



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:01 AM UTC

PDB ID : 8RJ8 / pdb_00008rj8
Title : CytK nanopore mutant
Authors : Whittaker, J.J.; Sauciuc, A.; Guskov, A.
Deposited on : 2023-12-20
Resolution : 4.32 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

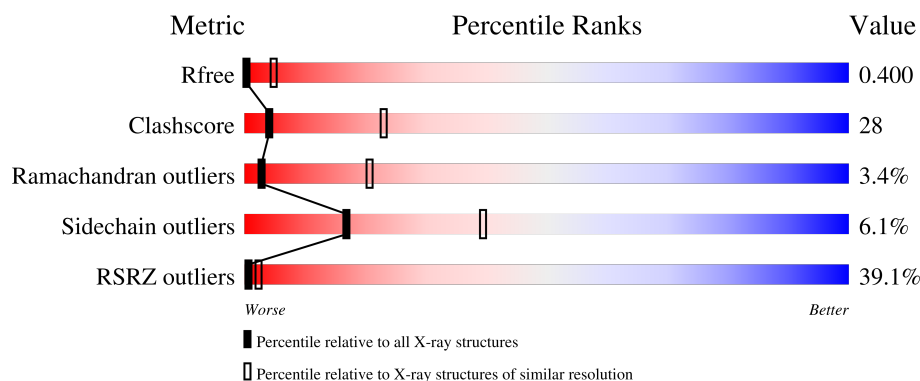
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.32 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	1056 (4.72-3.90)
Clashscore	190562	1101 (4.72-3.90)
Ramachandran outliers	187476	1003 (4.72-3.90)
Sidechain outliers	187428	1010 (4.76-3.88)
RSRZ outliers	180081	1053 (4.72-3.90)

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	310	35% 40% 45% 7% 6%
1	B	310	35% 45% 40% 12%
1	C	310	37% 49% 38% 5% 8%
1	D	310	45% 37% 43% 8% 10%
1	E	310	43% 49% 40% 6%

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Mol	Chain	Length	Quality of chain
1	F	310	27% 43% 49% • • •
1	G	310	32% 54% 38% • 6%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 15699 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 Cytotoxin K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2267	1419	381	460	7			
1	B	272	Total	C	N	O	S	0	0	0
			2119	1324	357	431	7			
1	C	284	Total	C	N	O	S	0	0	0
			2227	1396	376	448	7			
1	D	279	Total	C	N	O	S	0	0	0
			2184	1371	368	438	7			
1	E	292	Total	C	N	O	S	0	0	0
			2267	1420	380	460	7			
1	F	302	Total	C	N	O	S	0	0	0
			2351	1472	393	478	8			
1	G	292	Total	C	N	O	S	0	0	0
			2284	1432	382	463	7			

There are 49 discrepancies between the modelled and reference sequences:

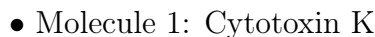
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q09KJ1
A	130	ASP	LYS	conflict	UNP Q09KJ1
A	149	ASP	THR	conflict	UNP Q09KJ1
A	157	ASP	LYS	conflict	UNP Q09KJ1
A	308	GLY	-	expression tag	UNP Q09KJ1
A	309	SER	-	expression tag	UNP Q09KJ1
A	310	ALA	-	expression tag	UNP Q09KJ1
B	1	MET	-	initiating methionine	UNP Q09KJ1
B	130	ASP	LYS	conflict	UNP Q09KJ1
B	149	ASP	THR	conflict	UNP Q09KJ1
B	157	ASP	LYS	conflict	UNP Q09KJ1
B	308	GLY	-	expression tag	UNP Q09KJ1
B	309	SER	-	expression tag	UNP Q09KJ1
B	310	ALA	-	expression tag	UNP Q09KJ1
C	1	MET	-	initiating methionine	UNP Q09KJ1

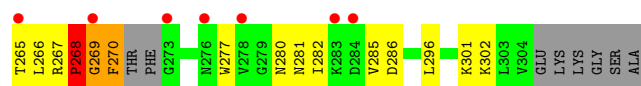
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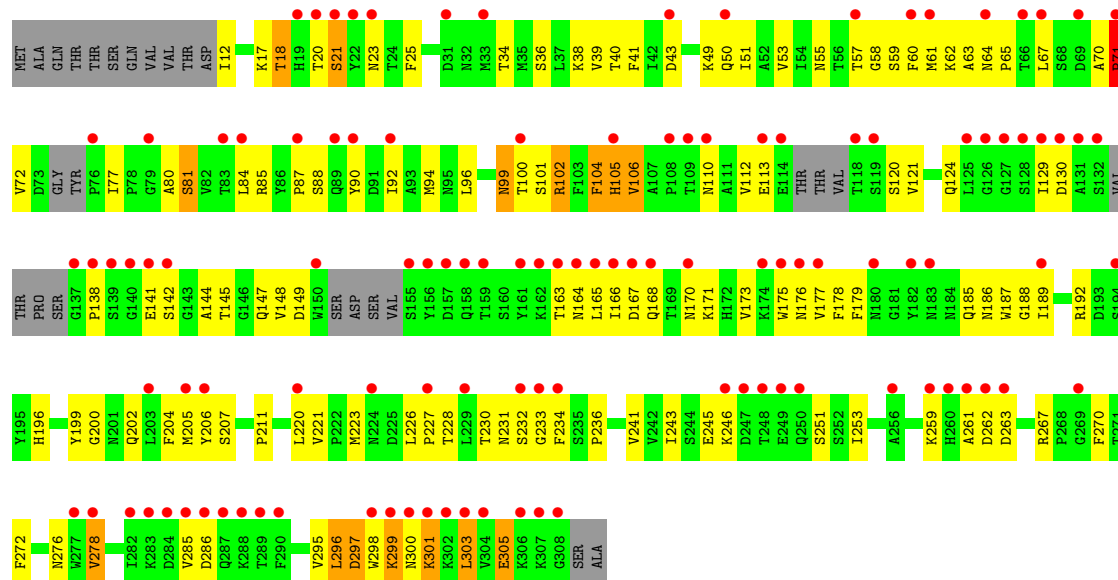
Chain	Residue	Modelled	Actual	Comment	Reference
C	130	ASP	LYS	conflict	UNP Q09KJ1
C	149	ASP	THR	conflict	UNP Q09KJ1
C	157	ASP	LYS	conflict	UNP Q09KJ1
C	308	GLY	-	expression tag	UNP Q09KJ1
C	309	SER	-	expression tag	UNP Q09KJ1
C	310	ALA	-	expression tag	UNP Q09KJ1
D	1	MET	-	initiating methionine	UNP Q09KJ1
D	130	ASP	LYS	conflict	UNP Q09KJ1
D	149	ASP	THR	conflict	UNP Q09KJ1
D	157	ASP	LYS	conflict	UNP Q09KJ1
D	308	GLY	-	expression tag	UNP Q09KJ1
D	309	SER	-	expression tag	UNP Q09KJ1
D	310	ALA	-	expression tag	UNP Q09KJ1
E	1	MET	-	initiating methionine	UNP Q09KJ1
E	130	ASP	LYS	conflict	UNP Q09KJ1
E	149	ASP	THR	conflict	UNP Q09KJ1
E	157	ASP	LYS	conflict	UNP Q09KJ1
E	308	GLY	-	expression tag	UNP Q09KJ1
E	309	SER	-	expression tag	UNP Q09KJ1
E	310	ALA	-	expression tag	UNP Q09KJ1
F	1	MET	-	initiating methionine	UNP Q09KJ1
F	130	ASP	LYS	conflict	UNP Q09KJ1
F	149	ASP	THR	conflict	UNP Q09KJ1
F	157	ASP	LYS	conflict	UNP Q09KJ1
F	308	GLY	-	expression tag	UNP Q09KJ1
F	309	SER	-	expression tag	UNP Q09KJ1
F	310	ALA	-	expression tag	UNP Q09KJ1
G	1	MET	-	initiating methionine	UNP Q09KJ1
G	130	ASP	LYS	conflict	UNP Q09KJ1
G	149	ASP	THR	conflict	UNP Q09KJ1
G	157	ASP	LYS	conflict	UNP Q09KJ1
G	308	GLY	-	expression tag	UNP Q09KJ1
G	309	SER	-	expression tag	UNP Q09KJ1
G	310	ALA	-	expression tag	UNP Q09KJ1

- Molecule 1: Cytotoxin K

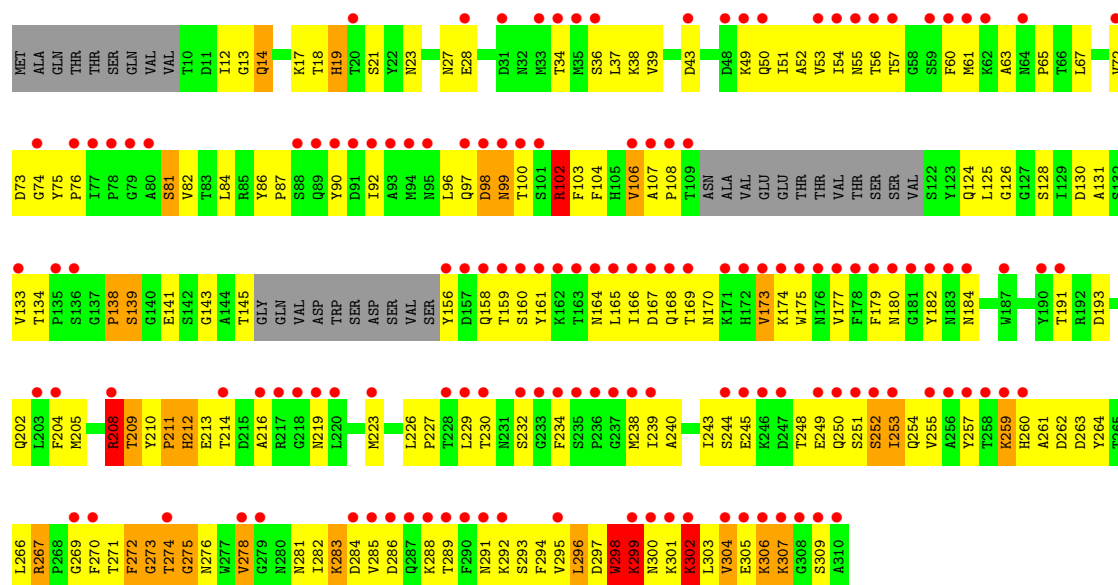




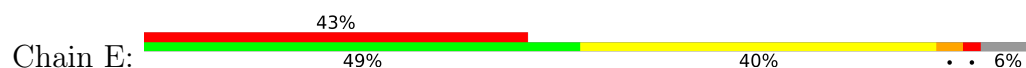
• Molecule 1: Cytotoxin K

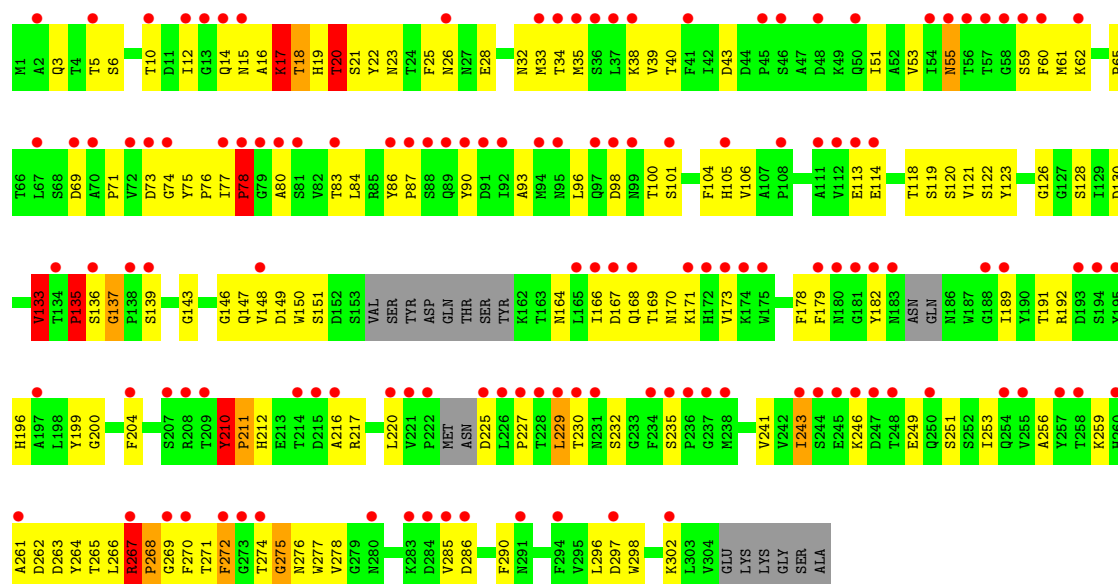


• Molecule 1: Cytotoxin K

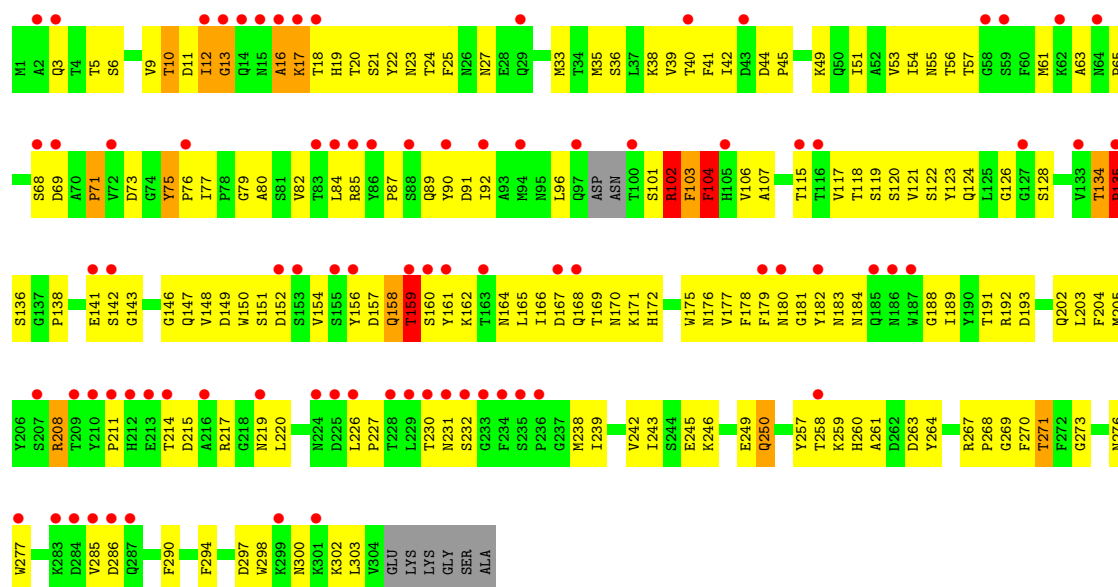


• Molecule 1: Cytotoxin K

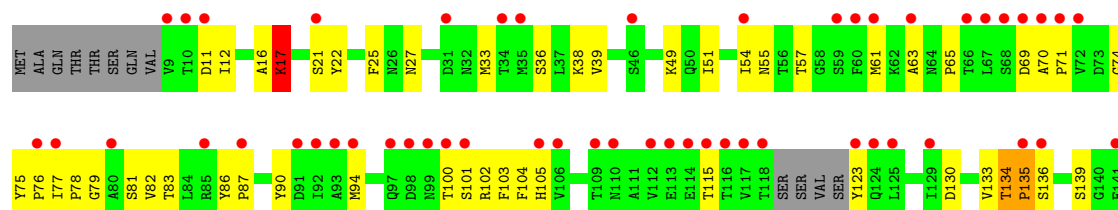


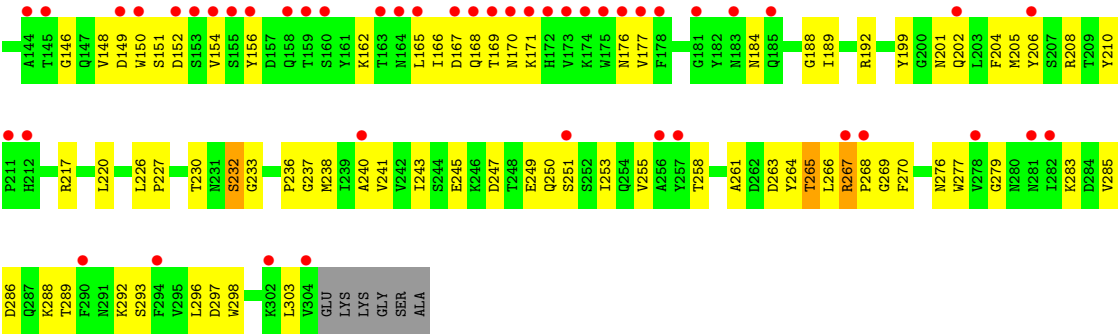


• Molecule 1: Cytotoxin K



• Molecule 1: Cytotoxin K





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.23Å 186.22Å 104.53Å 90.00° 115.85° 90.00°	Depositor
Resolution (Å)	94.07 – 4.32 94.07 – 4.32	Depositor EDS
% Data completeness (in resolution range)	95.5 (94.07-4.32) 97.0 (94.07-4.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 4.30Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.322 , 0.407 0.326 , 0.400	Depositor DCC
R_{free} test set	1277 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å ²)	84.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 178.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.059 for l,-k,h	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	15699	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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	0.53	0/2318	0.82	8/3153 (0.3%)
1	B	0.32	0/2161	0.69	4/2933 (0.1%)
1	C	0.40	0/2278	0.72	4/3093 (0.1%)
1	D	0.60	0/2237	0.91	5/3042 (0.2%)
1	E	0.43	0/2319	0.76	3/3159 (0.1%)
1	F	0.32	0/2407	0.74	9/3282 (0.3%)
1	G	0.32	0/2340	0.65	0/3191
All	All	0.43	0/16060	0.76	33/21853 (0.2%)

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	2
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	10

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	17	LYS	N-CA-C	10.09	121.86	111.07
1	B	209	THR	N-CA-C	10.08	121.96	110.97
1	F	250	GLN	N-CA-C	9.29	123.36	110.35
1	E	78	PRO	N-CA-CB	-8.76	94.05	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	135	PRO	N-CA-CB	-8.28	94.56	103.25
1	D	139	SER	CA-C-N	-8.18	114.89	122.17
1	D	139	SER	C-N-CA	-8.18	114.89	122.17
1	F	159	THR	N-CA-C	-7.48	102.06	112.45
1	C	71	PRO	N-CA-CB	-7.20	95.69	103.25
1	F	159	THR	CA-CB-OG1	-6.91	99.24	109.60
1	A	191	THR	N-CA-C	-6.37	103.63	111.40
1	C	81	SER	N-CA-C	6.28	120.31	111.52
1	B	209	THR	CB-CA-C	-5.87	101.92	110.96
1	F	250	GLN	CB-CA-C	-5.79	100.45	109.61
1	B	234	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	189	ILE	CA-C-O	-5.63	113.74	120.78
1	A	104	PHE	N-CA-CB	5.62	119.99	110.49
1	F	102	ARG	N-CA-CB	-5.62	101.75	110.29
1	D	81	SER	N-CA-C	5.61	119.38	111.52
1	A	103	PHE	CA-C-O	-5.58	112.52	120.51
1	C	297	ASP	CA-CB-CG	5.56	118.16	112.60
1	D	173	VAL	O-C-N	-5.55	117.35	123.18
1	F	104	PHE	CA-CB-CG	5.55	119.36	113.80
1	E	105	HIS	CB-CA-C	-5.50	100.84	109.70
1	D	82	VAL	N-CA-C	5.43	116.40	108.58
1	F	10	THR	N-CA-C	-5.33	105.58	111.71
1	A	103	PHE	CA-CB-CG	-5.27	108.53	113.80
1	C	104	PHE	CB-CA-C	-5.26	100.72	113.19
1	A	105	HIS	CA-C-N	-5.11	116.39	122.11
1	A	105	HIS	C-N-CA	-5.11	116.39	122.11
1	F	102	ARG	N-CA-C	5.11	118.04	110.48
1	A	184	ASN	CB-CA-C	5.08	118.89	109.54
1	B	268	PRO	N-CA-CB	-5.05	97.94	103.25

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	190	TYR	Mainchain
1	B	267	ARG	Sidechain
1	C	102	ARG	Sidechain
1	D	102	ARG	Sidechain
1	D	208	ARG	Sidechain
1	D	267	ARG	Sidechain
1	E	267	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	102	ARG	Sidechain
1	G	267	ARG	Sidechain

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	2267	0	2148	158	0
1	B	2119	0	2006	127	0
1	C	2227	0	2102	144	0
1	D	2184	0	2067	120	0
1	E	2267	0	2149	126	0
1	F	2351	0	2226	154	0
1	G	2284	0	2151	107	0
All	All	15699	0	14849	842	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 28.

All (842) 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:C:296:LEU:HA	1:C:303:LEU:HD23	1.28	1.12
1:D:87:PRO:HA	1:D:261:ALA:HA	1.12	1.11
1:A:72:VAL:HA	1:A:79:GLY:HA2	1.12	1.11
1:A:96:LEU:HD21	1:A:101:SER:H	1.21	1.05
1:G:265:THR:OG1	1:G:267:ARG:HG2	1.58	1.01
1:A:72:VAL:HA	1:A:79:GLY:CA	1.91	1.00
1:B:250:GLN:HA	1:B:296:LEU:O	1.64	0.97
1:E:270:PHE:HB2	1:E:278:VAL:HG21	1.47	0.96
1:C:20:THR:CB	1:C:301:LYS:HZ1	1.79	0.95
1:A:38:LYS:HB2	1:A:55:ASN:HB3	1.49	0.94
1:B:209:THR:O	1:B:210:TYR:HD1	1.49	0.94
1:C:251:SER:HB3	1:C:298:TRP:CZ3	2.06	0.90
1:C:20:THR:CB	1:C:301:LYS:NZ	2.35	0.90
1:D:81:SER:CB	1:D:267:ARG:HH21	1.84	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ASP:HB3	1:C:61:MET:HB2	1.55	0.88
1:C:20:THR:HG21	1:C:301:LYS:NZ	1.90	0.87
1:D:295:VAL:H	1:D:304:VAL:HB	1.39	0.86
1:F:39:VAL:HG12	1:F:54:ILE:HG13	1.58	0.84
1:D:87:PRO:HA	1:D:261:ALA:CA	2.03	0.84
1:B:87:PRO:HA	1:B:261:ALA:HA	1.59	0.84
1:D:108:PRO:HD2	1:D:175:TRP:CZ3	2.13	0.83
1:F:102:ARG:HB3	1:F:170:ASN:HB3	1.60	0.83
1:G:87:PRO:HA	1:G:261:ALA:HA	1.59	0.83
1:A:96:LEU:HD21	1:A:101:SER:N	1.94	0.83
1:C:20:THR:HB	1:C:301:LYS:HZ1	1.44	0.82
1:A:98:ASP:HA	1:A:171:LYS:HD3	1.59	0.82
1:B:209:THR:O	1:B:210:TYR:CD1	2.33	0.82
1:A:169:THR:HA	1:E:34:THR:HG21	1.62	0.82
1:D:81:SER:HB2	1:D:267:ARG:HH21	1.43	0.81
1:B:102:ARG:HD2	1:B:170:ASN:HB3	1.64	0.79
1:F:115:THR:HB	1:G:156:TYR:HB2	1.65	0.79
1:A:87:PRO:HA	1:A:261:ALA:HA	1.64	0.79
1:F:159:THR:HB	1:F:181:GLY:H	1.47	0.79
1:D:34:THR:HG21	1:G:169:THR:HA	1.62	0.79
1:E:80:ALA:HA	1:E:268:PRO:HD3	1.64	0.78
1:D:267:ARG:NH1	1:D:270:PHE:CE1	2.52	0.78
1:G:100:THR:HG21	1:G:251:SER:HA	1.66	0.78
1:F:79:GLY:HA3	1:F:268:PRO:HG2	1.63	0.77
1:C:20:THR:CG2	1:C:301:LYS:HZ1	1.97	0.77
1:C:20:THR:CG2	1:C:301:LYS:NZ	2.49	0.76
1:B:89:GLN:HB2	1:B:260:HIS:HB2	1.69	0.75
1:A:16:ALA:HB1	1:A:42:ILE:HD11	1.67	0.75
1:B:124:GLN:HG2	1:C:147:GLN:HG2	1.67	0.75
1:A:192:ARG:O	1:A:193:ASP:C	2.30	0.74
1:F:120:SER:HB2	1:F:149:ASP:HB3	1.68	0.74
1:A:110:ASN:HD21	1:A:164:ASN:HA	1.50	0.74
1:G:81:SER:HB2	1:G:267:ARG:HH11	1.51	0.74
1:A:72:VAL:CA	1:A:79:GLY:HA2	2.07	0.74
1:E:26:ASN:HD21	1:E:35:MET:HE3	1.53	0.74
1:F:71:PRO:HG3	1:F:217:ARG:HH22	1.53	0.73
1:F:87:PRO:HA	1:F:261:ALA:HA	1.70	0.73
1:G:130:ASP:HB2	1:G:139:SER:HB2	1.71	0.73
1:A:104:PHE:HA	1:E:25:PHE:CD2	2.23	0.73
1:E:121:VAL:HG22	1:E:148:VAL:HG13	1.70	0.73
1:A:133:VAL:HG11	1:E:137:GLY:HA2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:GLN:HB2	1:F:260:HIS:HB2	1.68	0.73
1:A:21:SER:HB3	1:C:12:ILE:HG22	1.70	0.73
1:G:265:THR:OG1	1:G:267:ARG:CG	2.37	0.73
1:B:124:GLN:HG3	1:C:147:GLN:HA	1.70	0.72
1:C:43:ASP:OD1	1:C:246:LYS:NZ	2.22	0.72
1:C:20:THR:HG21	1:C:301:LYS:HZ3	1.55	0.72
1:E:114:GLU:HA	1:F:157:ASP:HA	1.71	0.72
1:F:261:ALA:HB3	1:F:286:ASP:HB2	1.69	0.72
1:B:163:THR:HA	1:B:177:VAL:HG13	1.72	0.72
1:D:184:ASN:ND2	1:D:202:GLN:O	2.23	0.72
1:F:42:ILE:HG23	1:F:51:ILE:HB	1.72	0.72
1:D:164:ASN:O	1:D:175:TRP:HB3	1.91	0.71
1:B:134:THR:HB	1:B:135:PRO:HD3	1.72	0.71
1:C:87:PRO:HA	1:C:261:ALA:HA	1.71	0.70
1:C:251:SER:CB	1:C:298:TRP:CZ3	2.73	0.70
1:G:81:SER:HB2	1:G:267:ARG:NH1	2.05	0.70
1:F:84:LEU:HD21	1:F:220:LEU:HD22	1.73	0.70
1:E:6:SER:OG	1:F:13:GLY:HA3	1.92	0.70
1:B:181:GLY:HA3	1:B:191:THR:HA	1.74	0.69
1:F:69:ASP:HB3	1:F:217:ARG:HH21	1.56	0.69
1:G:226:LEU:HG	1:G:227:PRO:HD2	1.73	0.69
1:C:106:VAL:HG11	1:C:173:VAL:HG11	1.72	0.69
1:F:161:TYR:HB3	1:F:177:VAL:HG22	1.74	0.69
1:D:211:PRO:C	1:D:213:GLU:H	2.00	0.69
1:F:96:LEU:HD13	1:F:171:LYS:HZ2	1.58	0.69
1:F:267:ARG:HE	1:F:269:GLY:HA3	1.57	0.69
1:B:130:ASP:HB3	1:B:139:SER:HB2	1.74	0.69
1:G:77:ILE:HB	1:G:78:PRO:HD3	1.75	0.69
1:B:41:PHE:HB3	1:B:301:LYS:HE3	1.75	0.69
1:C:120:SER:HB3	1:C:149:ASP:HB2	1.75	0.68
1:C:165:LEU:HD21	1:C:168:GLN:HE22	1.56	0.68
1:B:96:LEU:HG	1:B:253:ILE:HG22	1.75	0.68
1:F:202:GLN:HB3	1:F:205:MET:HE2	1.75	0.68
1:G:103:PHE:HB2	1:G:170:ASN:HA	1.76	0.68
1:G:268:PRO:O	1:G:270:PHE:N	2.25	0.68
1:C:270:PHE:HB2	1:C:278:VAL:HG22	1.76	0.68
1:B:95:ASN:HB3	1:B:172:HIS:CE1	2.29	0.67
1:C:20:THR:OG1	1:C:301:LYS:NZ	2.26	0.67
1:C:202:GLN:NE2	1:C:205:MET:SD	2.68	0.67
1:G:115:THR:HA	1:G:154:VAL:HG12	1.77	0.67
1:G:263:ASP:HB2	1:G:285:VAL:HG11	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:HB3	1:A:139:SER:HB2	1.77	0.67
1:A:161:TYR:HB2	1:C:112:VAL:HG12	1.77	0.67
1:E:87:PRO:HA	1:E:261:ALA:HA	1.76	0.67
1:B:88:SER:HA	1:B:179:PHE:CE2	2.29	0.67
1:E:17:LYS:HB2	1:E:43:ASP:HB3	1.77	0.67
1:B:42:ILE:HB	1:B:51:ILE:HG23	1.77	0.66
1:C:251:SER:HB3	1:C:298:TRP:CH2	2.31	0.66
1:D:138:PRO:HG2	1:G:133:VAL:HG23	1.78	0.66
1:D:161:TYR:HA	1:D:179:PHE:HA	1.78	0.66
1:A:202:GLN:NE2	1:A:205:MET:SD	2.67	0.66
1:A:226:LEU:HB3	1:A:230:THR:HG21	1.77	0.66
1:B:38:LYS:HB3	1:B:55:ASN:HB2	1.78	0.66
1:C:168:GLN:HB2	1:C:173:VAL:HA	1.77	0.66
1:A:189:ILE:HB	1:A:196:HIS:NE2	2.11	0.65
1:F:169:THR:HB	1:F:172:HIS:H	1.62	0.65
1:D:100:THR:HB	1:D:251:SER:HA	1.79	0.65
1:A:80:ALA:HB3	1:A:268:PRO:HD3	1.78	0.65
1:A:109:THR:HB	1:E:235:SER:HB3	1.79	0.65
1:B:205:MET:HE1	1:B:266:LEU:HG	1.79	0.65
1:B:251:SER:HB3	1:B:296:LEU:HB2	1.78	0.64
1:A:133:VAL:HG13	1:A:134:THR:H	1.63	0.64
1:D:102:ARG:HB3	1:D:104:PHE:CE2	2.32	0.64
1:D:133:VAL:HG12	1:D:134:THR:H	1.62	0.64
1:F:63:ALA:O	1:F:85:ARG:NH2	2.31	0.64
1:A:120:SER:HB3	1:A:149:ASP:HB3	1.79	0.64
1:B:6:SER:HB3	1:C:12:ILE:HD11	1.80	0.64
1:G:133:VAL:HG12	1:G:134:THR:H	1.63	0.64
1:A:20:THR:HB	1:A:22:TYR:CE2	2.33	0.64
1:D:175:TRP:CZ3	1:D:238:MET:HB3	2.33	0.64
1:E:130:ASP:HB2	1:E:139:SER:HB2	1.80	0.64
1:F:184:ASN:ND2	1:F:205:MET:O	2.31	0.64
1:A:158:GLN:C	1:A:160:SER:H	2.06	0.63
1:A:160:SER:HB3	1:A:180:ASN:HB3	1.80	0.63
1:F:159:THR:O	1:F:160:SER:C	2.41	0.63
1:A:96:LEU:HD11	1:A:101:SER:HB3	1.81	0.63
1:B:166:ILE:HD11	1:C:61:MET:HE3	1.79	0.63
1:C:120:SER:N	1:C:149:ASP:O	2.27	0.63
1:E:261:ALA:HB3	1:E:286:ASP:HB2	1.79	0.63
1:F:123:TYR:HA	1:F:146:GLY:HA2	1.80	0.63
1:A:182:TYR:CE1	1:A:227:PRO:HD3	2.34	0.63
1:A:251:SER:HB3	1:A:296:LEU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:PHE:HD2	1:E:278:VAL:HG11	1.64	0.63
1:E:73:ASP:OD1	1:E:74:GLY:N	2.32	0.63
1:C:38:LYS:HB3	1:C:55:ASN:HB3	1.80	0.62
1:B:186:ASN:HB3	1:G:150:TRP:HH2	1.64	0.62
1:C:84:LEU:HD21	1:C:220:LEU:HD22	1.81	0.62
1:C:296:LEU:HB2	1:C:298:TRP:CZ3	2.34	0.62
1:D:106:VAL:HG21	1:D:173:VAL:HG21	1.81	0.62
1:F:267:ARG:HG2	1:F:269:GLY:H	1.64	0.62
1:A:90:TYR:HB2	1:A:177:VAL:HG23	1.82	0.62
1:B:191:THR:HG23	1:B:193:ASP:H	1.63	0.62
1:G:245:GLU:HG3	1:G:247:ASP:H	1.65	0.62
1:B:162:LYS:NZ	1:C:226:LEU:O	2.32	0.62
1:B:261:ALA:HB3	1:B:286:ASP:HB2	1.81	0.62
1:D:301:LYS:O	1:D:302:LYS:C	2.43	0.62
1:F:92:ILE:HG12	1:F:257:TYR:HD1	1.65	0.62
1:A:189:ILE:HD11	1:A:208:ARG:HE	1.65	0.62
1:C:81:SER:HB3	1:C:267:ARG:HE	1.64	0.62
1:F:165:LEU:HD21	1:F:168:GLN:HE21	1.65	0.62
1:F:257:TYR:HB2	1:F:290:PHE:CZ	2.35	0.62
1:A:189:ILE:HB	1:A:196:HIS:CE1	2.35	0.62
1:D:156:TYR:HB3	1:D:158:GLN:HG2	1.82	0.62
1:A:201:ASN:HD22	1:A:281:ASN:HB3	1.64	0.61
1:B:162:LYS:HB2	1:C:228:THR:HG22	1.81	0.61
1:E:216:ALA:HB2	1:E:277:TRP:CZ3	2.35	0.61
1:D:165:LEU:HG	1:D:175:TRP:CD1	2.35	0.61
1:C:20:THR:HG21	1:C:301:LYS:HZ1	1.60	0.61
1:G:134:THR:O	1:G:136:SER:N	2.33	0.61
1:B:100:THR:OG1	1:B:101:SER:N	2.34	0.61
1:A:68:SER:O	1:A:82:VAL:HA	2.01	0.61
1:E:122:SER:O	1:E:147:GLN:N	2.27	0.61
1:G:22:TYR:CE2	1:G:303:LEU:HB3	2.36	0.61
1:F:226:LEU:HB3	1:F:230:THR:HG21	1.83	0.61
1:A:42:ILE:HG23	1:A:51:ILE:HB	1.83	0.60
1:F:75:TYR:HB2	1:F:76:PRO:HD3	1.82	0.60
1:D:226:LEU:HB3	1:D:230:THR:HG21	1.82	0.60
1:D:174:LYS:C	1:D:175:TRP:CD1	2.80	0.60
1:F:27:ASN:ND2	1:F:33:MET:O	2.35	0.60
1:C:41:PHE:HE2	1:C:296:LEU:HD23	1.67	0.60
1:D:212:HIS:HB2	1:D:214:THR:HG22	1.84	0.60
1:C:21:SER:HA	1:C:40:THR:HG22	1.84	0.59
1:D:107:ALA:HB3	1:D:239:ILE:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:GLY:N	1:D:143:GLY:O	2.34	0.59
1:C:251:SER:CB	1:C:298:TRP:HZ3	2.15	0.59
1:A:267:ARG:HG3	1:A:268:PRO:HD2	1.83	0.59
1:B:53:VAL:HG13	1:B:241:VAL:HG22	1.83	0.59
1:B:122:SER:O	1:B:147:GLN:N	2.25	0.59
1:B:202:GLN:HG2	1:B:205:MET:HB3	1.84	0.59
1:E:38:LYS:HG3	1:E:55:ASN:HB2	1.83	0.59
1:E:123:TYR:HA	1:E:146:GLY:HA2	1.83	0.59
1:G:86:TYR:CE1	1:G:230:THR:HG23	2.37	0.59
1:A:184:ASN:H	1:A:190:TYR:HE1	1.48	0.59
1:D:159:THR:O	1:D:227:PRO:HG3	2.03	0.59
1:E:249:GLU:O	1:E:298:TRP:N	2.35	0.59
1:B:47:ALA:HA	1:C:21:SER:O	2.03	0.59
1:A:97:GLN:HB2	1:A:252:SER:OG	2.03	0.59
1:A:48:ASP:HB2	1:E:22:TYR:CD1	2.38	0.58
1:B:61:MET:HB2	1:D:167:ASP:CG	2.28	0.58
1:B:180:ASN:O	1:B:192:ARG:N	2.35	0.58
1:E:263:ASP:OD1	1:E:285:VAL:HG21	2.03	0.58
1:A:232:SER:HB3	1:C:165:LEU:O	2.02	0.58
1:F:165:LEU:HD11	1:F:168:GLN:HE21	1.69	0.58
1:G:292:LYS:NZ	1:G:293:SER:O	2.35	0.58
1:A:23:ASN:O	1:C:49:LYS:NZ	2.35	0.58
1:A:189:ILE:CG1	1:A:208:ARG:HH21	2.15	0.58
1:A:192:ARG:HD2	1:E:225:ASP:OD2	2.04	0.58
1:A:158:GLN:C	1:A:160:SER:N	2.60	0.58
1:B:103:PHE:N	1:B:170:ASN:O	2.34	0.58
1:B:213:GLU:HA	1:B:277:TRP:HZ2	1.69	0.58
1:F:36:SER:HB2	1:F:57:THR:O	2.04	0.58
1:A:103:PHE:N	1:A:170:ASN:OD1	2.36	0.57
1:A:190:TYR:HE2	1:A:208:ARG:HH22	1.51	0.57
1:D:81:SER:HB2	1:D:267:ARG:NH2	2.17	0.57
1:G:250:GLN:HG3	1:G:297:ASP:HA	1.86	0.57
1:B:46:SER:HB2	1:C:20:THR:HA	1.86	0.57
1:B:214:THR:HG22	1:B:215:ASP:H	1.69	0.57
1:A:103:PHE:O	1:A:242:VAL:HA	2.04	0.57
1:F:17:LYS:C	1:F:19:HIS:H	2.12	0.57
1:A:122:SER:O	1:A:147:GLN:N	2.31	0.57
1:B:204:PHE:CE2	1:B:264:TYR:HB3	2.39	0.57
1:D:294:PHE:HA	1:D:304:VAL:HG12	1.86	0.57
1:D:253:ILE:HG12	1:D:296:LEU:HD23	1.86	0.57
1:F:154:VAL:HB	1:F:156:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HE2	1:B:5:THR:CG2	2.34	0.57
1:A:249:GLU:HA	1:A:298:TRP:HB2	1.87	0.57
1:B:33:MET:HE3	1:B:259:LYS:HE3	1.86	0.57
1:F:208:ARG:HH11	1:F:208:ARG:HB2	1.69	0.57
1:B:61:MET:O	1:B:259:LYS:NZ	2.27	0.57
1:B:186:ASN:HB3	1:G:150:TRP:CH2	2.39	0.57
1:A:192:ARG:O	1:A:194:SER:N	2.38	0.57
1:D:175:TRP:CH2	1:D:238:MET:HB3	2.39	0.57
1:E:53:VAL:HG12	1:E:241:VAL:HG22	1.87	0.56
1:F:104:PHE:HB2	1:G:25:PHE:CE2	2.39	0.56
1:A:78:PRO:HD2	1:A:268:PRO:HG3	1.87	0.56
1:C:77:ILE:HB	1:C:80:ALA:HB3	1.88	0.56
1:D:251:SER:O	1:D:252:SER:C	2.48	0.56
1:F:38:LYS:HB3	1:F:55:ASN:HB2	1.88	0.56
1:F:121:VAL:HG22	1:F:148:VAL:HG13	1.87	0.56
1:C:297:ASP:O	1:C:298:TRP:C	2.49	0.56
1:E:10:THR:HA	1:F:40:THR:HG21	1.88	0.56
1:G:285:VAL:HG13	1:G:286:ASP:H	1.70	0.56
1:D:87:PRO:CA	1:D:261:ALA:HA	2.08	0.56
1:E:33:MET:HG3	1:E:60:PHE:HD1	1.70	0.56
1:E:120:SER:O	1:E:149:ASP:N	2.33	0.56
1:A:41:PHE:CG	1:A:301:LYS:HD2	2.40	0.56
1:G:75:TYR:O	1:G:79:GLY:HA2	2.05	0.56
1:F:80:ALA:O	1:F:267:ARG:HG3	2.06	0.56
1:G:27:ASN:ND2	1:G:33:MET:O	2.39	0.56
1:B:104:PHE:CE1	1:B:243:ILE:HG23	2.40	0.56
1:F:35:MET:HE1	1:F:294:PHE:CZ	2.40	0.56
1:A:123:TYR:HA	1:A:146:GLY:HA2	1.88	0.56
1:B:34:THR:HG21	1:D:169:THR:HA	1.88	0.56
1:B:168:GLN:HB3	1:C:34:THR:HG21	1.87	0.56
1:E:33:MET:HE1	1:E:290:PHE:CB	2.36	0.55
1:G:69:ASP:HA	1:G:82:VAL:HG22	1.87	0.55
1:F:73:ASP:HB3	1:F:77:ILE:HB	1.87	0.55
1:A:121:VAL:HG13	1:E:150:TRP:HB2	1.89	0.55
1:A:190:TYR:HE2	1:A:208:ARG:NH2	2.05	0.55
1:C:34:THR:HG23	1:C:59:SER:H	1.71	0.55
1:A:100:THR:C	1:A:102:ARG:H	2.14	0.55
1:D:90:TYR:CE1	1:D:259:LYS:HB2	2.41	0.55
1:D:244:SER:HB2	1:D:298:TRP:CD1	2.41	0.55
1:A:90:TYR:CE1	1:A:259:LYS:HG3	2.42	0.55
1:B:43:ASP:OD1	1:B:246:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:THR:OG1	1:B:172:HIS:O	2.21	0.55
1:C:88:SER:OG	1:C:192:ARG:NH2	2.39	0.55
1:D:92:ILE:HG23	1:D:257:TYR:CE1	2.42	0.55
1:G:123:TYR:HA	1:G:146:GLY:HA2	1.87	0.55
1:G:101:SER:OG	1:G:170:ASN:OD1	2.25	0.55
1:B:49:LYS:HD2	1:B:245:GLU:HA	1.87	0.55
1:B:204:PHE:HB2	1:B:220:LEU:HD23	1.89	0.55
1:B:269:GLY:O	1:B:270:PHE:C	2.49	0.55
1:E:84:LEU:HD22	1:E:220:LEU:HD13	1.88	0.55
1:E:113:GLU:OE1	1:E:113:GLU:N	2.39	0.55
1:A:260:HIS:HB3	1:A:284:ASP:OD1	2.07	0.55
1:B:33:MET:HB3	1:B:60:PHE:HD1	1.72	0.55
1:G:90:TYR:HB2	1:G:177:VAL:HG23	1.89	0.55
1:B:52:ALA:HB3	1:B:242:VAL:HG23	1.89	0.55
1:B:130:ASP:OD1	1:B:131:ALA:N	2.40	0.54
1:E:196:HIS:ND1	1:E:200:GLY:O	2.36	0.54
1:F:20:THR:OG1	1:F:41:PHE:HB2	2.07	0.54
1:G:51:ILE:HG22	1:G:243:ILE:HG12	1.88	0.54
1:E:106:VAL:HG21	1:E:168:GLN:OE1	2.07	0.54
1:C:65:PRO:HB2	1:C:67:LEU:HG	1.89	0.54
1:B:124:GLN:HG2	1:C:147:GLN:CG	2.37	0.54
1:A:166:ILE:HG12	1:A:167:ASP:H	1.72	0.54
1:C:36:SER:HB2	1:C:57:THR:C	2.33	0.54
1:G:82:VAL:HG11	1:G:217:ARG:HA	1.90	0.54
1:F:36:SER:HB2	1:F:57:THR:C	2.33	0.54
1:G:253:ILE:HG12	1:G:296:LEU:HD11	1.90	0.54
1:B:66:THR:HG21	1:B:217:ARG:HG3	1.90	0.54
1:D:275:GLY:O	1:D:276:ASN:C	2.50	0.54
1:F:25:PHE:CZ	1:F:36:SER:HB3	2.43	0.54
1:D:124:GLN:HG2	1:D:145:THR:HB	1.90	0.54
1:F:16:ALA:HB1	1:F:44:ASP:HA	1.90	0.54
1:F:68:SER:O	1:F:82:VAL:HA	2.08	0.54
1:A:107:ALA:HB3	1:A:239:ILE:HG13	1.89	0.53
1:C:196:HIS:N	1:C:200:GLY:O	2.38	0.53
1:F:184:ASN:HB3	1:F:208:ARG:NH2	2.23	0.53
1:G:94:MET:SD	1:G:255:VAL:HG12	2.49	0.53
1:A:80:ALA:C	1:A:82:VAL:H	2.15	0.53
1:F:65:PRO:HD2	1:F:85:ARG:HB3	1.91	0.53
1:A:70:ALA:HB3	1:A:71:PRO:HD3	1.90	0.53
1:C:96:LEU:HD13	1:C:100:THR:HG22	1.91	0.53
1:E:19:HIS:O	1:E:21:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:ALA:O	1:G:17:LYS:C	2.51	0.53
1:D:128:SER:HB3	1:D:141:GLU:HB3	1.90	0.53
1:C:92:ILE:HG23	1:C:175:TRP:CD1	2.44	0.53
1:F:38:LYS:N	1:F:55:ASN:O	2.42	0.53
1:F:166:ILE:HG13	1:F:176:ASN:HB2	1.90	0.53
1:G:74:GLY:HA3	1:G:78:PRO:HG2	1.89	0.53
1:B:93:ALA:HB3	1:B:256:ALA:HB3	1.89	0.53
1:D:97:GLN:O	1:D:99:ASN:N	2.42	0.53
1:F:120:SER:HA	1:G:150:TRP:O	2.09	0.53
1:D:56:THR:HG22	1:D:238:MET:O	2.09	0.52
1:A:160:SER:O	1:A:162:LYS:N	2.39	0.52
1:A:206:TYR:HB3	1:A:219:ASN:O	2.10	0.52
1:B:216:ALA:HB1	1:B:266:LEU:HD22	1.91	0.52
1:C:41:PHE:CE1	1:C:301:LYS:HB3	2.44	0.52
1:E:62:LYS:HG3	1:E:230:THR:HA	1.91	0.52
1:A:97:GLN:O	1:A:99:ASN:N	2.42	0.52
1:D:211:PRO:C	1:D:213:GLU:N	2.67	0.52
1:F:102:ARG:CB	1:F:170:ASN:HB3	2.37	0.52
1:F:165:LEU:HD21	1:F:168:GLN:HG3	1.92	0.52
1:A:28:GLU:N	1:A:28:GLU:OE1	2.42	0.52
1:A:38:LYS:CE	1:B:5:THR:HG22	2.40	0.52
1:C:23:ASN:HB3	1:C:25:PHE:CE1	2.44	0.52
1:C:81:SER:HB3	1:C:267:ARG:NE	2.23	0.52
1:G:286:ASP:OD1	1:G:288:LYS:NZ	2.43	0.52
1:A:229:LEU:HD23	1:A:234:PHE:HB2	1.90	0.52
1:E:274:THR:O	1:E:275:GLY:C	2.52	0.52
1:A:190:TYR:HD2	1:A:202:GLN:HB2	1.73	0.52
1:D:273:GLY:O	1:D:275:GLY:N	2.43	0.52
1:B:69:ASP:OD2	1:B:217:ARG:NH1	2.42	0.52
1:B:164:ASN:ND2	1:C:231:ASN:OD1	2.42	0.52
1:A:38:LYS:CB	1:A:55:ASN:HB3	2.33	0.52
1:A:187:TRP:HE1	1:A:191:THR:HA	1.75	0.52
1:C:39:VAL:HA	1:C:53:VAL:O	2.10	0.52
1:F:191:THR:HG23	1:F:193:ASP:H	1.75	0.52
1:B:68:SER:HB3	1:B:83:THR:HG22	1.91	0.52
1:C:63:ALA:O	1:C:65:PRO:HD3	2.10	0.52
1:D:108:PRO:HD2	1:D:175:TRP:CH2	2.45	0.52
1:C:96:LEU:HD13	1:C:100:THR:CG2	2.40	0.51
1:E:86:TYR:CZ	1:E:204:PHE:HD2	2.28	0.51
1:A:63:ALA:O	1:A:65:PRO:HD3	2.10	0.51
1:A:228:THR:HA	1:C:164:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ASP:HA	1:B:171:LYS:HD2	1.92	0.51
1:D:81:SER:OG	1:D:267:ARG:NH2	2.42	0.51
1:F:17:LYS:O	1:F:19:HIS:N	2.38	0.51
1:F:204:PHE:CE2	1:F:264:TYR:HB3	2.46	0.51
1:E:80:ALA:HA	1:E:268:PRO:CD	2.38	0.51
1:C:50:GLN:HG3	1:C:246:LYS:HG2	1.90	0.51
1:E:268:PRO:O	1:E:269:GLY:C	2.52	0.51
1:F:90:TYR:CE1	1:F:259:LYS:HG3	2.45	0.51
1:F:117:VAL:HB	1:G:156:TYR:CE1	2.45	0.51
1:G:184:ASN:ND2	1:G:202:GLN:O	2.39	0.51
1:C:57:THR:HG22	1:C:58:GLY:H	1.74	0.51
1:F:91:ASP:O	1:F:258:THR:OG1	2.23	0.51
1:D:216:ALA:HA	1:D:219:ASN:HB3	1.92	0.51
1:D:297:ASP:CG	1:D:300:ASN:HB3	2.36	0.51
1:D:305:GLU:C	1:D:307:LYS:H	2.19	0.51
1:G:81:SER:CB	1:G:267:ARG:HH11	2.20	0.51
1:B:127:GLY:O	1:C:144:ALA:N	2.44	0.51
1:F:227:PRO:O	1:F:231:ASN:ND2	2.44	0.51
1:E:266:LEU:HD11	1:E:277:TRP:HB3	1.93	0.51
1:F:126:GLY:N	1:F:143:GLY:O	2.44	0.51
1:E:169:THR:HG22	1:E:170:ASN:H	1.75	0.50
1:C:295:VAL:H	1:C:305:GLU:HA	1.76	0.50
1:F:157:ASP:O	1:F:158:GLN:C	2.54	0.50
1:A:38:LYS:HE2	1:B:5:THR:HG22	1.94	0.50
1:D:38:LYS:HB3	1:D:55:ASN:HB3	1.92	0.50
1:E:33:MET:HG3	1:E:60:PHE:CD1	2.46	0.50
1:F:22:TYR:CD2	1:F:303:LEU:HB3	2.46	0.50
1:B:63:ALA:O	1:B:65:PRO:HD3	2.11	0.50
1:C:251:SER:HG	1:C:298:TRP:HZ3	1.55	0.50
1:D:133:VAL:HG12	1:D:134:THR:N	2.27	0.50
1:G:39:VAL:HG22	1:G:54:ILE:HG22	1.93	0.50
1:A:10:THR:HG22	1:E:53:VAL:HG21	1.94	0.50
1:G:154:VAL:HG22	1:G:156:TYR:CE1	2.47	0.50
1:B:103:PHE:CE1	1:B:240:ALA:HB1	2.47	0.50
1:D:84:LEU:HD13	1:D:86:TYR:CD2	2.47	0.50
1:D:18:THR:O	1:D:19:HIS:HB3	2.12	0.50
1:D:175:TRP:HZ3	1:D:238:MET:SD	2.35	0.50
1:F:122:SER:HA	1:G:148:VAL:O	2.11	0.49
1:B:124:GLN:CG	1:C:147:GLN:HA	2.40	0.49
1:D:97:GLN:C	1:D:99:ASN:H	2.20	0.49
1:F:24:THR:C	1:F:25:PHE:HD1	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:TYR:HB2	1:C:177:VAL:HG23	1.92	0.49
1:C:166:ILE:HB	1:C:176:ASN:CG	2.37	0.49
1:G:22:TYR:CZ	1:G:39:VAL:HB	2.47	0.49
1:G:70:ALA:H	1:G:82:VAL:HG22	1.77	0.49
1:A:168:GLN:HG2	1:E:59:SER:HB3	1.94	0.49
1:C:41:PHE:CE2	1:C:296:LEU:HD23	2.47	0.49
1:E:76:PRO:O	1:E:80:ALA:HB2	2.12	0.49
1:B:66:THR:HB	1:B:84:LEU:HG	1.94	0.49
1:B:253:ILE:HG12	1:B:296:LEU:HD11	1.94	0.49
1:F:134:THR:O	1:F:135:PRO:C	2.56	0.49
1:F:270:PHE:O	1:F:271:THR:OG1	2.26	0.49
1:A:104:PHE:CE2	1:E:23:ASN:HB3	2.47	0.49
1:B:22:TYR:OH	1:B:302:LYS:HG2	2.13	0.49
1:B:48:ASP:C	1:B:49:LYS:HD3	2.37	0.49
1:B:57:THR:HA	1:B:236:PRO:O	2.13	0.49
1:C:186:ASN:OD1	1:C:186:ASN:O	2.31	0.49
1:F:106:VAL:HG13	1:F:175:TRP:CZ2	2.47	0.49
1:F:118:THR:HA	1:G:152:ASP:O	2.11	0.49
1:G:49:LYS:HG2	1:G:245:GLU:HA	1.95	0.49
1:A:133:VAL:HG13	1:A:134:THR:N	2.28	0.49
1:D:205:MET:HE3	1:D:208:ARG:HG3	1.93	0.49
1:F:250:GLN:HA	1:F:298:TRP:HD1	1.77	0.49
1:G:22:TYR:HE2	1:G:303:LEU:HD22	1.78	0.49
1:A:12:ILE:HD11	1:A:44:ASP:OD2	2.13	0.49
1:A:201:ASN:ND2	1:A:281:ASN:HB3	2.27	0.49
1:F:263:ASP:HB2	1:F:285:VAL:HG21	1.95	0.49
1:B:28:GLU:HG2	1:B:33:MET:HB2	1.95	0.48
1:E:120:SER:HB3	1:E:149:ASP:HB3	1.94	0.48
1:F:22:TYR:CG	1:F:23:ASN:N	2.81	0.48
1:F:63:ALA:O	1:F:65:PRO:HD3	2.13	0.48
1:F:90:TYR:HB2	1:F:177:VAL:HG13	1.94	0.48
1:G:210:TYR:HB3	1:G:277:TRP:HE1	1.76	0.48
1:F:54:ILE:HD13	1:F:242:VAL:HG23	1.93	0.48
1:C:105:HIS:HB3	1:C:241:VAL:CG1	2.43	0.48
1:G:296:LEU:HG	1:G:303:LEU:HD12	1.95	0.48
1:B:20:THR:OG1	1:B:41:PHE:HB2	2.12	0.48
1:C:296:LEU:HG	1:C:303:LEU:CD2	2.44	0.48
1:D:130:ASP:OD1	1:D:131:ALA:N	2.46	0.48
1:D:232:SER:HB3	1:G:165:LEU:O	2.13	0.48
1:E:121:VAL:HG13	1:E:148:VAL:HG22	1.94	0.48
1:E:251:SER:HB2	1:E:296:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:PHE:N	1:F:170:ASN:O	2.42	0.48
1:F:122:SER:O	1:F:147:GLN:N	2.26	0.48
1:A:96:LEU:HB3	1:A:171:LYS:HA	1.94	0.48
1:E:272:PHE:HD2	1:E:276:ASN:HB2	1.79	0.48
1:F:164:ASN:HD21	1:F:178:PHE:HD2	1.61	0.48
1:F:215:ASP:OD2	1:F:217:ARG:NH1	2.46	0.48
1:A:14:GLN:O	1:A:15:ASN:C	2.55	0.48
1:A:103:PHE:O	1:A:104:PHE:HB2	2.14	0.48
1:C:298:TRP:O	1:C:299:LYS:C	2.56	0.48
1:E:65:PRO:O	1:E:84:LEU:HD12	2.14	0.48
1:E:126:GLY:N	1:E:143:GLY:O	2.43	0.48
1:F:49:LYS:HG2	1:F:245:GLU:HA	1.96	0.48
1:A:48:ASP:HB2	1:E:22:TYR:CE1	2.49	0.48
1:A:165:LEU:O	1:E:232:SER:HB3	2.14	0.48
1:A:169:THR:HG1	1:A:172:HIS:H	1.58	0.48
1:B:164:ASN:HB3	1:C:232:SER:OG	2.14	0.48
1:C:61:MET:HG2	1:C:63:ALA:N	2.29	0.48
1:E:166:ILE:HG13	1:E:167:ASP:H	1.79	0.48
1:E:28:GLU:N	1:E:28:GLU:OE1	2.47	0.48
1:E:199:TYR:CE1	1:E:276:ASN:HB3	2.48	0.48
1:A:49:LYS:HG2	1:A:245:GLU:HA	1.96	0.48
1:C:49:LYS:HD3	1:C:245:GLU:HG3	1.94	0.48
1:C:206:TYR:HA	1:C:221:VAL:HG13	1.96	0.48
1:G:149:ASP:OD1	1:G:150:TRP:N	2.46	0.48
1:C:297:ASP:O	1:C:301:LYS:N	2.39	0.47
1:D:297:ASP:C	1:D:299:LYS:H	2.22	0.47
1:F:56:THR:HG22	1:F:238:MET:O	2.13	0.47
1:G:166:ILE:HG13	1:G:176:ASN:ND2	2.30	0.47
1:G:202:GLN:O	1:G:202:GLN:HG2	2.14	0.47
1:D:19:HIS:CE1	1:G:12:ILE:HA	2.50	0.47
1:D:297:ASP:HB3	1:D:300:ASN:C	2.40	0.47
1:E:212:HIS:O	1:E:212:HIS:CG	2.67	0.47
1:F:128:SER:HB3	1:F:141:GLU:HB3	1.94	0.47
1:G:202:GLN:HG3	1:G:205:MET:HB3	1.95	0.47
1:G:206:TYR:HB2	1:G:220:LEU:C	2.39	0.47
1:B:110:ASN:ND2	1:C:233:GLY:O	2.33	0.47
1:C:70:ALA:O	1:C:71:PRO:C	2.57	0.47
1:C:64:ASN:ND2	1:C:230:THR:O	2.47	0.47
1:D:51:ILE:HA	1:D:243:ILE:HG13	1.97	0.47
1:D:72:VAL:O	1:D:74:GLY:N	2.47	0.47
1:A:133:VAL:CG1	1:E:137:GLY:HA2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:PHE:CE1	1:C:243:ILE:HB	2.49	0.47
1:C:163:THR:HA	1:C:177:VAL:HG12	1.96	0.47
1:F:118:THR:HB	1:F:151:SER:HB2	1.96	0.47
1:F:159:THR:HG1	1:F:180:ASN:H	1.61	0.47
1:G:204:PHE:CE2	1:G:264:TYR:HB3	2.50	0.47
1:A:19:HIS:HD2	1:A:42:ILE:HD13	1.80	0.47
1:B:104:PHE:HA	1:B:168:GLN:NE2	2.29	0.47
1:E:83:THR:HG22	1:E:265:THR:HB	1.96	0.47
1:A:49:LYS:HB3	1:A:244:SER:O	2.15	0.47
1:A:267:ARG:HB3	1:A:278:VAL:HB	1.96	0.47
1:B:12:ILE:HG23	1:C:38:LYS:HZ1	1.80	0.47
1:B:77:ILE:HB	1:B:78:PRO:HD3	1.96	0.47
1:C:270:PHE:O	1:C:276:ASN:HB2	2.14	0.47
1:C:270:PHE:C	1:C:272:PHE:H	2.23	0.47
1:D:274:THR:O	1:D:275:GLY:C	2.56	0.47
1:E:169:THR:HG22	1:E:170:ASN:N	2.30	0.47
1:F:166:ILE:HG22	1:F:167:ASP:H	1.79	0.47
1:C:207:SER:HB3	1:C:211:PRO:HD3	1.96	0.47
1:D:75:TYR:N	1:D:76:PRO:HD3	2.30	0.47
1:D:158:GLN:C	1:D:160:SER:H	2.21	0.47
1:F:120:SER:O	1:F:149:ASP:N	2.33	0.47
1:B:261:ALA:N	1:B:286:ASP:O	2.48	0.47
1:E:168:GLN:O	1:F:61:MET:HE2	2.15	0.47
1:A:104:PHE:HB3	1:A:105:HIS:H	1.42	0.46
1:A:167:ASP:HB3	1:E:61:MET:SD	2.56	0.46
1:B:50:GLN:HB2	1:B:301:LYS:HE2	1.97	0.46
1:C:227:PRO:O	1:C:230:THR:HG22	2.15	0.46
1:D:61:MET:HG2	1:D:63:ALA:N	2.30	0.46
1:D:96:LEU:HD23	1:D:103:PHE:CE1	2.50	0.46
1:D:267:ARG:HG2	1:D:269:GLY:H	1.80	0.46
1:F:166:ILE:HG13	1:F:176:ASN:CG	2.40	0.46
1:G:285:VAL:HG13	1:G:286:ASP:N	2.29	0.46
1:A:140:GLY:O	1:C:130:ASP:HB3	2.14	0.46
1:A:307:LYS:HB3	1:A:308:GLY:H	1.55	0.46
1:E:43:ASP:OD1	1:E:246:LYS:NZ	2.25	0.46
1:F:6:SER:N	1:G:11:ASP:HB3	2.29	0.46
1:C:223:MET:HB3	1:C:231:ASN:HB3	1.98	0.46
1:A:190:TYR:CD2	1:A:202:GLN:HB2	2.50	0.46
1:B:164:ASN:ND2	1:C:228:THR:O	2.48	0.46
1:D:305:GLU:HB3	1:D:306:LYS:H	1.36	0.46
1:E:86:TYR:CE2	1:E:264:TYR:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:PHE:CZ	1:D:234:PHE:HD2	2.33	0.46
1:F:167:ASP:HB3	1:G:61:MET:SD	2.56	0.46
1:B:62:LYS:HE2	1:B:233:GLY:HA2	1.97	0.46
1:E:98:ASP:HA	1:E:171:LYS:HD3	1.98	0.46
1:A:184:ASN:O	1:A:186:ASN:N	2.48	0.46
1:A:227:PRO:O	1:A:230:THR:HG22	2.14	0.46
1:C:100:THR:OG1	1:C:101:SER:N	2.48	0.46
1:C:251:SER:CB	1:C:298:TRP:CH2	2.96	0.46
1:E:119:SER:OG	1:F:152:ASP:HB2	2.16	0.46
1:F:205:MET:HE3	1:F:208:ARG:HA	1.97	0.46
1:G:74:GLY:O	1:G:79:GLY:N	2.49	0.46
1:B:160:SER:O	1:B:179:PHE:HB2	2.16	0.46
1:C:17:LYS:O	1:C:18:THR:OG1	2.28	0.46
1:D:49:LYS:HZ1	1:D:104:PHE:HZ	1.58	0.46
1:F:203:LEU:HD11	1:F:264:TYR:CE2	2.51	0.46
1:E:168:GLN:HG2	1:E:173:VAL:HA	1.98	0.46
1:D:223:MET:SD	1:D:223:MET:N	2.90	0.45
1:E:33:MET:HE1	1:E:290:PHE:CG	2.51	0.45
1:F:211:PRO:HB2	1:F:277:TRP:CD1	2.51	0.45
1:A:16:ALA:CB	1:A:42:ILE:HD11	2.41	0.45
1:A:303:LEU:C	1:A:305:GLU:H	2.24	0.45
1:B:209:THR:C	1:B:210:TYR:HD1	2.21	0.45
1:C:60:PHE:HB2	1:C:259:LYS:HE2	1.98	0.45
1:E:199:TYR:HE1	1:E:276:ASN:HB3	1.82	0.45
1:A:91:ASP:HA	1:A:175:TRP:O	2.15	0.45
1:C:88:SER:HB2	1:C:262:ASP:OD2	2.16	0.45
1:E:128:SER:HA	1:F:142:SER:O	2.17	0.45
1:A:48:ASP:HB2	1:E:22:TYR:HD1	1.80	0.45
1:F:159:THR:HB	1:F:181:GLY:N	2.24	0.45
1:G:166:ILE:HG13	1:G:176:ASN:CG	2.42	0.45
1:B:7:GLN:HG3	1:C:105:HIS:CD2	2.51	0.45
1:C:94:MET:CG	1:C:173:VAL:HB	2.46	0.45
1:D:50:GLN:HG3	1:D:298:TRP:CZ3	2.51	0.45
1:E:84:LEU:HD23	1:E:86:TYR:OH	2.16	0.45
1:F:21:SER:HG	1:F:38:LYS:HZ2	1.58	0.45
1:F:69:ASP:HB3	1:F:217:ARG:HE	1.80	0.45
1:F:89:GLN:HG3	1:F:178:PHE:CD1	2.52	0.45
1:F:192:ARG:HG3	1:F:193:ASP:OD1	2.17	0.45
1:G:104:PHE:CE1	1:G:243:ILE:HB	2.52	0.45
1:A:80:ALA:C	1:A:82:VAL:N	2.75	0.45
1:F:102:ARG:HA	1:F:170:ASN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TYR:H	1:A:196:HIS:HE1	1.65	0.45
1:B:61:MET:HG2	1:B:63:ALA:N	2.31	0.45
1:C:285:VAL:HG23	1:C:286:ASP:H	1.81	0.45
1:D:52:ALA:HB2	1:D:298:TRP:CH2	2.52	0.45
1:D:273:GLY:O	1:D:274:THR:C	2.60	0.45
1:D:283:LYS:O	1:D:284:ASP:C	2.59	0.45
1:E:22:TYR:HB2	1:E:39:VAL:HG12	1.98	0.45
1:E:69:ASP:HB3	1:E:217:ARG:CZ	2.46	0.45
1:F:165:LEU:HD11	1:F:168:GLN:NE2	2.32	0.45
1:F:211:PRO:HD2	1:F:276:ASN:HA	1.98	0.45
1:A:59:SER:HB3	1:A:61:MET:HE1	1.98	0.45
1:B:80:ALA:H	1:B:268:PRO:HD3	1.80	0.45
1:B:184:ASN:O	1:B:185:GLN:C	2.59	0.45
1:C:166:ILE:HG13	1:C:167:ASP:H	1.82	0.45
1:F:128:SER:N	1:F:141:GLU:O	2.49	0.45
1:C:263:ASP:CG	1:C:285:VAL:HG21	2.42	0.45
1:C:301:LYS:HB2	1:C:301:LYS:HE3	1.36	0.45
1:D:229:LEU:HD23	1:D:234:PHE:HB2	1.99	0.45
1:E:274:THR:O	1:E:276:ASN:N	2.50	0.45
1:F:249:GLU:HB3	1:F:250:GLN:H	1.65	0.45
1:A:201:ASN:HD22	1:A:281:ASN:CB	2.28	0.45
1:D:17:LYS:C	1:D:18:THR:HG1	2.21	0.45
1:E:191:THR:OG1	1:E:192:ARG:N	2.50	0.45
1:E:270:PHE:CD2	1:E:278:VAL:HG11	2.48	0.45
1:F:159:THR:HB	1:F:181:GLY:O	2.17	0.45
1:A:182:TYR:CG	1:A:183:ASN:N	2.85	0.44
1:C:164:ASN:ND2	1:C:178:PHE:HE2	2.14	0.44
1:C:188:GLY:HA3	1:C:189:ILE:HA	1.63	0.44
1:D:27:ASN:HB3	1:G:170:ASN:ND2	2.32	0.44
1:E:33:MET:HE2	1:E:33:MET:HB3	1.73	0.44
1:B:17:LYS:NZ	1:B:43:ASP:O	2.47	0.44
1:B:167:ASP:CB	1:C:61:MET:HB2	2.37	0.44
1:D:165:LEU:HG	1:D:175:TRP:NE1	2.32	0.44
1:G:38:LYS:HB3	1:G:55:ASN:HB2	1.98	0.44
1:A:51:ILE:HA	1:A:243:ILE:HG13	1.99	0.44
1:A:149:ASP:O	1:A:150:TRP:HD1	2.00	0.44
1:E:122:SER:HA	1:F:148:VAL:O	2.18	0.44
1:F:35:MET:HG3	1:F:257:TYR:CE2	2.51	0.44
1:A:25:PHE:CE1	1:C:170:ASN:HB3	2.52	0.44
1:A:57:THR:HA	1:A:236:PRO:O	2.18	0.44
1:A:96:LEU:N	1:A:171:LYS:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG22	1:A:134:THR:HG23	1.99	0.44
1:D:244:SER:OG	1:D:248:THR:OG1	2.27	0.44
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.84	0.44
1:A:158:GLN:NE2	1:C:113:GLU:OE2	2.51	0.44
1:B:48:ASP:OD1	1:B:48:ASP:N	2.44	0.44
1:C:96:LEU:HB3	1:C:253:ILE:HD12	1.99	0.44
1:F:166:ILE:HG22	1:F:167:ASP:N	2.33	0.44
1:G:63:ALA:O	1:G:65:PRO:HD3	2.18	0.44
1:C:196:HIS:HB3	1:C:199:TYR:HB2	1.98	0.44
1:D:18:THR:HG21	1:D:43:ASP:H	1.82	0.44
1:D:159:THR:HG23	1:D:182:TYR:CD1	2.53	0.44
1:D:254:GLN:HA	1:D:293:SER:HA	2.00	0.44
1:E:229:LEU:O	1:E:230:THR:C	2.60	0.44
1:F:214:THR:HB	1:F:219:ASN:HD21	1.82	0.44
1:B:51:ILE:HA	1:B:243:ILE:HG22	2.00	0.44
1:B:205:MET:HE2	1:B:205:MET:HB2	1.82	0.44
1:B:83:THR:HA	1:B:265:THR:HA	2.00	0.44
1:D:54:ILE:HG13	1:D:240:ALA:O	2.18	0.44
1:E:210:TYR:HA	1:E:211:PRO:HD3	1.88	0.44
1:F:159:THR:HG1	1:F:179:PHE:HD1	1.60	0.44
1:F:160:SER:OG	1:F:161:TYR:N	2.51	0.44
1:A:94:MET:HE1	1:A:255:VAL:HG13	2.00	0.43
1:C:20:THR:OG1	1:C:41:PHE:HB2	2.18	0.43
1:E:96:LEU:HD21	1:E:101:SER:H	1.83	0.43
1:E:133:VAL:HG23	1:F:138:PRO:HG3	2.00	0.43
1:E:261:ALA:O	1:E:285:VAL:N	2.41	0.43
1:F:168:GLN:O	1:G:61:MET:HE2	2.17	0.43
1:F:227:PRO:O	1:F:230:THR:HG22	2.18	0.43
1:F:268:PRO:HA	1:F:273:GLY:HA3	2.00	0.43
1:G:54:ILE:HG13	1:G:240:ALA:O	2.18	0.43
1:A:86:TYR:N	1:A:262:ASP:O	2.50	0.43
1:B:96:LEU:O	1:B:172:HIS:NE2	2.52	0.43
1:F:183:ASN:HB3	1:F:189:ILE:HD13	2.00	0.43
1:G:21:SER:HA	1:G:39:VAL:O	2.18	0.43
1:C:165:LEU:HD12	1:C:175:TRP:CZ3	2.54	0.43
1:G:199:TYR:CE1	1:G:276:ASN:HB3	2.53	0.43
1:A:93:ALA:HB3	1:A:256:ALA:HB3	2.00	0.43
1:A:124:GLN:HA	1:E:147:GLN:HA	2.00	0.43
1:A:168:GLN:O	1:E:61:MET:HE2	2.18	0.43
1:B:33:MET:HB3	1:B:60:PHE:CD1	2.51	0.43
1:C:96:LEU:HG	1:C:171:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:VAL:HG12	1:C:148:VAL:HG22	1.99	0.43
1:C:124:GLN:HG2	1:C:145:THR:HB	1.99	0.43
1:D:204:PHE:HD1	1:D:226:LEU:HD21	1.83	0.43
1:G:201:ASN:N	1:G:279:GLY:O	2.52	0.43
1:A:182:TYR:CD1	1:A:227:PRO:HD3	2.53	0.43
1:B:216:ALA:O	1:B:266:LEU:HD13	2.19	0.43
1:D:67:LEU:HD23	1:D:67:LEU:HA	1.79	0.43
1:E:86:TYR:N	1:E:262:ASP:O	2.51	0.43
1:E:267:ARG:HE	1:E:267:ARG:HB2	1.36	0.43
1:F:96:LEU:HD12	1:F:171:LYS:HA	1.99	0.43
1:F:191:THR:OG1	1:F:192:ARG:N	2.51	0.43
1:A:60:PHE:CZ	1:A:234:PHE:HD2	2.36	0.43
1:B:84:LEU:HD13	1:B:220:LEU:HD21	2.01	0.43
1:D:166:ILE:HB	1:D:174:LYS:O	2.19	0.43
1:D:227:PRO:O	1:D:230:THR:HG22	2.19	0.43
1:E:22:TYR:CE2	1:E:302:LYS:HA	2.53	0.43
1:E:90:TYR:CE1	1:E:259:LYS:HG3	2.53	0.43
1:F:101:SER:HB3	1:F:243:ILE:O	2.18	0.43
1:A:189:ILE:HD11	1:A:208:ARG:NE	2.34	0.43
1:B:6:SER:O	1:C:53:VAL:HB	2.19	0.43
1:B:25:PHE:HB2	1:D:104:PHE:CD1	2.54	0.43
1:D:103:PHE:HB2	1:D:170:ASN:HA	2.00	0.43
1:E:84:LEU:HD12	1:E:84:LEU:HA	1.84	0.43
1:G:57:THR:HA	1:G:236:PRO:O	2.18	0.43
1:G:188:GLY:HA3	1:G:189:ILE:HA	1.79	0.43
1:B:103:PHE:HD1	1:B:104:PHE:H	1.66	0.43
1:D:208:ARG:O	1:D:209:THR:C	2.62	0.43
1:F:165:LEU:O	1:G:232:SER:HB3	2.18	0.43
1:B:145:THR:HA	1:D:125:LEU:O	2.19	0.43
1:B:280:ASN:OD1	1:B:281:ASN:N	2.52	0.43
1:C:92:ILE:HG23	1:C:175:TRP:HD1	1.84	0.43
1:D:271:THR:HG22	1:D:278:VAL:HG22	2.00	0.43
1:G:250:GLN:HA	1:G:298:TRP:HD1	1.83	0.43
1:A:189:ILE:C	1:A:190:TYR:CD2	2.97	0.43
1:A:189:ILE:HG12	1:A:208:ARG:HH21	1.84	0.43
1:A:285:VAL:HG23	1:A:286:ASP:H	1.84	0.43
1:C:58:GLY:O	1:C:236:PRO:HD2	2.18	0.43
1:C:70:ALA:O	1:C:72:VAL:N	2.52	0.43
1:D:49:LYS:HG2	1:D:245:GLU:HA	2.00	0.43
1:G:263:ASP:CB	1:G:285:VAL:HG11	2.45	0.43
1:A:256:ALA:HA	1:A:291:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:PHE:CE1	1:E:34:THR:HB	2.54	0.42
1:E:71:PRO:HG3	1:E:80:ALA:O	2.18	0.42
1:E:272:PHE:CD2	1:E:276:ASN:HB2	2.54	0.42
1:A:104:PHE:CE2	1:E:25:PHE:HB2	2.54	0.42
1:A:192:ARG:CZ	1:A:193:ASP:HB2	2.49	0.42
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.93	0.42
1:F:107:ALA:HB3	1:F:239:ILE:HB	2.00	0.42
1:G:83:THR:HB	1:G:263:ASP:OD1	2.19	0.42
1:G:166:ILE:HG22	1:G:167:ASP:OD1	2.19	0.42
1:A:100:THR:OG1	1:A:171:LYS:NZ	2.52	0.42
1:A:162:LYS:HE2	1:A:162:LYS:HB2	1.43	0.42
1:A:180:ASN:O	1:A:192:ARG:HB2	2.19	0.42
1:B:34:THR:HG21	1:D:168:GLN:O	2.18	0.42
1:E:20:THR:O	1:E:40:THR:HA	2.18	0.42
1:E:32:ASN:OD1	1:E:61:MET:HB2	2.19	0.42
1:F:162:LYS:O	1:F:177:VAL:HA	2.19	0.42
1:G:134:THR:O	1:G:135:PRO:C	2.62	0.42
1:A:62:LYS:HE2	1:A:233:GLY:HA2	2.01	0.42
1:B:185:GLN:HE21	1:B:185:GLN:HB2	1.48	0.42
1:C:61:MET:HE2	1:C:63:ALA:HA	2.01	0.42
1:E:199:TYR:O	1:E:278:VAL:HG13	2.20	0.42
1:G:102:ARG:HB3	1:G:243:ILE:O	2.20	0.42
1:A:20:THR:HG21	1:A:41:PHE:HB2	2.01	0.42
1:A:205:MET:HE1	1:A:277:TRP:HB3	2.01	0.42
1:C:204:PHE:CE1	1:C:226:LEU:HD22	2.54	0.42
1:D:63:ALA:O	1:D:65:PRO:HD3	2.18	0.42
1:F:119:SER:HA	1:F:150:TRP:CD1	2.54	0.42
1:F:250:GLN:HG3	1:F:297:ASP:HA	2.00	0.42
1:G:51:ILE:HG22	1:G:243:ILE:CG1	2.49	0.42
1:B:49:LYS:HB3	1:B:244:SER:O	2.19	0.42
1:B:127:GLY:HA2	1:B:141:GLU:O	2.20	0.42
1:C:57:THR:HA	1:C:236:PRO:O	2.20	0.42
1:D:209:THR:HB	1:D:210:TYR:H	1.67	0.42
1:D:267:ARG:NH1	1:D:270:PHE:CZ	2.87	0.42
1:E:120:SER:HA	1:F:151:SER:HA	2.01	0.42
1:E:168:GLN:NE2	1:E:173:VAL:HB	2.34	0.42
1:F:124:GLN:HA	1:G:146:GLY:O	2.20	0.42
1:C:38:LYS:N	1:C:55:ASN:O	2.53	0.42
1:D:160:SER:HB3	1:D:227:PRO:HB3	2.01	0.42
1:E:75:TYR:N	1:E:76:PRO:HD3	2.35	0.42
1:A:28:GLU:HB2	1:A:33:MET:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:SER:OG	1:B:244:SER:HA	2.19	0.42
1:C:90:TYR:CE2	1:C:259:LYS:HG2	2.54	0.42
1:D:158:GLN:OE1	1:D:180:ASN:HB2	2.20	0.42
1:E:14:GLN:HB2	1:F:19:HIS:CD2	2.54	0.42
1:A:17:LYS:O	1:A:18:THR:C	2.63	0.42
1:D:36:SER:HB3	1:D:57:THR:C	2.44	0.42
1:D:84:LEU:HD11	1:D:264:TYR:HB3	2.02	0.42
1:D:272:PHE:O	1:D:274:THR:N	2.53	0.42
1:D:302:LYS:HD2	1:D:302:LYS:HA	1.48	0.42
1:F:91:ASP:HA	1:F:175:TRP:O	2.20	0.42
1:C:51:ILE:HA	1:C:243:ILE:HG13	2.02	0.42
1:C:166:ILE:HB	1:C:176:ASN:OD1	2.20	0.42
1:C:179:PHE:C	1:C:192:ARG:HH12	2.27	0.42
1:D:23:ASN:ND2	1:D:37:LEU:O	2.46	0.42
1:F:300:ASN:HD21	1:F:302:LYS:HD3	1.85	0.42
1:A:95:ASN:HA	1:A:172:HIS:HA	2.01	0.41
1:A:297:ASP:HB3	1:A:302:LYS:H	1.84	0.41
1:B:82:VAL:HG11	1:B:217:ARG:HA	2.01	0.41
1:C:41:PHE:CD1	1:C:301:LYS:HB3	2.55	0.41
1:C:164:ASN:HB2	1:C:176:ASN:OD1	2.20	0.41
1:F:89:GLN:HB2	1:F:260:HIS:CB	2.43	0.41
1:F:182:TYR:CE1	1:F:227:PRO:HD3	2.56	0.41
1:G:226:LEU:HD23	1:G:230:THR:HG21	2.02	0.41
1:G:237:GLY:H	1:G:238:MET:CE	2.32	0.41
1:A:204:PHE:CE2	1:A:264:TYR:HB3	2.56	0.41
1:D:18:THR:O	1:D:19:HIS:CB	2.67	0.41
1:G:22:TYR:CZ	1:G:303:LEU:HB3	2.54	0.41
1:G:36:SER:HB2	1:G:57:THR:C	2.45	0.41
1:A:12:ILE:HD13	1:E:21:SER:HB2	2.02	0.41
1:A:166:ILE:HD12	1:A:176:ASN:ND2	2.35	0.41
1:B:86:TYR:HB2	1:B:264:TYR:CD1	2.55	0.41
1:B:129:ILE:HG13	1:C:142:SER:HB2	2.02	0.41
1:C:270:PHE:O	1:C:272:PHE:N	2.53	0.41
1:C:296:LEU:HG	1:C:303:LEU:HD23	2.01	0.41
1:D:191:THR:HG22	1:D:193:ASP:H	1.85	0.41
1:F:9:VAL:C	1:F:11:ASP:N	2.77	0.41
1:F:161:TYR:CE2	1:F:179:PHE:HB2	2.55	0.41
1:A:100:THR:C	1:A:102:ARG:N	2.77	0.41
1:A:107:ALA:HB3	1:A:239:ILE:CG1	2.51	0.41
1:A:189:ILE:CG2	1:A:196:HIS:NE2	2.84	0.41
1:B:98:ASP:HA	1:B:171:LYS:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:HD2	1:B:170:ASN:CB	2.42	0.41
1:B:191:THR:OG1	1:B:192:ARG:N	2.54	0.41
1:B:205:MET:SD	1:B:277:TRP:HB3	2.60	0.41
1:C:199:TYR:HE1	1:C:276:ASN:HB3	1.85	0.41
1:E:253:ILE:CG1	1:E:296:LEU:HD11	2.50	0.41
1:B:50:GLN:NE2	1:B:245:GLU:O	2.52	0.41
1:C:185:GLN:HE21	1:C:187:TRP:HB3	1.84	0.41
1:E:164:ASN:HB3	1:F:232:SER:OG	2.20	0.41
1:E:167:ASP:OD1	1:E:167:ASP:N	2.46	0.41
1:G:258:THR:HG22	1:G:289:THR:HG22	2.01	0.41
1:A:192:ARG:C	1:A:194:SER:N	2.78	0.41
1:B:103:PHE:HE1	1:B:240:ALA:HB1	1.83	0.41
1:B:215:ASP:OD1	1:B:216:ALA:N	2.54	0.41
1:D:61:MET:HB2	1:G:167:ASP:HB3	2.02	0.41
1:E:51:ILE:HG13	1:E:243:ILE:HD11	2.03	0.41
1:F:102:ARG:HB3	1:F:170:ASN:CB	2.41	0.41
1:F:165:LEU:HD21	1:F:168:GLN:NE2	2.35	0.41
1:G:38:LYS:N	1:G:55:ASN:O	2.54	0.41
1:G:70:ALA:HA	1:G:71:PRO:HD3	1.94	0.41
1:G:205:MET:HE3	1:G:208:ARG:HD3	2.01	0.41
1:A:86:TYR:HD2	1:A:264:TYR:CE2	2.39	0.41
1:D:283:LYS:HB2	1:D:284:ASP:H	1.77	0.41
1:E:93:ALA:HB3	1:E:256:ALA:HB3	2.03	0.41
1:E:118:THR:N	1:E:151:SER:O	2.45	0.41
1:G:232:SER:HB2	1:G:233:GLY:H	1.64	0.41
1:A:128:SER:HB2	1:A:141:GLU:HB3	2.02	0.41
1:A:188:GLY:O	1:A:189:ILE:HG23	2.21	0.41
1:A:206:TYR:HB2	1:A:221:VAL:N	2.35	0.41
1:B:282:ILE:HD12	1:B:285:VAL:HG22	2.02	0.41
1:C:101:SER:O	1:C:102:ARG:HB2	2.21	0.41
1:C:270:PHE:C	1:C:272:PHE:N	2.75	0.41
1:D:23:ASN:O	1:G:49:LYS:NZ	2.53	0.41
1:D:34:THR:CG2	1:G:169:THR:HA	2.42	0.41
1:E:182:TYR:HE1	1:E:227:PRO:HG2	1.86	0.41
1:F:39:VAL:HA	1:F:53:VAL:O	2.20	0.41
1:A:17:LYS:HD3	1:A:17:LYS:HA	1.37	0.41
1:A:60:PHE:CE1	1:A:234:PHE:HB3	2.56	0.41
1:A:71:PRO:HB2	1:A:81:SER:HB2	2.03	0.41
1:B:104:PHE:HE1	1:B:243:ILE:HG23	1.83	0.41
1:B:214:THR:HG22	1:B:215:ASP:N	2.35	0.41
1:D:28:GLU:OE1	1:D:28:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:VAL:HA	1:D:53:VAL:O	2.21	0.41
1:E:86:TYR:CE2	1:E:204:PHE:HD2	2.39	0.41
1:F:5:THR:C	1:G:11:ASP:HB3	2.45	0.41
1:F:35:MET:HE1	1:F:294:PHE:HZ	1.83	0.41
1:F:169:THR:HG22	1:F:170:ASN:N	2.35	0.41
1:E:86:TYR:CD2	1:E:264:TYR:HB3	2.56	0.41
1:E:100:THR:HB	1:E:251:SER:OG	2.21	0.41
1:F:3:GLN:OE1	1:G:241:VAL:HG21	2.21	0.41
1:F:35:MET:HG2	1:F:36:SER:N	2.36	0.41
1:F:91:ASP:OD1	1:F:91:ASP:N	2.53	0.41
1:G:101:SER:OG	1:G:171:LYS:HD3	2.21	0.41
1:G:192:ARG:NH1	1:G:283:LYS:HG2	2.36	0.41
1:C:60:PHE:CE1	1:C:234:PHE:HB3	2.56	0.40
1:C:105:HIS:HB3	1:C:241:VAL:HG12	2.03	0.40
1:D:96:LEU:HA	1:D:253:ILE:HA	2.02	0.40
1:E:178:PHE:CG	1:E:179:PHE:N	2.89	0.40
1:E:296:LEU:O	1:E:297:ASP:C	2.64	0.40
1:F:120:SER:N	1:F:149:ASP:O	2.33	0.40
1:G:168:GLN:HG2	1:G:169:THR:N	2.36	0.40
1:B:82:VAL:HB	1:B:216:ALA:HB3	2.03	0.40
1:C:110:ASN:OD1	1:C:165:LEU:N	2.55	0.40
1:C:226:LEU:HB3	1:C:227:PRO:HD2	2.02	0.40
1:D:14:GLN:HE21	1:D:14:GLN:H	1.69	0.40
1:E:14:GLN:O	1:E:15:ASN:C	2.63	0.40
1:E:16:ALA:O	1:E:18:THR:N	2.54	0.40
1:E:104:PHE:HA	1:F:25:PHE:CE2	2.56	0.40
1:E:274:THR:O	1:E:276:ASN:ND2	2.54	0.40
1:F:134:THR:O	1:F:136:SER:N	2.55	0.40
1:A:190:TYR:H	1:A:196:HIS:CE1	2.40	0.40
1:C:62:LYS:HE2	1:C:233:GLY:HA2	2.03	0.40
1:C:85:ARG:HA	1:C:262:ASP:O	2.21	0.40
1:E:179:PHE:HE2	1:E:182:TYR:HH	1.66	0.40
1:F:12:ILE:HD11	1:G:38:LYS:HE2	2.04	0.40
1:F:119:SER:O	1:G:151:SER:HA	2.21	0.40
1:F:188:GLY:HA3	1:F:189:ILE:HA	1.83	0.40
1:G:249:GLU:OE1	1:G:250:GLN:HB2	2.21	0.40
1:B:96:LEU:HD13	1:B:171:LYS:O	2.22	0.40
1:C:168:GLN:CB	1:C:173:VAL:HA	2.48	0.40
1:D:211:PRO:HB2	1:D:219:ASN:CG	2.46	0.40
1:E:261:ALA:N	1:E:286:ASP:O	2.52	0.40
1:F:96:LEU:HD13	1:F:171:LYS:NZ	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:SER:HA	1:A:150:TRP:CD1	2.56	0.40
1:A:189:ILE:HD12	1:A:202:GLN:HG3	2.03	0.40
1:B:202:GLN:CG	1:B:205:MET:HB3	2.51	0.40
1:D:263:ASP:OD1	1:D:263:ASP:N	2.55	0.40
1:E:3:GLN:O	1:E:5:THR:HG23	2.21	0.40
1:E:22:TYR:HB2	1:E:39:VAL:CG1	2.52	0.40
1:E:130:ASP:CB	1:E:139:SER:HB2	2.51	0.40
1:F:45:PRO:HA	1:F:246:LYS:NZ	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	283/310 (91%)	222 (78%)	42 (15%)	19 (7%)	1	12
1	B	258/310 (83%)	223 (86%)	31 (12%)	4 (2%)	7	36
1	C	274/310 (88%)	231 (84%)	37 (14%)	6 (2%)	5	29
1	D	273/310 (88%)	206 (76%)	52 (19%)	15 (6%)	1	15
1	E	284/310 (92%)	235 (83%)	38 (13%)	11 (4%)	2	19
1	F	298/310 (96%)	257 (86%)	34 (11%)	7 (2%)	5	28
1	G	288/310 (93%)	247 (86%)	36 (12%)	5 (2%)	7	35
All	All	1958/2170 (90%)	1621 (83%)	270 (14%)	67 (3%)	3	21

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	98	ASP
1	A	103	PHE

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Mol	Chain	Res	Type
1	A	104	PHE
1	A	135	PRO
1	A	189	ILE
1	A	193	ASP
1	B	185	GLN
1	C	71	PRO
1	C	105	HIS
1	D	19	HIS
1	D	98	ASP
1	D	274	THR
1	D	299	LYS
1	D	302	LYS
1	E	20	THR
1	E	78	PRO
1	E	135	PRO
1	E	275	GLY
1	F	18	THR
1	F	75	TYR
1	F	135	PRO
1	G	17	LYS
1	G	105	HIS
1	A	190	TYR
1	D	73	ASP
1	D	273	GLY
1	F	16	ALA
1	G	135	PRO
1	A	70	ALA
1	A	80	ALA
1	A	99	ASN
1	A	101	SER
1	A	185	GLN
1	B	177	VAL
1	D	212	HIS
1	D	252	SER
1	E	211	PRO
1	F	271	THR
1	A	156	TYR
1	B	105	HIS
1	C	305	GLU
1	D	13	GLY
1	D	275	GLY
1	D	306	LYS

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Mol	Chain	Res	Type
1	E	17	LYS
1	E	18	THR
1	E	136	SER
1	E	137	GLY
1	F	13	GLY
1	G	269	GLY
1	A	13	GLY
1	A	72	VAL
1	C	18	THR
1	C	99	ASN
1	D	138	PRO
1	D	298	TRP
1	G	76	PRO
1	A	18	THR
1	A	155	SER
1	E	133	VAL
1	E	210	TYR
1	B	269	GLY
1	C	138	PRO
1	D	211	PRO
1	A	71	PRO
1	F	71	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	254/270 (94%)	234 (92%)	20 (8%)	11	32
1	B	237/270 (88%)	231 (98%)	6 (2%)	42	62
1	C	247/270 (92%)	235 (95%)	12 (5%)	22	45
1	D	242/270 (90%)	204 (84%)	38 (16%)	2	13
1	E	254/270 (94%)	238 (94%)	16 (6%)	16	38
1	F	264/270 (98%)	255 (97%)	9 (3%)	32	54
1	G	255/270 (94%)	249 (98%)	6 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1753/1890 (93%)	1646 (94%)	107 (6%)	17	39

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	77	ILE
1	A	95	ASN
1	A	97	GLN
1	A	100	THR
1	A	103	PHE
1	A	106	VAL
1	A	136	SER
1	A	162	LYS
1	A	183	ASN
1	A	184	ASN
1	A	189	ILE
1	A	190	TYR
1	A	191	THR
1	A	192	ARG
1	A	194	SER
1	A	280	ASN
1	A	283	LYS
1	A	306	LYS
1	A	307	LYS
1	B	21	SER
1	B	68	SER
1	B	77	ILE
1	B	185	GLN
1	B	268	PRO
1	B	270	PHE
1	C	21	SER
1	C	71	PRO
1	C	99	ASN
1	C	106	VAL
1	C	129	ILE
1	C	141	GLU
1	C	278	VAL
1	C	296	LEU
1	C	299	LYS
1	C	300	ASN
1	C	301	LYS

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Mol	Chain	Res	Type
1	C	303	LEU
1	D	12	ILE
1	D	14	GLN
1	D	21	SER
1	D	98	ASP
1	D	99	ASN
1	D	102	ARG
1	D	106	VAL
1	D	139	SER
1	D	177	VAL
1	D	208	ARG
1	D	209	THR
1	D	249	GLU
1	D	250	GLN
1	D	253	ILE
1	D	255	VAL
1	D	259	LYS
1	D	260	HIS
1	D	262	ASP
1	D	266	LEU
1	D	272	PHE
1	D	278	VAL
1	D	281	ASN
1	D	282	ILE
1	D	283	LYS
1	D	285	VAL
1	D	286	ASP
1	D	288	LYS
1	D	289	THR
1	D	291	ASN
1	D	292	LYS
1	D	296	LEU
1	D	298	TRP
1	D	299	LYS
1	D	302	LYS
1	D	303	LEU
1	D	304	VAL
1	D	307	LYS
1	D	309	SER
1	E	12	ILE
1	E	17	LYS
1	E	20	THR

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Mol	Chain	Res	Type
1	E	55	ASN
1	E	77	ILE
1	E	78	PRO
1	E	133	VAL
1	E	135	PRO
1	E	189	ILE
1	E	210	TYR
1	E	229	LEU
1	E	243	ILE
1	E	267	ARG
1	E	268	PRO
1	E	271	THR
1	E	272	PHE
1	F	10	THR
1	F	12	ILE
1	F	103	PHE
1	F	104	PHE
1	F	134	THR
1	F	135	PRO
1	F	158	GLN
1	F	159	THR
1	F	208	ARG
1	G	17	LYS
1	G	134	THR
1	G	162	LYS
1	G	232	SER
1	G	265	THR
1	G	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	176	ASN
1	A	180	ASN
1	A	185	GLN
1	A	201	ASN
1	A	291	ASN
1	B	26	ASN
1	B	164	ASN
1	B	185	GLN
1	B	202	GLN

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Mol	Chain	Res	Type
1	C	185	GLN
1	C	186	ASN
1	C	231	ASN
1	D	14	GLN
1	D	32	ASN
1	D	97	GLN
1	D	219	ASN
1	D	276	ASN
1	D	300	ASN
1	E	276	ASN
1	F	14	GLN
1	F	15	ASN
1	F	158	GLN
1	F	168	GLN
1	F	180	ASN
1	F	212	HIS
1	G	14	GLN
1	G	15	ASN
1	G	291	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	291/310 (93%)	2.08	108 (37%)  	30, 84, 154, 262	0
1	B	272/310 (87%)	2.26	107 (39%)  	39, 89, 150, 256	0
1	C	284/310 (91%)	2.53	115 (40%)  	30, 93, 166, 237	0
1	D	279/310 (90%)	3.10	141 (50%)  	30, 82, 141, 167	0
1	E	292/310 (94%)	2.51	133 (45%)  	30, 80, 134, 204	0
1	F	302/310 (97%)	1.65	84 (27%)  	30, 85, 137, 197	0
1	G	292/310 (94%)	2.10	99 (33%)  	43, 80, 137, 203	0
All	All	2012/2170 (92%)	2.31	787 (39%)  	30, 85, 145, 262	0

All (787) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	SER	25.0
1	C	140	GLY	21.3
1	C	130	ASP	20.6
1	C	141	GLU	20.1
1	D	165	LEU	18.2
1	C	129	ILE	17.5
1	G	110	ASN	17.4
1	D	176	ASN	17.2
1	D	109	THR	15.8
1	C	138	PRO	15.2
1	D	175	TRP	15.1
1	D	166	ILE	14.6
1	E	231	ASN	14.6
1	D	163	THR	14.3
1	E	59	SER	14.3
1	D	177	VAL	14.2
1	C	127	GLY	13.7

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Mol	Chain	Res	Type	RSRZ
1	C	139	SER	13.7
1	D	229	LEU	13.7
1	E	56	THR	13.1
1	D	167	ASP	13.1
1	G	165	LEU	13.0
1	F	232	SER	12.7
1	B	235	SER	12.7
1	C	113	GLU	12.6
1	C	283	LYS	12.5
1	D	90	TYR	12.5
1	A	192	ARG	12.4
1	G	164	ASN	12.2
1	E	237	GLY	12.2
1	E	60	PHE	12.0
1	D	161	TYR	11.8
1	E	174	LYS	11.5
1	B	233	GLY	11.4
1	B	234	PHE	11.3
1	D	60	PHE	11.0
1	B	137	GLY	10.9
1	D	157	ASP	10.5
1	D	230	THR	10.5
1	C	131	ALA	10.4
1	C	137	GLY	10.4
1	D	159	THR	10.3
1	E	235	SER	10.3
1	C	288	LYS	10.3
1	B	232	SER	10.1
1	D	237	GLY	10.1
1	E	173	VAL	10.1
1	B	31	ASP	10.1
1	D	239	ILE	10.1
1	C	167	ASP	10.0
1	G	113	GLU	10.0
1	G	98	ASP	10.0
1	B	161	TYR	9.9
1	G	97	GLN	9.8
1	E	58	GLY	9.7
1	F	233	GLY	9.7
1	A	191	THR	9.6
1	B	228	THR	9.5
1	D	174	LYS	9.4

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Mol	Chain	Res	Type	RSRZ
1	D	158	GLN	9.4
1	G	167	ASP	9.3
1	B	229	LEU	9.3
1	B	32	ASN	9.3
1	B	60	PHE	9.3
1	G	71	PRO	9.2
1	D	91	ASP	9.0
1	D	178	PHE	8.8
1	D	92	ILE	8.8
1	E	234	PHE	8.8
1	D	172	HIS	8.8
1	E	172	HIS	8.7
1	G	9	VAL	8.7
1	B	163	THR	8.7
1	D	234	PHE	8.6
1	F	86	TYR	8.6
1	D	156	TYR	8.6
1	E	238	MET	8.6
1	D	238	MET	8.5
1	B	236	PRO	8.5
1	D	168	GLN	8.5
1	B	133	VAL	8.4
1	C	287	GLN	8.4
1	D	235	SER	8.4
1	G	156	TYR	8.4
1	A	284	ASP	8.3
1	A	162	LYS	8.3
1	B	64	ASN	8.2
1	E	86	TYR	8.2
1	D	173	VAL	8.1
1	B	61	MET	8.1
1	D	56	THR	8.1
1	B	182	TYR	8.1
1	F	234	PHE	8.0
1	C	166	ILE	7.9
1	A	157	ASP	7.9
1	G	105	HIS	7.9
1	F	231	ASN	7.8
1	E	225	ASP	7.8
1	F	69	ASP	7.7
1	A	163	THR	7.7
1	B	62	LYS	7.7

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Mol	Chain	Res	Type	RSRZ
1	E	165	LEU	7.6
1	G	172	HIS	7.6
1	E	88	SER	7.5
1	A	310	ALA	7.5
1	G	109	THR	7.5
1	A	31	ASP	7.5
1	E	55	ASN	7.4
1	E	35	MET	7.4
1	B	30	ALA	7.3
1	D	160	SER	7.3
1	C	125	LEU	7.3
1	C	114	GLU	7.2
1	B	86	TYR	7.2
1	A	179	PHE	7.2
1	A	309	SER	7.2
1	G	145	THR	7.1
1	F	225	ASP	7.1
1	G	114	GLU	7.1
1	G	99	ASN	7.0
1	F	228	THR	7.0
1	F	155	SER	7.0
1	D	31	ASP	7.0
1	E	36	SER	7.0
1	B	136	SER	6.9
1	B	224	ASN	6.9
1	F	180	ASN	6.9
1	A	285	VAL	6.8
1	G	112	VAL	6.8
1	F	229	LEU	6.8
1	D	287	GLN	6.8
1	G	106	VAL	6.8
1	G	116	THR	6.7
1	A	260	HIS	6.6
1	A	283	LYS	6.6
1	A	90	TYR	6.6
1	D	260	HIS	6.5
1	F	68	SER	6.5
1	B	231	ASN	6.5
1	E	285	VAL	6.5
1	G	93	ALA	6.5
1	F	235	SER	6.5
1	G	10	THR	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	257	TYR	6.4
1	E	257	TYR	6.4
1	C	182	TYR	6.4
1	E	38	LYS	6.3
1	G	169	THR	6.3
1	C	284	ASP	6.3
1	E	90	TYR	6.3
1	D	108	PRO	6.3
1	C	260	HIS	6.2
1	A	193	ASP	6.2
1	B	90	TYR	6.2
1	E	99	ASN	6.2
1	F	152	ASP	6.2
1	C	156	TYR	6.2
1	E	114	GLU	6.2
1	E	182	TYR	6.2
1	D	171	LYS	6.2
1	C	163	THR	6.1
1	C	142	SER	6.1
1	C	155	SER	6.1
1	E	57	THR	6.1
1	D	183	ASN	6.0
1	E	92	ILE	6.0
1	A	105	HIS	6.0
1	C	308	GLY	6.0
1	A	307	LYS	6.0
1	E	37	LEU	6.0
1	E	204	PHE	5.9
1	E	112	VAL	5.9
1	B	203	LEU	5.8
1	G	202	GLN	5.7
1	G	124	GLN	5.7
1	G	153	SER	5.7
1	A	257	TYR	5.7
1	G	117	VAL	5.7
1	A	39	VAL	5.6
1	G	240	ALA	5.6
1	A	190	TYR	5.6
1	A	156	TYR	5.6
1	A	165	LEU	5.6
1	A	189	ILE	5.6
1	D	62	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	113	GLU	5.5
1	B	139	SER	5.5
1	D	34	THR	5.5
1	D	236	PRO	5.5
1	E	138	PRO	5.5
1	C	233	GLY	5.4
1	D	182	TYR	5.4
1	A	176	ASN	5.4
1	D	250	GLN	5.4
1	C	83	THR	5.4
1	E	105	HIS	5.4
1	F	85	ARG	5.3
1	D	284	ASP	5.3
1	G	154	VAL	5.3
1	C	161	TYR	5.3
1	E	255	VAL	5.3
1	D	169	THR	5.3
1	F	3	GLN	5.3
1	E	236	PRO	5.3
1	F	76	PRO	5.2
1	G	94	MET	5.2
1	B	46	SER	5.2
1	D	89	GLN	5.1
1	G	173	VAL	5.1
1	B	59	SER	5.1
1	E	94	MET	5.1
1	A	180	ASN	5.1
1	G	59	SER	5.1
1	G	170	ASN	5.1
1	B	230	THR	5.1
1	G	163	THR	5.1
1	C	176	ASN	5.1
1	D	107	ALA	5.1
1	E	230	THR	5.1
1	A	164	ASN	5.0
1	B	260	HIS	5.0
1	A	308	GLY	5.0
1	A	210	TYR	5.0
1	C	259	LYS	5.0
1	F	92	ILE	5.0
1	F	287	GLN	5.0
1	C	224	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	77	ILE	5.0
1	G	70	ALA	5.0
1	C	89	GLN	5.0
1	A	306	LYS	5.0
1	D	94	MET	5.0
1	E	34	THR	4.9
1	G	135	PRO	4.9
1	F	2	ALA	4.9
1	E	95	ASN	4.9
1	G	176	ASN	4.9
1	C	261	ALA	4.8
1	E	97	GLN	4.8
1	A	152	ASP	4.8
1	A	178	PHE	4.8
1	B	89	GLN	4.8
1	F	209	THR	4.8
1	D	55	ASN	4.8
1	B	48	ASP	4.8
1	D	286	ASP	4.8
1	D	228	THR	4.8
1	A	187	TRP	4.8
1	C	298	TRP	4.7
1	D	80	ALA	4.7
1	G	171	LYS	4.7
1	C	165	LEU	4.7
1	A	66	THR	4.7
1	D	300	ASN	4.7
1	D	233	GLY	4.7
1	F	185	GLN	4.7
1	A	168	GLN	4.6
1	E	168	GLN	4.6
1	A	277	TRP	4.6
1	F	116	THR	4.6
1	E	111	ALA	4.6
1	D	218	GLY	4.6
1	E	167	ASP	4.6
1	C	66	THR	4.6
1	D	98	ASP	4.6
1	G	34	THR	4.6
1	C	189	ILE	4.6
1	A	37	LEU	4.6
1	C	299	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	7	GLN	4.6
1	D	285	VAL	4.6
1	B	226	LEU	4.5
1	D	259	LYS	4.5
1	G	290	PHE	4.5
1	D	79	GLY	4.5
1	D	106	VAL	4.5
1	E	286	ASP	4.5
1	D	258	THR	4.5
1	D	252	SER	4.5
1	E	175	TRP	4.5
1	D	255	VAL	4.5
1	A	154	VAL	4.4
1	B	8	VAL	4.4
1	B	130	ASP	4.4
1	A	86	TYR	4.4
1	E	222	PRO	4.4
1	A	282	ILE	4.4
1	B	223	MET	4.4
1	D	33	MET	4.4
1	E	220	LEU	4.4
1	B	138	PRO	4.3
1	F	90	TYR	4.3
1	D	61	MET	4.3
1	B	87	PRO	4.3
1	E	14	GLN	4.3
1	B	10	THR	4.3
1	D	164	ASN	4.3
1	D	203	LEU	4.2
1	B	214	THR	4.2
1	D	101	SER	4.2
1	E	98	ASP	4.2
1	E	13	GLY	4.2
1	F	210	TYR	4.2
1	G	185	GLN	4.2
1	A	111	ALA	4.1
1	A	159	THR	4.1
1	B	238	MET	4.1
1	F	163	THR	4.1
1	G	150	TRP	4.1
1	E	183	ASN	4.1
1	D	299	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	89	GLN	4.1
1	F	97	GLN	4.1
1	D	249	GLU	4.0
1	A	4	THR	4.0
1	D	95	ASN	4.0
1	C	234	PHE	4.0
1	A	175	TRP	4.0
1	G	175	TRP	4.0
1	A	52	ALA	4.0
1	G	257	TYR	4.0
1	B	88	SER	4.0
1	B	135	PRO	4.0
1	B	11	ASP	4.0
1	A	185	GLN	4.0
1	F	186	ASN	3.9
1	B	132	SER	3.9
1	B	12	ILE	3.9
1	B	166	ILE	3.9
1	G	61	MET	3.9
1	A	158	GLN	3.9
1	D	93	ALA	3.9
1	A	88	SER	3.9
1	D	309	SER	3.9
1	F	207	SER	3.9
1	G	168	GLN	3.9
1	G	178	PHE	3.9
1	E	62	LYS	3.9
1	D	136	SER	3.9
1	F	83	THR	3.9
1	E	227	PRO	3.9
1	A	182	TYR	3.9
1	C	307	LYS	3.9
1	E	226	LEU	3.8
1	D	35	MET	3.8
1	C	183	ASN	3.8
1	E	166	ILE	3.8
1	C	300	ASN	3.8
1	D	244	SER	3.8
1	F	13	GLY	3.8
1	B	177	VAL	3.8
1	B	257	TYR	3.8
1	E	291	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	285	VAL	3.8
1	C	31	ASP	3.8
1	B	227	PRO	3.8
1	A	48	ASP	3.8
1	E	46	SER	3.7
1	F	182	TYR	3.7
1	A	233	GLY	3.7
1	C	269	GLY	3.7
1	D	135	PRO	3.7
1	D	247	ASP	3.7
1	G	21	SER	3.7
1	F	40	THR	3.7
1	B	225	ASP	3.7
1	C	23	ASN	3.7
1	C	132	SER	3.7
1	F	100	THR	3.7
1	E	254	GLN	3.7
1	F	286	ASP	3.7
1	F	142	SER	3.6
1	B	5	THR	3.6
1	G	118	THR	3.6
1	C	164	ASN	3.6
1	C	109	THR	3.6
1	E	134	THR	3.6
1	F	214	THR	3.6
1	D	307	LYS	3.6
1	E	244	SER	3.6
1	E	250	GLN	3.6
1	E	26	ASN	3.6
1	G	174	LYS	3.6
1	C	64	ASN	3.6
1	F	285	VAL	3.6
1	G	72	VAL	3.5
1	C	61	MET	3.5
1	E	33	MET	3.5
1	F	64	ASN	3.5
1	E	67	LEU	3.5
1	G	101	SER	3.5
1	G	256	ALA	3.5
1	G	141	GLU	3.5
1	C	84	LEU	3.5
1	C	43	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	245	GLU	3.5
1	B	50	GLN	3.5
1	E	81	SER	3.5
1	D	78	PRO	3.5
1	G	92	ILE	3.5
1	G	159	THR	3.5
1	F	94	MET	3.4
1	E	195	TYR	3.4
1	E	269	GLY	3.4
1	E	215	ASP	3.4
1	A	194	SER	3.4
1	B	216	ALA	3.4
1	F	14	GLN	3.4
1	C	229	LEU	3.4
1	E	79	GLY	3.4
1	A	51	ILE	3.4
1	F	135	PRO	3.4
1	G	67	LEU	3.4
1	C	306	LYS	3.4
1	E	273	GLY	3.4
1	D	256	ALA	3.4
1	C	250	GLN	3.4
1	F	160	SER	3.4
1	F	141	GLU	3.4
1	E	247	ASP	3.4
1	E	189	ILE	3.4
1	D	50	GLN	3.4
1	D	288	LYS	3.4
1	C	282	ILE	3.4
1	D	77	ILE	3.4
1	G	66	THR	3.3
1	A	161	TYR	3.3
1	E	91	ASP	3.3
1	B	56	THR	3.3
1	F	115	THR	3.3
1	F	230	THR	3.3
1	G	123	TYR	3.3
1	D	220	LEU	3.3
1	C	246	LYS	3.3
1	G	35	MET	3.3
1	C	50	GLN	3.3
1	F	43	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	245	GLU	3.3
1	B	247	ASP	3.3
1	C	290	PHE	3.3
1	A	54	ILE	3.3
1	B	49	LYS	3.3
1	A	261	ALA	3.3
1	C	286	ASP	3.3
1	F	12	ILE	3.3
1	F	213	GLU	3.2
1	D	278	VAL	3.2
1	C	263	ASP	3.2
1	F	277	TRP	3.2
1	C	301	LYS	3.2
1	E	228	THR	3.2
1	B	237	GLY	3.2
1	E	77	ILE	3.2
1	D	88	SER	3.2
1	E	15	ASN	3.2
1	D	289	THR	3.2
1	E	197	ALA	3.2
1	D	54	ILE	3.2
1	D	48	ASP	3.2
1	C	256	ALA	3.2
1	A	205	MET	3.2
1	E	283	LYS	3.2
1	D	187	TRP	3.2
1	E	261	ALA	3.2
1	G	152	ASP	3.2
1	C	248	THR	3.1
1	D	57	THR	3.1
1	B	179	PHE	3.1
1	G	60	PHE	3.1
1	E	208	ARG	3.1
1	C	67	LEU	3.1
1	F	153	SER	3.1
1	G	91	ASP	3.1
1	E	89	GLN	3.1
1	D	204	PHE	3.1
1	E	180	ASN	3.1
1	C	203	LEU	3.1
1	B	175	TRP	3.1
1	B	243	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	127	GLY	3.1
1	B	265	THR	3.1
1	G	278	VAL	3.1
1	B	108	PRO	3.1
1	C	118	THR	3.1
1	E	5	THR	3.1
1	E	280	ASN	3.1
1	E	179	PHE	3.1
1	D	304	VAL	3.1
1	A	202	GLN	3.0
1	A	235	SER	3.0
1	D	301	LYS	3.0
1	A	94	MET	3.0
1	G	181	GLY	3.0
1	C	232	SER	3.0
1	C	247	ASP	3.0
1	E	10	THR	3.0
1	E	139	SER	3.0
1	F	72	VAL	3.0
1	D	246	LYS	3.0
1	B	242	VAL	3.0
1	A	262	ASP	3.0
1	A	188	GLY	3.0
1	D	74	GLY	3.0
1	A	170	ASN	3.0
1	A	204	PHE	3.0
1	D	49	LYS	3.0
1	D	251	SER	2.9
1	E	274	THR	2.9
1	A	224	ASN	2.9
1	A	305	GLU	2.9
1	C	302	LYS	2.9
1	A	69	ASP	2.9
1	C	20	THR	2.9
1	A	91	ASP	2.9
1	B	91	ASP	2.9
1	E	284	ASP	2.9
1	C	289	THR	2.9
1	D	162	LYS	2.9
1	C	168	GLN	2.9
1	A	40	THR	2.8
1	B	34	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	125	LEU	2.8
1	A	32	ASN	2.8
1	C	87	PRO	2.8
1	F	62	LYS	2.8
1	C	277	TRP	2.8
1	B	183	ASN	2.8
1	C	110	ASN	2.8
1	B	100	THR	2.8
1	B	284	ASP	2.8
1	C	158	GLN	2.8
1	G	158	GLN	2.8
1	B	192	ARG	2.8
1	A	232	SER	2.8
1	C	21	SER	2.8
1	D	308	GLY	2.8
1	C	206	TYR	2.8
1	B	276	ASN	2.8
1	B	273	GLY	2.8
1	C	119	SER	2.8
1	A	216	ALA	2.8
1	E	73	ASP	2.8
1	F	167	ASP	2.8
1	A	220	LEU	2.8
1	D	290	PHE	2.8
1	E	12	ILE	2.8
1	E	246	LYS	2.8
1	C	262	ASP	2.8
1	D	72	VAL	2.7
1	D	217	ARG	2.7
1	A	302	LYS	2.7
1	E	171	LYS	2.7
1	B	16	ALA	2.7
1	C	220	LEU	2.7
1	F	211	PRO	2.7
1	G	268	PRO	2.7
1	F	284	ASP	2.7
1	D	184	ASN	2.7
1	D	302	LYS	2.7
1	D	190	TYR	2.7
1	C	227	PRO	2.7
1	B	81	SER	2.7
1	B	244	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	243	ILE	2.7
1	D	180	ASN	2.7
1	G	80	ALA	2.7
1	E	270	PHE	2.7
1	E	209	THR	2.7
1	F	84	LEU	2.7
1	G	144	ALA	2.7
1	A	104	PHE	2.7
1	G	76	PRO	2.7
1	E	54	ILE	2.7
1	C	174	LYS	2.7
1	D	208	ARG	2.7
1	A	155	SER	2.7
1	A	75	TYR	2.7
1	C	105	HIS	2.7
1	E	258	THR	2.7
1	A	294	PHE	2.7
1	B	283	LYS	2.6
1	F	161	TYR	2.6
1	A	203	LEU	2.6
1	D	181	GLY	2.6
1	D	53	VAL	2.6
1	C	19	HIS	2.6
1	B	110	ASN	2.6
1	A	259	LYS	2.6
1	D	274	THR	2.6
1	E	48	ASP	2.6
1	E	297	ASP	2.6
1	E	294	PHE	2.6
1	D	36	SER	2.6
1	C	76	PRO	2.6
1	D	76	PRO	2.6
1	A	181	GLY	2.6
1	C	162	LYS	2.6
1	D	279	GLY	2.6
1	E	87	PRO	2.6
1	E	248	THR	2.6
1	A	122	SER	2.6
1	B	246	LYS	2.6
1	C	177	VAL	2.6
1	A	209	THR	2.6
1	F	105	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	69	ASP	2.5
1	C	126	GLY	2.5
1	D	28	GLU	2.5
1	D	291	ASN	2.5
1	F	219	ASN	2.5
1	A	174	LYS	2.5
1	B	115	THR	2.5
1	A	303	LEU	2.5
1	C	194	SER	2.5
1	F	133	VAL	2.5
1	B	73	ASP	2.5
1	B	80	ALA	2.5
1	C	22	TYR	2.5
1	C	170	ASN	2.5
1	G	183	ASN	2.5
1	A	5	THR	2.5
1	C	159	THR	2.5
1	D	214	THR	2.5
1	E	245	GLU	2.5
1	F	29	GLN	2.5
1	D	292	LYS	2.5
1	D	306	LYS	2.5
1	G	281	ASN	2.5
1	C	150	TRP	2.5
1	B	13	GLY	2.5
1	E	50	GLN	2.5
1	F	299	LYS	2.5
1	A	137	GLY	2.5
1	A	70	ALA	2.5
1	B	248	THR	2.5
1	E	260	HIS	2.5
1	C	60	PHE	2.5
1	G	31	ASP	2.5
1	A	87	PRO	2.5
1	A	64	ASN	2.5
1	B	35	MET	2.5
1	E	113	GLU	2.4
1	E	78	PRO	2.4
1	G	63	ALA	2.4
1	D	179	PHE	2.4
1	A	92	ILE	2.4
1	E	181	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	100	THR	2.4
1	D	59	SER	2.4
1	E	267	ARG	2.4
1	A	304	VAL	2.4
1	G	304	VAL	2.4
1	B	167	ASP	2.4
1	G	282	ILE	2.4
1	A	214	THR	2.4
1	D	310	ALA	2.4
1	D	305	GLU	2.4
1	E	188	GLY	2.4
1	G	100	THR	2.4
1	A	84	LEU	2.4
1	G	87	PRO	2.3
1	B	269	GLY	2.3
1	G	115	THR	2.3
1	G	251	SER	2.3
1	G	211	PRO	2.3
1	A	197	ALA	2.3
1	D	253	ILE	2.3
1	E	2	ALA	2.3
1	A	266	LEU	2.3
1	C	90	TYR	2.3
1	E	229	LEU	2.3
1	E	193	ASP	2.3
1	C	92	ILE	2.3
1	F	18	THR	2.3
1	G	267	ARG	2.3
1	D	295	VAL	2.3
1	B	134	THR	2.3
1	D	20	THR	2.3
1	A	207	SER	2.3
1	F	88	SER	2.3
1	B	41	PHE	2.3
1	C	71	PRO	2.3
1	G	54	ILE	2.3
1	F	17	LYS	2.3
1	G	177	VAL	2.3
1	F	15	ASN	2.3
1	E	207	SER	2.3
1	E	108	PRO	2.3
1	B	9	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	148	VAL	2.3
1	A	208	ARG	2.3
1	F	159	THR	2.3
1	F	59	SER	2.3
1	C	108	PRO	2.3
1	F	58	GLY	2.3
1	B	47	ALA	2.3
1	C	304	VAL	2.3
1	E	72	VAL	2.3
1	A	246	LYS	2.2
1	D	232	SER	2.2
1	G	136	SER	2.2
1	G	302	LYS	2.2
1	E	70	ALA	2.2
1	A	35	MET	2.2
1	B	43	ASP	2.2
1	G	11	ASP	2.2
1	F	156	TYR	2.2
1	E	101	SER	2.2
1	F	16	ALA	2.2
1	F	216	ALA	2.2
1	B	33	MET	2.2
1	G	85	ARG	2.2
1	G	160	SER	2.2
1	B	19	HIS	2.2
1	C	157	ASP	2.2
1	A	123	TYR	2.2
1	F	187	TRP	2.2
1	C	180	ASN	2.2
1	B	101	SER	2.2
1	D	219	ASN	2.2
1	E	80	ALA	2.2
1	A	46	SER	2.2
1	G	46	SER	2.2
1	E	41	PHE	2.2
1	C	303	LEU	2.2
1	D	97	GLN	2.2
1	G	206	TYR	2.2
1	E	45	PRO	2.2
1	D	100	THR	2.2
1	A	252	SER	2.2
1	E	194	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	179	PHE	2.2
1	B	264	TYR	2.2
1	C	249	GLU	2.2
1	E	69	ASP	2.2
1	D	64	ASN	2.2
1	B	18	THR	2.2
1	B	178	PHE	2.2
1	D	191	THR	2.2
1	F	226	LEU	2.2
1	A	173	VAL	2.2
1	B	77	ILE	2.1
1	F	301	LYS	2.1
1	E	136	SER	2.1
1	C	205	MET	2.1
1	D	216	ALA	2.1
1	D	43	ASP	2.1
1	D	270	PHE	2.1
1	E	302	LYS	2.1
1	D	99	ASN	2.1
1	E	214	THR	2.1
1	D	133	VAL	2.1
1	C	33	MET	2.1
1	B	58	GLY	2.1
1	C	175	TRP	2.1
1	E	272	PHE	2.1
1	F	258	THR	2.1
1	G	212	HIS	2.1
1	A	60	PHE	2.1
1	F	236	PRO	2.1
1	G	129	ILE	2.1
1	B	209	THR	2.1
1	B	165	LEU	2.1
1	E	74	GLY	2.1
1	G	155	SER	2.1
1	G	294	PHE	2.1
1	C	278	VAL	2.1
1	E	221	VAL	2.1
1	G	149	ASP	2.1
1	F	212	HIS	2.1
1	C	79	GLY	2.1
1	F	168	GLN	2.1
1	F	283	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	243	ILE	2.1
1	B	109	THR	2.1
1	B	169	THR	2.1
1	C	57	THR	2.1
1	A	245	GLU	2.1
1	B	278	VAL	2.1
1	D	269	GLY	2.0
1	E	216	ALA	2.0
1	E	83	THR	2.0
1	F	224	ASN	2.0
1	G	68	SER	2.0
1	G	69	ASP	2.0
1	A	148	VAL	2.0
1	D	223	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.