CA-C-N	7.47	129.97	120.56
1	D	208	LYS	C-N-CA	7.47	129.97	120.56
1	B	853	SER	CA-C-N	7.44	135.76	121.54
1	B	853	SER	C-N-CA	7.44	135.76	121.54
1	D	1174	ASN	CA-C-N	7.43	135.73	121.54
1	D	1174	ASN	C-N-CA	7.43	135.73	121.54
1	D	97	ASN	CA-CB-CG	7.41	120.01	112.60
1	E	109	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	208	LYS	CA-C-N	7.38	129.85	120.56
1	A	208	LYS	C-N-CA	7.38	129.85	120.56
1	C	208	LYS	CA-C-N	7.20	129.63	120.56
1	C	208	LYS	C-N-CA	7.20	129.63	120.56
1	A	1093	THR	CA-C-N	7.15	135.21	121.54
1	A	1093	THR	C-N-CA	7.15	135.21	121.54
1	E	476	MET	CB-CG-SD	7.07	133.92	112.70
1	D	1260	ASP	CA-CB-CG	7.02	119.62	112.60
1	F	110	ASP	CA-C-N	7.00	134.91	121.54
1	F	110	ASP	C-N-CA	7.00	134.91	121.54
1	A	100	ILE	N-CA-C	-6.99	103.92	113.00
1	D	99	ASN	CA-CB-CG	6.91	119.51	112.60
1	A	143	ILE	N-CA-C	-6.80	95.19	109.34
1	D	812	ASN	CA-C-N	6.80	134.53	121.54
1	D	812	ASN	C-N-CA	6.80	134.53	121.54
1	D	1174	ASN	CA-CB-CG	6.79	119.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	95	ASN	CA-CB-CG	6.72	119.32	112.60
1	C	95	ASN	CA-CB-CG	6.66	119.26	112.60
1	A	855	ASN	CA-CB-CG	6.66	119.25	112.60
1	B	1260	ASP	CA-CB-CG	6.63	119.23	112.60
1	D	944	THR	CA-C-N	6.62	130.38	120.31
1	D	944	THR	C-N-CA	6.62	130.38	120.31
1	F	95	ASN	CA-CB-CG	6.61	119.21	112.60
1	D	647	THR	CA-C-N	6.55	129.06	120.28
1	D	647	THR	C-N-CA	6.55	129.06	120.28
1	D	1070	ASP	CA-C-N	6.50	129.87	120.38
1	D	1070	ASP	C-N-CA	6.50	129.87	120.38
1	C	647	THR	CA-C-N	6.50	128.99	120.28
1	C	647	THR	C-N-CA	6.50	128.99	120.28
1	C	107	SER	CA-C-N	6.49	129.63	120.28
1	C	107	SER	C-N-CA	6.49	129.63	120.28
1	B	806	MET	N-CA-C	6.46	120.08	112.72
1	E	110	ASP	N-CA-C	6.45	120.39	111.55
1	A	944	THR	CA-C-N	6.44	130.09	120.31
1	A	944	THR	C-N-CA	6.44	130.09	120.31
1	F	1260	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	1138	THR	CA-C-N	6.41	128.77	120.44
1	A	1138	THR	C-N-CA	6.41	128.77	120.44
1	A	1260	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	1089	ASN	CA-CB-CG	6.36	118.96	112.60
1	A	807	ILE	CA-C-N	6.35	133.67	121.54
1	A	807	ILE	C-N-CA	6.35	133.67	121.54
1	C	1260	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	944	THR	CA-C-N	6.31	129.90	120.31
1	B	944	THR	C-N-CA	6.31	129.90	120.31
1	C	99	ASN	CA-CB-CG	6.29	118.89	112.60
1	A	1095	ASP	CA-C-N	6.27	133.52	121.54
1	A	1095	ASP	C-N-CA	6.27	133.52	121.54
1	D	816	THR	CA-C-N	-6.27	111.97	120.87
1	D	816	THR	C-N-CA	-6.27	111.97	120.87
1	A	647	THR	CA-C-N	6.25	128.65	120.28
1	A	647	THR	C-N-CA	6.25	128.65	120.28
1	E	1070	ASP	CA-C-N	6.25	129.50	120.38
1	E	1070	ASP	C-N-CA	6.25	129.50	120.38
1	C	944	THR	CA-C-N	6.21	129.74	120.31
1	C	944	THR	C-N-CA	6.21	129.74	120.31
1	E	647	THR	CA-C-N	6.19	128.57	120.28
1	E	647	THR	C-N-CA	6.19	128.57	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	PRO	CA-C-N	6.17	128.55	120.28
1	A	372	PRO	C-N-CA	6.17	128.55	120.28
1	D	1139	SER	CA-C-N	6.16	128.82	120.44
1	D	1139	SER	C-N-CA	6.16	128.82	120.44
1	D	1238	ASN	CA-CB-CG	6.16	118.76	112.60
1	B	647	THR	CA-C-N	6.16	128.53	120.28
1	B	647	THR	C-N-CA	6.16	128.53	120.28
1	B	789	SER	CA-C-N	6.15	133.29	121.54
1	B	789	SER	C-N-CA	6.15	133.29	121.54
1	D	1097	ASN	CA-CB-CG	6.15	118.75	112.60
1	B	1309	VAL	CA-C-N	6.15	129.33	120.79
1	B	1309	VAL	C-N-CA	6.15	129.33	120.79
1	F	647	THR	CA-C-N	6.14	128.51	120.28
1	F	647	THR	C-N-CA	6.14	128.51	120.28
1	C	1138	THR	CA-C-N	6.12	128.40	120.44
1	C	1138	THR	C-N-CA	6.12	128.40	120.44
1	A	927	GLY	CA-C-N	6.12	129.40	120.71
1	A	927	GLY	C-N-CA	6.12	129.40	120.71
1	C	372	PRO	CA-C-N	6.12	128.48	120.28
1	C	372	PRO	C-N-CA	6.12	128.48	120.28
1	E	874	SER	CA-C-N	6.09	133.17	121.54
1	E	874	SER	C-N-CA	6.09	133.17	121.54
1	A	1322	ASP	CA-CB-CG	6.06	118.66	112.60
1	F	944	THR	CA-C-N	6.05	129.51	120.31
1	F	944	THR	C-N-CA	6.05	129.51	120.31
1	F	1088	PRO	N-CA-C	6.04	122.58	113.81
1	B	372	PRO	CA-C-N	6.04	128.38	120.28
1	B	372	PRO	C-N-CA	6.04	128.38	120.28
1	E	944	THR	CA-C-N	6.04	129.50	120.31
1	E	944	THR	C-N-CA	6.04	129.50	120.31
1	B	1139	SER	CA-C-N	6.04	128.65	120.44
1	B	1139	SER	C-N-CA	6.04	128.65	120.44
1	D	1095	ASP	CA-C-N	6.03	133.06	121.54
1	D	1095	ASP	C-N-CA	6.03	133.06	121.54
1	B	1070	ASP	CA-C-N	6.02	129.17	120.38
1	B	1070	ASP	C-N-CA	6.02	129.17	120.38
1	B	1090	SER	CA-C-N	6.01	128.26	120.44
1	B	1090	SER	C-N-CA	6.01	128.26	120.44
1	D	130	ILE	CA-C-N	-6.01	113.20	122.09
1	D	130	ILE	C-N-CA	-6.01	113.20	122.09
1	D	812	ASN	N-CA-C	-6.01	105.91	113.72
1	C	562	THR	CA-C-N	6.00	125.13	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	562	THR	C-N-CA	6.00	125.13	120.33
1	C	1070	ASP	CA-C-N	6.00	129.13	120.38
1	C	1070	ASP	C-N-CA	6.00	129.13	120.38
1	C	814	GLU	CB-CG-CD	5.97	122.75	112.60
1	F	1070	ASP	CA-C-N	5.97	129.09	120.38
1	F	1070	ASP	C-N-CA	5.97	129.09	120.38
1	D	372	PRO	CA-C-N	5.96	128.27	120.28
1	D	372	PRO	C-N-CA	5.96	128.27	120.28
1	F	372	PRO	CA-C-N	5.95	128.26	120.28
1	F	372	PRO	C-N-CA	5.95	128.26	120.28
1	A	57	HIS	CA-C-N	5.93	128.82	120.28
1	A	57	HIS	C-N-CA	5.93	128.82	120.28
1	E	1260	ASP	CA-CB-CG	5.93	118.53	112.60
1	D	929	SER	N-CA-C	-5.92	101.28	110.10
1	C	1322	ASP	CA-CB-CG	5.91	118.51	112.60
1	C	57	HIS	CA-C-N	5.90	128.46	120.38
1	C	57	HIS	C-N-CA	5.90	128.46	120.38
1	E	99	ASN	CA-CB-CG	5.89	118.49	112.60
1	F	735	ASN	CA-CB-CG	5.89	118.49	112.60
1	F	874	SER	CA-C-N	5.89	132.78	121.54
1	F	874	SER	C-N-CA	5.89	132.78	121.54
1	C	855	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	562	THR	CA-C-N	5.88	125.03	120.33
1	A	562	THR	C-N-CA	5.88	125.03	120.33
1	B	1072	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	1138	THR	CA-C-N	5.86	128.06	120.44
1	B	1138	THR	C-N-CA	5.86	128.06	120.44
1	C	100	ILE	CA-C-N	5.86	128.72	120.28
1	C	100	ILE	C-N-CA	5.86	128.72	120.28
1	D	1072	ASP	CA-CB-CG	5.85	118.45	112.60
1	D	1309	VAL	CA-C-N	5.85	128.92	120.79
1	D	1309	VAL	C-N-CA	5.85	128.92	120.79
1	E	1088	PRO	N-CA-C	5.85	122.29	113.81
1	A	1070	ASP	CA-C-N	5.84	128.91	120.38
1	A	1070	ASP	C-N-CA	5.84	128.91	120.38
1	C	931	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	99	ASN	CA-CB-CG	5.83	118.43	112.60
1	F	1095	ASP	CA-C-N	5.83	132.68	121.54
1	F	1095	ASP	C-N-CA	5.83	132.68	121.54
1	F	1138	THR	CA-C-N	5.83	128.02	120.44
1	F	1138	THR	C-N-CA	5.83	128.02	120.44
1	A	1072	ASP	CA-CB-CG	5.80	118.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	980	ASP	CA-CB-CG	5.80	118.40	112.60
1	F	855	ASN	CA-CB-CG	5.80	118.40	112.60
1	E	1095	ASP	CA-C-N	5.80	132.62	121.54
1	E	1095	ASP	C-N-CA	5.80	132.62	121.54
1	D	433	ASP	CA-CB-CG	5.79	118.39	112.60
1	D	1208	LYS	CA-C-N	5.78	128.03	120.28
1	D	1208	LYS	C-N-CA	5.78	128.03	120.28
1	C	927	GLY	CA-C-N	5.78	128.91	120.71
1	C	927	GLY	C-N-CA	5.78	128.91	120.71
1	F	380	ASN	CA-CB-CG	5.78	118.38	112.60
1	E	380	ASN	CA-CB-CG	5.77	118.37	112.60
1	E	735	ASN	CA-CB-CG	5.76	118.36	112.60
1	C	109	ASP	CA-CB-CG	5.76	118.36	112.60
1	C	980	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	110	ASP	CA-C-N	5.74	128.29	120.54
1	A	110	ASP	C-N-CA	5.74	128.29	120.54
1	B	451	PHE	CA-CB-CG	-5.74	108.06	113.80
1	B	735	ASN	CA-CB-CG	5.74	118.34	112.60
1	E	1208	LYS	CA-C-N	5.73	127.96	120.28
1	E	1208	LYS	C-N-CA	5.73	127.96	120.28
1	A	1268	PRO	CA-C-N	5.71	128.29	120.46
1	A	1268	PRO	C-N-CA	5.71	128.29	120.46
1	E	855	ASN	CA-CB-CG	5.71	118.31	112.60
1	C	380	ASN	CA-CB-CG	5.70	118.30	112.60
1	E	372	PRO	CA-C-N	5.70	127.91	120.28
1	E	372	PRO	C-N-CA	5.70	127.91	120.28
1	F	1309	VAL	CA-C-N	5.69	128.70	120.79
1	F	1309	VAL	C-N-CA	5.69	128.70	120.79
1	F	1322	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	967	HIS	CA-C-N	5.69	128.17	120.38
1	B	967	HIS	C-N-CA	5.69	128.17	120.38
1	E	1268	PRO	CA-C-N	5.68	128.25	120.46
1	E	1268	PRO	C-N-CA	5.68	128.25	120.46
1	E	433	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	1208	LYS	CA-C-N	5.67	127.88	120.28
1	A	1208	LYS	C-N-CA	5.67	127.88	120.28
1	A	931	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	380	ASN	CA-CB-CG	5.66	118.26	112.60
1	F	433	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	562	THR	CA-C-N	5.66	124.85	120.33
1	D	562	THR	C-N-CA	5.66	124.85	120.33
1	F	99	ASN	CA-CB-CG	5.66	118.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	ASN	CA-CB-CG	5.65	118.25	112.60
1	F	1208	LYS	CA-C-N	5.65	127.85	120.28
1	F	1208	LYS	C-N-CA	5.65	127.85	120.28
1	D	1268	PRO	CA-C-N	5.64	128.19	120.46
1	D	1268	PRO	C-N-CA	5.64	128.19	120.46
1	A	848	GLU	CB-CG-CD	5.64	122.19	112.60
1	B	143	ILE	CB-CG1-CD1	5.63	125.63	113.80
1	C	142	ASP	N-CA-C	5.63	120.16	113.12
1	D	967	HIS	CA-C-N	5.63	127.83	120.28
1	D	967	HIS	C-N-CA	5.63	127.83	120.28
1	A	253	GLY	N-CA-C	-5.61	108.50	114.67
1	B	142	ASP	N-CA-C	5.61	120.13	113.12
1	F	341	VAL	CA-C-N	5.60	128.79	120.95
1	F	341	VAL	C-N-CA	5.60	128.79	120.95
1	A	1095	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	100	ILE	CA-C-N	5.59	128.33	120.28
1	B	100	ILE	C-N-CA	5.59	128.33	120.28
1	B	1268	PRO	CA-C-N	5.59	128.12	120.46
1	B	1268	PRO	C-N-CA	5.59	128.12	120.46
1	C	341	VAL	CA-C-N	5.59	128.78	120.95
1	C	341	VAL	C-N-CA	5.59	128.78	120.95
1	D	142	ASP	N-CA-C	5.58	120.10	113.12
1	F	1072	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	980	ASP	CA-CB-CG	5.58	118.18	112.60
1	F	100	ILE	CA-C-N	5.58	128.31	120.28
1	F	100	ILE	C-N-CA	5.58	128.31	120.28
1	B	380	ASN	CA-CB-CG	5.57	118.17	112.60
1	F	1268	PRO	CA-C-N	5.57	128.09	120.46
1	F	1268	PRO	C-N-CA	5.57	128.09	120.46
1	C	1268	PRO	CA-C-N	5.56	128.08	120.46
1	C	1268	PRO	C-N-CA	5.56	128.08	120.46
1	D	735	ASN	CA-CB-CG	5.56	118.16	112.60
1	E	142	ASP	N-CA-C	5.56	120.07	113.12
1	C	1097	ASN	CA-CB-CG	5.55	118.16	112.60
1	C	253	GLY	N-CA-C	-5.54	108.06	115.32
1	E	1263	ARG	CA-C-N	5.54	131.25	122.61
1	E	1263	ARG	C-N-CA	5.54	131.25	122.61
1	E	100	ILE	CA-C-N	5.53	128.24	120.28
1	E	100	ILE	C-N-CA	5.53	128.24	120.28
1	E	927	GLY	CA-C-N	5.53	128.56	120.71
1	E	927	GLY	C-N-CA	5.53	128.56	120.71
1	C	1139	SER	CA-C-N	5.52	127.95	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1139	SER	C-N-CA	5.52	127.95	120.44
1	C	1208	LYS	CA-C-N	5.52	127.68	120.28
1	C	1208	LYS	C-N-CA	5.52	127.68	120.28
1	F	530	TRP	N-CA-C	-5.52	99.53	108.41
1	D	774	GLY	N-CA-C	-5.51	107.72	115.32
1	F	931	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	96	ASP	CA-CB-CG	5.50	118.11	112.60
1	C	530	TRP	N-CA-C	-5.49	99.57	108.41
1	C	433	ASP	CA-CB-CG	5.49	118.09	112.60
1	E	980	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	341	VAL	CA-C-N	5.49	128.63	120.95
1	A	341	VAL	C-N-CA	5.49	128.63	120.95
1	B	128	PHE	CA-CB-CG	5.48	119.28	113.80
1	F	774	GLY	N-CA-C	-5.48	107.76	115.32
1	E	1138	THR	CA-C-N	5.47	127.88	120.44
1	E	1138	THR	C-N-CA	5.47	127.88	120.44
1	F	142	ASP	N-CA-C	5.47	119.96	113.12
1	B	980	ASP	CA-CB-CG	5.47	118.07	112.60
1	C	872	GLY	N-CA-C	5.46	120.39	113.24
1	A	774	GLY	N-CA-C	-5.45	107.80	115.32
1	A	678	LEU	CA-C-N	5.45	131.25	121.66
1	A	678	LEU	C-N-CA	5.45	131.25	121.66
1	F	927	GLY	CA-C-N	5.45	128.44	120.71
1	F	927	GLY	C-N-CA	5.45	128.44	120.71
1	C	630	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	530	TRP	N-CA-C	-5.44	99.65	108.41
1	E	562	THR	CA-C-N	5.44	124.68	120.33
1	E	562	THR	C-N-CA	5.44	124.68	120.33
1	A	853	SER	CA-C-O	-5.43	115.10	121.07
1	D	927	GLY	CA-C-N	5.43	128.42	120.71
1	D	927	GLY	C-N-CA	5.43	128.42	120.71
1	B	1208	LYS	CA-C-N	5.43	127.55	120.28
1	B	1208	LYS	C-N-CA	5.43	127.55	120.28
1	B	700	GLU	CB-CG-CD	5.42	121.82	112.60
1	A	967	HIS	CA-C-N	5.42	127.80	120.38
1	A	967	HIS	C-N-CA	5.42	127.80	120.38
1	B	562	THR	CA-C-N	5.41	124.66	120.33
1	B	562	THR	C-N-CA	5.41	124.66	120.33
1	A	530	TRP	N-CA-C	-5.41	99.70	108.41
1	E	57	HIS	CA-C-N	5.40	128.06	120.28
1	E	57	HIS	C-N-CA	5.40	128.06	120.28
1	D	509	PHE	CA-CB-CG	5.40	119.20	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	970	GLY	CA-C-N	5.39	127.51	120.28
1	D	970	GLY	C-N-CA	5.39	127.51	120.28
1	D	530	TRP	N-CA-C	-5.39	99.73	108.41
1	E	967	HIS	CA-C-N	5.39	127.50	120.28
1	E	967	HIS	C-N-CA	5.39	127.50	120.28
1	E	931	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	530	TRP	N-CA-C	-5.38	99.75	108.41
1	B	217	ASN	CA-C-N	5.38	128.23	120.38
1	B	217	ASN	C-N-CA	5.38	128.23	120.38
1	A	1309	VAL	CA-C-N	5.37	128.26	120.79
1	A	1309	VAL	C-N-CA	5.37	128.26	120.79
1	D	807	ILE	N-CA-C	-5.37	98.17	109.34
1	E	1322	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	678	LEU	CA-C-N	5.37	131.11	121.66
1	B	678	LEU	C-N-CA	5.37	131.11	121.66
1	E	1072	ASP	CA-CB-CG	5.37	117.97	112.60
1	F	345	ASP	N-CA-C	5.37	116.83	107.49
1	B	433	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	345	ASP	N-CA-C	5.36	116.81	107.49
1	D	1138	THR	CA-C-N	5.35	127.72	120.44
1	D	1138	THR	C-N-CA	5.35	127.72	120.44
1	D	1262	ASN	CA-CB-CG	5.34	117.94	112.60
1	B	774	GLY	N-CA-C	-5.34	107.95	115.32
1	F	253	GLY	N-CA-C	-5.34	108.32	115.32
1	C	683	VAL	N-CA-C	-5.34	98.27	107.24
1	A	451	PHE	CA-CB-CG	-5.34	108.46	113.80
1	A	1139	SER	CA-C-N	5.34	127.70	120.44
1	A	1139	SER	C-N-CA	5.34	127.70	120.44
1	D	945	GLU	CB-CG-CD	5.32	121.65	112.60
1	C	130	ILE	CA-C-N	-5.32	112.97	122.07
1	C	130	ILE	C-N-CA	-5.32	112.97	122.07
1	A	433	ASP	CA-CB-CG	5.31	117.91	112.60
1	F	980	ASP	CA-CB-CG	5.31	117.91	112.60
1	F	967	HIS	CA-C-N	5.31	127.39	120.28
1	F	967	HIS	C-N-CA	5.31	127.39	120.28
1	D	683	VAL	N-CA-C	-5.30	98.34	107.24
1	F	130	ILE	CA-C-N	-5.30	113.01	122.07
1	F	130	ILE	C-N-CA	-5.30	113.01	122.07
1	B	927	GLY	CA-C-N	5.30	128.75	120.75
1	B	927	GLY	C-N-CA	5.30	128.75	120.75
1	D	345	ASP	N-CA-C	5.29	116.70	107.49
1	F	82	GLY	CA-C-N	5.29	127.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	82	GLY	C-N-CA	5.29	127.63	120.38
1	A	683	VAL	N-CA-C	-5.29	98.36	107.24
1	E	774	GLY	N-CA-C	-5.29	108.02	115.32
1	F	1139	SER	CA-C-N	5.29	127.63	120.44
1	F	1139	SER	C-N-CA	5.29	127.63	120.44
1	F	562	THR	CA-C-N	5.28	124.56	120.33
1	F	562	THR	C-N-CA	5.28	124.56	120.33
1	B	253	GLY	N-CA-C	-5.28	108.40	115.32
1	E	345	ASP	N-CA-C	5.28	116.68	107.49
1	D	855	ASN	CA-C-N	5.28	129.84	122.08
1	D	855	ASN	C-N-CA	5.28	129.84	122.08
1	A	239	ARG	CA-C-N	5.28	128.36	120.87
1	A	239	ARG	C-N-CA	5.28	128.36	120.87
1	C	268	MET	CA-C-N	5.28	128.72	120.75
1	C	268	MET	C-N-CA	5.28	128.72	120.75
1	E	100	ILE	N-CA-C	-5.28	106.06	112.76
1	C	217	ASN	CA-C-N	5.27	128.08	120.38
1	C	217	ASN	C-N-CA	5.27	128.08	120.38
1	B	149	GLU	CB-CG-CD	5.27	121.56	112.60
1	C	110	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	1322	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	130	ILE	CA-C-N	-5.27	113.06	122.07
1	E	130	ILE	C-N-CA	-5.27	113.06	122.07
1	E	1335	SER	CA-C-N	5.27	127.87	120.28
1	E	1335	SER	C-N-CA	5.27	127.87	120.28
1	A	100	ILE	CA-C-N	5.26	127.86	120.28
1	A	100	ILE	C-N-CA	5.26	127.86	120.28
1	B	1322	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	341	VAL	CA-C-N	5.26	128.31	120.95
1	E	341	VAL	C-N-CA	5.26	128.31	120.95
1	A	724	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	345	ASP	N-CA-C	5.26	116.64	107.49
1	A	380	ASN	CA-CB-CG	5.25	117.85	112.60
1	C	1072	ASP	CA-CB-CG	5.25	117.85	112.60
1	F	509	PHE	CA-CB-CG	5.25	119.05	113.80
1	E	724	ASP	CA-C-N	5.25	127.57	120.38
1	E	724	ASP	C-N-CA	5.25	127.57	120.38
1	A	99	ASN	CA-CB-CG	5.24	117.84	112.60
1	E	1309	VAL	CA-C-N	5.24	128.08	120.79
1	E	1309	VAL	C-N-CA	5.24	128.08	120.79
1	F	451	PHE	CA-CB-CG	-5.24	108.56	113.80
1	E	1139	SER	CA-C-N	5.24	127.56	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1139	SER	C-N-CA	5.24	127.56	120.44
1	F	100	ILE	N-CA-C	-5.24	106.11	112.76
1	C	967	HIS	CA-C-N	5.23	127.29	120.28
1	C	967	HIS	C-N-CA	5.23	127.29	120.28
1	C	774	GLY	N-CA-C	-5.23	108.10	115.32
1	D	253	GLY	N-CA-C	-5.22	108.48	115.32
1	E	253	GLY	N-CA-C	-5.21	108.49	115.32
1	A	130	ILE	CA-C-N	-5.20	113.17	122.07
1	A	130	ILE	C-N-CA	-5.20	113.17	122.07
1	D	1134	ALA	CA-C-N	5.20	127.51	120.38
1	D	1134	ALA	C-N-CA	5.20	127.51	120.38
1	B	1309	VAL	N-CA-C	-5.20	105.43	110.42
1	C	1093	THR	CA-C-N	5.20	131.47	121.54
1	C	1093	THR	C-N-CA	5.20	131.47	121.54
1	D	341	VAL	CA-C-N	5.19	128.22	120.95
1	D	341	VAL	C-N-CA	5.19	128.22	120.95
1	F	724	ASP	CA-C-N	5.19	127.49	120.38
1	F	724	ASP	C-N-CA	5.19	127.49	120.38
1	D	807	ILE	CA-C-N	5.18	131.43	121.54
1	D	807	ILE	C-N-CA	5.18	131.43	121.54
1	E	509	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	130	ILE	CA-C-N	-5.17	113.22	122.07
1	B	130	ILE	C-N-CA	-5.17	113.22	122.07
1	B	1134	ALA	CA-C-N	5.17	127.46	120.38
1	B	1134	ALA	C-N-CA	5.17	127.46	120.38
1	C	700	GLU	CB-CG-CD	5.15	121.36	112.60
1	D	1144	LEU	CA-C-N	5.15	129.45	122.19
1	D	1144	LEU	C-N-CA	5.15	129.45	122.19
1	B	945	GLU	CB-CG-CD	5.15	121.35	112.60
1	D	700	GLU	CB-CG-CD	5.14	121.34	112.60
1	D	942	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	509	PHE	CA-CB-CG	5.14	118.94	113.80
1	B	71	ASN	CA-CB-CG	5.14	117.74	112.60
1	C	333	GLU	CA-C-N	5.14	127.42	120.38
1	C	333	GLU	C-N-CA	5.14	127.42	120.38
1	E	128	PHE	CA-CB-CG	5.13	118.94	113.80
1	E	678	LEU	CA-C-N	5.13	130.69	121.66
1	E	678	LEU	C-N-CA	5.13	130.69	121.66
1	D	217	ASN	CA-C-N	5.12	127.86	120.38
1	D	217	ASN	C-N-CA	5.12	127.86	120.38
1	C	735	ASN	CA-CB-CG	5.12	117.72	112.60
1	D	109	ASP	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1188	GLU	CA-C-N	5.12	131.32	121.54
1	E	1188	GLU	C-N-CA	5.12	131.32	121.54
1	C	509	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	1144	LEU	CA-C-N	5.11	129.40	122.19
1	B	1144	LEU	C-N-CA	5.11	129.40	122.19
1	C	942	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	345	ASP	N-CA-C	5.10	116.37	107.49
1	A	1335	SER	CA-C-N	5.10	127.63	120.28
1	A	1335	SER	C-N-CA	5.10	127.63	120.28
1	B	1238	ASN	CB-CA-C	-5.10	103.65	111.66
1	D	333	GLU	CA-C-N	5.09	127.36	120.38
1	D	333	GLU	C-N-CA	5.09	127.36	120.38
1	D	854	ASN	CA-C-N	5.09	130.04	122.82
1	D	854	ASN	C-N-CA	5.09	130.04	122.82
1	F	128	PHE	CA-CB-CG	5.09	118.89	113.80
1	C	1335	SER	CA-C-N	5.08	127.59	120.28
1	C	1335	SER	C-N-CA	5.08	127.59	120.28
1	D	451	PHE	CA-CB-CG	-5.08	108.72	113.80
1	B	812	ASN	CA-C-N	5.07	127.59	120.28
1	B	812	ASN	C-N-CA	5.07	127.59	120.28
1	B	1093	THR	CA-C-N	5.07	131.21	121.54
1	B	1093	THR	C-N-CA	5.07	131.21	121.54
1	D	1335	SER	CA-C-N	5.07	127.58	120.28
1	D	1335	SER	C-N-CA	5.07	127.58	120.28
1	F	678	LEU	CA-C-N	5.05	130.56	121.66
1	F	678	LEU	C-N-CA	5.05	130.56	121.66
1	A	1144	LEU	CA-C-N	5.05	129.31	122.19
1	A	1144	LEU	C-N-CA	5.05	129.31	122.19
1	C	100	ILE	N-CA-C	-5.05	106.35	112.76
1	C	724	ASP	CA-C-N	5.04	127.28	120.38
1	C	724	ASP	C-N-CA	5.04	127.28	120.38
1	B	341	VAL	CA-C-N	5.04	128.00	120.95
1	B	341	VAL	C-N-CA	5.04	128.00	120.95
1	B	1238	ASN	CA-CB-CG	5.03	117.63	112.60
1	C	871	SER	CA-C-N	5.03	126.43	120.14
1	C	871	SER	C-N-CA	5.03	126.43	120.14
1	E	383	GLY	N-CA-C	5.03	120.11	110.86
1	F	1263	ARG	CA-C-N	5.02	130.45	122.61
1	F	1263	ARG	C-N-CA	5.02	130.45	122.61
1	B	383	GLY	N-CA-C	5.02	120.09	110.86
1	C	699	ASN	CA-C-N	5.01	127.31	120.54
1	C	699	ASN	C-N-CA	5.01	127.31	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	451	PHE	CA-CB-CG	-5.01	108.79	113.80
1	B	109	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	249	SER	CA-C-N	5.01	127.30	120.54
1	C	249	SER	C-N-CA	5.01	127.30	120.54
1	F	942	ASP	CA-CB-CG	5.00	117.61	112.60
1	C	239	ARG	CA-C-N	5.00	127.97	120.87
1	C	239	ARG	C-N-CA	5.00	127.97	120.87
1	D	991	SER	N-CA-C	5.00	116.79	109.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	926	SER	Mainchain
1	C	926	SER	Mainchain

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	10016	0	9726	186	0
1	B	9999	0	9707	187	0
1	C	9993	0	9706	184	0
1	D	9976	0	9687	208	0
1	E	9886	0	9597	159	0
1	F	9897	0	9610	164	0
All	All	59767	0	58033	1046	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1046) 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:D:100:ILE:CG1	1:D:100:ILE:CD1	1.76	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:812:ASN:ND2	1:D:815:ASN:HD22	1.28	1.31
1:F:1279:PHE:CE2	1:F:1301:ARG:HD2	1.78	1.18
1:A:1266:THR:HG21	1:C:1264:LEU:HD11	1.19	1.15
1:A:1264:LEU:HG	1:C:1283:GLN:HB2	1.30	1.09
1:F:1279:PHE:HE2	1:F:1301:ARG:HD2	1.09	1.05
1:A:1134:ALA:HA	1:A:1137:MET:HE2	1.38	1.05
1:C:1279:PHE:CE2	1:C:1301:ARG:HD2	1.93	1.02
1:F:1279:PHE:CE2	1:F:1301:ARG:CD	2.42	1.01
1:D:812:ASN:ND2	1:D:815:ASN:ND2	2.09	1.00
1:D:1279:PHE:CE1	1:D:1301:ARG:HD2	2.00	0.96
1:E:1279:PHE:CE1	1:E:1301:ARG:HD2	2.00	0.96
1:A:1287:LEU:HD22	1:D:158:LEU:HD21	1.46	0.96
1:B:1279:PHE:CE1	1:B:1301:ARG:HD2	2.01	0.96
1:A:1279:PHE:CE1	1:A:1301:ARG:HD2	2.01	0.93
1:F:1301:ARG:HG2	1:F:1328:PHE:CE2	2.03	0.92
1:A:528:ASN:HD22	1:A:530:TRP:HE3	1.15	0.92
1:F:1301:ARG:HG2	1:F:1328:PHE:CD2	2.04	0.92
1:E:528:ASN:HD22	1:E:530:TRP:HE3	1.17	0.90
1:F:528:ASN:HD22	1:F:530:TRP:HE3	1.17	0.90
1:C:667:PHE:HE2	1:D:815:ASN:O	1.53	0.90
1:C:808:THR:HB	1:D:634:ASN:OD1	1.72	0.90
1:C:528:ASN:HD22	1:C:530:TRP:HE3	1.18	0.89
1:D:528:ASN:HD22	1:D:530:TRP:HE3	1.18	0.89
1:D:277:LEU:HD13	1:D:620:HIS:NE2	1.87	0.89
1:B:528:ASN:HD22	1:B:530:TRP:HE3	1.17	0.89
1:B:277:LEU:HD13	1:B:620:HIS:NE2	1.89	0.88
1:A:387:TYR:CE2	1:A:425:VAL:HG21	2.09	0.87
1:D:812:ASN:HD21	1:D:815:ASN:HD22	1.21	0.87
1:D:813:LYS:H	1:D:817:ARG:HH12	1.23	0.86
1:A:1134:ALA:HA	1:A:1137:MET:CE	2.07	0.85
1:C:667:PHE:CE2	1:D:815:ASN:O	2.29	0.85
1:A:1274:ASP:HB3	1:A:1277:THR:HG22	1.59	0.84
1:F:1274:ASP:HB3	1:F:1277:THR:HG22	1.58	0.84
1:A:1264:LEU:HD13	1:A:1284:TYR:HE1	1.42	0.83
1:D:1274:ASP:HB3	1:D:1277:THR:HG22	1.60	0.83
1:E:1274:ASP:HB3	1:E:1277:THR:HG22	1.60	0.83
1:B:1226:THR:H	1:B:1238:ASN:HD21	1.25	0.83
1:B:1274:ASP:HB3	1:B:1277:THR:HG22	1.59	0.83
1:A:1266:THR:CG2	1:C:1264:LEU:HD11	2.07	0.82
1:C:1274:ASP:HB3	1:C:1277:THR:HG22	1.63	0.80
1:E:1264:LEU:HD13	1:E:1284:TYR:HE2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:THR:HG21	1:D:814:GLU:OE2	1.81	0.80
1:A:109:ASP:HB2	1:A:113:LYS:HD2	1.64	0.79
1:C:820:PHE:HE2	1:D:682:PHE:HE2	1.30	0.79
1:B:237:THR:HG22	1:B:1108:GLN:HG3	1.66	0.78
1:C:1264:LEU:HD13	1:C:1284:TYR:HE1	1.47	0.77
1:F:1264:LEU:HD13	1:F:1284:TYR:HE1	1.49	0.77
1:F:523:LEU:HG	1:F:557:MET:HE1	1.66	0.77
1:A:1264:LEU:HG	1:C:1283:GLN:CB	2.13	0.76
1:E:237:THR:HG22	1:E:1108:GLN:HG3	1.68	0.76
1:F:237:THR:HG22	1:F:1108:GLN:HG3	1.68	0.76
1:C:237:THR:HG22	1:C:1108:GLN:HG3	1.68	0.75
1:D:237:THR:HG22	1:D:1108:GLN:HG3	1.69	0.75
1:E:994:SER:HB2	1:E:1137:MET:HE2	1.70	0.74
1:D:810:HIS:CG	1:D:818:TRP:CZ3	2.76	0.74
1:A:1097:ASN:HB3	1:A:1098:PRO:CD	2.17	0.74
1:B:1264:LEU:HD13	1:B:1284:TYR:HE1	1.52	0.74
1:D:811:LEU:CD1	1:D:894:ILE:HG13	2.17	0.74
1:D:1264:LEU:HD13	1:D:1284:TYR:HE1	1.52	0.73
1:D:813:LYS:H	1:D:817:ARG:NH1	1.86	0.73
1:D:813:LYS:N	1:D:817:ARG:HH12	1.87	0.73
1:F:994:SER:HB2	1:F:1137:MET:HE2	1.71	0.72
1:E:869:THR:HG23	1:E:875:SER:H	1.54	0.72
1:A:237:THR:HG22	1:A:1108:GLN:HG3	1.69	0.72
1:D:1097:ASN:HB2	1:D:1098:PRO:HD3	1.70	0.72
1:A:528:ASN:ND2	1:A:530:TRP:HE3	1.86	0.72
1:C:994:SER:HB2	1:C:1137:MET:HE2	1.69	0.72
1:C:1279:PHE:HE2	1:C:1301:ARG:HD2	1.48	0.72
1:E:528:ASN:ND2	1:E:530:TRP:HE3	1.88	0.71
1:F:869:THR:HG23	1:F:875:SER:H	1.53	0.71
1:B:923:ILE:HG22	1:B:1140:LEU:HD23	1.72	0.71
1:C:528:ASN:ND2	1:C:530:TRP:HE3	1.88	0.71
1:D:1305:ILE:HD11	1:D:1317:ARG:HB3	1.73	0.71
1:A:923:ILE:HG22	1:A:1140:LEU:HD23	1.72	0.71
1:B:617:PHE:CD2	1:B:859:PHE:HD2	2.09	0.71
1:C:820:PHE:HE2	1:D:682:PHE:CE2	2.09	0.71
1:D:923:ILE:HG22	1:D:1140:LEU:HD23	1.72	0.71
1:B:987:ALA:HB1	1:B:1115:TYR:CD2	2.25	0.71
1:D:528:ASN:ND2	1:D:530:TRP:HE3	1.89	0.71
1:A:1264:LEU:HD13	1:A:1284:TYR:CE1	2.25	0.70
1:B:528:ASN:ND2	1:B:530:TRP:HE3	1.89	0.70
1:D:810:HIS:CD2	1:D:818:TRP:CZ3	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:769:PRO:HA	1:C:776:PRO:HA	1.74	0.69
1:A:98:LEU:HD12	1:A:125:GLN:HG2	1.73	0.69
1:A:109:ASP:CB	1:A:113:LYS:HD2	2.22	0.69
1:A:387:TYR:HE2	1:A:425:VAL:HG21	1.58	0.69
1:D:194:SER:HB2	1:D:200:LEU:HD23	1.74	0.69
1:B:994:SER:HB2	1:B:1137:MET:HE2	1.74	0.69
1:F:923:ILE:HG22	1:F:1140:LEU:HD23	1.75	0.69
1:A:1305:ILE:HD11	1:A:1317:ARG:HB3	1.75	0.68
1:B:769:PRO:HA	1:B:776:PRO:HA	1.76	0.68
1:B:1305:ILE:HD11	1:B:1317:ARG:HB3	1.74	0.68
1:B:277:LEU:HD13	1:B:620:HIS:CD2	2.29	0.68
1:C:923:ILE:HG22	1:C:1140:LEU:HD23	1.74	0.68
1:F:1305:ILE:HD11	1:F:1317:ARG:HB3	1.75	0.68
1:F:769:PRO:HA	1:F:776:PRO:HA	1.76	0.68
1:E:194:SER:HB2	1:E:200:LEU:HD23	1.76	0.68
1:B:148:MET:HE1	1:B:355:PHE:CZ	2.29	0.67
1:A:1287:LEU:HD22	1:D:158:LEU:CD2	2.21	0.67
1:F:528:ASN:ND2	1:F:530:TRP:HE3	1.89	0.67
1:F:988:ASP:OD2	1:F:991:SER:O	2.12	0.67
1:D:994:SER:HB2	1:D:1137:MET:HE2	1.75	0.67
1:F:194:SER:HB2	1:F:200:LEU:HD23	1.75	0.67
1:A:1266:THR:HG21	1:C:1264:LEU:CD1	2.13	0.67
1:C:1264:LEU:HD13	1:C:1284:TYR:CE1	2.28	0.67
1:E:923:ILE:HG22	1:E:1140:LEU:HD23	1.76	0.67
1:A:769:PRO:HA	1:A:776:PRO:HA	1.76	0.67
1:F:1263:ARG:HG3	1:F:1264:LEU:HD12	1.76	0.67
1:E:1264:LEU:HD13	1:E:1284:TYR:CE2	2.30	0.67
1:E:1305:ILE:HD11	1:E:1317:ARG:HB3	1.76	0.67
1:B:1263:ARG:HG3	1:B:1264:LEU:HD12	1.77	0.67
1:B:194:SER:HB2	1:B:200:LEU:HD23	1.77	0.66
1:A:1263:ARG:HG3	1:A:1264:LEU:HD12	1.78	0.66
1:D:1263:ARG:HG3	1:D:1264:LEU:HD12	1.77	0.66
1:A:809:GLN:HG2	1:B:634:ASN:HB2	1.76	0.66
1:C:1305:ILE:HD11	1:C:1317:ARG:HB3	1.77	0.66
1:C:570:GLN:HG2	1:C:596:GLY:HA2	1.77	0.66
1:E:1263:ARG:HG3	1:E:1264:LEU:HD12	1.77	0.66
1:D:769:PRO:HA	1:D:776:PRO:HA	1.76	0.66
1:D:617:PHE:CD2	1:D:859:PHE:HD2	2.14	0.65
1:E:646:ASN:HB2	1:F:823:ASN:HA	1.77	0.65
1:E:988:ASP:OD2	1:E:991:SER:O	2.13	0.65
1:A:570:GLN:HG2	1:A:596:GLY:HA2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:769:PRO:HA	1:E:776:PRO:HA	1.77	0.65
1:D:95:ASN:HD21	1:D:125:GLN:HG3	1.62	0.65
1:F:1264:LEU:HD13	1:F:1284:TYR:CE1	2.31	0.65
1:A:194:SER:HB2	1:A:200:LEU:HD23	1.79	0.65
1:C:194:SER:HB2	1:C:200:LEU:HD23	1.78	0.65
1:B:777:PHE:O	1:B:795:THR:HG22	1.98	0.64
1:A:1097:ASN:HB3	1:A:1098:PRO:HD3	1.80	0.64
1:D:277:LEU:HD13	1:D:620:HIS:CD2	2.32	0.64
1:A:777:PHE:O	1:A:795:THR:HG22	1.98	0.63
1:D:217:ASN:HB3	1:D:220:VAL:HG23	1.80	0.63
1:D:244:SER:HB2	1:D:568:TYR:O	1.99	0.63
1:B:570:GLN:HG2	1:B:596:GLY:HA2	1.80	0.63
1:D:1264:LEU:HD13	1:D:1284:TYR:CE1	2.33	0.63
1:F:570:GLN:HG2	1:F:596:GLY:HA2	1.80	0.63
1:B:217:ASN:HB3	1:B:220:VAL:HG23	1.81	0.63
1:C:820:PHE:CE2	1:D:682:PHE:HE2	2.13	0.63
1:B:681:ASN:HB2	1:B:730:LEU:HD22	1.80	0.63
1:D:570:GLN:HG2	1:D:596:GLY:HA2	1.79	0.63
1:B:58:GLN:NE2	1:B:149:GLU:O	2.32	0.63
1:C:777:PHE:O	1:C:795:THR:HG22	1.99	0.63
1:C:1263:ARG:HG3	1:C:1264:LEU:HD12	1.80	0.63
1:A:244:SER:HB3	1:A:571:LEU:HB2	1.80	0.62
1:D:777:PHE:O	1:D:795:THR:HG22	1.99	0.62
1:B:244:SER:HB3	1:B:571:LEU:HB2	1.82	0.62
1:B:1264:LEU:HD13	1:B:1284:TYR:CE1	2.33	0.62
1:D:812:ASN:HD21	1:D:815:ASN:ND2	1.86	0.62
1:A:808:THR:HB	1:B:634:ASN:OD1	1.99	0.62
1:C:809:GLN:HE22	1:C:811:LEU:HD23	1.64	0.62
1:E:777:PHE:O	1:E:795:THR:HG22	2.00	0.62
1:F:1279:PHE:CE2	1:F:1301:ARG:HD3	2.33	0.62
1:B:834:TYR:OH	1:B:945:GLU:HG2	2.00	0.62
1:C:681:ASN:HB2	1:C:730:LEU:HD22	1.80	0.62
1:F:79:LYS:HD3	1:F:1232:PRO:HA	1.82	0.62
1:C:244:SER:HB3	1:C:571:LEU:HB2	1.82	0.62
1:E:1003:ASN:HB3	1:E:1102:PRO:HG2	1.82	0.62
1:B:244:SER:HB2	1:B:568:TYR:O	2.00	0.61
1:A:1003:ASN:HB3	1:A:1102:PRO:HG2	1.82	0.61
1:B:1248:THR:HB	1:B:1331:VAL:HG13	1.82	0.61
1:E:1279:PHE:HE1	1:E:1301:ARG:HD2	1.64	0.61
1:E:570:GLN:HG2	1:E:596:GLY:HA2	1.81	0.61
1:B:1033:ASP:OD1	1:B:1038:ARG:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1248:THR:HB	1:C:1331:VAL:HG13	1.83	0.61
1:D:1248:THR:HB	1:D:1331:VAL:HG13	1.82	0.61
1:C:217:ASN:HB3	1:C:220:VAL:HG23	1.82	0.61
1:E:244:SER:HB3	1:E:571:LEU:HB2	1.82	0.61
1:E:79:LYS:HD3	1:E:1232:PRO:HA	1.83	0.61
1:C:244:SER:HB2	1:C:568:TYR:O	2.01	0.61
1:A:1248:THR:HB	1:A:1331:VAL:HG13	1.83	0.61
1:C:1033:ASP:OD1	1:C:1038:ARG:HG3	2.00	0.61
1:F:1248:THR:HB	1:F:1331:VAL:HG13	1.83	0.61
1:A:217:ASN:HB3	1:A:220:VAL:HG23	1.82	0.61
1:C:811:LEU:HD11	1:C:895:ASN:O	2.01	0.61
1:F:244:SER:HB2	1:F:568:TYR:O	2.01	0.61
1:F:244:SER:HB3	1:F:571:LEU:HB2	1.82	0.61
1:F:1301:ARG:HG2	1:F:1328:PHE:HD2	1.63	0.61
1:F:777:PHE:O	1:F:795:THR:HG22	2.00	0.60
1:B:277:LEU:HD13	1:B:620:HIS:HE2	1.66	0.60
1:C:1003:ASN:HB3	1:C:1102:PRO:HG2	1.83	0.60
1:D:244:SER:HB3	1:D:571:LEU:HB2	1.83	0.60
1:C:537:MET:HE1	1:C:551:LEU:HD21	1.83	0.60
1:D:935:LYS:HB3	1:D:972:PHE:HD2	1.66	0.60
1:D:1003:ASN:HB3	1:D:1102:PRO:HG2	1.84	0.60
1:E:537:MET:HE1	1:E:551:LEU:HD21	1.82	0.60
1:E:742:ARG:HH12	1:F:1036:ARG:HH21	1.50	0.60
1:A:244:SER:HB2	1:A:568:TYR:O	2.01	0.60
1:D:79:LYS:HD3	1:D:1232:PRO:HA	1.84	0.60
1:E:852:PRO:HA	1:E:858:PRO:HA	1.84	0.60
1:F:1003:ASN:HB3	1:F:1102:PRO:HG2	1.83	0.60
1:C:94:GLN:HA	1:C:94:GLN:HE21	1.67	0.59
1:C:457:MET:HA	1:C:465:PHE:O	2.02	0.59
1:C:817:ARG:HG2	1:C:817:ARG:HH21	1.67	0.59
1:E:457:MET:HA	1:E:465:PHE:O	2.02	0.59
1:F:217:ASN:HB3	1:F:220:VAL:HG23	1.84	0.59
1:B:148:MET:HE1	1:B:355:PHE:HZ	1.66	0.59
1:A:79:LYS:HD3	1:A:1232:PRO:HA	1.85	0.59
1:C:105:LYS:HZ2	1:C:105:LYS:HB2	1.66	0.59
1:D:614:GLY:HA3	1:D:854:ASN:HD21	1.67	0.59
1:F:457:MET:HA	1:F:465:PHE:O	2.01	0.59
1:E:244:SER:HB2	1:E:568:TYR:O	2.02	0.59
1:C:810:HIS:NE2	1:C:814:GLU:HA	2.18	0.59
1:F:1301:ARG:HG2	1:F:1328:PHE:HE2	1.64	0.59
1:B:457:MET:HA	1:B:465:PHE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:834:TYR:OH	1:D:945:GLU:HG2	2.03	0.59
1:F:1033:ASP:OD1	1:F:1038:ARG:HG3	2.02	0.59
1:A:817:ARG:HG2	1:A:817:ARG:HH21	1.68	0.59
1:F:537:MET:HE1	1:F:551:LEU:HD21	1.85	0.59
1:B:1003:ASN:HB3	1:B:1102:PRO:HG2	1.85	0.58
1:E:217:ASN:HB3	1:E:220:VAL:HG23	1.84	0.58
1:C:122:LEU:HB3	1:C:126:GLN:HE21	1.68	0.58
1:E:742:ARG:HH12	1:F:1036:ARG:NH2	2.01	0.58
1:A:681:ASN:HB2	1:A:730:LEU:HD22	1.85	0.58
1:A:852:PRO:HA	1:A:858:PRO:HA	1.85	0.58
1:C:852:PRO:HA	1:C:858:PRO:HA	1.84	0.58
1:A:667:PHE:CE2	1:B:816:THR:HG23	2.38	0.58
1:A:59:GLN:HB2	1:A:142:ASP:O	2.03	0.58
1:D:457:MET:HA	1:D:465:PHE:O	2.03	0.58
1:D:811:LEU:HA	1:D:817:ARG:HH11	1.67	0.58
1:F:852:PRO:HA	1:F:858:PRO:HA	1.84	0.58
1:B:79:LYS:HD3	1:B:1232:PRO:HA	1.85	0.58
1:E:476:MET:HE3	1:E:479:THR:HG21	1.84	0.58
1:F:681:ASN:HB2	1:F:730:LEU:HD22	1.86	0.58
1:E:681:ASN:HB2	1:E:730:LEU:HD22	1.85	0.58
1:A:457:MET:HA	1:A:465:PHE:O	2.04	0.58
1:C:513:ILE:HD12	1:C:515:PRO:HD2	1.86	0.58
1:D:813:LYS:HA	1:D:817:ARG:HH12	1.69	0.58
1:F:1261:PHE:HE1	1:F:1345:PRO:HA	1.69	0.57
1:B:852:PRO:HA	1:B:858:PRO:HA	1.85	0.57
1:D:646:ASN:HD22	1:D:651:LYS:HA	1.70	0.57
1:D:809:GLN:CG	1:D:894:ILE:HG21	2.34	0.57
1:C:105:LYS:HB2	1:C:105:LYS:NZ	2.19	0.57
1:D:852:PRO:HA	1:D:858:PRO:HA	1.87	0.57
1:B:804:LYS:H	1:B:804:LYS:HD3	1.70	0.57
1:C:834:TYR:OH	1:C:945:GLU:HG2	2.05	0.57
1:D:95:ASN:ND2	1:D:125:GLN:HG3	2.18	0.57
1:D:277:LEU:HD13	1:D:620:HIS:HE2	1.64	0.57
1:E:834:TYR:OH	1:E:945:GLU:HG2	2.05	0.57
1:C:939:GLN:HE21	1:C:950:ASN:HD22	1.53	0.57
1:B:1295:PHE:HE2	1:B:1300:ILE:HG12	1.69	0.57
1:C:79:LYS:HD3	1:C:1232:PRO:HA	1.86	0.57
1:C:819:VAL:HG23	1:C:820:PHE:HD1	1.70	0.57
1:D:614:GLY:HA3	1:D:854:ASN:ND2	2.20	0.57
1:F:58:GLN:OE1	1:F:149:GLU:HB3	2.04	0.56
1:F:834:TYR:OH	1:F:945:GLU:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:THR:CG2	1:D:814:GLU:OE2	2.52	0.56
1:D:804:LYS:H	1:D:804:LYS:HD3	1.68	0.56
1:A:646:ASN:HD22	1:A:651:LYS:HA	1.71	0.56
1:C:199:ASN:O	1:C:344:TYR:HA	2.05	0.56
1:D:681:ASN:HB2	1:D:730:LEU:HD22	1.86	0.56
1:D:1295:PHE:HE2	1:D:1300:ILE:HG12	1.69	0.56
1:C:1096:THR:HG22	1:C:1098:PRO:HD2	1.87	0.56
1:A:834:TYR:OH	1:A:945:GLU:HG2	2.05	0.56
1:A:939:GLN:HE21	1:A:950:ASN:HD22	1.53	0.56
1:C:820:PHE:CE2	1:D:682:PHE:CE2	2.93	0.56
1:E:1295:PHE:HE2	1:E:1300:ILE:HG12	1.71	0.56
1:F:646:ASN:HD22	1:F:651:LYS:HA	1.71	0.56
1:A:1264:LEU:CG	1:C:1283:GLN:HB2	2.20	0.56
1:B:646:ASN:HD22	1:B:651:LYS:HA	1.71	0.56
1:C:646:ASN:HD22	1:C:651:LYS:HA	1.71	0.56
1:D:513:ILE:HD12	1:D:515:PRO:HD2	1.86	0.56
1:F:1335:SER:HB3	1:F:1338:GLY:O	2.06	0.56
1:D:1030:THR:HB	1:D:1045:THR:OG1	2.06	0.56
1:D:122:LEU:HB3	1:D:126:GLN:HE21	1.71	0.56
1:E:1248:THR:HB	1:E:1331:VAL:HG13	1.86	0.56
1:B:1261:PHE:HE1	1:B:1345:PRO:HA	1.71	0.55
1:E:646:ASN:HD22	1:E:651:LYS:HA	1.71	0.55
1:F:1218:PHE:HE2	1:F:1220:LYS:HG2	1.71	0.55
1:B:770:TRP:HE3	1:B:773:ASN:HB2	1.71	0.55
1:E:58:GLN:OE1	1:E:149:GLU:HB3	2.05	0.55
1:E:255:LYS:HD2	1:E:609:LEU:HB2	1.89	0.55
1:A:255:LYS:HD2	1:A:609:LEU:HB2	1.89	0.55
1:A:813:LYS:HA	1:B:817:ARG:HG2	1.88	0.55
1:E:695:ALA:HB3	1:E:751:THR:HG22	1.89	0.55
1:F:134:ASP:HB3	1:F:140:LEU:HD21	1.89	0.55
1:F:695:ALA:HB3	1:F:751:THR:HG22	1.89	0.55
1:F:939:GLN:HE21	1:F:950:ASN:HD22	1.55	0.55
1:A:1109:PRO:CG	1:A:1137:MET:HE1	2.37	0.55
1:D:813:LYS:CA	1:D:817:ARG:HH12	2.18	0.55
1:B:1115:TYR:HE1	1:B:1125:ILE:HG21	1.72	0.55
1:A:122:LEU:HB3	1:A:126:GLN:HE21	1.71	0.55
1:C:255:LYS:HD2	1:C:609:LEU:HB2	1.88	0.55
1:F:770:TRP:HE3	1:F:773:ASN:HB2	1.72	0.55
1:A:77:SER:HA	1:A:89:GLY:HA2	1.89	0.54
1:B:199:ASN:O	1:B:344:TYR:HA	2.07	0.54
1:C:1030:THR:HB	1:C:1045:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:TRP:HE3	1:A:773:ASN:HB2	1.72	0.54
1:B:1335:SER:HB3	1:B:1338:GLY:O	2.07	0.54
1:E:1335:SER:HB3	1:E:1338:GLY:O	2.07	0.54
1:F:255:LYS:HD2	1:F:609:LEU:HB2	1.88	0.54
1:A:1295:PHE:HE2	1:A:1300:ILE:HG12	1.71	0.54
1:E:68:TRP:CD1	1:E:92:ARG:HB2	2.43	0.54
1:A:58:GLN:OE1	1:A:149:GLU:HB3	2.06	0.54
1:B:924:ASN:HB2	1:B:985:PHE:HA	1.90	0.54
1:D:770:TRP:HE3	1:D:773:ASN:HB2	1.72	0.54
1:E:134:ASP:HB3	1:E:140:LEU:HD21	1.89	0.54
1:C:614:GLY:HA3	1:C:854:ASN:HD21	1.73	0.54
1:A:199:ASN:O	1:A:344:TYR:HA	2.07	0.54
1:A:1335:SER:HB3	1:A:1338:GLY:O	2.08	0.54
1:C:1335:SER:HB3	1:C:1338:GLY:O	2.08	0.54
1:F:122:LEU:HB3	1:F:126:GLN:HE21	1.73	0.54
1:C:924:ASN:HB2	1:C:985:PHE:HA	1.89	0.54
1:E:770:TRP:HE3	1:E:773:ASN:HB2	1.72	0.54
1:E:939:GLN:HE21	1:E:950:ASN:HD22	1.55	0.54
1:B:65:LEU:HB3	1:B:91:VAL:HG13	1.90	0.54
1:E:823:ASN:HA	1:F:646:ASN:HB2	1.90	0.54
1:A:98:LEU:O	1:A:99:ASN:C	2.49	0.53
1:B:122:LEU:HB3	1:B:126:GLN:HE21	1.72	0.53
1:E:199:ASN:O	1:E:344:TYR:HA	2.08	0.53
1:F:1295:PHE:HE2	1:F:1300:ILE:HG12	1.72	0.53
1:B:1143:LEU:HD23	1:B:1149:ILE:HG12	1.89	0.53
1:B:1030:THR:HB	1:B:1045:THR:OG1	2.08	0.53
1:A:529:ARG:HB2	1:A:715:GLU:O	2.08	0.53
1:A:1218:PHE:HE2	1:A:1220:LYS:HG2	1.73	0.53
1:D:134:ASP:HB3	1:D:140:LEU:HD21	1.91	0.53
1:E:321:TRP:HE1	1:E:476:MET:CE	2.21	0.53
1:E:321:TRP:HE1	1:E:476:MET:HE1	1.73	0.53
1:A:134:ASP:HB3	1:A:140:LEU:HD21	1.91	0.53
1:B:939:GLN:HE21	1:B:950:ASN:HD22	1.55	0.53
1:B:1218:PHE:HE2	1:B:1220:LYS:HG2	1.73	0.53
1:C:77:SER:HA	1:C:89:GLY:HA2	1.91	0.53
1:C:614:GLY:HA3	1:C:854:ASN:ND2	2.24	0.53
1:C:770:TRP:HE3	1:C:773:ASN:HB2	1.73	0.53
1:D:924:ASN:HB2	1:D:985:PHE:HA	1.89	0.53
1:E:1218:PHE:HE2	1:E:1220:LYS:HG2	1.73	0.53
1:D:255:LYS:HD2	1:D:609:LEU:HB2	1.90	0.53
1:B:134:ASP:HB3	1:B:140:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:ALA:HB3	1:B:751:THR:HG22	1.91	0.53
1:C:668:ASN:ND2	1:D:816:THR:OG1	2.36	0.53
1:D:812:ASN:H	1:D:817:ARG:HH11	1.56	0.53
1:D:846:PRO:HG2	1:D:849:GLN:HE22	1.73	0.53
1:C:1143:LEU:HD23	1:C:1149:ILE:HG12	1.91	0.53
1:D:939:GLN:HE21	1:D:950:ASN:HD22	1.56	0.53
1:F:65:LEU:HB3	1:F:91:VAL:HG13	1.91	0.53
1:F:924:ASN:HB2	1:F:985:PHE:HA	1.91	0.53
1:A:924:ASN:HB2	1:A:985:PHE:HA	1.91	0.52
1:C:134:ASP:HB3	1:C:140:LEU:HD21	1.91	0.52
1:D:396:THR:HG21	1:D:404:ARG:HE	1.75	0.52
1:E:1030:THR:HB	1:E:1045:THR:OG1	2.09	0.52
1:F:817:ARG:HG2	1:F:817:ARG:HH21	1.73	0.52
1:A:513:ILE:HD12	1:A:515:PRO:HD2	1.91	0.52
1:D:695:ALA:HB3	1:D:751:THR:HG22	1.92	0.52
1:C:808:THR:CB	1:D:634:ASN:OD1	2.53	0.52
1:D:1335:SER:HB3	1:D:1338:GLY:O	2.09	0.52
1:E:77:SER:HA	1:E:89:GLY:HA2	1.91	0.52
1:E:924:ASN:HB2	1:E:985:PHE:HA	1.91	0.52
1:F:513:ILE:HD12	1:F:515:PRO:HD2	1.91	0.52
1:F:1030:THR:HB	1:F:1045:THR:OG1	2.09	0.52
1:B:255:LYS:HD2	1:B:609:LEU:HB2	1.90	0.52
1:C:248:ASP:HB2	1:C:301:LYS:HB2	1.92	0.52
1:D:199:ASN:O	1:D:344:TYR:HA	2.08	0.52
1:E:1003:ASN:HD21	1:E:1146:THR:HG21	1.74	0.52
1:F:199:ASN:O	1:F:344:TYR:HA	2.09	0.52
1:D:816:THR:HB	1:D:819:VAL:HG22	1.92	0.52
1:D:1218:PHE:HE2	1:D:1220:LYS:HG2	1.73	0.52
1:C:846:PRO:HG2	1:C:849:GLN:HE22	1.73	0.52
1:C:892:ASP:HA	1:C:900:THR:HG23	1.92	0.52
1:D:248:ASP:HB2	1:D:301:LYS:HB2	1.92	0.52
1:B:228:LYS:HE2	1:B:230:THR:HB	1.91	0.52
1:B:248:ASP:HB2	1:B:301:LYS:HB2	1.92	0.52
1:D:1313:THR:HG22	1:D:1344:GLN:HG3	1.91	0.52
1:A:695:ALA:HB3	1:A:751:THR:HG22	1.92	0.51
1:C:1295:PHE:HE2	1:C:1300:ILE:HG12	1.73	0.51
1:F:68:TRP:CD1	1:F:92:ARG:HB2	2.45	0.51
1:F:846:PRO:HG2	1:F:849:GLN:HE22	1.74	0.51
1:A:68:TRP:CD1	1:A:92:ARG:HB2	2.45	0.51
1:B:529:ARG:HB2	1:B:715:GLU:O	2.10	0.51
1:D:77:SER:HA	1:D:89:GLY:HA2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:ARG:HB2	1:D:715:GLU:O	2.10	0.51
1:D:809:GLN:HG3	1:D:894:ILE:HG21	1.92	0.51
1:E:846:PRO:HG2	1:E:849:GLN:HE22	1.74	0.51
1:A:65:LEU:HB3	1:A:91:VAL:HG13	1.92	0.51
1:B:846:PRO:HG2	1:B:849:GLN:HE22	1.74	0.51
1:C:695:ALA:HB3	1:C:751:THR:HG22	1.91	0.51
1:F:529:ARG:HB2	1:F:715:GLU:O	2.09	0.51
1:B:59:GLN:HB2	1:B:143:ILE:H	1.76	0.51
1:F:1003:ASN:HD21	1:F:1146:THR:HG21	1.76	0.51
1:A:1261:PHE:HE1	1:A:1345:PRO:HA	1.76	0.51
1:B:68:TRP:CD1	1:B:92:ARG:HB2	2.46	0.51
1:E:513:ILE:HD12	1:E:515:PRO:HD2	1.93	0.51
1:A:897:LEU:CD2	1:B:816:THR:HG21	2.41	0.51
1:B:834:TYR:CZ	1:B:945:GLU:HG2	2.46	0.51
1:C:1003:ASN:HD21	1:C:1146:THR:HG21	1.76	0.51
1:E:122:LEU:HB3	1:E:126:GLN:HE21	1.74	0.51
1:B:1014:VAL:O	1:B:1069:LEU:HD22	2.11	0.51
1:C:529:ARG:HB2	1:C:715:GLU:O	2.11	0.51
1:B:817:ARG:HB3	1:B:818:TRP:CD1	2.46	0.51
1:D:58:GLN:OE1	1:D:149:GLU:HB3	2.11	0.51
1:D:65:LEU:HB3	1:D:91:VAL:HG13	1.93	0.50
1:D:834:TYR:CZ	1:D:945:GLU:HG2	2.47	0.50
1:F:77:SER:HA	1:F:89:GLY:HA2	1.93	0.50
1:B:112:LEU:HD11	1:B:333:GLU:HG2	1.92	0.50
1:D:68:TRP:CD1	1:D:92:ARG:HB2	2.46	0.50
1:F:1027:TRP:CE3	1:F:1046:LEU:HB3	2.47	0.50
1:A:1003:ASN:HD21	1:A:1146:THR:HG21	1.75	0.50
1:C:65:LEU:HB3	1:C:91:VAL:HG13	1.92	0.50
1:D:809:GLN:HG3	1:D:894:ILE:CG2	2.41	0.50
1:D:812:ASN:CG	1:D:815:ASN:ND2	2.69	0.50
1:E:529:ARG:HB2	1:E:715:GLU:O	2.10	0.50
1:E:834:TYR:CZ	1:E:945:GLU:HG2	2.47	0.50
1:B:892:ASP:HA	1:B:900:THR:HG23	1.93	0.50
1:C:98:LEU:O	1:C:98:LEU:HD12	2.11	0.50
1:D:186:LYS:HB3	1:D:205:LEU:HB3	1.94	0.50
1:A:154:VAL:HG23	1:A:170:PHE:HB3	1.94	0.50
1:A:504:PRO:HG2	1:A:507:VAL:HG23	1.94	0.50
1:E:1027:TRP:CE3	1:E:1046:LEU:HB3	2.46	0.50
1:E:1261:PHE:HE1	1:E:1345:PRO:HA	1.77	0.50
1:A:377:PRO:HG3	1:A:443:ILE:HG13	1.94	0.50
1:A:396:THR:HG21	1:A:404:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:ASP:HA	1:A:900:THR:HG23	1.93	0.50
1:A:1027:TRP:CE3	1:A:1046:LEU:HB3	2.46	0.50
1:B:513:ILE:HD12	1:B:515:PRO:HD2	1.93	0.50
1:B:869:THR:HG22	1:B:875:SER:OG	2.11	0.50
1:C:1261:PHE:HE1	1:C:1345:PRO:HA	1.76	0.50
1:D:276:ALA:HB2	1:D:655:PRO:HD3	1.93	0.50
1:D:810:HIS:CD2	1:D:818:TRP:HZ3	2.26	0.50
1:E:614:GLY:HA3	1:E:854:ASN:HD21	1.77	0.50
1:E:742:ARG:NH1	1:F:1036:ARG:HH21	2.09	0.50
1:C:1027:TRP:CE3	1:C:1046:LEU:HB3	2.46	0.50
1:A:186:LYS:HB3	1:A:205:LEU:HB3	1.94	0.50
1:A:254:GLU:O	1:A:297:LYS:HB3	2.12	0.50
1:C:396:THR:HG21	1:C:404:ARG:HE	1.77	0.50
1:C:674:THR:CB	1:D:814:GLU:OE2	2.59	0.50
1:E:892:ASP:HA	1:E:900:THR:HG23	1.93	0.50
1:F:892:ASP:HA	1:F:900:THR:HG23	1.93	0.50
1:F:254:GLU:O	1:F:297:LYS:HB3	2.12	0.49
1:E:371:PRO:HD2	1:E:374:TRP:CD2	2.47	0.49
1:B:77:SER:HA	1:B:89:GLY:HA2	1.94	0.49
1:B:396:THR:HG21	1:B:404:ARG:HE	1.77	0.49
1:E:65:LEU:HB3	1:E:91:VAL:HG13	1.92	0.49
1:A:926:SER:O	1:A:983:ILE:HG12	2.12	0.49
1:B:813:LYS:HA	1:B:817:ARG:HH22	1.78	0.49
1:C:254:GLU:O	1:C:297:LYS:HB3	2.12	0.49
1:F:614:GLY:HA3	1:F:854:ASN:HD21	1.77	0.49
1:A:112:LEU:HD11	1:A:333:GLU:HG2	1.93	0.49
1:A:327:THR:HG21	1:A:367:VAL:HG21	1.95	0.49
1:A:834:TYR:CZ	1:A:945:GLU:HG2	2.48	0.49
1:B:1226:THR:H	1:B:1238:ASN:ND2	2.03	0.49
1:C:58:GLN:OE1	1:C:149:GLU:HB3	2.13	0.49
1:C:834:TYR:CZ	1:C:945:GLU:HG2	2.47	0.49
1:D:327:THR:HG21	1:D:367:VAL:HG21	1.94	0.49
1:D:812:ASN:H	1:D:817:ARG:NH1	2.10	0.49
1:D:1143:LEU:HD23	1:D:1149:ILE:HG12	1.95	0.49
1:E:59:GLN:HB2	1:E:143:ILE:H	1.78	0.49
1:A:1143:LEU:HD23	1:A:1149:ILE:HG12	1.94	0.49
1:D:112:LEU:HD11	1:D:333:GLU:HG2	1.93	0.49
1:A:846:PRO:HG2	1:A:849:GLN:HE22	1.77	0.49
1:C:68:TRP:CD1	1:C:92:ARG:HB2	2.47	0.49
1:B:1003:ASN:HD21	1:B:1146:THR:HG21	1.77	0.49
1:C:391:ASN:HD22	1:C:418:ASN:HD22	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:811:LEU:CD1	1:D:894:ILE:CG1	2.88	0.49
1:D:1027:TRP:CE3	1:D:1046:LEU:HB3	2.47	0.49
1:F:777:PHE:HB3	1:F:795:THR:CG2	2.43	0.49
1:B:466:ILE:HB	1:B:487:PHE:HB2	1.94	0.49
1:C:371:PRO:HD2	1:C:374:TRP:CD2	2.48	0.49
1:D:254:GLU:O	1:D:297:LYS:HB3	2.12	0.49
1:D:275:LYS:HG2	1:D:644:TYR:HE1	1.78	0.49
1:B:186:LYS:HB3	1:B:205:LEU:HB3	1.95	0.49
1:B:987:ALA:HA	1:B:1115:TYR:CE2	2.48	0.49
1:E:466:ILE:HB	1:E:487:PHE:HB2	1.95	0.49
1:F:396:THR:HG21	1:F:404:ARG:HE	1.78	0.49
1:D:777:PHE:HB3	1:D:795:THR:CG2	2.43	0.48
1:E:557:MET:HB3	1:E:557:MET:HE2	1.50	0.48
1:C:777:PHE:HB3	1:C:795:THR:CG2	2.43	0.48
1:E:1143:LEU:HD23	1:E:1149:ILE:HG12	1.95	0.48
1:F:59:GLN:HB2	1:F:143:ILE:H	1.78	0.48
1:F:834:TYR:CZ	1:F:945:GLU:HG2	2.47	0.48
1:D:391:ASN:HD22	1:D:418:ASN:HD22	1.62	0.48
1:A:651:LYS:CE	1:B:823:ASN:HD21	2.26	0.48
1:B:987:ALA:CB	1:B:1115:TYR:CD2	2.96	0.48
1:E:112:LEU:HD11	1:E:333:GLU:HG2	1.95	0.48
1:B:809:GLN:HB3	1:B:826:PRO:HB2	1.95	0.48
1:C:277:LEU:HB2	1:C:653:VAL:HB	1.96	0.48
1:D:1003:ASN:HD21	1:D:1146:THR:HG21	1.79	0.48
1:E:154:VAL:HG23	1:E:170:PHE:HB3	1.96	0.48
1:E:777:PHE:HB3	1:E:795:THR:CG2	2.44	0.48
1:B:617:PHE:CE2	1:B:859:PHE:HB2	2.48	0.48
1:B:1312:GLN:O	1:B:1345:PRO:HD2	2.13	0.48
1:C:466:ILE:HB	1:C:487:PHE:HB2	1.95	0.48
1:C:1143:LEU:O	1:C:1149:ILE:HD11	2.14	0.48
1:E:524:PRO:HD2	1:E:557:MET:HE1	1.95	0.48
1:F:276:ALA:HB2	1:F:655:PRO:HD3	1.96	0.48
1:A:1097:ASN:CB	1:A:1098:PRO:CD	2.90	0.48
1:A:1109:PRO:HG3	1:A:1137:MET:HE1	1.95	0.48
1:A:277:LEU:HB2	1:A:653:VAL:HB	1.96	0.48
1:B:58:GLN:OE1	1:B:149:GLU:HB3	2.13	0.48
1:B:520:LEU:HD23	1:B:757:ASP:HA	1.95	0.48
1:C:186:LYS:HB3	1:C:205:LEU:HB3	1.96	0.48
1:D:154:VAL:HG23	1:D:170:PHE:HB3	1.95	0.48
1:D:892:ASP:HA	1:D:900:THR:HG23	1.95	0.48
1:F:112:LEU:HD11	1:F:333:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:GLU:O	1:E:297:LYS:HB3	2.13	0.48
1:F:1312:GLN:O	1:F:1345:PRO:HD2	2.14	0.48
1:B:806:MET:HB2	1:B:843:ASN:OD1	2.13	0.48
1:B:1027:TRP:CE3	1:B:1046:LEU:HB3	2.48	0.48
1:C:889:PRO:HD2	1:C:951:LEU:HD21	1.95	0.48
1:F:377:PRO:HB2	1:F:400:PHE:O	2.14	0.48
1:C:154:VAL:HG23	1:C:170:PHE:HB3	1.94	0.47
1:C:276:ALA:HB2	1:C:655:PRO:HD3	1.96	0.47
1:C:377:PRO:HG3	1:C:443:ILE:HG13	1.95	0.47
1:E:396:THR:HG21	1:E:404:ARG:HE	1.79	0.47
1:A:245:PRO:HG2	1:A:568:TYR:HB2	1.96	0.47
1:C:327:THR:HG21	1:C:367:VAL:HG21	1.96	0.47
1:D:371:PRO:HD2	1:D:374:TRP:CD2	2.49	0.47
1:F:186:LYS:HB3	1:F:205:LEU:HB3	1.96	0.47
1:A:391:ASN:HD22	1:A:418:ASN:HD22	1.62	0.47
1:B:276:ALA:HB2	1:B:655:PRO:HD3	1.96	0.47
1:B:377:PRO:HB2	1:B:400:PHE:O	2.14	0.47
1:C:112:LEU:HD11	1:C:333:GLU:HG2	1.96	0.47
1:C:994:SER:HB2	1:C:1137:MET:CE	2.42	0.47
1:E:231:GLN:HG3	1:E:1096:THR:HA	1.97	0.47
1:F:371:PRO:HD2	1:F:374:TRP:CD2	2.48	0.47
1:C:245:PRO:HG2	1:C:568:TYR:HB2	1.97	0.47
1:C:520:LEU:HD23	1:C:757:ASP:HA	1.97	0.47
1:C:845:ILE:HG22	1:C:883:LEU:O	2.15	0.47
1:D:994:SER:HB2	1:D:1137:MET:CE	2.43	0.47
1:E:994:SER:HB2	1:E:1137:MET:CE	2.43	0.47
1:E:276:ALA:HB2	1:E:655:PRO:HD3	1.96	0.47
1:F:277:LEU:HB2	1:F:653:VAL:HB	1.96	0.47
1:A:614:GLY:HA3	1:A:854:ASN:HD21	1.80	0.47
1:B:254:GLU:O	1:B:297:LYS:HB3	2.14	0.47
1:D:59:GLN:HB2	1:D:143:ILE:H	1.79	0.47
1:F:377:PRO:HG3	1:F:443:ILE:HG13	1.97	0.47
1:A:277:LEU:HD21	1:A:610:GLN:HG3	1.97	0.47
1:B:777:PHE:HB3	1:B:795:THR:CG2	2.45	0.47
1:D:811:LEU:HD13	1:D:894:ILE:HG13	1.95	0.47
1:B:277:LEU:HD21	1:B:610:GLN:CG	2.45	0.47
1:E:186:LYS:HB3	1:E:205:LEU:HB3	1.97	0.47
1:E:277:LEU:HB2	1:E:653:VAL:HB	1.96	0.47
1:E:377:PRO:HB2	1:E:400:PHE:O	2.15	0.47
1:E:520:LEU:HD23	1:E:757:ASP:HA	1.96	0.47
1:E:614:GLY:HA3	1:E:854:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:PHE:HB3	1:A:795:THR:CG2	2.45	0.47
1:C:793:LEU:HD22	1:C:801:VAL:HG13	1.96	0.47
1:D:889:PRO:HD2	1:D:951:LEU:HD21	1.96	0.47
1:F:994:SER:HB2	1:F:1137:MET:CE	2.43	0.47
1:F:1261:PHE:CE1	1:F:1345:PRO:HA	2.50	0.47
1:A:570:GLN:HG2	1:A:596:GLY:CA	2.45	0.47
1:B:178:THR:O	1:B:358:VAL:HG11	2.15	0.47
1:B:391:ASN:HD22	1:B:418:ASN:HD22	1.62	0.47
1:E:889:PRO:HD2	1:E:951:LEU:HD21	1.97	0.47
1:E:1036:ARG:HH21	1:F:742:ARG:HH12	1.63	0.47
1:A:1143:LEU:O	1:A:1149:ILE:HD11	2.16	0.46
1:C:377:PRO:HB2	1:C:400:PHE:O	2.15	0.46
1:A:178:THR:O	1:A:358:VAL:HG11	2.15	0.46
1:A:371:PRO:HD2	1:A:374:TRP:CD2	2.50	0.46
1:A:466:ILE:HB	1:A:487:PHE:HB2	1.96	0.46
1:A:1013:VAL:HG11	1:A:1075:PRO:HB3	1.98	0.46
1:B:154:VAL:HG23	1:B:170:PHE:HB3	1.96	0.46
1:B:275:LYS:HG3	1:B:644:TYR:HE1	1.81	0.46
1:D:520:LEU:HD23	1:D:757:ASP:HA	1.97	0.46
1:E:448:GLU:H	1:E:448:GLU:HG2	1.48	0.46
1:F:1143:LEU:HD23	1:F:1149:ILE:HG12	1.95	0.46
1:A:559:ASP:OD2	1:A:562:THR:HB	2.16	0.46
1:E:1143:LEU:O	1:E:1149:ILE:HD11	2.15	0.46
1:F:889:PRO:HD2	1:F:951:LEU:HD21	1.97	0.46
1:B:1345:PRO:O	1:B:1346:PHE:HB2	2.15	0.46
1:D:845:ILE:HG22	1:D:883:LEU:O	2.16	0.46
1:A:770:TRP:CE3	1:A:773:ASN:HB2	2.51	0.46
1:A:793:LEU:HD22	1:A:801:VAL:HG13	1.97	0.46
1:B:277:LEU:HB2	1:B:653:VAL:HB	1.98	0.46
1:B:327:THR:HG21	1:B:367:VAL:HG21	1.97	0.46
1:B:373:SER:HB2	1:B:374:TRP:HD1	1.79	0.46
1:C:570:GLN:HG2	1:C:596:GLY:CA	2.46	0.46
1:C:710:ILE:HD11	1:C:712:TYR:CZ	2.49	0.46
1:C:1191:SER:HB2	1:C:1196:THR:HG23	1.98	0.46
1:E:228:LYS:NZ	1:E:1096:THR:HG21	2.30	0.46
1:E:327:THR:HG21	1:E:367:VAL:HG21	1.97	0.46
1:E:1036:ARG:NH2	1:F:742:ARG:HH12	2.13	0.46
1:A:92:ARG:HG3	1:A:128:PHE:CE1	2.51	0.46
1:C:945:GLU:H	1:C:945:GLU:HG3	1.24	0.46
1:D:277:LEU:HD21	1:D:610:GLN:CG	2.45	0.46
1:F:162:PRO:HG3	1:F:344:TYR:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:HG3	1:A:644:TYR:HE1	1.81	0.46
1:A:276:ALA:HB2	1:A:655:PRO:HD3	1.97	0.46
1:F:614:GLY:HA3	1:F:854:ASN:ND2	2.31	0.46
1:A:983:ILE:HD11	1:A:1152:LYS:HD2	1.98	0.46
1:C:281:VAL:HG22	1:C:293:ASN:HA	1.98	0.46
1:D:281:VAL:HG22	1:D:293:ASN:HA	1.98	0.46
1:D:373:SER:HB2	1:D:374:TRP:HD1	1.81	0.46
1:E:177:PRO:HG2	1:E:180:TRP:CE3	2.51	0.46
1:F:1143:LEU:O	1:F:1149:ILE:HD11	2.15	0.46
1:A:377:PRO:HB2	1:A:400:PHE:O	2.16	0.46
1:A:1286:PRO:HG2	1:D:158:LEU:HD22	1.97	0.46
1:D:817:ARG:N	1:D:817:ARG:HD2	2.30	0.46
1:E:275:LYS:HG3	1:E:644:TYR:HE1	1.81	0.46
1:E:504:PRO:HG2	1:E:507:VAL:HG23	1.97	0.46
1:F:245:PRO:HG2	1:F:568:TYR:HB2	1.98	0.46
1:F:504:PRO:HG2	1:F:507:VAL:HG23	1.98	0.46
1:A:1134:ALA:CA	1:A:1137:MET:HE2	2.26	0.46
1:B:377:PRO:HG3	1:B:443:ILE:HG13	1.98	0.46
1:D:524:PRO:HD3	1:D:905:PRO:HG3	1.98	0.46
1:E:391:ASN:HD22	1:E:418:ASN:HD22	1.64	0.46
1:A:277:LEU:HD21	1:A:610:GLN:CG	2.47	0.45
1:B:277:LEU:HD21	1:B:610:GLN:HG3	1.98	0.45
1:B:770:TRP:CE3	1:B:773:ASN:HB2	2.50	0.45
1:B:889:PRO:HD2	1:B:951:LEU:HD21	1.98	0.45
1:D:377:PRO:HB2	1:D:400:PHE:O	2.16	0.45
1:D:861:PRO:HB3	1:D:879:THR:HG21	1.98	0.45
1:E:1274:ASP:CB	1:E:1277:THR:HG22	2.41	0.45
1:F:154:VAL:HG23	1:F:170:PHE:HB3	1.97	0.45
1:F:520:LEU:HD23	1:F:757:ASP:HA	1.96	0.45
1:A:614:GLY:HA3	1:A:854:ASN:ND2	2.30	0.45
1:A:845:ILE:HG22	1:A:883:LEU:O	2.17	0.45
1:A:889:PRO:HD2	1:A:951:LEU:HD21	1.98	0.45
1:B:371:PRO:HD2	1:B:374:TRP:CD2	2.51	0.45
1:C:749:ARG:NH1	1:C:1034:PHE:O	2.49	0.45
1:D:396:THR:CG2	1:D:404:ARG:HE	2.29	0.45
1:D:570:GLN:HG2	1:D:596:GLY:CA	2.44	0.45
1:E:178:THR:O	1:E:358:VAL:HG11	2.16	0.45
1:F:277:LEU:HD21	1:F:610:GLN:HG3	1.98	0.45
1:F:841:GLN:HE22	1:F:843:ASN:HB2	1.81	0.45
1:A:115:LEU:HD11	1:A:324:LEU:HD13	1.99	0.45
1:C:524:PRO:HD3	1:C:905:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1008:ASP:HB3	1:E:1061:TRP:CD1	2.52	0.45
1:F:1112:VAL:HA	1:F:1127:PRO:HA	1.99	0.45
1:B:115:LEU:HD11	1:B:324:LEU:HD13	1.98	0.45
1:B:277:LEU:HD22	1:B:620:HIS:CD2	2.51	0.45
1:D:770:TRP:CE3	1:D:773:ASN:HB2	2.51	0.45
1:D:1013:VAL:HG11	1:D:1075:PRO:HB3	1.99	0.45
1:D:377:PRO:HG3	1:D:443:ILE:HG13	1.98	0.45
1:D:466:ILE:HB	1:D:487:PHE:HB2	1.97	0.45
1:F:1269:VAL:HA	1:F:1272:LEU:HD12	1.99	0.45
1:A:448:GLU:H	1:A:448:GLU:HG2	1.46	0.45
1:B:245:PRO:HG2	1:B:568:TYR:HB2	1.99	0.45
1:B:281:VAL:HG22	1:B:293:ASN:HA	1.99	0.45
1:B:1112:VAL:HA	1:B:1127:PRO:HA	1.99	0.45
1:B:1191:SER:HB2	1:B:1196:THR:HG23	1.98	0.45
1:D:1312:GLN:O	1:D:1345:PRO:HD2	2.17	0.45
1:E:377:PRO:HG3	1:E:443:ILE:HG13	1.97	0.45
1:E:770:TRP:CE3	1:E:773:ASN:HB2	2.50	0.45
1:F:391:ASN:HD22	1:F:418:ASN:HD22	1.64	0.45
1:A:281:VAL:HG22	1:A:293:ASN:HA	1.99	0.45
1:B:504:PRO:HG2	1:B:507:VAL:HG23	1.99	0.45
1:C:275:LYS:HG3	1:C:644:TYR:HE1	1.80	0.45
1:C:1269:VAL:HA	1:C:1272:LEU:HD12	1.98	0.45
1:D:277:LEU:HD22	1:D:620:HIS:CD2	2.52	0.45
1:E:162:PRO:HG3	1:E:344:TYR:CE2	2.52	0.45
1:E:524:PRO:HD3	1:E:905:PRO:HG3	1.97	0.45
1:E:841:GLN:HE22	1:E:843:ASN:HB2	1.82	0.45
1:F:1321:LYS:HB2	1:F:1328:PHE:CE1	2.52	0.45
1:C:115:LEU:HD11	1:C:324:LEU:HD13	1.98	0.45
1:C:841:GLN:HE22	1:C:843:ASN:HB2	1.81	0.45
1:D:793:LEU:HD22	1:D:801:VAL:HG13	1.98	0.45
1:E:245:PRO:HG2	1:E:568:TYR:HB2	1.98	0.45
1:F:793:LEU:HD22	1:F:801:VAL:HG13	1.99	0.45
1:A:520:LEU:HD23	1:A:757:ASP:HA	1.99	0.45
1:C:651:LYS:HE3	1:D:823:ASN:HD21	1.82	0.45
1:D:1143:LEU:O	1:D:1149:ILE:HD11	2.17	0.45
1:E:277:LEU:HD21	1:E:610:GLN:HG3	1.98	0.45
1:F:570:GLN:HG2	1:F:596:GLY:CA	2.46	0.45
1:C:770:TRP:CE3	1:C:773:ASN:HB2	2.51	0.45
1:F:178:THR:O	1:F:358:VAL:HG11	2.16	0.45
1:F:277:LEU:HD21	1:F:610:GLN:CG	2.46	0.45
1:A:732:LEU:HD13	1:A:732:LEU:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:PHE:CG	1:B:542:VAL:HG21	2.52	0.44
1:D:811:LEU:HD23	1:D:817:ARG:CZ	2.48	0.44
1:E:277:LEU:HD21	1:E:610:GLN:CG	2.46	0.44
1:E:1269:VAL:HA	1:E:1272:LEU:HD12	1.99	0.44
1:F:845:ILE:HG22	1:F:883:LEU:O	2.17	0.44
1:A:525:LEU:HD21	1:A:557:MET:HG2	1.98	0.44
1:A:749:ARG:NH1	1:A:1034:PHE:O	2.51	0.44
1:A:1003:ASN:ND2	1:A:1146:THR:HG21	2.32	0.44
1:B:628:ILE:HD12	1:B:657:ARG:HD3	1.99	0.44
1:D:162:PRO:HG3	1:D:344:TYR:CE2	2.52	0.44
1:F:373:SER:HB2	1:F:374:TRP:HD1	1.82	0.44
1:F:466:ILE:HB	1:F:487:PHE:HB2	1.97	0.44
1:F:1013:VAL:HG11	1:F:1075:PRO:HB3	1.99	0.44
1:A:524:PRO:HD3	1:A:905:PRO:HG3	2.00	0.44
1:A:710:ILE:HD11	1:A:712:TYR:CZ	2.52	0.44
1:A:792:PRO:HG3	1:A:967:HIS:CE1	2.53	0.44
1:A:1112:VAL:HA	1:A:1127:PRO:HA	1.98	0.44
1:B:162:PRO:HG3	1:B:344:TYR:CE2	2.53	0.44
1:B:994:SER:HB2	1:B:1137:MET:CE	2.44	0.44
1:C:667:PHE:HE2	1:D:815:ASN:C	2.24	0.44
1:F:165:ASP:HB3	1:F:168:LYS:HB2	1.98	0.44
1:F:238:GLN:HE21	1:F:239:ARG:HG2	1.81	0.44
1:F:1191:SER:HB2	1:F:1196:THR:HG23	1.99	0.44
1:A:177:PRO:HG2	1:A:180:TRP:CE3	2.53	0.44
1:B:177:PRO:HG2	1:B:180:TRP:CE3	2.53	0.44
1:B:710:ILE:HD11	1:B:712:TYR:CZ	2.52	0.44
1:B:1269:VAL:HA	1:B:1272:LEU:HD12	1.98	0.44
1:C:58:GLN:OE1	1:C:149:GLU:CB	2.65	0.44
1:C:1013:VAL:HG11	1:C:1075:PRO:HB3	1.99	0.44
1:D:277:LEU:HB2	1:D:653:VAL:HB	1.98	0.44
1:F:275:LYS:HG3	1:F:644:TYR:HE1	1.82	0.44
1:A:92:ARG:HG3	1:A:128:PHE:CD1	2.53	0.44
1:A:1269:VAL:HA	1:A:1272:LEU:HD12	1.99	0.44
1:A:1334:ALA:HB3	1:A:1339:PRO:HA	2.00	0.44
1:B:570:GLN:HG2	1:B:596:GLY:CA	2.46	0.44
1:B:1109:PRO:HB3	1:B:1137:MET:SD	2.57	0.44
1:C:926:SER:O	1:C:983:ILE:HG12	2.18	0.44
1:A:378:LYS:O	1:A:397:THR:HG23	2.17	0.44
1:B:749:ARG:NH1	1:B:1034:PHE:O	2.51	0.44
1:E:91:VAL:HG21	1:E:131:ARG:CZ	2.47	0.44
1:E:524:PRO:HD2	1:E:557:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1003:ASN:ND2	1:E:1146:THR:HG21	2.32	0.44
1:F:228:LYS:NZ	1:F:1096:THR:HG21	2.31	0.44
1:F:525:LEU:HD21	1:F:557:MET:HG2	2.00	0.44
1:F:749:ARG:NH1	1:F:1034:PHE:O	2.50	0.44
1:A:651:LYS:HE3	1:B:823:ASN:HD21	1.83	0.44
1:B:1334:ALA:HB3	1:B:1339:PRO:HA	2.00	0.44
1:C:178:THR:O	1:C:358:VAL:HG11	2.18	0.44
1:C:793:LEU:HD12	1:C:941:TRP:HE3	1.82	0.44
1:C:1008:ASP:HB3	1:C:1061:TRP:CD1	2.51	0.44
1:D:749:ARG:NH1	1:D:1034:PHE:O	2.51	0.44
1:A:72:ASN:HB2	1:A:473:ALA:HB2	1.99	0.44
1:A:396:THR:CG2	1:A:404:ARG:HE	2.30	0.44
1:A:1008:ASP:HB3	1:A:1061:TRP:CD1	2.52	0.44
1:B:470:ASN:OD1	1:B:472:HIS:HB2	2.18	0.44
1:B:861:PRO:HB3	1:B:879:THR:HG21	2.00	0.44
1:B:1143:LEU:O	1:B:1149:ILE:HD11	2.18	0.44
1:C:1112:VAL:HA	1:C:1127:PRO:HA	1.99	0.44
1:E:152:SER:OG	1:E:172:LEU:HB3	2.18	0.44
1:F:1292:PRO:HG2	1:F:1295:PHE:HB2	2.00	0.44
1:D:100:ILE:HD12	1:D:100:ILE:H	1.83	0.44
1:D:245:PRO:HG2	1:D:568:TYR:HB2	2.00	0.44
1:E:845:ILE:HG22	1:E:883:LEU:O	2.17	0.44
1:E:1191:SER:HB2	1:E:1196:THR:HG23	2.00	0.44
1:B:536:ARG:NH1	1:B:686:ASN:HB3	2.33	0.43
1:C:135:ASN:HD22	1:C:1330:PRO:HD2	1.83	0.43
1:D:115:LEU:HD11	1:D:324:LEU:HD13	2.00	0.43
1:D:200:LEU:HD12	1:D:344:TYR:CE2	2.53	0.43
1:D:277:LEU:HD21	1:D:610:GLN:HG3	2.00	0.43
1:D:381:HIS:HD1	1:D:532:GLU:CD	2.25	0.43
1:D:628:ILE:HD12	1:D:657:ARG:HD3	2.00	0.43
1:F:524:PRO:HD3	1:F:905:PRO:HG3	2.00	0.43
1:F:628:ILE:HD12	1:F:657:ARG:HD3	2.00	0.43
1:F:1008:ASP:HB3	1:F:1061:TRP:CD1	2.52	0.43
1:A:238:GLN:HE21	1:A:239:ARG:HG2	1.84	0.43
1:B:559:ASP:OD2	1:B:562:THR:HB	2.18	0.43
1:D:177:PRO:HG2	1:D:180:TRP:CE3	2.53	0.43
1:D:1112:VAL:HA	1:D:1127:PRO:HA	2.00	0.43
1:D:1269:VAL:HA	1:D:1272:LEU:HD12	1.99	0.43
1:E:793:LEU:HD22	1:E:801:VAL:HG13	1.99	0.43
1:F:470:ASN:OD1	1:F:472:HIS:HB2	2.18	0.43
1:A:373:SER:HB2	1:A:374:TRP:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:HIS:HE1	1:A:686:ASN:O	2.01	0.43
1:B:237:THR:HG21	1:B:575:LEU:HD13	2.01	0.43
1:C:237:THR:HG21	1:C:575:LEU:HD13	2.00	0.43
1:C:628:ILE:HD12	1:C:657:ARG:HD3	2.00	0.43
1:D:504:PRO:HG2	1:D:507:VAL:HG23	1.99	0.43
1:D:732:LEU:HD13	1:D:732:LEU:HA	1.87	0.43
1:A:200:LEU:HD12	1:A:344:TYR:CE2	2.52	0.43
1:D:152:SER:OG	1:D:172:LEU:HB3	2.18	0.43
1:E:238:GLN:HE21	1:E:239:ARG:HG2	1.83	0.43
1:E:628:ILE:HD12	1:E:657:ARG:HD3	2.01	0.43
1:E:1112:VAL:HA	1:E:1127:PRO:HA	1.99	0.43
1:E:1261:PHE:CE1	1:E:1345:PRO:HA	2.54	0.43
1:F:115:LEU:HD11	1:F:324:LEU:HD13	2.00	0.43
1:F:177:PRO:HG2	1:F:180:TRP:CE3	2.52	0.43
1:F:1193:GLN:HE21	1:F:1193:GLN:HB3	1.59	0.43
1:B:524:PRO:HD3	1:B:905:PRO:HG3	2.00	0.43
1:B:599:ASN:HB2	1:B:658:TYR:O	2.18	0.43
1:B:987:ALA:CA	1:B:1115:TYR:CD2	3.02	0.43
1:C:72:ASN:HB2	1:C:473:ALA:HB2	2.01	0.43
1:C:1003:ASN:ND2	1:C:1146:THR:HG21	2.32	0.43
1:E:467:PHE:CG	1:E:542:VAL:HG21	2.54	0.43
1:F:327:THR:HG21	1:F:367:VAL:HG21	1.99	0.43
1:F:770:TRP:CE3	1:F:773:ASN:HB2	2.51	0.43
1:A:793:LEU:HD12	1:A:941:TRP:HE3	1.83	0.43
1:B:92:ARG:HG3	1:B:128:PHE:CE1	2.54	0.43
1:C:271:SER:HB2	1:C:868:VAL:HG22	2.01	0.43
1:C:373:SER:HB2	1:C:374:TRP:HD1	1.82	0.43
1:D:72:ASN:HB2	1:D:473:ALA:HB2	2.00	0.43
1:D:237:THR:HG21	1:D:575:LEU:HD13	2.01	0.43
1:F:945:GLU:H	1:F:945:GLU:HG3	1.24	0.43
1:A:699:ASN:ND2	1:A:702:LEU:HB2	2.34	0.43
1:B:793:LEU:HD12	1:B:941:TRP:HE3	1.83	0.43
1:C:1334:ALA:HB3	1:C:1339:PRO:HA	2.01	0.43
1:E:1301:ARG:HG2	1:E:1328:PHE:CD2	2.54	0.43
1:F:91:VAL:HG21	1:F:131:ARG:CZ	2.48	0.43
1:F:374:TRP:CD1	1:F:374:TRP:N	2.87	0.43
1:F:1321:LYS:HA	1:F:1328:PHE:CD1	2.53	0.43
1:C:1041:TYR:CE1	1:C:1181:ASN:HB2	2.54	0.43
1:F:381:HIS:HD1	1:F:532:GLU:CD	2.27	0.43
1:A:467:PHE:CG	1:A:542:VAL:HG21	2.54	0.43
1:A:470:ASN:OD1	1:A:472:HIS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:THR:CG2	1:C:404:ARG:HE	2.31	0.43
1:C:599:ASN:HB2	1:C:658:TYR:O	2.19	0.43
1:D:165:ASP:HB3	1:D:168:LYS:HB2	2.01	0.43
1:D:273:ARG:HD3	1:D:619:PRO:HB3	2.01	0.43
1:D:1097:ASN:HB2	1:D:1098:PRO:CD	2.43	0.43
1:F:523:LEU:HG	1:F:557:MET:CE	2.42	0.43
1:A:1191:SER:HB2	1:A:1196:THR:HG23	2.00	0.43
1:B:277:LEU:HD22	1:B:620:HIS:HD2	1.84	0.43
1:B:1003:ASN:ND2	1:B:1146:THR:HG21	2.33	0.43
1:C:277:LEU:HD21	1:C:610:GLN:CG	2.49	0.43
1:C:277:LEU:HD21	1:C:610:GLN:HG3	2.00	0.43
1:E:165:ASP:HB3	1:E:168:LYS:HB2	2.01	0.43
1:E:200:LEU:HD12	1:E:344:TYR:CE2	2.53	0.43
1:E:396:THR:CG2	1:E:404:ARG:HE	2.32	0.43
1:E:570:GLN:HG2	1:E:596:GLY:CA	2.47	0.43
1:A:162:PRO:HG3	1:A:344:TYR:CE2	2.54	0.42
1:B:273:ARG:HD3	1:B:619:PRO:HB3	2.01	0.42
1:B:396:THR:CG2	1:B:404:ARG:HE	2.31	0.42
1:B:793:LEU:HD22	1:B:801:VAL:HG13	2.01	0.42
1:B:913:ARG:NH2	1:B:920:PRO:HD3	2.34	0.42
1:B:1008:ASP:HB3	1:B:1061:TRP:CD1	2.54	0.42
1:C:172:LEU:HD11	1:C:351:ASN:HB3	2.01	0.42
1:C:504:PRO:HG2	1:C:507:VAL:HG23	2.01	0.42
1:C:811:LEU:HD21	1:C:895:ASN:O	2.19	0.42
1:C:1070:ASP:HB3	1:C:1072:ASP:OD1	2.19	0.42
1:D:811:LEU:HD23	1:D:817:ARG:NE	2.34	0.42
1:E:72:ASN:HB2	1:E:473:ALA:HB2	2.01	0.42
1:E:281:VAL:HG22	1:E:293:ASN:HA	2.00	0.42
1:A:861:PRO:HB3	1:A:879:THR:HG21	2.01	0.42
1:A:913:ARG:NH2	1:A:920:PRO:HD3	2.34	0.42
1:C:228:LYS:NZ	1:C:239:ARG:HH12	2.17	0.42
1:C:983:ILE:HD11	1:C:1152:LYS:HD2	2.00	0.42
1:D:92:ARG:HG3	1:D:128:PHE:CD1	2.54	0.42
1:D:194:SER:CB	1:D:200:LEU:HD23	2.48	0.42
1:D:1191:SER:HB2	1:D:1196:THR:HG23	2.00	0.42
1:E:381:HIS:HD1	1:E:532:GLU:CD	2.27	0.42
1:F:152:SER:OG	1:F:172:LEU:HB3	2.18	0.42
1:F:467:PHE:CG	1:F:542:VAL:HG21	2.54	0.42
1:A:1319:GLU:HB3	1:A:1328:PHE:HB3	2.00	0.42
1:B:525:LEU:HD21	1:B:557:MET:HG2	2.00	0.42
1:C:59:GLN:HB2	1:C:143:ILE:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:THR:O	1:D:358:VAL:HG11	2.19	0.42
1:D:1319:GLU:HB3	1:D:1328:PHE:HB3	2.01	0.42
1:E:373:SER:HB2	1:E:374:TRP:HD1	1.84	0.42
1:E:1292:PRO:HG2	1:E:1295:PHE:HB2	2.00	0.42
1:F:281:VAL:HG22	1:F:293:ASN:HA	2.00	0.42
1:F:396:THR:CG2	1:F:404:ARG:HE	2.31	0.42
1:A:381:HIS:HD1	1:A:532:GLU:CD	2.27	0.42
1:A:1070:ASP:HB3	1:A:1072:ASP:OD1	2.20	0.42
1:B:792:PRO:HG3	1:B:967:HIS:CE1	2.54	0.42
1:C:448:GLU:H	1:C:448:GLU:HG2	1.48	0.42
1:C:651:LYS:CE	1:D:823:ASN:HD21	2.32	0.42
1:D:405:HIS:HE1	1:D:686:ASN:O	2.02	0.42
1:D:811:LEU:HD11	1:D:895:ASN:OD1	2.20	0.42
1:D:841:GLN:HE22	1:D:843:ASN:HB2	1.85	0.42
1:E:470:ASN:OD1	1:E:472:HIS:HB2	2.20	0.42
1:E:749:ARG:NH1	1:E:1034:PHE:O	2.52	0.42
1:A:244:SER:HA	1:A:571:LEU:HD22	2.01	0.42
1:A:628:ILE:HD12	1:A:657:ARG:HD3	2.00	0.42
1:B:72:ASN:HB2	1:B:473:ALA:HB2	2.00	0.42
1:B:165:ASP:HB3	1:B:168:LYS:HB2	2.02	0.42
1:B:381:HIS:HD1	1:B:532:GLU:CD	2.26	0.42
1:D:92:ARG:HG3	1:D:128:PHE:CE1	2.55	0.42
1:D:467:PHE:CG	1:D:542:VAL:HG21	2.54	0.42
1:D:1334:ALA:HB3	1:D:1339:PRO:HA	2.01	0.42
1:F:201:TYR:CE1	1:F:345:ASP:HB3	2.55	0.42
1:F:1274:ASP:CB	1:F:1277:THR:HG22	2.40	0.42
1:A:98:LEU:O	1:A:121:TYR:OH	2.31	0.42
1:A:165:ASP:HB3	1:A:168:LYS:HB2	2.02	0.42
1:B:1261:PHE:CE1	1:B:1345:PRO:HA	2.52	0.42
1:C:177:PRO:HG2	1:C:180:TRP:CE3	2.54	0.42
1:C:817:ARG:NE	1:C:817:ARG:HA	2.34	0.42
1:D:1070:ASP:HB3	1:D:1072:ASP:OD1	2.19	0.42
1:D:1092:THR:C	1:D:1094:TYR:H	2.28	0.42
1:E:1013:VAL:HG11	1:E:1075:PRO:HB3	2.02	0.42
1:F:1301:ARG:CG	1:F:1328:PHE:HE2	2.32	0.42
1:A:749:ARG:HG3	1:A:749:ARG:HH21	1.84	0.42
1:A:817:ARG:NE	1:A:817:ARG:HA	2.35	0.42
1:A:841:GLN:HE22	1:A:843:ASN:HB2	1.84	0.42
1:B:405:HIS:HE1	1:B:686:ASN:O	2.03	0.42
1:D:710:ILE:HD11	1:D:712:TYR:CZ	2.54	0.42
1:F:72:ASN:HB2	1:F:473:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:536:ARG:NH1	1:F:686:ASN:HB3	2.35	0.42
1:F:1003:ASN:ND2	1:F:1146:THR:HG21	2.33	0.42
1:A:1189:GLU:OE2	1:B:729:LEU:HD11	2.20	0.42
1:B:152:SER:OG	1:B:172:LEU:HB3	2.20	0.42
1:B:732:LEU:HD13	1:B:732:LEU:HA	1.90	0.42
1:B:987:ALA:HA	1:B:1115:TYR:CD2	2.55	0.42
1:C:244:SER:HA	1:C:571:LEU:HD22	2.02	0.42
1:C:536:ARG:NH1	1:C:686:ASN:HB3	2.34	0.42
1:D:122:LEU:HB3	1:D:126:GLN:NE2	2.35	0.42
1:D:617:PHE:CE2	1:D:859:PHE:HB2	2.54	0.42
1:D:773:ASN:HB3	1:D:775:LYS:HB2	2.01	0.42
1:E:543:LYS:HD2	1:E:1012:LEU:HB3	2.02	0.42
1:E:1097:ASN:HB3	1:E:1098:PRO:HD3	2.02	0.42
1:F:543:LYS:HD2	1:F:1012:LEU:HB3	2.02	0.42
1:F:599:ASN:HB2	1:F:658:TYR:O	2.20	0.42
1:A:1312:GLN:O	1:A:1345:PRO:HD2	2.20	0.42
1:B:587:GLU:HG3	1:B:1107:TYR:HE1	1.85	0.42
1:B:1070:ASP:HB3	1:B:1072:ASP:OD1	2.19	0.42
1:C:152:SER:OG	1:C:172:LEU:HB3	2.20	0.42
1:D:1003:ASN:ND2	1:D:1146:THR:HG21	2.34	0.42
1:E:115:LEU:HD11	1:E:324:LEU:HD13	2.01	0.42
1:A:1141:LEU:HD12	1:A:1141:LEU:HA	1.93	0.42
1:B:92:ARG:HG3	1:B:128:PHE:CD1	2.54	0.42
1:B:374:TRP:N	1:B:374:TRP:CD1	2.87	0.42
1:B:1319:GLU:HB3	1:B:1328:PHE:HB3	2.01	0.42
1:C:467:PHE:CG	1:C:542:VAL:HG21	2.55	0.42
1:C:470:ASN:OD1	1:C:472:HIS:HB2	2.18	0.42
1:E:92:ARG:HG3	1:E:128:PHE:CE2	2.54	0.42
1:F:237:THR:HG21	1:F:575:LEU:HD13	2.02	0.42
1:F:793:LEU:HD12	1:F:941:TRP:HE3	1.85	0.42
1:F:983:ILE:HD11	1:F:1152:LYS:HD2	2.02	0.42
1:A:1097:ASN:HB3	1:A:1098:PRO:HD2	1.99	0.41
1:B:238:GLN:HE21	1:B:239:ARG:HG2	1.85	0.41
1:C:661:LEU:HD13	1:C:901:ASN:HD21	1.85	0.41
1:D:536:ARG:NH1	1:D:686:ASN:HB3	2.35	0.41
1:D:923:ILE:HD13	1:D:923:ILE:HA	1.85	0.41
1:E:109:ASP:HB3	1:E:113:LYS:HD3	2.02	0.41
1:F:543:LYS:HB2	1:F:1012:LEU:HD13	2.02	0.41
1:C:391:ASN:ND2	1:C:418:ASN:HD22	2.18	0.41
1:C:850:VAL:CG2	1:C:851:LYS:N	2.83	0.41
1:D:599:ASN:HB2	1:D:658:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:ASN:OD1	1:D:633:ASN:HB2	2.20	0.41
1:A:588:ASP:C	1:A:909:GLN:HE22	2.28	0.41
1:A:1279:PHE:HE1	1:A:1301:ARG:HD2	1.72	0.41
1:B:244:SER:HA	1:B:571:LEU:HD22	2.03	0.41
1:B:888:SER:HB2	1:B:889:PRO:HD2	2.02	0.41
1:B:1013:VAL:HG11	1:B:1075:PRO:HB3	2.02	0.41
1:C:162:PRO:HG3	1:C:344:TYR:CE2	2.54	0.41
1:C:164:PHE:CZ	1:C:166:PRO:HA	2.55	0.41
1:C:810:HIS:CE1	1:C:814:GLU:HG2	2.54	0.41
1:E:172:LEU:HD11	1:E:351:ASN:HB3	2.03	0.41
1:E:374:TRP:N	1:E:374:TRP:CD1	2.87	0.41
1:B:696:ALA:HB1	1:B:747:VAL:HG12	2.01	0.41
1:C:200:LEU:HD12	1:C:344:TYR:CE2	2.55	0.41
1:C:939:GLN:HE21	1:C:950:ASN:HB2	1.84	0.41
1:D:100:ILE:CD1	1:D:100:ILE:H	2.33	0.41
1:D:924:ASN:CB	1:D:985:PHE:HA	2.51	0.41
1:D:945:GLU:H	1:D:945:GLU:HG3	1.25	0.41
1:E:588:ASP:C	1:E:909:GLN:HE22	2.29	0.41
1:E:983:ILE:HD11	1:E:1152:LYS:HD2	2.03	0.41
1:A:237:THR:HG21	1:A:575:LEU:HD13	2.01	0.41
1:B:194:SER:CB	1:B:200:LEU:HD23	2.49	0.41
1:B:923:ILE:HD13	1:B:923:ILE:HA	1.87	0.41
1:C:122:LEU:HB3	1:C:126:GLN:NE2	2.33	0.41
1:C:588:ASP:C	1:C:909:GLN:HE22	2.28	0.41
1:E:237:THR:HG21	1:E:575:LEU:HD13	2.02	0.41
1:E:710:ILE:HD11	1:E:712:TYR:CZ	2.55	0.41
1:F:835:ARG:HB3	1:F:1122:ASN:HA	2.02	0.41
1:A:135:ASN:HD22	1:A:1330:PRO:HD2	1.86	0.41
1:A:599:ASN:HB2	1:A:658:TYR:O	2.20	0.41
1:B:810:HIS:ND1	1:B:817:ARG:HD3	2.35	0.41
1:C:631:ASN:OD1	1:C:633:ASN:HB2	2.20	0.41
1:C:846:PRO:HG2	1:C:849:GLN:NE2	2.36	0.41
1:C:1312:GLN:O	1:C:1345:PRO:HD2	2.21	0.41
1:C:1319:GLU:HB3	1:C:1328:PHE:HB3	2.01	0.41
1:D:846:PRO:HG2	1:D:849:GLN:NE2	2.35	0.41
1:F:135:ASN:HD22	1:F:1330:PRO:HD2	1.84	0.41
1:F:1097:ASN:HB3	1:F:1098:PRO:HD3	2.03	0.41
1:A:164:PHE:CZ	1:A:166:PRO:HA	2.55	0.41
1:B:845:ILE:HG22	1:B:883:LEU:O	2.21	0.41
1:B:1301:ARG:HG2	1:B:1328:PHE:CD2	2.56	0.41
1:C:91:VAL:HG21	1:C:131:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:LEU:HD21	1:C:557:MET:HG2	2.03	0.41
1:C:861:PRO:HB3	1:C:879:THR:HG21	2.03	0.41
1:D:135:ASN:HD22	1:D:1330:PRO:HD2	1.85	0.41
1:E:271:SER:HB2	1:E:868:VAL:HG22	2.02	0.41
1:E:1036:ARG:HH21	1:F:742:ARG:NH1	2.19	0.41
1:E:1312:GLN:O	1:E:1345:PRO:HD2	2.19	0.41
1:A:850:VAL:CG2	1:A:851:LYS:N	2.84	0.41
1:B:99:ASN:ND2	1:B:102:SER:HB3	2.35	0.41
1:B:122:LEU:HB3	1:B:126:GLN:NE2	2.35	0.41
1:B:467:PHE:CD1	1:B:542:VAL:HG21	2.56	0.41
1:C:374:TRP:N	1:C:374:TRP:CD1	2.88	0.41
1:C:702:LEU:HD12	1:C:702:LEU:HA	1.87	0.41
1:D:696:ALA:HB1	1:D:747:VAL:HG12	2.02	0.41
1:F:527:THR:HB	1:F:533:TYR:HB3	2.03	0.41
1:A:122:LEU:HB3	1:A:126:GLN:NE2	2.34	0.41
1:A:243:ASP:HB2	1:A:309:VAL:HG11	2.03	0.41
1:A:271:SER:HB2	1:A:868:VAL:HG22	2.03	0.41
1:A:1137:MET:HB2	1:A:1137:MET:HE3	1.63	0.41
1:B:149:GLU:O	1:B:150:ASN:C	2.63	0.41
1:B:543:LYS:HD2	1:B:1012:LEU:HB3	2.03	0.41
1:B:615:SER:N	1:B:854:ASN:HD21	2.18	0.41
1:B:749:ARG:HH21	1:B:749:ARG:HG3	1.85	0.41
1:B:809:GLN:HB2	1:B:828:ILE:CD1	2.50	0.41
1:B:939:GLN:HE21	1:B:950:ASN:HB2	1.85	0.41
1:C:405:HIS:HE1	1:C:686:ASN:O	2.03	0.41
1:C:587:GLU:HG3	1:C:1107:TYR:HE1	1.86	0.41
1:C:835:ARG:HB3	1:C:1122:ASN:HA	2.02	0.41
1:C:926:SER:O	1:C:983:ILE:HG23	2.20	0.41
1:C:1261:PHE:CE1	1:C:1345:PRO:HA	2.56	0.41
1:D:1032:THR:OG1	1:D:1043:GLY:HA2	2.20	0.41
1:E:92:ARG:HG3	1:E:128:PHE:CD2	2.56	0.41
1:E:661:LEU:HD13	1:E:901:ASN:HD21	1.85	0.41
1:E:1334:ALA:HB3	1:E:1339:PRO:HA	2.02	0.41
1:F:92:ARG:HG3	1:F:128:PHE:CE2	2.55	0.41
1:F:122:LEU:HB3	1:F:126:GLN:NE2	2.36	0.41
1:F:1248:THR:HA	1:F:1251:ILE:HD12	2.03	0.41
1:F:1319:GLU:HB3	1:F:1328:PHE:HB3	2.02	0.41
1:F:1321:LYS:HA	1:F:1328:PHE:HD1	1.86	0.41
1:A:172:LEU:HD11	1:A:351:ASN:HB3	2.03	0.41
1:A:696:ALA:HB1	1:A:747:VAL:HG12	2.03	0.41
1:B:987:ALA:CA	1:B:1115:TYR:HD2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:LYS:HB2	1:C:1012:LEU:HD13	2.03	0.41
1:D:201:TYR:CE1	1:D:345:ASP:HB3	2.56	0.41
1:D:244:SER:HA	1:D:571:LEU:HD22	2.03	0.41
1:E:702:LEU:HD12	1:E:702:LEU:HA	1.92	0.41
1:E:793:LEU:HD12	1:E:941:TRP:HE3	1.86	0.41
1:E:945:GLU:H	1:E:945:GLU:HG3	1.24	0.41
1:E:1319:GLU:HB3	1:E:1328:PHE:HB3	2.02	0.41
1:F:244:SER:HA	1:F:571:LEU:HD22	2.03	0.41
1:A:130:ILE:HG13	1:A:143:ILE:HG23	2.03	0.40
1:A:543:LYS:HD2	1:A:1012:LEU:HB3	2.03	0.40
1:A:661:LEU:HD13	1:A:901:ASN:HD21	1.86	0.40
1:B:773:ASN:HB3	1:B:775:LYS:HB2	2.03	0.40
1:B:983:ILE:HD11	1:B:1152:LYS:HD2	2.01	0.40
1:C:792:PRO:HG3	1:C:967:HIS:CE1	2.56	0.40
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.88	0.40
1:D:391:ASN:ND2	1:D:418:ASN:HD22	2.19	0.40
1:E:99:ASN:C	1:E:101:SER:N	2.79	0.40
1:F:273:ARG:HD3	1:F:619:PRO:HB3	2.03	0.40
1:A:91:VAL:HG21	1:A:131:ARG:CZ	2.52	0.40
1:A:397:THR:HG22	1:A:418:ASN:OD1	2.21	0.40
1:A:579:ALA:HA	1:A:582:GLN:HB2	2.04	0.40
1:A:923:ILE:HD13	1:A:923:ILE:HA	1.87	0.40
1:B:527:THR:HB	1:B:533:TYR:HB3	2.02	0.40
1:C:682:PHE:HE2	1:D:820:PHE:CE1	2.40	0.40
1:C:1031:PHE:CE1	1:C:1044:ILE:HD11	2.56	0.40
1:D:809:GLN:NE2	1:D:828:ILE:HD12	2.36	0.40
1:D:888:SER:HB2	1:D:889:PRO:HD2	2.04	0.40
1:E:1141:LEU:HD12	1:E:1141:LEU:HA	1.95	0.40
1:A:109:ASP:HB3	1:A:113:LYS:HD2	2.00	0.40
1:A:467:PHE:CD1	1:A:542:VAL:HG21	2.55	0.40
1:A:823:ASN:HD21	1:B:651:LYS:HE3	1.86	0.40
1:B:631:ASN:OD1	1:B:633:ASN:HB2	2.22	0.40
1:C:151:PRO:HG3	1:C:180:TRP:CE2	2.57	0.40
1:D:527:THR:HB	1:D:533:TYR:HB3	2.03	0.40
1:D:570:GLN:HG3	1:D:573:LYS:HE2	2.03	0.40
1:D:792:PRO:HG3	1:D:967:HIS:CE1	2.56	0.40
1:D:811:LEU:HD13	1:D:894:ILE:CG1	2.51	0.40
1:D:983:ILE:HD11	1:D:1152:LYS:HD2	2.03	0.40
1:D:1301:ARG:HG2	1:D:1328:PHE:CD2	2.56	0.40
1:E:123:ASP:OD1	1:E:208:LYS:HE2	2.20	0.40
1:E:536:ARG:NH1	1:E:686:ASN:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:599:ASN:HB2	1:E:658:TYR:O	2.20	0.40
1:E:835:ARG:HB3	1:E:1122:ASN:HA	2.02	0.40
1:F:231:GLN:HG3	1:F:1096:THR:HA	2.02	0.40
1:F:1318:LEU:HB3	1:F:1331:VAL:HB	2.03	0.40
1:A:374:TRP:CD1	1:A:374:TRP:N	2.86	0.40
1:A:536:ARG:NH1	1:A:686:ASN:HB3	2.36	0.40
1:B:835:ARG:HB3	1:B:1122:ASN:HA	2.03	0.40
1:D:661:LEU:HD13	1:D:901:ASN:HD21	1.85	0.40
1:D:702:LEU:HD12	1:D:702:LEU:HA	1.87	0.40
1:D:749:ARG:HH21	1:D:749:ARG:HG3	1.86	0.40
1:E:939:GLN:HE21	1:E:950:ASN:HB2	1.87	0.40
1:F:200:LEU:HD12	1:F:344:TYR:CE2	2.55	0.40
1:F:661:LEU:HD13	1:F:901:ASN:HD21	1.85	0.40
1:A:817:ARG:HG2	1:A:817:ARG:NH2	2.35	0.40
1:B:145:LEU:HA	1:B:148:MET:HE2	2.04	0.40
1:B:661:LEU:HD13	1:B:901:ASN:HD21	1.87	0.40
1:D:467:PHE:CD1	1:D:542:VAL:HG21	2.56	0.40
1:D:579:ALA:HA	1:D:582:GLN:HB2	2.03	0.40
1:E:559:ASP:OD2	1:E:562:THR:HB	2.22	0.40
1:F:710:ILE:HD11	1:F:712:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1270/1304 (97%)	1128 (89%)	122 (10%)	20 (2%)	7	33
1	B	1267/1304 (97%)	1136 (90%)	114 (9%)	17 (1%)	9	37
1	C	1266/1304 (97%)	1128 (89%)	123 (10%)	15 (1%)	10	38
1	D	1263/1304 (97%)	1127 (89%)	117 (9%)	19 (2%)	8	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1252/1304 (96%)	1118 (89%)	117 (9%)	17 (1%)	9	35
1	F	1252/1304 (96%)	1114 (89%)	119 (10%)	19 (2%)	8	34
All	All	7570/7824 (97%)	6751 (89%)	712 (9%)	107 (1%)	9	35

All (107) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	A	1094	TYR
1	A	1097	ASN
1	A	1241	GLY
1	B	811	LEU
1	B	926	SER
1	B	1241	GLY
1	C	926	SER
1	C	1240	GLN
1	D	874	SER
1	D	926	SER
1	D	1096	THR
1	D	1097	ASN
1	D	1175	THR
1	D	1240	GLN
1	E	926	SER
1	E	1241	GLY
1	F	111	ASN
1	F	926	SER
1	F	1241	GLY
1	A	99	ASN
1	A	618	GLY
1	A	827	ASP
1	A	926	SER
1	A	1057	ALA
1	A	1096	THR
1	A	1346	PHE
1	B	618	GLY
1	B	854	ASN
1	B	1057	ALA
1	C	143	ILE
1	C	618	GLY
1	C	827	ASP
1	C	1057	ALA

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Mol	Chain	Res	Type
1	D	618	GLY
1	D	807	ILE
1	D	1057	ALA
1	E	618	GLY
1	E	874	SER
1	E	875	SER
1	E	1057	ALA
1	E	1096	THR
1	E	1346	PHE
1	F	108	SER
1	F	618	GLY
1	F	874	SER
1	F	875	SER
1	F	1057	ALA
1	F	1096	THR
1	F	1346	PHE
1	A	662	TYR
1	A	927	GLY
1	A	1133	ALA
1	B	662	TYR
1	C	662	TYR
1	C	927	GLY
1	C	1094	TYR
1	C	1346	PHE
1	D	662	TYR
1	D	808	THR
1	D	1090	SER
1	E	662	TYR
1	F	662	TYR
1	A	823	ASN
1	B	143	ILE
1	B	808	THR
1	B	823	ASN
1	B	1133	ALA
1	C	1133	ALA
1	D	143	ILE
1	D	823	ASN
1	E	143	ILE
1	E	1097	ASN
1	E	1133	ALA
1	F	143	ILE
1	F	1092	THR

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Mol	Chain	Res	Type
1	F	1097	ASN
1	F	1133	ALA
1	A	232	SER
1	B	568	TYR
1	B	1089	ASN
1	C	568	TYR
1	C	809	GLN
1	C	823	ASN
1	D	568	TYR
1	D	813	LYS
1	D	1133	ALA
1	E	568	TYR
1	E	823	ASN
1	E	1092	THR
1	F	568	TYR
1	F	823	ASN
1	A	816	THR
1	A	852	PRO
1	B	227	VAL
1	B	790	SER
1	B	1094	TYR
1	C	852	PRO
1	A	1268	PRO
1	B	852	PRO
1	D	852	PRO
1	E	852	PRO
1	E	1268	PRO
1	F	852	PRO
1	F	1268	PRO
1	A	143	ILE
1	D	1268	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1121/1146 (98%)	957 (85%)	164 (15%)	3 14
1	B	1120/1146 (98%)	961 (86%)	159 (14%)	3 16
1	C	1118/1146 (98%)	961 (86%)	157 (14%)	3 16
1	D	1117/1146 (98%)	958 (86%)	159 (14%)	3 16
1	E	1107/1146 (97%)	957 (86%)	150 (14%)	3 17
1	F	1108/1146 (97%)	958 (86%)	150 (14%)	4 17
All	All	6691/6876 (97%)	5752 (86%)	939 (14%)	3 16

All (939) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	88	PHE
1	A	91	VAL
1	A	98	LEU
1	A	101	SER
1	A	106	ASN
1	A	119	GLU
1	A	125	GLN
1	A	127	ASN
1	A	130	ILE
1	A	142	ASP
1	A	143	ILE
1	A	156	ARG
1	A	158	LEU
1	A	178	THR
1	A	182	GLU
1	A	184	LYS
1	A	187	VAL
1	A	197	SER
1	A	203	VAL
1	A	204	LEU
1	A	209	VAL
1	A	218	ASN
1	A	220	VAL
1	A	223	GLU
1	A	225	LEU
1	A	228	LYS

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Mol	Chain	Res	Type
1	A	238	GLN
1	A	239	ARG
1	A	242	LYS
1	A	251	LYS
1	A	257	SER
1	A	259	THR
1	A	268	MET
1	A	272	THR
1	A	300	LEU
1	A	301	LYS
1	A	314	GLU
1	A	315	LYS
1	A	324	LEU
1	A	333	GLU
1	A	334	LYS
1	A	342	SER
1	A	350	GLU
1	A	353	THR
1	A	358	VAL
1	A	373	SER
1	A	376	THR
1	A	380	ASN
1	A	384	ILE
1	A	393	LEU
1	A	396	THR
1	A	404	ARG
1	A	405	HIS
1	A	415	LYS
1	A	425	VAL
1	A	431	LYS
1	A	436	LYS
1	A	437	LYS
1	A	457	MET
1	A	458	VAL
1	A	492	THR
1	A	508	LEU
1	A	513	ILE
1	A	523	LEU
1	A	529	ARG
1	A	567	LYS
1	A	569	ASP
1	A	572	GLU

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Mol	Chain	Res	Type
1	A	573	LYS
1	A	587	GLU
1	A	609	LEU
1	A	613	MET
1	A	642	SER
1	A	662	TYR
1	A	673	LEU
1	A	707	SER
1	A	710	ILE
1	A	714	LYS
1	A	725	ARG
1	A	732	LEU
1	A	735	ASN
1	A	746	VAL
1	A	747	VAL
1	A	756	LEU
1	A	771	ILE
1	A	790	SER
1	A	806	MET
1	A	807	ILE
1	A	808	THR
1	A	810	HIS
1	A	813	LYS
1	A	814	GLU
1	A	819	VAL
1	A	828	ILE
1	A	835	ARG
1	A	840	ASN
1	A	841	GLN
1	A	853	SER
1	A	869	THR
1	A	871	SER
1	A	874	SER
1	A	883	LEU
1	A	887	ILE
1	A	897	LEU
1	A	908	ASN
1	A	923	ILE
1	A	924	ASN
1	A	929	SER
1	A	943	LYS
1	A	944	THR

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Mol	Chain	Res	Type
1	A	945	GLU
1	A	965	LEU
1	A	974	THR
1	A	986	LYS
1	A	989	SER
1	A	1002	LEU
1	A	1012	LEU
1	A	1030	THR
1	A	1038	ARG
1	A	1039	THR
1	A	1042	LEU
1	A	1061	TRP
1	A	1067	SER
1	A	1089	ASN
1	A	1092	THR
1	A	1096	THR
1	A	1100	LEU
1	A	1106	LEU
1	A	1117	THR
1	A	1120	THR
1	A	1141	LEU
1	A	1144	LEU
1	A	1150	LYS
1	A	1152	LYS
1	A	1178	THR
1	A	1179	THR
1	A	1192	ILE
1	A	1215	ASP
1	A	1220	LYS
1	A	1221	MET
1	A	1226	THR
1	A	1244	SER
1	A	1246	SER
1	A	1259	ILE
1	A	1260	ASP
1	A	1263	ARG
1	A	1267	LEU
1	A	1270	THR
1	A	1276	ASN
1	A	1282	ASP
1	A	1287	LEU
1	A	1300	ILE

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Mol	Chain	Res	Type
1	A	1310	GLU
1	A	1314	LEU
1	A	1318	LEU
1	A	1326	GLN
1	A	1327	GLN
1	A	1329	ILE
1	A	1336	SER
1	A	1340	GLN
1	A	1341	THR
1	A	1342	VAL
1	A	1346	PHE
1	B	57	HIS
1	B	78	LEU
1	B	88	PHE
1	B	91	VAL
1	B	94	GLN
1	B	97	ASN
1	B	99	ASN
1	B	101	SER
1	B	105	LYS
1	B	108	SER
1	B	111	ASN
1	B	119	GLU
1	B	125	GLN
1	B	127	ASN
1	B	130	ILE
1	B	142	ASP
1	B	143	ILE
1	B	149	GLU
1	B	156	ARG
1	B	158	LEU
1	B	178	THR
1	B	182	GLU
1	B	184	LYS
1	B	187	VAL
1	B	197	SER
1	B	203	VAL
1	B	204	LEU
1	B	209	VAL
1	B	218	ASN
1	B	220	VAL
1	B	223	GLU

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Mol	Chain	Res	Type
1	B	225	LEU
1	B	238	GLN
1	B	239	ARG
1	B	242	LYS
1	B	251	LYS
1	B	257	SER
1	B	259	THR
1	B	268	MET
1	B	272	THR
1	B	300	LEU
1	B	301	LYS
1	B	315	LYS
1	B	324	LEU
1	B	334	LYS
1	B	342	SER
1	B	350	GLU
1	B	353	THR
1	B	358	VAL
1	B	373	SER
1	B	376	THR
1	B	380	ASN
1	B	384	ILE
1	B	393	LEU
1	B	396	THR
1	B	404	ARG
1	B	405	HIS
1	B	415	LYS
1	B	431	LYS
1	B	436	LYS
1	B	437	LYS
1	B	457	MET
1	B	458	VAL
1	B	486	VAL
1	B	492	THR
1	B	508	LEU
1	B	513	ILE
1	B	523	LEU
1	B	529	ARG
1	B	567	LYS
1	B	569	ASP
1	B	572	GLU
1	B	573	LYS

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Mol	Chain	Res	Type
1	B	587	GLU
1	B	609	LEU
1	B	613	MET
1	B	628	ILE
1	B	642	SER
1	B	662	TYR
1	B	673	LEU
1	B	707	SER
1	B	710	ILE
1	B	725	ARG
1	B	732	LEU
1	B	735	ASN
1	B	746	VAL
1	B	747	VAL
1	B	756	LEU
1	B	771	ILE
1	B	804	LYS
1	B	806	MET
1	B	807	ILE
1	B	811	LEU
1	B	828	ILE
1	B	835	ARG
1	B	840	ASN
1	B	841	GLN
1	B	854	ASN
1	B	883	LEU
1	B	887	ILE
1	B	908	ASN
1	B	923	ILE
1	B	943	LYS
1	B	944	THR
1	B	945	GLU
1	B	965	LEU
1	B	974	THR
1	B	986	LYS
1	B	989	SER
1	B	993	SER
1	B	1002	LEU
1	B	1012	LEU
1	B	1038	ARG
1	B	1039	THR
1	B	1042	LEU

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Mol	Chain	Res	Type
1	B	1061	TRP
1	B	1067	SER
1	B	1091	SER
1	B	1092	THR
1	B	1096	THR
1	B	1100	LEU
1	B	1106	LEU
1	B	1117	THR
1	B	1120	THR
1	B	1141	LEU
1	B	1144	LEU
1	B	1150	LYS
1	B	1152	LYS
1	B	1178	THR
1	B	1179	THR
1	B	1192	ILE
1	B	1215	ASP
1	B	1220	LYS
1	B	1221	MET
1	B	1226	THR
1	B	1244	SER
1	B	1246	SER
1	B	1259	ILE
1	B	1260	ASP
1	B	1263	ARG
1	B	1267	LEU
1	B	1270	THR
1	B	1276	ASN
1	B	1282	ASP
1	B	1283	GLN
1	B	1287	LEU
1	B	1300	ILE
1	B	1310	GLU
1	B	1311	ASN
1	B	1314	LEU
1	B	1318	LEU
1	B	1326	GLN
1	B	1327	GLN
1	B	1329	ILE
1	B	1336	SER
1	B	1340	GLN
1	B	1341	THR

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Mol	Chain	Res	Type
1	B	1342	VAL
1	B	1346	PHE
1	C	58	GLN
1	C	78	LEU
1	C	88	PHE
1	C	91	VAL
1	C	94	GLN
1	C	99	ASN
1	C	101	SER
1	C	105	LYS
1	C	106	ASN
1	C	119	GLU
1	C	127	ASN
1	C	130	ILE
1	C	142	ASP
1	C	156	ARG
1	C	158	LEU
1	C	178	THR
1	C	182	GLU
1	C	184	LYS
1	C	187	VAL
1	C	197	SER
1	C	203	VAL
1	C	204	LEU
1	C	209	VAL
1	C	218	ASN
1	C	220	VAL
1	C	223	GLU
1	C	225	LEU
1	C	238	GLN
1	C	242	LYS
1	C	251	LYS
1	C	257	SER
1	C	259	THR
1	C	272	THR
1	C	275	LYS
1	C	300	LEU
1	C	301	LYS
1	C	314	GLU
1	C	315	LYS
1	C	324	LEU
1	C	330	ILE

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Mol	Chain	Res	Type
1	C	332	ARG
1	C	334	LYS
1	C	342	SER
1	C	350	GLU
1	C	353	THR
1	C	358	VAL
1	C	373	SER
1	C	376	THR
1	C	380	ASN
1	C	384	ILE
1	C	393	LEU
1	C	396	THR
1	C	404	ARG
1	C	405	HIS
1	C	415	LYS
1	C	431	LYS
1	C	436	LYS
1	C	437	LYS
1	C	457	MET
1	C	458	VAL
1	C	486	VAL
1	C	492	THR
1	C	508	LEU
1	C	513	ILE
1	C	523	LEU
1	C	529	ARG
1	C	543	LYS
1	C	562	THR
1	C	567	LYS
1	C	569	ASP
1	C	572	GLU
1	C	573	LYS
1	C	587	GLU
1	C	609	LEU
1	C	628	ILE
1	C	642	SER
1	C	662	TYR
1	C	673	LEU
1	C	707	SER
1	C	710	ILE
1	C	725	ARG
1	C	732	LEU

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Mol	Chain	Res	Type
1	C	735	ASN
1	C	746	VAL
1	C	747	VAL
1	C	756	LEU
1	C	771	ILE
1	C	789	SER
1	C	804	LYS
1	C	806	MET
1	C	807	ILE
1	C	808	THR
1	C	811	LEU
1	C	813	LYS
1	C	814	GLU
1	C	828	ILE
1	C	835	ARG
1	C	840	ASN
1	C	841	GLN
1	C	855	ASN
1	C	869	THR
1	C	883	LEU
1	C	887	ILE
1	C	908	ASN
1	C	923	ILE
1	C	924	ASN
1	C	943	LYS
1	C	944	THR
1	C	945	GLU
1	C	965	LEU
1	C	974	THR
1	C	986	LYS
1	C	988	ASP
1	C	989	SER
1	C	1002	LEU
1	C	1012	LEU
1	C	1038	ARG
1	C	1039	THR
1	C	1042	LEU
1	C	1061	TRP
1	C	1067	SER
1	C	1089	ASN
1	C	1092	THR
1	C	1100	LEU

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Mol	Chain	Res	Type
1	C	1106	LEU
1	C	1117	THR
1	C	1120	THR
1	C	1141	LEU
1	C	1144	LEU
1	C	1150	LYS
1	C	1152	LYS
1	C	1178	THR
1	C	1179	THR
1	C	1192	ILE
1	C	1215	ASP
1	C	1226	THR
1	C	1240	GLN
1	C	1243	THR
1	C	1259	ILE
1	C	1260	ASP
1	C	1263	ARG
1	C	1267	LEU
1	C	1270	THR
1	C	1276	ASN
1	C	1282	ASP
1	C	1287	LEU
1	C	1300	ILE
1	C	1309	VAL
1	C	1314	LEU
1	C	1318	LEU
1	C	1326	GLN
1	C	1327	GLN
1	C	1329	ILE
1	C	1336	SER
1	C	1340	GLN
1	C	1341	THR
1	C	1342	VAL
1	D	78	LEU
1	D	88	PHE
1	D	91	VAL
1	D	100	ILE
1	D	101	SER
1	D	105	LYS
1	D	106	ASN
1	D	119	GLU
1	D	125	GLN

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Mol	Chain	Res	Type
1	D	127	ASN
1	D	130	ILE
1	D	142	ASP
1	D	156	ARG
1	D	158	LEU
1	D	178	THR
1	D	182	GLU
1	D	184	LYS
1	D	187	VAL
1	D	197	SER
1	D	203	VAL
1	D	204	LEU
1	D	209	VAL
1	D	218	ASN
1	D	220	VAL
1	D	223	GLU
1	D	225	LEU
1	D	228	LYS
1	D	231	GLN
1	D	238	GLN
1	D	239	ARG
1	D	242	LYS
1	D	251	LYS
1	D	257	SER
1	D	259	THR
1	D	272	THR
1	D	300	LEU
1	D	301	LYS
1	D	315	LYS
1	D	330	ILE
1	D	333	GLU
1	D	342	SER
1	D	350	GLU
1	D	353	THR
1	D	358	VAL
1	D	373	SER
1	D	376	THR
1	D	380	ASN
1	D	384	ILE
1	D	393	LEU
1	D	396	THR
1	D	404	ARG

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Mol	Chain	Res	Type
1	D	405	HIS
1	D	415	LYS
1	D	431	LYS
1	D	436	LYS
1	D	437	LYS
1	D	458	VAL
1	D	486	VAL
1	D	492	THR
1	D	508	LEU
1	D	513	ILE
1	D	523	LEU
1	D	529	ARG
1	D	543	LYS
1	D	562	THR
1	D	567	LYS
1	D	569	ASP
1	D	572	GLU
1	D	573	LYS
1	D	587	GLU
1	D	609	LEU
1	D	613	MET
1	D	642	SER
1	D	662	TYR
1	D	673	LEU
1	D	707	SER
1	D	710	ILE
1	D	725	ARG
1	D	732	LEU
1	D	735	ASN
1	D	746	VAL
1	D	747	VAL
1	D	756	LEU
1	D	771	ILE
1	D	804	LYS
1	D	807	ILE
1	D	809	GLN
1	D	814	GLU
1	D	816	THR
1	D	817	ARG
1	D	819	VAL
1	D	828	ILE
1	D	835	ARG

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Mol	Chain	Res	Type
1	D	840	ASN
1	D	841	GLN
1	D	842	LYS
1	D	883	LEU
1	D	887	ILE
1	D	897	LEU
1	D	908	ASN
1	D	923	ILE
1	D	924	ASN
1	D	943	LYS
1	D	944	THR
1	D	945	GLU
1	D	965	LEU
1	D	974	THR
1	D	986	LYS
1	D	989	SER
1	D	993	SER
1	D	1002	LEU
1	D	1012	LEU
1	D	1038	ARG
1	D	1039	THR
1	D	1042	LEU
1	D	1067	SER
1	D	1092	THR
1	D	1097	ASN
1	D	1100	LEU
1	D	1106	LEU
1	D	1117	THR
1	D	1120	THR
1	D	1139	SER
1	D	1141	LEU
1	D	1144	LEU
1	D	1150	LYS
1	D	1152	LYS
1	D	1175	THR
1	D	1177	THR
1	D	1179	THR
1	D	1192	ILE
1	D	1204	LYS
1	D	1215	ASP
1	D	1220	LYS
1	D	1221	MET

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Mol	Chain	Res	Type
1	D	1226	THR
1	D	1243	THR
1	D	1244	SER
1	D	1259	ILE
1	D	1260	ASP
1	D	1263	ARG
1	D	1267	LEU
1	D	1270	THR
1	D	1276	ASN
1	D	1282	ASP
1	D	1283	GLN
1	D	1287	LEU
1	D	1300	ILE
1	D	1310	GLU
1	D	1311	ASN
1	D	1314	LEU
1	D	1318	LEU
1	D	1326	GLN
1	D	1327	GLN
1	D	1329	ILE
1	D	1336	SER
1	D	1340	GLN
1	D	1341	THR
1	D	1342	VAL
1	E	57	HIS
1	E	78	LEU
1	E	88	PHE
1	E	91	VAL
1	E	99	ASN
1	E	101	SER
1	E	105	LYS
1	E	106	ASN
1	E	109	ASP
1	E	119	GLU
1	E	125	GLN
1	E	127	ASN
1	E	130	ILE
1	E	142	ASP
1	E	156	ARG
1	E	158	LEU
1	E	178	THR
1	E	182	GLU

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Mol	Chain	Res	Type
1	E	184	LYS
1	E	187	VAL
1	E	197	SER
1	E	203	VAL
1	E	204	LEU
1	E	209	VAL
1	E	218	ASN
1	E	220	VAL
1	E	223	GLU
1	E	225	LEU
1	E	228	LYS
1	E	238	GLN
1	E	239	ARG
1	E	242	LYS
1	E	251	LYS
1	E	257	SER
1	E	259	THR
1	E	268	MET
1	E	272	THR
1	E	300	LEU
1	E	301	LYS
1	E	315	LYS
1	E	324	LEU
1	E	330	ILE
1	E	333	GLU
1	E	334	LYS
1	E	342	SER
1	E	350	GLU
1	E	353	THR
1	E	358	VAL
1	E	373	SER
1	E	376	THR
1	E	380	ASN
1	E	384	ILE
1	E	393	LEU
1	E	396	THR
1	E	404	ARG
1	E	405	HIS
1	E	415	LYS
1	E	431	LYS
1	E	436	LYS
1	E	437	LYS

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Mol	Chain	Res	Type
1	E	457	MET
1	E	458	VAL
1	E	492	THR
1	E	508	LEU
1	E	513	ILE
1	E	523	LEU
1	E	529	ARG
1	E	567	LYS
1	E	569	ASP
1	E	572	GLU
1	E	573	LYS
1	E	587	GLU
1	E	609	LEU
1	E	628	ILE
1	E	642	SER
1	E	662	TYR
1	E	673	LEU
1	E	707	SER
1	E	710	ILE
1	E	725	ARG
1	E	732	LEU
1	E	735	ASN
1	E	746	VAL
1	E	747	VAL
1	E	756	LEU
1	E	771	ILE
1	E	790	SER
1	E	807	ILE
1	E	828	ILE
1	E	835	ARG
1	E	840	ASN
1	E	841	GLN
1	E	869	THR
1	E	883	LEU
1	E	887	ILE
1	E	908	ASN
1	E	923	ILE
1	E	924	ASN
1	E	929	SER
1	E	943	LYS
1	E	944	THR
1	E	945	GLU

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Mol	Chain	Res	Type
1	E	965	LEU
1	E	974	THR
1	E	986	LYS
1	E	989	SER
1	E	1002	LEU
1	E	1012	LEU
1	E	1038	ARG
1	E	1039	THR
1	E	1042	LEU
1	E	1061	TRP
1	E	1067	SER
1	E	1100	LEU
1	E	1106	LEU
1	E	1117	THR
1	E	1120	THR
1	E	1141	LEU
1	E	1144	LEU
1	E	1150	LYS
1	E	1152	LYS
1	E	1178	THR
1	E	1179	THR
1	E	1188	GLU
1	E	1192	ILE
1	E	1215	ASP
1	E	1220	LYS
1	E	1221	MET
1	E	1226	THR
1	E	1243	THR
1	E	1244	SER
1	E	1259	ILE
1	E	1260	ASP
1	E	1263	ARG
1	E	1267	LEU
1	E	1270	THR
1	E	1276	ASN
1	E	1282	ASP
1	E	1287	LEU
1	E	1300	ILE
1	E	1310	GLU
1	E	1311	ASN
1	E	1314	LEU
1	E	1318	LEU

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Mol	Chain	Res	Type
1	E	1326	GLN
1	E	1329	ILE
1	E	1336	SER
1	E	1340	GLN
1	E	1342	VAL
1	E	1346	PHE
1	F	78	LEU
1	F	88	PHE
1	F	91	VAL
1	F	94	GLN
1	F	99	ASN
1	F	101	SER
1	F	106	ASN
1	F	110	ASP
1	F	119	GLU
1	F	125	GLN
1	F	127	ASN
1	F	130	ILE
1	F	142	ASP
1	F	156	ARG
1	F	158	LEU
1	F	178	THR
1	F	182	GLU
1	F	184	LYS
1	F	187	VAL
1	F	197	SER
1	F	203	VAL
1	F	204	LEU
1	F	209	VAL
1	F	218	ASN
1	F	220	VAL
1	F	223	GLU
1	F	225	LEU
1	F	228	LYS
1	F	238	GLN
1	F	239	ARG
1	F	242	LYS
1	F	251	LYS
1	F	257	SER
1	F	259	THR
1	F	268	MET
1	F	272	THR

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Mol	Chain	Res	Type
1	F	300	LEU
1	F	301	LYS
1	F	315	LYS
1	F	324	LEU
1	F	330	ILE
1	F	333	GLU
1	F	334	LYS
1	F	342	SER
1	F	353	THR
1	F	358	VAL
1	F	373	SER
1	F	376	THR
1	F	380	ASN
1	F	384	ILE
1	F	393	LEU
1	F	396	THR
1	F	404	ARG
1	F	405	HIS
1	F	415	LYS
1	F	431	LYS
1	F	436	LYS
1	F	437	LYS
1	F	457	MET
1	F	458	VAL
1	F	486	VAL
1	F	492	THR
1	F	508	LEU
1	F	513	ILE
1	F	523	LEU
1	F	529	ARG
1	F	567	LYS
1	F	569	ASP
1	F	572	GLU
1	F	573	LYS
1	F	587	GLU
1	F	609	LEU
1	F	628	ILE
1	F	642	SER
1	F	662	TYR
1	F	673	LEU
1	F	707	SER
1	F	710	ILE

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Mol	Chain	Res	Type
1	F	725	ARG
1	F	732	LEU
1	F	735	ASN
1	F	746	VAL
1	F	747	VAL
1	F	756	LEU
1	F	771	ILE
1	F	807	ILE
1	F	819	VAL
1	F	828	ILE
1	F	835	ARG
1	F	840	ASN
1	F	841	GLN
1	F	855	ASN
1	F	869	THR
1	F	883	LEU
1	F	887	ILE
1	F	908	ASN
1	F	923	ILE
1	F	924	ASN
1	F	929	SER
1	F	943	LYS
1	F	944	THR
1	F	945	GLU
1	F	965	LEU
1	F	974	THR
1	F	986	LYS
1	F	989	SER
1	F	1002	LEU
1	F	1012	LEU
1	F	1038	ARG
1	F	1039	THR
1	F	1042	LEU
1	F	1061	TRP
1	F	1067	SER
1	F	1100	LEU
1	F	1106	LEU
1	F	1117	THR
1	F	1120	THR
1	F	1141	LEU
1	F	1144	LEU
1	F	1150	LYS

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Mol	Chain	Res	Type
1	F	1152	LYS
1	F	1179	THR
1	F	1188	GLU
1	F	1192	ILE
1	F	1215	ASP
1	F	1220	LYS
1	F	1221	MET
1	F	1226	THR
1	F	1243	THR
1	F	1244	SER
1	F	1246	SER
1	F	1259	ILE
1	F	1260	ASP
1	F	1263	ARG
1	F	1267	LEU
1	F	1270	THR
1	F	1276	ASN
1	F	1282	ASP
1	F	1283	GLN
1	F	1287	LEU
1	F	1300	ILE
1	F	1310	GLU
1	F	1311	ASN
1	F	1314	LEU
1	F	1318	LEU
1	F	1326	GLN
1	F	1329	ILE
1	F	1336	SER
1	F	1340	GLN
1	F	1342	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (224) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	111	ASN
1	A	125	GLN
1	A	126	GLN
1	A	175	ASN
1	A	199	ASN
1	A	217	ASN
1	A	235	ASN

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Mol	Chain	Res	Type
1	A	238	GLN
1	A	391	ASN
1	A	395	GLN
1	A	576	ASN
1	A	620	HIS
1	A	629	GLN
1	A	646	ASN
1	A	652	HIS
1	A	668	ASN
1	A	681	ASN
1	A	699	ASN
1	A	727	ASN
1	A	728	GLN
1	A	735	ASN
1	A	737	ASN
1	A	841	GLN
1	A	849	GLN
1	A	854	ASN
1	A	855	ASN
1	A	885	ASN
1	A	908	ASN
1	A	909	GLN
1	A	924	ASN
1	A	939	GLN
1	A	947	ASN
1	A	1003	ASN
1	A	1122	ASN
1	A	1171	GLN
1	A	1326	GLN
1	A	1344	GLN
1	B	71	ASN
1	B	97	ASN
1	B	99	ASN
1	B	111	ASN
1	B	125	GLN
1	B	126	GLN
1	B	175	ASN
1	B	235	ASN
1	B	238	GLN
1	B	391	ASN
1	B	395	GLN
1	B	547	ASN

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Mol	Chain	Res	Type
1	B	548	GLN
1	B	576	ASN
1	B	629	GLN
1	B	646	ASN
1	B	681	ASN
1	B	727	ASN
1	B	735	ASN
1	B	737	ASN
1	B	823	ASN
1	B	841	GLN
1	B	849	GLN
1	B	854	ASN
1	B	885	ASN
1	B	908	ASN
1	B	909	GLN
1	B	932	GLN
1	B	939	GLN
1	B	947	ASN
1	B	1003	ASN
1	B	1097	ASN
1	B	1122	ASN
1	B	1148	ASN
1	B	1171	GLN
1	B	1238	ASN
1	B	1311	ASN
1	B	1326	GLN
1	B	1327	GLN
1	C	71	ASN
1	C	94	GLN
1	C	99	ASN
1	C	111	ASN
1	C	126	GLN
1	C	235	ASN
1	C	241	GLN
1	C	391	ASN
1	C	395	GLN
1	C	528	ASN
1	C	576	ASN
1	C	620	HIS
1	C	646	ASN
1	C	652	HIS
1	C	681	ASN

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Mol	Chain	Res	Type
1	C	727	ASN
1	C	728	GLN
1	C	735	ASN
1	C	809	GLN
1	C	841	GLN
1	C	843	ASN
1	C	849	GLN
1	C	854	ASN
1	C	908	ASN
1	C	909	GLN
1	C	924	ASN
1	C	939	GLN
1	C	947	ASN
1	C	1003	ASN
1	C	1097	ASN
1	C	1148	ASN
1	C	1235	ASN
1	C	1344	GLN
1	D	71	ASN
1	D	97	ASN
1	D	111	ASN
1	D	125	GLN
1	D	126	GLN
1	D	155	GLN
1	D	175	ASN
1	D	235	ASN
1	D	238	GLN
1	D	391	ASN
1	D	395	GLN
1	D	528	ASN
1	D	576	ASN
1	D	646	ASN
1	D	652	HIS
1	D	681	ASN
1	D	727	ASN
1	D	735	ASN
1	D	737	ASN
1	D	810	HIS
1	D	812	ASN
1	D	841	GLN
1	D	843	ASN
1	D	849	GLN

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Mol	Chain	Res	Type
1	D	854	ASN
1	D	885	ASN
1	D	909	GLN
1	D	924	ASN
1	D	939	GLN
1	D	947	ASN
1	D	1003	ASN
1	D	1122	ASN
1	D	1171	GLN
1	D	1235	ASN
1	D	1311	ASN
1	D	1326	GLN
1	E	71	ASN
1	E	99	ASN
1	E	111	ASN
1	E	125	GLN
1	E	126	GLN
1	E	175	ASN
1	E	217	ASN
1	E	235	ASN
1	E	238	GLN
1	E	391	ASN
1	E	395	GLN
1	E	528	ASN
1	E	576	ASN
1	E	620	HIS
1	E	646	ASN
1	E	652	HIS
1	E	681	ASN
1	E	727	ASN
1	E	735	ASN
1	E	737	ASN
1	E	841	GLN
1	E	843	ASN
1	E	849	GLN
1	E	854	ASN
1	E	885	ASN
1	E	908	ASN
1	E	909	GLN
1	E	924	ASN
1	E	939	GLN
1	E	947	ASN

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Mol	Chain	Res	Type
1	E	1003	ASN
1	E	1105	GLN
1	E	1122	ASN
1	E	1148	ASN
1	E	1171	GLN
1	E	1235	ASN
1	E	1312	GLN
1	E	1326	GLN
1	E	1344	GLN
1	F	71	ASN
1	F	97	ASN
1	F	99	ASN
1	F	125	GLN
1	F	126	GLN
1	F	175	ASN
1	F	217	ASN
1	F	235	ASN
1	F	238	GLN
1	F	391	ASN
1	F	395	GLN
1	F	528	ASN
1	F	576	ASN
1	F	620	HIS
1	F	629	GLN
1	F	646	ASN
1	F	652	HIS
1	F	681	ASN
1	F	727	ASN
1	F	735	ASN
1	F	841	GLN
1	F	843	ASN
1	F	849	GLN
1	F	854	ASN
1	F	885	ASN
1	F	908	ASN
1	F	909	GLN
1	F	924	ASN
1	F	939	GLN
1	F	947	ASN
1	F	1003	ASN
1	F	1122	ASN
1	F	1148	ASN

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Mol	Chain	Res	Type
1	F	1171	GLN
1	F	1193	GLN
1	F	1235	ASN
1	F	1311	ASN
1	F	1326	GLN
1	F	1344	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 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	1278/1304 (98%)	-0.32	11 (0%)	81 64	13, 49, 106, 165	0
1	B	1275/1304 (97%)	-0.18	25 (1%)	65 45	24, 60, 127, 238	0
1	C	1274/1304 (97%)	-0.23	17 (1%)	75 56	11, 50, 128, 234	0
1	D	1271/1304 (97%)	-0.17	18 (1%)	73 54	18, 58, 132, 228	0
1	E	1262/1304 (96%)	0.81	136 (10%)	11 8	25, 156, 238, 252	0
1	F	1262/1304 (96%)	0.71	113 (8%)	15 10	21, 149, 229, 244	0
All	All	7622/7824 (97%)	0.10	320 (4%)	40 26	11, 68, 224, 252	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	295	PHE	5.9
1	C	807	ILE	5.6
1	E	920	PRO	5.6
1	E	957	VAL	5.5
1	E	604	PRO	5.2
1	A	1264	LEU	4.9
1	D	807	ILE	4.8
1	F	392	LEU	4.8
1	E	1106	LEU	4.6
1	E	1212	GLY	4.6
1	F	659	SER	4.6
1	F	604	PRO	4.6
1	F	695	ALA	4.6
1	E	1100	LEU	4.4
1	F	961	TYR	4.3
1	F	719	ALA	4.2
1	E	807	ILE	4.1
1	F	1106	LEU	4.1
1	F	603	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	1125	ILE	4.0
1	F	972	PHE	4.0
1	F	826	PRO	3.9
1	E	1000	SER	3.9
1	E	963	ALA	3.9
1	F	807	ILE	3.8
1	A	807	ILE	3.8
1	F	878	THR	3.7
1	F	589	LEU	3.7
1	E	849	GLN	3.7
1	F	836	VAL	3.7
1	C	811	LEU	3.7
1	F	566	LEU	3.7
1	B	1259	ILE	3.6
1	E	953	GLY	3.6
1	E	961	TYR	3.6
1	E	826	PRO	3.6
1	E	532	GLU	3.6
1	F	1000	SER	3.6
1	A	811	LEU	3.6
1	B	809	GLN	3.6
1	E	227	VAL	3.6
1	A	816	THR	3.6
1	D	1257	ASN	3.5
1	E	295	PHE	3.5
1	E	626	PRO	3.5
1	F	884	PRO	3.5
1	E	695	ALA	3.5
1	E	885	ASN	3.5
1	F	582	GLN	3.5
1	F	398	GLY	3.4
1	F	974	THR	3.4
1	D	810	HIS	3.4
1	F	877	PRO	3.4
1	E	876	LYS	3.4
1	C	1269	VAL	3.4
1	E	1125	ILE	3.4
1	F	851	LYS	3.4
1	E	1146	THR	3.4
1	F	828	ILE	3.3
1	F	885	ASN	3.3
1	E	658	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	599	ASN	3.3
1	E	1156	GLY	3.3
1	E	820	PHE	3.3
1	D	1309	VAL	3.3
1	B	1097	ASN	3.3
1	F	1264	LEU	3.2
1	C	1270	THR	3.2
1	B	262	SER	3.2
1	E	903	ASN	3.2
1	F	580	GLN	3.2
1	B	270	THR	3.2
1	D	808	THR	3.2
1	F	641	ILE	3.2
1	B	269	ALA	3.2
1	F	309	VAL	3.2
1	E	799	ILE	3.2
1	E	959	GLY	3.2
1	F	227	VAL	3.2
1	D	1265	PHE	3.1
1	E	828	ILE	3.1
1	E	1264	LEU	3.1
1	E	580	GLN	3.1
1	E	582	GLN	3.1
1	E	1099	THR	3.1
1	E	1124	LEU	3.1
1	D	1269	VAL	3.1
1	F	434	GLY	3.0
1	E	591	ILE	3.0
1	F	279	VAL	3.0
1	E	577	LEU	3.0
1	F	957	VAL	3.0
1	C	1268	PRO	3.0
1	F	225	LEU	3.0
1	E	1115	TYR	2.9
1	C	618	GLY	2.9
1	E	669	TRP	2.9
1	B	1265	PHE	2.9
1	F	1241	GLY	2.9
1	C	812	ASN	2.9
1	E	797	SER	2.8
1	F	879	THR	2.8
1	D	1264	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	764	PHE	2.8
1	E	960	LEU	2.8
1	E	985	PHE	2.8
1	F	621	TYR	2.8
1	F	723	ALA	2.8
1	E	619	PRO	2.8
1	E	958	ASN	2.8
1	A	1158	ALA	2.8
1	E	919	ILE	2.8
1	E	923	ILE	2.8
1	F	1110	ASN	2.8
1	F	876	LYS	2.8
1	E	583	GLY	2.7
1	F	862	ASN	2.7
1	F	769	PRO	2.7
1	F	420	SER	2.7
1	F	624	ASN	2.7
1	E	922	LEU	2.7
1	B	807	ILE	2.7
1	E	974	THR	2.7
1	B	1264	LEU	2.7
1	E	1021	GLY	2.7
1	E	893	TRP	2.7
1	E	1170	SER	2.7
1	A	809	GLN	2.6
1	E	1109	PRO	2.6
1	F	881	PRO	2.6
1	F	956	GLU	2.6
1	B	1270	THR	2.6
1	F	994	SER	2.6
1	F	656	TYR	2.6
1	E	396	THR	2.6
1	F	818	TRP	2.6
1	E	393	LEU	2.6
1	E	1104	PHE	2.6
1	F	598	ALA	2.6
1	B	1257	ASN	2.6
1	F	394	LEU	2.6
1	F	565	ARG	2.6
1	F	1015	ILE	2.5
1	B	1346	PHE	2.5
1	E	769	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	1241	GLY	2.5
1	C	261	ALA	2.5
1	F	593	THR	2.5
1	B	1268	PRO	2.5
1	D	1293	SER	2.5
1	E	1153	LEU	2.5
1	F	383	GLY	2.5
1	F	1240	GLN	2.5
1	E	962	ASN	2.5
1	C	1293	SER	2.5
1	E	886	SER	2.5
1	E	792	PRO	2.5
1	F	920	PRO	2.5
1	E	392	LEU	2.5
1	E	1087	LEU	2.5
1	E	618	GLY	2.5
1	B	1269	VAL	2.5
1	F	552	ALA	2.5
1	F	443	ILE	2.5
1	E	968	THR	2.5
1	E	965	LEU	2.5
1	B	1289	VAL	2.5
1	E	780	SER	2.4
1	F	720	GLU	2.4
1	E	1004	TRP	2.4
1	C	781	PRO	2.4
1	F	632	VAL	2.4
1	F	799	ILE	2.4
1	E	790	SER	2.4
1	E	879	THR	2.4
1	E	918	THR	2.4
1	D	267	GLY	2.4
1	D	1227	GLY	2.4
1	E	434	GLY	2.4
1	F	639	ALA	2.4
1	F	629	GLN	2.4
1	E	612	GLU	2.4
1	E	667	PHE	2.4
1	D	815	ASN	2.4
1	F	561	ALA	2.4
1	C	1265	PHE	2.4
1	E	659	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	978	SER	2.4
1	B	1098	PRO	2.4
1	F	752	THR	2.4
1	E	243	ASP	2.4
1	E	1213	ILE	2.4
1	B	1314	LEU	2.4
1	C	1287	LEU	2.4
1	E	884	PRO	2.4
1	F	792	PRO	2.4
1	C	1096	THR	2.3
1	F	1226	THR	2.3
1	B	851	LYS	2.3
1	F	640	LEU	2.3
1	E	642	SER	2.3
1	F	1109	PRO	2.3
1	E	1001	GLY	2.3
1	F	791	THR	2.3
1	F	729	LEU	2.3
1	E	1081	PRO	2.3
1	F	441	SER	2.3
1	F	893	TRP	2.3
1	E	971	PHE	2.3
1	F	847	PHE	2.3
1	F	1286	PRO	2.3
1	E	1180	GLY	2.3
1	E	1192	ILE	2.3
1	F	963	ALA	2.3
1	C	1283	GLN	2.3
1	F	648	ASP	2.3
1	F	605	VAL	2.3
1	F	1127	PRO	2.3
1	E	713	GLY	2.3
1	E	802	GLY	2.3
1	F	1124	LEU	2.3
1	E	1195	GLU	2.2
1	C	1288	LEU	2.2
1	E	571	LEU	2.2
1	F	221	VAL	2.2
1	E	510	GLY	2.2
1	E	609	LEU	2.2
1	F	618	GLY	2.2
1	F	660	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	851	LYS	2.2
1	F	396	THR	2.2
1	E	420	SER	2.2
1	F	692	SER	2.2
1	D	1285	VAL	2.2
1	E	921	VAL	2.2
1	B	815	ASN	2.2
1	D	1259	ILE	2.2
1	B	268	MET	2.2
1	E	1098	PRO	2.2
1	F	999	GLY	2.2
1	E	1131	THR	2.2
1	D	1289	VAL	2.2
1	C	828	ILE	2.2
1	E	803	VAL	2.2
1	E	1107	TYR	2.2
1	E	670	SER	2.2
1	F	793	LEU	2.2
1	A	1262	ASN	2.2
1	E	312	GLU	2.2
1	D	851	LYS	2.2
1	E	1110	ASN	2.2
1	E	1122	ASN	2.2
1	F	229	ALA	2.2
1	E	545	VAL	2.1
1	E	890	THR	2.1
1	E	1211	ILE	2.1
1	D	809	GLN	2.1
1	E	256	LEU	2.1
1	F	955	GLY	2.1
1	E	779	ASN	2.1
1	C	865	ASP	2.1
1	B	810	HIS	2.1
1	E	279	VAL	2.1
1	E	605	VAL	2.1
1	F	803	VAL	2.1
1	E	821	ILE	2.1
1	E	729	LEU	2.1
1	E	261	ALA	2.1
1	F	558	GLY	2.1
1	F	583	GLY	2.1
1	E	221	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	683	VAL	2.1
1	F	1027	TRP	2.1
1	E	768	LEU	2.1
1	E	1182	ILE	2.1
1	F	897	LEU	2.1
1	B	261	ALA	2.1
1	E	696	ALA	2.1
1	E	781	PRO	2.1
1	E	889	PRO	2.1
1	F	722	GLU	2.1
1	A	1097	ASN	2.1
1	E	1112	VAL	2.1
1	E	1144	LEU	2.1
1	F	387	TYR	2.1
1	E	680	ALA	2.1
1	E	858	PRO	2.1
1	F	601	PRO	2.1
1	F	1098	PRO	2.1
1	F	311	LEU	2.1
1	F	1100	LEU	2.1
1	E	892	ASP	2.1
1	F	630	ASP	2.1
1	E	1010	GLY	2.1
1	F	581	GLY	2.1
1	E	956	GLU	2.1
1	E	1111	LYS	2.0
1	A	790	SER	2.0
1	E	731	SER	2.0
1	D	1288	LEU	2.0
1	E	950	ASN	2.0
1	E	1055	ILE	2.0
1	F	727	ASN	2.0
1	E	996	THR	2.0
1	F	1133	ALA	2.0
1	F	753	GLY	2.0
1	F	564	PRO	2.0
1	F	905	PRO	2.0
1	B	720	GLU	2.0
1	F	612	GLU	2.0
1	F	575	LEU	2.0
1	E	782	SER	2.0
1	F	1173	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	1097	ASN	2.0
1	B	230	THR	2.0
1	E	237	THR	2.0
1	A	1098	PRO	2.0
1	B	1255	PRO	2.0
1	E	601	PRO	2.0
1	E	902	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.