



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:26 AM UTC

PDB ID : 1AL0 / pdb_00001al0
Title : PROCAPSID OF BACTERIOPHAGE PHIX174
Authors : Rossmann, M.G.; Dokland, T.
Deposited on : 1997-06-06
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

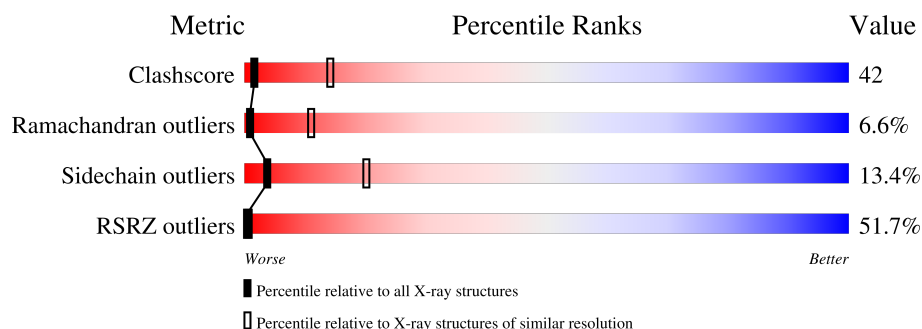
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	1	152	57% 36% 44% 11% 6%
1	2	152	49% 29% 40% 16% 12%
1	3	152	26% 32% 41% 19% 8%
1	4	152	39% 34% 47% 13% •
2	F	426	56% 29% 44% 20% 6% •
3	G	175	53% 50% 39% 10% •
4	B	120	28% 8% 14% 12% 7% 59%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9521 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 SCAFFOLDING PROTEIN GPD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	143	Total	C	N	O	S	0	0	0
			1125	716	194	211	4			
1	2	133	Total	C	N	O	S	0	0	0
			1039	665	175	195	4			
1	3	140	Total	C	N	O	S	0	0	0
			1099	699	187	209	4			
1	4	146	Total	C	N	O	S	0	0	0
			1145	728	197	215	5			

- Molecule 2 is a protein called CAPSID PROTEIN GPF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	418	Total	C	N	O	S	0	0	0
			3358	2139	581	625	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	216	ARG	HIS	conflict	UNP P03641

- Molecule 3 is a protein called SPIKE PROTEIN GPG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	175	Total	C	N	O	S	0	0	0
			1340	856	221	255	8			

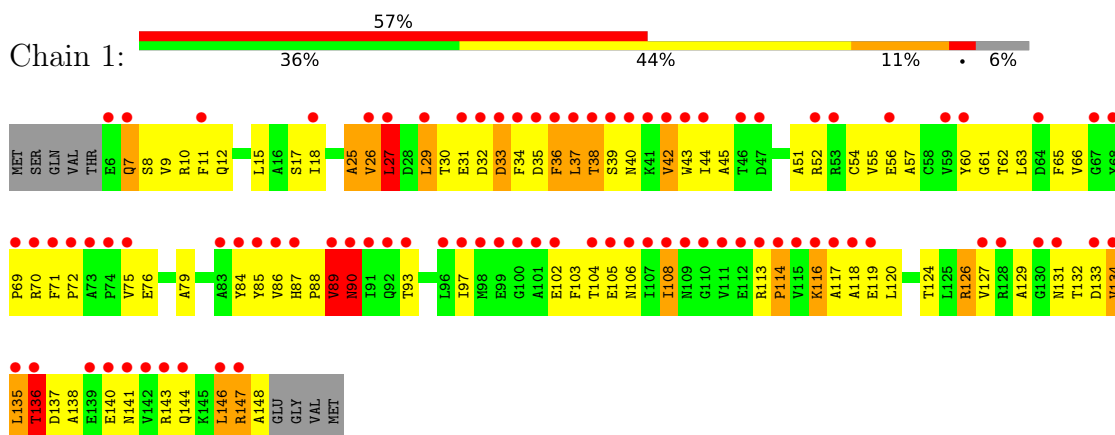
- Molecule 4 is a protein called SCAFFOLDING PROTEIN GPB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	49	Total	C	N	O	S	0	0	0
			415	262	71	80	2			

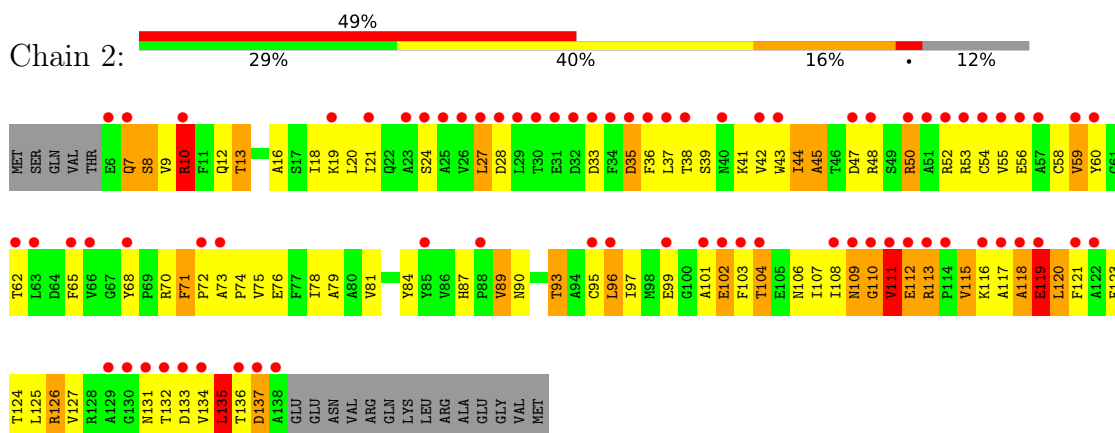
3 Residue-property plots [i](#)

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

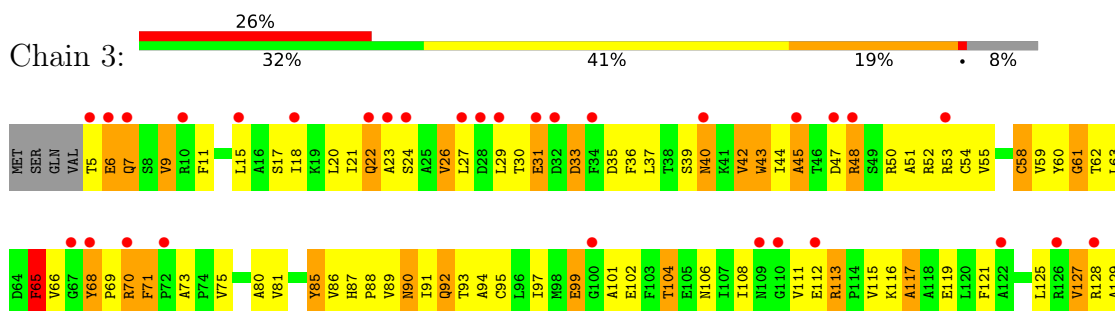
• Molecule 1: SCAFFOLDING PROTEIN GPD

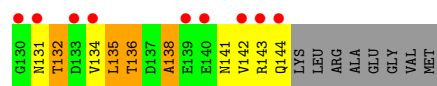


• Molecule 1: SCAFFOLDING PROTEIN GPD

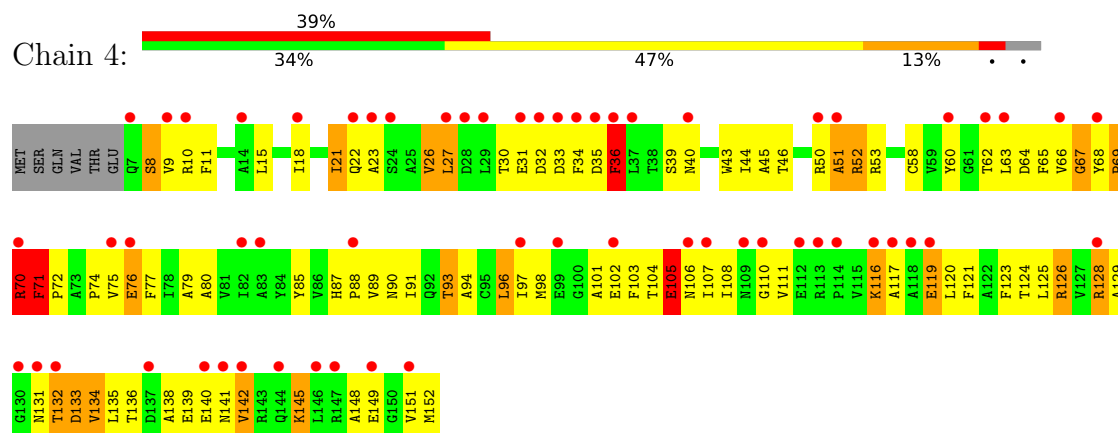


• Molecule 1: SCAFFOLDING PROTEIN GPD

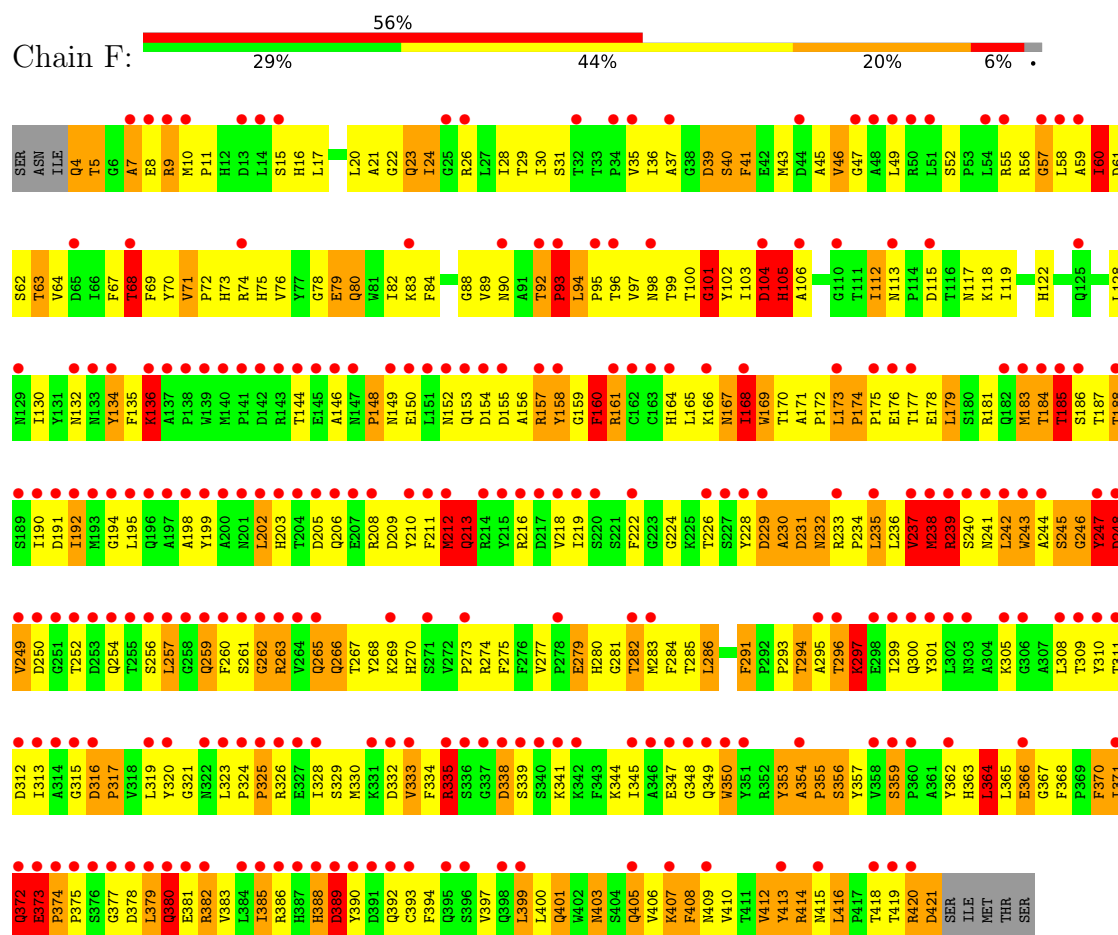




• Molecule 1: SCAFFOLDING PROTEIN GPD

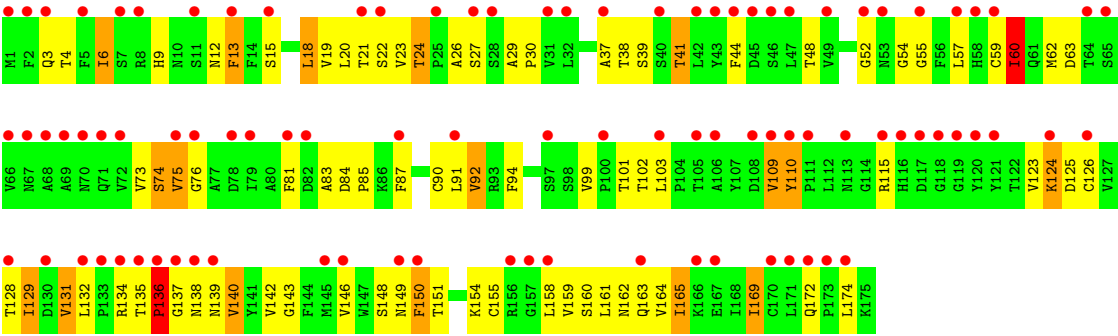


• Molecule 2: CAPSID PROTEIN GPF

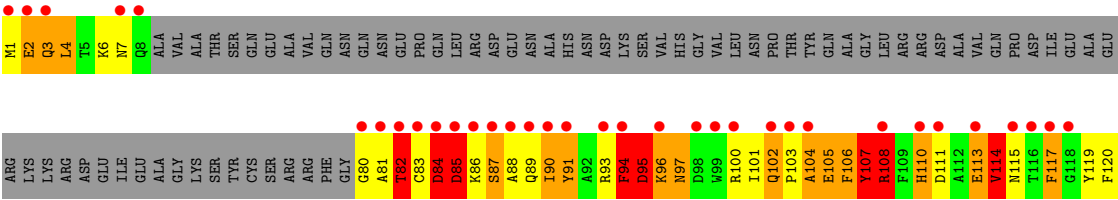


• Molecule 3: SPIKE PROTEIN GPG





● Molecule 4: SCAFFOLDING PROTEIN GPB



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	774.00Å 774.00Å 774.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 8.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.50) 52.7 (8.00-3.50)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.316 , (Not available) 0.489 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.004 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.07	EDS
Total number of atoms	9521	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.75% 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	1	1.38	4/1145 (0.3%)	1.50	28/1557 (1.8%)
1	2	1.29	1/1059 (0.1%)	1.51	23/1443 (1.6%)
1	3	1.44	8/1119 (0.7%)	1.56	27/1524 (1.8%)
1	4	1.38	6/1165 (0.5%)	1.46	25/1582 (1.6%)
2	F	1.40	19/3454 (0.6%)	1.62	90/4702 (1.9%)
3	G	1.18	2/1372 (0.1%)	1.42	28/1872 (1.5%)
4	B	1.44	3/425 (0.7%)	1.86	18/569 (3.2%)
All	All	1.36	43/9739 (0.4%)	1.55	239/13249 (1.8%)

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	3	0	1
1	4	0	1
2	F	0	1
4	B	0	3
All	All	0	6

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	71	VAL	CA-CB	-7.87	1.47	1.54
2	F	219	ILE	CA-CB	-7.65	1.45	1.54
2	F	40	SER	C-O	7.09	1.32	1.24
1	4	131	ASN	CA-C	-6.64	1.46	1.53
1	4	134	VAL	CA-CB	-6.51	1.46	1.54
1	3	90	ASN	CA-CB	-6.48	1.44	1.53
2	F	218	VAL	CA-CB	-6.40	1.47	1.54
1	4	9	VAL	CA-CB	-6.39	1.46	1.54
1	3	127	VAL	CA-CB	-6.32	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	18	ILE	CA-CB	-6.30	1.46	1.54
3	G	6	ILE	CA-CB	-6.25	1.46	1.54
2	F	76	VAL	CA-CB	-6.14	1.48	1.55
2	F	59	ALA	CA-CB	-6.06	1.43	1.54
1	2	59	VAL	CA-CB	-6.01	1.47	1.54
2	F	17	LEU	CA-C	-6.00	1.45	1.52
2	F	119	ILE	CA-CB	-5.94	1.46	1.54
1	3	141	ASN	CA-C	-5.90	1.48	1.53
1	3	55	VAL	CA-CB	-5.74	1.47	1.54
1	1	127	VAL	CA-CB	-5.72	1.48	1.54
4	B	80	GLY	N-CA	5.68	1.54	1.45
4	B	95	ASP	CA-C	-5.66	1.45	1.52
1	4	26	VAL	CA-CB	-5.66	1.48	1.54
4	B	90	ILE	CA-CB	-5.64	1.48	1.54
2	F	252	THR	CA-CB	-5.64	1.46	1.54
2	F	385	ILE	CA-CB	-5.61	1.48	1.54
1	1	108	ILE	CA-CB	-5.59	1.47	1.54
1	3	81	VAL	CA-CB	-5.59	1.48	1.54
3	G	99	VAL	CA-CB	-5.49	1.47	1.54
2	F	45	ALA	CA-CB	-5.46	1.46	1.53
2	F	412	VAL	CA-CB	-5.37	1.47	1.54
2	F	156	ALA	CA-CB	-5.34	1.45	1.53
1	3	142	VAL	CA-CB	5.29	1.61	1.54
1	3	73	ALA	CA-CB	-5.24	1.47	1.53
2	F	192	ILE	CA-CB	-5.24	1.47	1.54
2	F	374	PRO	CA-C	-5.21	1.47	1.52
2	F	46	VAL	CA-CB	-5.21	1.47	1.55
2	F	4	GLN	C-N	5.18	1.41	1.33
2	F	5	THR	CA-C	-5.17	1.45	1.52
1	4	26	VAL	CA-C	5.14	1.58	1.52
1	1	55	VAL	CA-CB	-5.13	1.48	1.54
2	F	24	ILE	C-O	-5.09	1.19	1.24
1	4	104	THR	CA-CB	5.07	1.61	1.53
1	1	134	VAL	CA-CB	5.01	1.61	1.54

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	80	GLN	N-CA-C	-13.99	94.57	112.90
2	F	421	ASP	CA-CB-CG	-13.76	98.84	112.60
1	2	135	LEU	N-CA-C	13.61	130.31	108.41
2	F	106	ALA	N-CA-C	-12.37	96.92	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	74	SER	N-CA-C	12.18	129.12	112.93
4	B	95	ASP	N-CA-C	-12.05	85.14	110.80
1	1	136	THR	N-CA-C	-11.05	87.27	110.80
2	F	291	PHE	N-CA-C	-10.85	96.28	110.39
1	3	90	ASN	N-CA-C	10.77	125.73	112.59
2	F	161	ARG	N-CA-C	10.34	125.44	110.24
2	F	92	THR	CA-C-N	10.16	132.53	119.84
2	F	92	THR	C-N-CA	10.16	132.53	119.84
1	3	68	TYR	N-CA-C	-10.03	98.28	110.31
2	F	238	MET	N-CA-C	9.93	126.13	111.34
1	3	26	VAL	N-CA-C	9.92	122.76	109.37
2	F	416	LEU	N-CA-C	-9.81	96.37	110.40
1	4	9	VAL	N-CA-C	-9.63	94.61	108.48
2	F	231	ASP	N-CA-C	-9.57	101.60	113.18
2	F	421	ASP	N-CA-CB	9.43	126.53	110.50
1	2	39	SER	N-CA-C	9.13	123.56	110.14
1	3	42	VAL	CB-CA-C	-9.09	101.60	111.59
1	4	104	THR	N-CA-C	9.09	123.89	110.17
1	1	146	LEU	N-CA-C	8.93	121.92	111.02
1	1	89	VAL	N-CA-C	-8.87	97.39	109.37
2	F	296	THR	N-CA-C	-8.86	102.46	113.18
2	F	39	ASP	N-CA-C	8.58	124.95	113.97
1	2	24	SER	N-CA-C	8.50	120.55	111.28
1	1	25	ALA	N-CA-C	-8.46	103.48	113.88
1	1	38	THR	N-CA-C	8.39	123.52	113.28
4	B	86	LYS	N-CA-C	-8.39	99.96	112.04
3	G	60	ILE	N-CA-C	-8.37	97.30	108.35
4	B	105	GLU	N-CA-C	-8.30	96.83	109.79
4	B	113	GLU	N-CA-C	-8.28	97.42	109.59
3	G	59	CYS	N-CA-C	8.20	122.65	110.52
2	F	420	ARG	O-C-N	8.12	132.47	123.22
1	4	110	GLY	N-CA-C	-8.09	103.83	115.64
1	2	137	ASP	N-CA-C	8.06	127.96	110.80
3	G	139	ASN	N-CA-C	-8.02	96.82	109.50
2	F	356	SER	N-CA-C	-7.97	93.83	110.80
4	B	107	TYR	N-CA-C	7.90	127.62	110.80
1	2	12	GLN	N-CA-C	7.88	120.86	111.33
3	G	150	PHE	N-CA-C	7.81	120.98	110.35
2	F	354	ALA	CA-C-N	7.63	129.37	119.84
2	F	354	ALA	C-N-CA	7.63	129.37	119.84
2	F	93	PRO	N-CA-C	7.60	128.12	112.47
2	F	254	GLN	N-CA-C	7.59	120.52	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	252	THR	N-CA-C	7.57	124.64	114.12
2	F	246	GLY	N-CA-C	7.56	119.13	111.95
4	B	111	ASP	N-CA-C	-7.52	96.47	108.73
3	G	138	ASN	N-CA-C	7.42	120.59	110.35
2	F	388	HIS	N-CA-C	7.40	120.79	111.69
4	B	91	TYR	N-CA-C	-7.39	104.26	113.20
2	F	315	GLY	N-CA-C	-7.25	105.22	115.30
2	F	184	THR	N-CA-C	7.22	121.02	112.93
2	F	160	PHE	N-CA-C	7.13	121.09	109.76
1	1	32	ASP	N-CA-C	7.09	119.09	111.36
1	4	46	THR	N-CA-C	-7.01	104.61	113.72
1	1	40	ASN	N-CA-C	-7.00	104.73	113.28
1	3	73	ALA	CA-C-N	7.00	126.92	119.85
1	3	73	ALA	C-N-CA	7.00	126.92	119.85
2	F	245	SER	N-CA-C	6.99	117.21	108.19
1	4	104	THR	CB-CA-C	-6.98	97.64	111.60
2	F	380	GLN	N-CA-C	-6.98	95.94	110.80
1	3	143	ARG	N-CA-C	6.95	119.91	108.99
1	4	142	VAL	CB-CA-C	-6.95	103.07	111.97
2	F	297	LYS	N-CA-C	6.84	121.01	111.56
2	F	335	ARG	N-CA-C	-6.83	99.41	110.20
1	3	86	VAL	N-CA-C	6.83	118.31	108.48
2	F	392	GLN	CB-CA-C	-6.74	98.16	110.63
1	4	85	TYR	N-CA-C	6.71	121.17	112.92
1	1	33	ASP	N-CA-C	-6.70	104.01	111.71
1	4	71	PHE	CA-C-N	-6.68	113.91	120.52
1	4	71	PHE	C-N-CA	-6.68	113.91	120.52
2	F	269	LYS	N-CA-C	-6.62	98.60	109.40
2	F	407	LYS	N-CA-CB	-6.62	100.78	110.84
2	F	4	GLN	O-C-N	6.60	133.56	123.00
2	F	377	GLY	N-CA-C	-6.58	105.44	112.08
3	G	101	THR	N-CA-C	-6.58	106.20	114.56
1	4	69	PRO	N-CA-C	-6.58	98.92	112.47
1	4	148	ALA	N-CA-C	-6.56	104.21	111.82
2	F	294	THR	N-CA-C	-6.54	97.59	108.32
3	G	129	ILE	CB-CA-C	-6.54	100.87	110.81
2	F	101	GLY	N-CA-C	6.50	128.59	113.18
1	1	136	THR	N-CA-CB	6.48	121.44	110.49
2	F	405	GLN	N-CA-C	-6.46	98.74	109.46
1	2	54	CYS	N-CA-C	6.41	119.51	111.24
1	3	66	VAL	N-CA-C	-6.41	99.19	108.36
1	2	120	LEU	N-CA-C	-6.39	104.24	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	GLN	CB-CA-C	6.38	122.23	110.10
3	G	124	LYS	N-CA-C	-6.38	97.21	110.80
2	F	190	ILE	CB-CA-C	-6.37	102.08	111.19
3	G	92	VAL	CB-CA-C	-6.37	101.01	110.82
1	2	131	ASN	N-CA-C	6.34	119.34	109.52
4	B	102	GLN	CA-C-N	6.33	125.90	119.19
4	B	102	GLN	C-N-CA	6.33	125.90	119.19
1	3	33	ASP	N-CA-C	-6.31	104.48	111.36
2	F	243	TRP	N-CA-C	-6.30	96.99	108.02
2	F	420	ARG	CB-CA-C	6.29	120.12	109.80
1	4	36	PHE	CB-CA-C	-6.25	97.99	110.42
2	F	403	ASN	CB-CA-C	-6.24	99.65	110.45
2	F	366	GLU	N-CA-C	6.23	120.70	111.04
4	B	97	ASN	N-CA-C	6.22	120.07	112.23
2	F	96	THR	N-CA-C	-6.18	100.35	109.81
3	G	137	GLY	N-CA-C	6.18	121.47	114.67
1	4	132	THR	N-CA-C	6.16	119.90	112.38
1	3	23	ALA	N-CA-C	6.14	117.98	111.28
4	B	82	THR	CB-CA-C	-6.14	98.21	110.42
1	1	132	THR	N-CA-C	-6.06	106.15	112.93
3	G	172	GLN	N-CA-C	-6.05	95.49	108.93
2	F	173	LEU	N-CA-C	-6.05	101.49	110.20
2	F	24	ILE	N-CA-C	6.05	116.82	108.84
1	2	115	VAL	N-CA-C	6.04	116.81	108.84
1	1	136	THR	CB-CA-C	-6.01	98.46	110.42
1	1	140	GLU	CA-C-N	6.01	128.61	120.38
1	1	140	GLU	C-N-CA	6.01	128.61	120.38
1	2	119	GLU	N-CA-C	-6.00	105.03	112.90
3	G	24	THR	CA-C-N	5.99	127.33	119.84
3	G	24	THR	C-N-CA	5.99	127.33	119.84
3	G	151	THR	N-CA-C	-5.99	100.14	109.72
2	F	40	SER	O-C-N	-5.97	114.66	122.59
4	B	110	HIS	CA-C-N	-5.96	114.85	122.77
4	B	110	HIS	C-N-CA	-5.96	114.85	122.77
1	4	129	ALA	N-CA-C	-5.95	101.72	110.52
3	G	146	VAL	N-CA-C	-5.91	99.91	108.89
1	1	39	SER	N-CA-C	5.86	117.46	110.19
2	F	408	PHE	N-CA-C	5.86	118.30	107.99
1	2	110	GLY	N-CA-C	-5.83	99.35	113.18
3	G	172	GLN	CA-C-N	5.83	126.23	119.47
3	G	172	GLN	C-N-CA	5.83	126.23	119.47
1	1	27	LEU	N-CA-C	-5.82	98.79	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	60	ILE	CB-CA-C	-5.82	101.71	110.55
2	F	338	ASP	N-CA-C	5.81	118.22	107.99
1	1	86	VAL	N-CA-C	5.79	117.67	108.87
1	2	74	PRO	N-CA-C	5.76	119.90	111.03
1	3	59	VAL	CB-CA-C	-5.76	105.97	111.44
1	1	71	PHE	N-CA-C	-5.75	100.20	109.58
3	G	135	THR	CA-C-N	5.74	127.02	119.84
3	G	135	THR	C-N-CA	5.74	127.02	119.84
2	F	7	ALA	N-CA-C	-5.73	105.95	113.17
2	F	104	ASP	N-CA-C	-5.73	99.91	109.24
3	G	76	GLY	N-CA-C	-5.70	99.67	113.18
1	3	144	GLN	N-CA-C	5.68	126.92	111.00
2	F	7	ALA	O-C-N	5.67	129.42	122.34
3	G	165	ILE	N-CA-C	-5.66	107.47	112.90
2	F	382	ARG	N-CA-C	-5.65	106.93	113.88
2	F	265	GLN	N-CA-C	5.65	123.22	114.64
2	F	247	TYR	N-CA-C	5.64	122.81	110.80
2	F	212	MET	N-CA-C	-5.63	98.81	110.80
4	B	104	ALA	N-CA-C	-5.62	106.26	113.01
1	3	101	ALA	N-CA-C	-5.61	99.12	108.32
4	B	87	SER	N-CA-C	-5.60	104.18	111.02
1	4	8	SER	N-CA-C	5.60	122.73	110.80
1	4	70	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	1	42	VAL	N-CA-C	5.58	117.25	109.55
3	G	110	TYR	CA-C-N	5.57	125.33	119.76
3	G	110	TYR	C-N-CA	5.57	125.33	119.76
1	3	40	ASN	N-CA-C	-5.55	106.51	113.28
1	3	48	ARG	NE-CZ-NH2	5.54	124.18	119.20
2	F	222	PHE	N-CA-C	-5.54	106.52	113.28
1	3	22	GLN	N-CA-C	-5.53	104.27	111.02
3	G	27	SER	N-CA-C	-5.53	105.33	111.36
2	F	103	ILE	CB-CA-C	-5.50	104.71	112.14
2	F	169	TRP	N-CA-C	5.50	119.98	113.16
1	4	69	PRO	CB-CA-C	5.49	120.62	111.56
2	F	4	GLN	N-CA-C	-5.49	95.63	111.00
2	F	160	PHE	N-CA-CB	5.48	118.45	109.95
2	F	112	ILE	N-CA-C	-5.48	100.69	108.58
1	4	101	ALA	N-CA-C	5.47	118.27	107.98
2	F	291	PHE	CA-C-N	-5.47	115.72	119.66
2	F	291	PHE	C-N-CA	-5.47	115.72	119.66
1	1	36	PHE	N-CA-C	-5.44	107.30	114.04
1	3	70	ARG	NE-CZ-NH2	5.44	124.09	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	92	GLN	N-CA-C	5.43	117.63	111.11
2	F	174	PRO	N-CA-C	-5.43	104.07	110.70
1	2	45	ALA	N-CA-C	5.42	117.89	111.33
2	F	185	THR	CB-CA-C	-5.42	99.63	110.42
1	3	68	TYR	N-CA-CB	5.42	115.90	109.72
1	2	42	VAL	CB-CA-C	-5.42	103.65	111.34
1	2	112	GLU	N-CA-C	-5.42	97.68	107.75
1	1	35	ASP	N-CA-C	-5.41	105.91	113.37
1	2	10	ARG	N-CA-C	5.41	119.72	113.18
2	F	134	TYR	N-CA-C	5.40	120.14	113.50
1	4	27	LEU	N-CA-C	-5.40	103.50	110.19
4	B	107	TYR	CB-CA-C	-5.39	99.69	110.42
2	F	420	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	4	131	ASN	CB-CA-C	-5.37	102.90	111.86
1	3	113	ARG	CA-C-N	5.35	125.25	119.85
1	3	113	ARG	C-N-CA	5.35	125.25	119.85
1	2	38	THR	CA-C-N	-5.34	113.49	123.05
1	2	38	THR	C-N-CA	-5.34	113.49	123.05
1	4	51	ALA	N-CA-C	-5.34	105.10	111.03
1	3	80	ALA	N-CA-C	-5.33	105.36	111.07
1	1	90	ASN	N-CA-C	5.33	122.14	110.80
1	2	38	THR	N-CA-C	5.32	119.64	113.20
2	F	381	GLU	N-CA-C	-5.32	106.86	113.19
1	3	129	ALA	N-CA-C	5.30	117.13	111.36
1	1	42	VAL	CB-CA-C	-5.28	104.34	111.63
2	F	244	ALA	N-CA-C	5.28	117.35	108.96
2	F	232	ASN	N-CA-C	5.27	119.29	112.86
1	1	135	LEU	CA-C-N	5.26	131.58	121.54
1	1	135	LEU	C-N-CA	5.26	131.58	121.54
1	3	70	ARG	N-CA-C	5.26	118.51	110.36
2	F	174	PRO	CA-C-N	5.23	126.38	119.84
2	F	174	PRO	C-N-CA	5.23	126.38	119.84
2	F	71	VAL	CB-CA-C	-5.21	106.13	111.08
3	G	131	VAL	N-CA-C	5.21	119.78	113.00
1	4	116	LYS	N-CA-C	-5.21	103.16	110.50
1	1	72	PRO	N-CA-C	5.20	119.03	111.03
3	G	132	LEU	CA-C-N	5.18	125.43	119.83
3	G	132	LEU	C-N-CA	5.18	125.43	119.83
2	F	224	GLY	N-CA-C	-5.18	103.40	111.12
2	F	185	THR	N-CA-C	5.18	121.83	110.80
4	B	85	ASP	N-CA-C	5.15	121.78	110.80
2	F	399	LEU	N-CA-C	-5.14	105.25	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	65	PHE	N-CA-C	-5.14	104.75	111.02
1	4	108	ILE	N-CA-C	5.13	120.02	109.34
2	F	43	MET	N-CA-C	5.13	117.61	109.50
1	2	127	VAL	N-CA-C	-5.12	105.72	110.53
2	F	5	THR	N-CA-C	-5.11	99.92	110.80
2	F	382	ARG	N-CA-CB	-5.11	103.80	110.59
1	2	118	ALA	N-CA-C	-5.09	99.96	110.80
1	1	148	ALA	N-CA-C	5.08	125.21	111.00
2	F	237	VAL	CA-C-N	-5.07	115.51	121.90
2	F	237	VAL	C-N-CA	-5.07	115.51	121.90
1	2	104	THR	N-CA-C	5.07	117.39	110.55
1	3	61	GLY	N-CA-C	5.06	125.18	113.18
2	F	401	GLN	N-CA-C	5.06	119.17	112.89
2	F	95	PRO	N-CA-C	5.06	119.16	111.11
1	1	129	ALA	N-CA-C	5.05	117.52	111.71
1	1	114	PRO	N-CA-C	-5.05	103.35	111.38
1	4	107	ILE	N-CA-C	5.04	116.09	109.58
1	4	94	ALA	N-CA-C	-5.03	105.26	111.40
2	F	263	ARG	N-CA-C	-5.03	101.76	109.76
2	F	267	THR	N-CA-C	-5.03	103.08	110.52
2	F	157	ARG	NE-CZ-NH2	5.03	123.72	119.20
4	B	108	ARG	N-CA-C	-5.02	100.10	110.80
2	F	373	GLU	CA-C-N	5.02	125.55	120.38
2	F	373	GLU	C-N-CA	5.02	125.55	120.38
1	2	71	PHE	O-C-N	-5.01	115.56	121.32

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	68	TYR	Sidechain
1	4	36	PHE	Sidechain
4	B	107	TYR	Sidechain
4	B	119	TYR	Sidechain
4	B	82	THR	Mainchain
2	F	160	PHE	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	1	1125	0	1121	79	0
1	2	1039	0	1031	106	0
1	3	1099	0	1086	98	0
1	4	1145	0	1142	106	0
2	F	3358	0	3242	319	0
3	G	1340	0	1323	69	0
4	B	415	0	376	78	0
All	All	9521	0	9321	786	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 42.

All (786) 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)
2:F:7:ALA:CB	4:B:100:ARG:CD	1.79	1.58
2:F:7:ALA:HB3	4:B:100:ARG:CD	1.42	1.41
2:F:7:ALA:CB	4:B:100:ARG:HD2	1.44	1.32
1:4:151:VAL:O	1:4:152:MET:HG2	1.13	1.29
2:F:7:ALA:CB	4:B:100:ARG:HD3	1.51	1.23
1:4:10:ARG:NH2	1:4:139:GLU:HB2	1.60	1.14
1:4:10:ARG:NH1	1:4:11:PHE:HB2	1.63	1.13
2:F:274:ARG:HH22	4:B:96:LYS:HA	1.07	1.11
1:4:151:VAL:O	1:4:152:MET:CG	1.99	1.11
2:F:157:ARG:NE	2:F:158:TYR:OH	1.84	1.10
2:F:7:ALA:HB1	4:B:100:ARG:CB	1.81	1.09
2:F:181:ARG:HG3	2:F:202:LEU:HD21	1.33	1.09
2:F:7:ALA:HB1	4:B:100:ARG:CD	1.60	1.08
2:F:341:LYS:HB3	2:F:382:ARG:HH22	1.13	1.07
2:F:68:THR:HG22	2:F:285:THR:HG22	1.37	1.05
2:F:154:ASP:O	2:F:158:TYR:HD1	1.36	1.04
2:F:154:ASP:HA	2:F:158:TYR:CE1	1.93	1.03
2:F:7:ALA:HB1	4:B:100:ARG:HD3	1.20	1.02
1:4:126:ARG:HG3	1:4:126:ARG:HH11	1.25	1.00
1:2:52:ARG:HH21	1:2:101:ALA:HA	1.26	1.00
1:3:43:TRP:HE1	1:3:90:ASN:HB3	1.25	0.99
2:F:7:ALA:HB1	4:B:100:ARG:HA	1.44	0.98
2:F:7:ALA:CA	4:B:100:ARG:HD3	1.93	0.98
2:F:7:ALA:C	4:B:100:ARG:HD3	1.90	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:7:ALA:HB1	4:B:100:ARG:CA	1.95	0.96
1:3:43:TRP:HE1	1:3:90:ASN:CB	1.78	0.96
2:F:157:ARG:CG	2:F:158:TYR:CE1	2.49	0.96
4:B:6:LYS:HG2	4:B:83:CYS:SG	2.06	0.95
1:3:58:CYS:SG	1:3:85:TYR:CD2	2.59	0.94
2:F:154:ASP:O	2:F:158:TYR:CD1	2.19	0.94
4:B:113:GLU:O	4:B:114:VAL:HB	1.66	0.94
3:G:60:ILE:HD13	3:G:161:LEU:HB2	1.50	0.93
2:F:153:GLN:O	2:F:157:ARG:HG2	1.69	0.92
2:F:157:ARG:HG3	2:F:158:TYR:CE1	2.04	0.92
2:F:7:ALA:HB1	4:B:100:ARG:CG	1.99	0.92
1:1:15:LEU:HA	1:1:18:ILE:HD12	1.51	0.92
1:2:27:LEU:H	1:2:27:LEU:HD23	1.35	0.92
1:4:10:ARG:HH11	1:4:11:PHE:H	1.12	0.91
2:F:212:MET:SD	2:F:213:GLN:N	2.44	0.90
2:F:157:ARG:HG3	2:F:158:TYR:CZ	2.05	0.90
3:G:169:ILE:H	3:G:169:ILE:HD13	1.36	0.90
4:B:7:ASN:HA	4:B:110:HIS:O	1.73	0.89
2:F:72:PRO:HD2	2:F:75:HIS:ND1	1.89	0.87
2:F:154:ASP:HA	2:F:158:TYR:HE1	1.37	0.87
3:G:38:THR:HG23	3:G:163:GLN:HE21	1.40	0.87
1:2:52:ARG:NH2	1:2:101:ALA:HA	1.88	0.87
4:B:3:GLN:HG2	4:B:87:SER:HB2	1.56	0.86
2:F:274:ARG:NH2	4:B:96:LYS:HA	1.89	0.86
1:3:60:TYR:CD2	1:3:70:ARG:HD3	2.10	0.86
1:2:16:ALA:HB1	1:3:42:VAL:HG21	1.59	0.85
3:G:15:SER:HA	3:G:41:THR:HG23	1.56	0.84
2:F:309:THR:HG22	2:F:310:TYR:H	1.40	0.84
1:2:87:HIS:HD2	1:2:89:VAL:HB	1.42	0.84
1:2:13:THR:HG23	1:3:89:VAL:O	1.77	0.84
2:F:297:LYS:HG2	2:F:335:ARG:HB3	1.60	0.84
2:F:166:LYS:HG2	4:B:117:PHE:CE2	2.13	0.83
2:F:70:TYR:CE2	2:F:72:PRO:HG3	2.14	0.82
1:1:134:VAL:HG12	1:1:136:THR:N	1.92	0.82
1:2:73:ALA:O	1:2:104:THR:HG22	1.78	0.82
3:G:39:SER:HB2	3:G:162:ASN:HD22	1.44	0.82
2:F:341:LYS:CB	2:F:382:ARG:HH22	1.92	0.82
1:3:43:TRP:HE1	1:3:90:ASN:CG	1.87	0.81
2:F:247:TYR:HD1	2:F:248:ASP:H	1.25	0.81
1:1:7:GLN:HG3	1:1:126:ARG:NH1	1.96	0.81
4:B:6:LYS:HE2	4:B:83:CYS:SG	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:341:LYS:HB3	2:F:382:ARG:NH2	1.95	0.81
2:F:309:THR:HG22	2:F:310:TYR:N	1.96	0.80
2:F:157:ARG:HG2	2:F:158:TYR:CE1	2.16	0.80
2:F:414:ARG:NH1	2:F:414:ARG:HB3	1.96	0.80
1:4:151:VAL:C	1:4:152:MET:HG2	2.07	0.79
2:F:256:SER:HB2	2:F:259:GLN:HB2	1.61	0.79
2:F:7:ALA:C	4:B:100:ARG:CD	2.55	0.79
1:4:35:ASP:O	1:4:39:SER:HB3	1.82	0.79
1:4:145:LYS:HZ3	1:4:149:GLU:HB2	1.48	0.79
2:F:250:ASP:HA	2:F:260:PHE:HD1	1.48	0.79
2:F:35:VAL:HG11	2:F:277:VAL:HG21	1.64	0.79
2:F:75:HIS:CD2	2:F:232:ASN:HA	2.18	0.78
1:4:128:ARG:CG	1:4:128:ARG:HH11	1.95	0.78
2:F:68:THR:CG2	2:F:285:THR:HG22	2.11	0.78
2:F:311:THR:HG22	2:F:319:LEU:HD13	1.64	0.78
1:3:121:PHE:CE1	1:3:125:LEU:HD11	2.19	0.78
2:F:68:THR:HA	2:F:285:THR:HA	1.65	0.78
2:F:20:LEU:HD11	2:F:30:ILE:HG12	1.64	0.77
4:B:4:LEU:HB2	4:B:110:HIS:HE1	1.49	0.77
1:1:30:THR:HA	1:1:147:ARG:NE	1.99	0.77
2:F:256:SER:O	2:F:257:LEU:HB2	1.84	0.77
3:G:83:ALA:O	3:G:85:PRO:HD3	1.84	0.77
2:F:7:ALA:O	4:B:100:ARG:HD3	1.82	0.77
1:2:87:HIS:CD2	1:2:89:VAL:H	2.03	0.77
1:1:31:GLU:N	1:1:147:ARG:HH21	1.82	0.77
1:2:99:GLU:HB2	1:2:117:ALA:HB2	1.66	0.76
1:2:44:ILE:HG12	1:2:45:ALA:N	1.98	0.76
1:2:44:ILE:HG12	1:2:45:ALA:H	1.50	0.76
1:3:43:TRP:NE1	1:3:90:ASN:HB3	2.00	0.76
2:F:7:ALA:CB	4:B:100:ARG:CB	2.60	0.76
4:B:3:GLN:HG2	4:B:87:SER:CB	2.15	0.76
1:4:10:ARG:HH11	1:4:11:PHE:N	1.82	0.76
1:2:84:TYR:CE1	1:2:135:LEU:HB2	2.21	0.75
2:F:208:ARG:HA	2:F:212:MET:HG3	1.67	0.75
1:3:115:VAL:HG13	1:3:119:GLU:HB3	1.68	0.75
2:F:135:PHE:O	2:F:136:LYS:HB3	1.86	0.75
4:B:6:LYS:CG	4:B:83:CYS:SG	2.75	0.75
4:B:106:PHE:O	4:B:107:TYR:HB2	1.83	0.74
3:G:143:GLY:HA2	3:G:161:LEU:HD21	1.70	0.74
2:F:363:HIS:O	2:F:364:LEU:HG	1.87	0.74
3:G:38:THR:HG23	3:G:163:GLN:NE2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:250:ASP:HA	2:F:260:PHE:CD1	2.23	0.73
1:2:10:ARG:HG2	1:2:10:ARG:HH11	1.54	0.73
1:1:143:ARG:HA	1:1:146:LEU:HG	1.71	0.73
1:2:68:TYR:HE1	1:3:93:THR:HG22	1.53	0.73
1:1:69:PRO:HG2	1:2:96:LEU:HD11	1.71	0.73
2:F:30:ILE:CG2	2:F:408:PHE:HZ	2.02	0.72
2:F:212:MET:SD	2:F:213:GLN:CA	2.77	0.72
2:F:273:PRO:HD2	4:B:107:TYR:OH	1.88	0.72
2:F:247:TYR:CE2	2:F:263:ARG:HD3	2.23	0.72
2:F:328:ILE:HG22	2:F:329:SER:H	1.55	0.72
1:2:84:TYR:CE1	1:2:133:ASP:HA	2.24	0.72
2:F:7:ALA:CB	4:B:100:ARG:CG	2.63	0.72
1:2:10:ARG:HH12	1:2:76:GLU:CD	1.97	0.72
1:3:89:VAL:HG12	1:3:90:ASN:OD1	1.88	0.72
2:F:30:ILE:HG22	2:F:408:PHE:HZ	1.53	0.72
1:3:44:ILE:HG22	1:3:45:ALA:H	1.55	0.71
2:F:49:LEU:HD23	2:F:64:VAL:HG21	1.70	0.71
1:1:66:VAL:HG11	1:2:44:ILE:HA	1.72	0.71
2:F:75:HIS:HD2	2:F:232:ASN:HA	1.55	0.71
3:G:90:CYS:SG	3:G:109:VAL:HG22	2.29	0.71
2:F:9:ARG:NH2	2:F:40:SER:HB2	2.06	0.71
3:G:12:ASN:HD22	3:G:13:PHE:N	1.88	0.71
1:3:102:GLU:OE1	1:3:112:GLU:HA	1.90	0.71
2:F:64:VAL:HB	2:F:242:LEU:HD12	1.72	0.71
1:2:10:ARG:HH11	1:2:10:ARG:CG	2.05	0.70
1:1:79:ALA:HA	1:1:124:THR:HG22	1.73	0.70
1:2:71:PHE:HB3	1:2:72:PRO:HD3	1.72	0.70
1:4:67:GLY:O	1:4:69:PRO:HD3	1.90	0.70
4:B:3:GLN:HG2	4:B:87:SER:HA	1.71	0.70
1:3:106:ASN:HB3	1:3:111:VAL:O	1.92	0.70
2:F:15:SER:HB3	2:F:410:VAL:H	1.57	0.70
1:3:71:PHE:CE1	1:4:96:LEU:HG	2.27	0.70
1:1:7:GLN:HA	1:1:10:ARG:HD2	1.74	0.69
1:4:74:PRO:HD2	1:4:77:PHE:CD2	2.27	0.69
2:F:414:ARG:CG	2:F:414:ARG:HH11	2.05	0.69
1:4:10:ARG:HH12	1:4:11:PHE:HB2	1.53	0.69
2:F:7:ALA:CB	4:B:100:ARG:HA	2.20	0.69
4:B:3:GLN:CG	4:B:87:SER:HA	2.22	0.69
2:F:414:ARG:HB3	2:F:414:ARG:HH11	1.57	0.69
2:F:181:ARG:CG	2:F:202:LEU:HD21	2.20	0.69
2:F:406:VAL:HG12	2:F:407:LYS:N	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:56:GLU:HG2	1:2:103:PHE:CZ	2.28	0.69
1:4:128:ARG:HH11	1:4:128:ARG:HG2	1.55	0.69
3:G:158:LEU:HD23	3:G:158:LEU:H	1.58	0.69
1:2:107:ILE:HG23	1:2:110:GLY:O	1.93	0.69
2:F:57:GLY:HA2	2:F:261:SER:O	1.93	0.69
4:B:3:GLN:HG2	4:B:87:SER:CA	2.23	0.68
2:F:301:TYR:HE1	2:F:328:ILE:HG23	1.58	0.68
4:B:95:ASP:C	4:B:97:ASN:N	2.50	0.68
2:F:7:ALA:CA	4:B:100:ARG:CD	2.59	0.68
2:F:309:THR:CG2	2:F:310:TYR:H	2.06	0.68
1:2:16:ALA:HB1	1:3:42:VAL:CG2	2.24	0.68
1:2:21:ILE:HD11	1:2:62:THR:HA	1.74	0.68
1:1:108:ILE:HG23	1:2:123:PHE:CE1	2.29	0.68
2:F:295:ALA:HA	2:F:371:ILE:HG22	1.74	0.68
1:2:27:LEU:HD23	1:2:27:LEU:N	2.08	0.68
1:4:126:ARG:HG3	1:4:126:ARG:NH1	1.97	0.67
2:F:82:ILE:N	2:F:82:ILE:HD12	2.10	0.67
2:F:166:LYS:HG2	4:B:117:PHE:CZ	2.29	0.67
3:G:169:ILE:HD13	3:G:169:ILE:N	2.09	0.67
2:F:9:ARG:NH1	4:B:101:ILE:HG13	2.09	0.67
1:4:10:ARG:NH1	1:4:11:PHE:CB	2.53	0.67
1:4:133:ASP:HB2	2:F:118:LYS:NZ	2.09	0.67
2:F:30:ILE:HG22	2:F:408:PHE:CZ	2.30	0.67
2:F:211:PHE:O	2:F:212:MET:HB3	1.95	0.66
1:4:105:GLU:CG	1:4:106:ASN:H	2.08	0.66
1:2:18:ILE:HG21	1:2:84:TYR:CD2	2.30	0.66
2:F:7:ALA:CB	4:B:100:ARG:HB3	2.25	0.66
2:F:413:TYR:N	2:F:413:TYR:CD1	2.64	0.66
1:4:27:LEU:HD13	1:4:58:CYS:SG	2.35	0.66
1:4:67:GLY:O	1:4:68:TYR:C	2.36	0.66
2:F:414:ARG:HH11	2:F:414:ARG:CB	2.09	0.66
2:F:79:GLU:HA	2:F:82:ILE:HD13	1.76	0.66
2:F:247:TYR:CD2	2:F:263:ARG:HD3	2.30	0.66
1:2:113:ARG:NH2	1:2:119:GLU:CD	2.53	0.65
1:3:127:VAL:CG1	1:3:131:ASN:HD21	2.10	0.65
2:F:158:TYR:CD1	2:F:158:TYR:N	2.65	0.65
3:G:12:ASN:HD22	3:G:13:PHE:H	1.44	0.65
1:4:10:ARG:NH1	1:4:11:PHE:H	1.88	0.65
1:4:10:ARG:CZ	1:4:139:GLU:HB2	2.25	0.65
1:1:108:ILE:HG12	1:2:123:PHE:HE1	1.61	0.65
1:3:60:TYR:CE2	1:3:70:ARG:HD3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:27:LEU:HD11	1:3:85:TYR:HE2	1.62	0.65
4:B:6:LYS:HE3	4:B:82:THR:HA	1.77	0.65
1:1:135:LEU:HB2	1:1:137:ASP:HB2	1.77	0.65
3:G:74:SER:O	3:G:125:ASP:O	2.15	0.64
1:1:31:GLU:H	1:1:147:ARG:HH21	1.44	0.64
1:3:43:TRP:NE1	1:3:90:ASN:CG	2.55	0.64
1:4:68:TYR:OH	1:4:139:GLU:CD	2.40	0.64
3:G:63:ASP:H	3:G:163:GLN:HE22	1.45	0.64
2:F:238:MET:SD	2:F:238:MET:C	2.80	0.64
1:4:68:TYR:C	1:4:69:PRO:O	2.35	0.64
1:4:124:THR:O	1:4:128:ARG:HB2	1.98	0.64
2:F:328:ILE:HG22	2:F:332:ASP:HB2	1.80	0.64
1:4:44:ILE:HG22	1:4:45:ALA:N	2.13	0.64
2:F:212:MET:SD	2:F:212:MET:C	2.81	0.64
2:F:29:THR:HA	2:F:286:LEU:HD23	1.79	0.64
1:3:63:LEU:HD23	1:4:93:THR:HG22	1.80	0.63
1:3:121:PHE:HE1	1:3:125:LEU:HD11	1.63	0.63
1:2:93:THR:O	1:2:97:ILE:HG13	1.98	0.63
2:F:418:THR:HG22	2:F:419:THR:N	2.13	0.63
1:3:87:HIS:CG	1:3:88:PRO:HD2	2.34	0.63
2:F:308:LEU:HD13	2:F:313:ILE:HD11	1.80	0.63
2:F:328:ILE:HD11	2:F:345:ILE:HG21	1.81	0.63
2:F:9:ARG:HA	2:F:415:ASN:HD22	1.64	0.62
1:2:108:ILE:O	1:2:111:VAL:HG22	1.99	0.62
2:F:41:PHE:HA	2:F:412:VAL:HG13	1.81	0.62
2:F:418:THR:HG22	2:F:419:THR:H	1.64	0.62
4:B:105:GLU:O	4:B:106:PHE:HB2	1.98	0.62
1:2:78:ILE:CD1	1:2:104:THR:HG21	2.29	0.62
2:F:40:SER:OG	2:F:274:ARG:HG2	1.99	0.62
1:3:5:THR:O	1:3:6:GLU:HB2	1.98	0.62
1:4:10:ARG:NH2	1:4:139:GLU:CB	2.52	0.62
2:F:228:TYR:CZ	2:F:230:ALA:HB3	2.35	0.62
1:1:116:LYS:NZ	1:1:119:GLU:HB2	2.15	0.62
1:1:66:VAL:CG1	1:2:44:ILE:HA	2.30	0.62
1:3:42:VAL:HG12	1:3:43:TRP:N	2.14	0.62
1:3:26:VAL:HG13	1:3:65:PHE:CD2	2.35	0.61
1:4:10:ARG:HH21	1:4:139:GLU:HB2	1.54	0.61
1:1:30:THR:HA	1:1:147:ARG:HE	1.61	0.61
2:F:274:ARG:HB3	4:B:105:GLU:HG2	1.83	0.61
2:F:414:ARG:HD3	2:F:416:LEU:HG	1.83	0.61
1:1:9:VAL:HG21	1:2:7:GLN:OE1	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:30:THR:HB	1:1:147:ARG:NH2	2.16	0.61
1:3:37:LEU:HD21	1:3:58:CYS:SG	2.40	0.61
1:2:18:ILE:HG21	1:2:84:TYR:HD2	1.64	0.61
1:3:36:PHE:CE2	1:3:50:ARG:HB2	2.36	0.61
1:1:108:ILE:HG12	1:2:123:PHE:CE1	2.36	0.60
1:4:93:THR:O	1:4:97:ILE:HG13	2.01	0.60
1:3:26:VAL:HG13	1:3:65:PHE:HD2	1.67	0.60
1:1:134:VAL:HG12	1:1:136:THR:H	1.65	0.60
2:F:206:GLN:O	2:F:210:TYR:HD1	1.85	0.60
2:F:309:THR:CG2	2:F:310:TYR:N	2.63	0.60
1:4:21:ILE:O	1:4:23:ALA:N	2.34	0.60
1:4:68:TYR:OH	1:4:139:GLU:OE2	2.19	0.60
2:F:69:PHE:CE1	2:F:134:TYR:CD2	2.89	0.60
2:F:285:THR:O	2:F:286:LEU:HB2	2.01	0.60
1:2:7:GLN:C	1:2:9:VAL:H	2.09	0.60
1:3:71:PHE:CE1	1:4:117:ALA:HB1	2.37	0.60
3:G:60:ILE:CD1	3:G:161:LEU:HB2	2.30	0.60
1:2:109:ASN:O	1:2:111:VAL:HG13	2.01	0.60
1:4:66:VAL:O	1:4:66:VAL:HG12	2.01	0.60
1:4:116:LYS:HD2	1:4:119:GLU:OE1	2.02	0.60
2:F:169:TRP:CZ3	2:F:375:PRO:HG3	2.37	0.60
1:3:27:LEU:HD13	1:3:29:LEU:HD12	1.83	0.59
2:F:49:LEU:HD22	2:F:64:VAL:HG11	1.83	0.59
1:2:78:ILE:HD11	1:2:104:THR:CG2	2.32	0.59
1:2:78:ILE:HD11	1:2:104:THR:HG21	1.83	0.59
1:3:116:LYS:HG3	1:3:117:ALA:H	1.67	0.59
1:1:87:HIS:CG	1:1:88:PRO:HD2	2.37	0.59
1:2:87:HIS:CD2	1:2:89:VAL:HB	2.31	0.59
1:4:67:GLY:O	1:4:69:PRO:CD	2.49	0.59
1:3:75:VAL:HG23	1:3:102:GLU:C	2.28	0.59
2:F:67:PHE:O	2:F:68:THR:HG23	2.03	0.59
3:G:9:HIS:HD2	3:G:74:SER:OG	1.85	0.59
4:B:114:VAL:HG12	4:B:115:ASN:N	2.17	0.59
2:F:36:ILE:HG22	2:F:37:ALA:N	2.16	0.58
3:G:13:PHE:N	3:G:13:PHE:HD1	2.01	0.58
1:4:10:ARG:NH1	1:4:139:GLU:OE2	2.36	0.58
2:F:354:ALA:HB1	2:F:355:PRO:HD2	1.85	0.58
3:G:81:PHE:CD1	3:G:155:CYS:HB3	2.37	0.58
1:1:141:ASN:O	1:1:144:GLN:HB2	2.02	0.58
1:2:113:ARG:HH21	1:2:119:GLU:CD	2.11	0.58
2:F:202:LEU:HD13	2:F:206:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:397:VAL:HG12	2:F:397:VAL:O	2.03	0.58
1:1:108:ILE:HG23	1:2:123:PHE:HE1	1.69	0.58
3:G:13:PHE:N	3:G:13:PHE:CD1	2.72	0.58
2:F:168:ILE:HG13	2:F:353:TYR:CD2	2.39	0.58
2:F:154:ASP:CA	2:F:158:TYR:HE1	2.14	0.58
1:3:60:TYR:HD2	1:3:70:ARG:HD3	1.63	0.58
1:2:71:PHE:O	1:2:73:ALA:N	2.37	0.58
1:3:87:HIS:CD2	1:3:88:PRO:HD2	2.38	0.58
2:F:24:ILE:HD11	2:F:291:PHE:HD2	1.68	0.58
2:F:35:VAL:HG21	2:F:283:MET:HG3	1.86	0.57
2:F:73:HIS:ND1	2:F:281:GLY:HA2	2.19	0.57
2:F:414:ARG:HH11	2:F:414:ARG:HG2	1.69	0.57
1:1:79:ALA:CB	1:1:124:THR:HG22	2.34	0.57
1:1:84:TYR:HE1	1:1:134:VAL:HB	1.69	0.57
1:2:71:PHE:HB3	1:2:72:PRO:CD	2.33	0.57
2:F:49:LEU:CD2	2:F:64:VAL:HG21	2.33	0.57
2:F:55:ARG:HH12	2:F:366:GLU:CD	2.12	0.57
1:1:90:ASN:C	1:1:90:ASN:HD22	2.12	0.57
2:F:26:ARG:HD3	2:F:159:GLY:O	2.05	0.57
2:F:240:SER:OG	2:F:270:HIS:HD2	1.86	0.57
2:F:249:VAL:HG12	2:F:249:VAL:O	2.04	0.57
3:G:74:SER:O	3:G:75:VAL:HG12	2.05	0.57
3:G:110:TYR:CE2	3:G:129:ILE:HD12	2.40	0.57
2:F:104:ASP:O	2:F:105:HIS:HB2	2.04	0.57
1:1:8:SER:O	1:1:12:GLN:HG2	2.04	0.57
1:2:7:GLN:HE22	1:2:126:ARG:HH21	1.52	0.57
1:2:68:TYR:CE1	1:3:93:THR:HG22	2.36	0.57
2:F:23:GLN:HE22	2:F:401:GLN:NE2	2.02	0.57
1:4:71:PHE:CD2	1:4:72:PRO:O	2.57	0.57
2:F:23:GLN:NE2	2:F:24:ILE:HG22	2.20	0.57
2:F:328:ILE:HG22	2:F:329:SER:N	2.19	0.57
1:1:133:ASP:O	1:1:134:VAL:HG23	2.05	0.56
1:3:36:PHE:HE2	1:3:50:ARG:HB2	1.70	0.56
1:3:43:TRP:N	1:3:43:TRP:CD1	2.71	0.56
3:G:44:PHE:HD1	3:G:44:PHE:O	1.87	0.56
1:2:20:LEU:HD13	1:2:65:PHE:HE1	1.70	0.56
1:4:64:ASP:OD1	1:4:70:ARG:NH2	2.36	0.56
2:F:23:GLN:HE22	2:F:401:GLN:CD	2.13	0.56
2:F:239:ARG:O	2:F:239:ARG:HG3	1.96	0.56
2:F:39:ASP:O	2:F:40:SER:HB3	2.04	0.56
2:F:320:TYR:HE2	2:F:348:GLY:HA2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:41:THR:HB	3:G:160:SER:HB2	1.86	0.56
1:3:71:PHE:CZ	1:4:117:ALA:HB1	2.40	0.56
1:4:145:LYS:NZ	1:4:149:GLU:HB2	2.18	0.56
2:F:167:ASN:OD1	2:F:168:ILE:N	2.38	0.56
4:B:95:ASP:C	4:B:97:ASN:H	2.12	0.56
1:1:31:GLU:H	1:1:147:ARG:NH2	2.03	0.56
3:G:158:LEU:HD23	3:G:158:LEU:N	2.19	0.56
1:3:7:GLN:HB3	1:3:11:PHE:CD1	2.40	0.56
2:F:152:ASN:HB2	2:F:155:ASP:HB2	1.87	0.56
1:3:127:VAL:HG13	1:3:131:ASN:HD21	1.69	0.56
4:B:1:MET:O	4:B:2:GLU:HB2	2.06	0.56
1:2:36:PHE:HZ	1:2:47:ASP:HB3	1.70	0.56
1:3:71:PHE:HE1	1:4:96:LEU:HG	1.71	0.56
2:F:7:ALA:HB3	4:B:100:ARG:HD2	0.63	0.55
2:F:26:ARG:HB3	2:F:159:GLY:O	2.06	0.55
4:B:87:SER:OG	4:B:88:ALA:N	2.35	0.55
2:F:420:ARG:C	2:F:421:ASP:O	2.45	0.55
1:3:127:VAL:HG12	1:3:131:ASN:ND2	2.22	0.55
2:F:36:ILE:CG2	2:F:37:ALA:N	2.69	0.55
2:F:263:ARG:HH21	2:F:265:GLN:NE2	2.03	0.55
1:1:38:THR:HG22	1:1:85:TYR:O	2.07	0.55
1:2:56:GLU:HG2	1:2:103:PHE:CE1	2.41	0.55
2:F:212:MET:SD	2:F:213:GLN:HA	2.47	0.55
1:1:76:GLU:OE1	1:1:104:THR:HG23	2.06	0.55
1:2:10:ARG:NH1	1:2:76:GLU:CD	2.64	0.55
1:2:35:ASP:HB3	1:2:41:LYS:NZ	2.22	0.55
2:F:353:TYR:OH	2:F:355:PRO:HA	2.07	0.55
2:F:367:GLY:O	2:F:368:PHE:CG	2.60	0.55
1:1:25:ALA:HB3	1:1:62:THR:CG2	2.37	0.55
1:2:111:VAL:CG2	1:2:111:VAL:O	2.55	0.54
2:F:8:GLU:N	4:B:100:ARG:NH1	2.55	0.54
4:B:85:ASP:O	4:B:89:GLN:HG3	2.07	0.54
1:3:44:ILE:HG22	1:3:45:ALA:N	2.21	0.54
1:4:76:GLU:OE1	1:4:123:PHE:HE2	1.91	0.54
2:F:154:ASP:CA	2:F:158:TYR:CE1	2.80	0.54
4:B:3:GLN:NE2	4:B:90:ILE:HB	2.22	0.54
1:3:135:LEU:O	1:3:136:THR:C	2.51	0.54
1:4:36:PHE:CE2	1:4:50:ARG:HB2	2.41	0.54
1:4:145:LYS:HD3	1:4:145:LYS:C	2.32	0.54
2:F:102:TYR:HD2	2:F:105:HIS:CE1	2.26	0.54
2:F:157:ARG:CG	2:F:158:TYR:CZ	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:94:PHE:CD2	3:G:103:LEU:HD12	2.43	0.54
1:4:43:TRP:CZ3	1:4:51:ALA:HB1	2.43	0.54
2:F:56:ARG:HH22	2:F:366:GLU:H	1.55	0.54
2:F:386:ARG:HG3	2:F:389:ASP:OD2	2.08	0.54
3:G:90:CYS:SG	3:G:109:VAL:CG2	2.95	0.54
1:1:30:THR:O	1:1:31:GLU:C	2.50	0.54
1:3:26:VAL:HB	1:3:62:THR:HG22	1.90	0.54
2:F:78:GLY:O	2:F:80:GLN:N	2.40	0.54
2:F:236:LEU:O	2:F:238:MET:N	2.40	0.54
1:1:79:ALA:CA	1:1:124:THR:HG22	2.36	0.54
1:4:138:ALA:O	1:4:142:VAL:HG23	2.08	0.54
3:G:38:THR:HG23	3:G:163:GLN:HB3	1.90	0.54
1:2:60:TYR:CD1	1:2:70:ARG:HD3	2.43	0.53
1:3:29:LEU:HD22	1:3:33:ASP:HB3	1.88	0.53
1:4:67:GLY:O	1:4:69:PRO:N	2.41	0.53
1:2:20:LEU:HD13	1:2:65:PHE:CE1	2.43	0.53
1:3:42:VAL:HG12	1:3:43:TRP:H	1.74	0.53
2:F:259:GLN:O	2:F:260:PHE:CD1	2.61	0.53
2:F:195:LEU:O	2:F:198:ALA:HB3	2.08	0.53
3:G:15:SER:CA	3:G:41:THR:HG23	2.33	0.53
1:1:43:TRP:CZ3	1:1:51:ALA:HB1	2.43	0.53
1:3:65:PHE:CD1	1:3:65:PHE:C	2.87	0.53
2:F:56:ARG:NH2	2:F:366:GLU:H	2.07	0.53
2:F:187:THR:C	2:F:188:THR:HG23	2.32	0.53
1:2:106:ASN:HB2	1:2:115:VAL:HG22	1.89	0.53
2:F:202:LEU:HD13	2:F:206:GLN:HE21	1.73	0.53
2:F:285:THR:O	2:F:286:LEU:CB	2.55	0.53
2:F:199:TYR:O	2:F:202:LEU:HB2	2.08	0.53
1:1:119:GLU:HG3	3:G:134:ARG:O	2.09	0.53
1:3:60:TYR:O	1:3:63:LEU:HB2	2.09	0.53
2:F:40:SER:O	2:F:41:PHE:C	2.51	0.53
2:F:98:ASN:O	2:F:148:PRO:HD2	2.09	0.53
2:F:357:TYR:CE1	2:F:359:SER:HA	2.43	0.53
2:F:35:VAL:CG2	2:F:283:MET:HG3	2.39	0.52
2:F:413:TYR:H	2:F:413:TYR:HD1	1.56	0.52
1:4:139:GLU:O	1:4:142:VAL:HB	2.09	0.52
2:F:175:PRO:HG2	2:F:176:GLU:HG3	1.91	0.52
1:3:69:PRO:O	1:4:96:LEU:HD11	2.09	0.52
3:G:44:PHE:O	3:G:44:PHE:CD1	2.61	0.52
1:3:58:CYS:SG	1:3:85:TYR:CE2	2.93	0.52
1:3:75:VAL:HG12	1:3:75:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:36:PHE:HE2	1:3:50:ARG:HD2	1.75	0.52
2:F:56:ARG:HH12	2:F:365:LEU:HB3	1.74	0.52
2:F:265:GLN:O	2:F:266:GLN:C	2.51	0.52
2:F:362:TYR:HD1	2:F:368:PHE:CE2	2.27	0.52
2:F:413:TYR:N	2:F:413:TYR:HD1	2.04	0.52
3:G:41:THR:CB	3:G:160:SER:HB2	2.40	0.52
4:B:113:GLU:O	4:B:114:VAL:CB	2.48	0.52
1:1:116:LYS:NZ	1:1:119:GLU:CD	2.67	0.52
1:1:34:PHE:C	1:1:36:PHE:H	2.16	0.52
1:3:65:PHE:C	1:3:65:PHE:HD1	2.18	0.52
2:F:153:GLN:HB3	2:F:157:ARG:HD3	1.91	0.52
2:F:157:ARG:NE	2:F:158:TYR:CZ	2.64	0.52
2:F:406:VAL:C	2:F:407:LYS:HG3	2.35	0.52
1:1:102:GLU:HG2	1:1:113:ARG:O	2.10	0.51
2:F:7:ALA:C	4:B:100:ARG:NE	2.67	0.51
2:F:112:ILE:HD12	2:F:112:ILE:N	2.24	0.51
2:F:235:LEU:N	2:F:235:LEU:HD23	2.25	0.51
2:F:238:MET:SD	2:F:238:MET:O	2.69	0.51
2:F:414:ARG:NH1	2:F:414:ARG:CB	2.69	0.51
1:1:87:HIS:CE1	1:1:88:PRO:HG2	2.45	0.51
2:F:239:ARG:NH1	4:B:120:PHE:CD1	2.78	0.51
1:2:58:CYS:HB2	1:2:81:VAL:HG11	1.92	0.51
1:3:33:ASP:OD2	1:3:53:ARG:NH2	2.42	0.51
1:4:128:ARG:HH11	1:4:128:ARG:HG3	1.76	0.51
1:3:115:VAL:CG1	1:3:119:GLU:HB3	2.39	0.51
2:F:69:PHE:CE1	2:F:134:TYR:HD2	2.28	0.51
2:F:311:THR:HG22	2:F:319:LEU:CD1	2.37	0.51
2:F:406:VAL:CG1	2:F:407:LYS:N	2.73	0.51
2:F:363:HIS:O	2:F:364:LEU:CG	2.58	0.51
1:1:29:LEU:HD21	1:1:57:ALA:HB3	1.92	0.51
1:3:26:VAL:CG1	1:3:65:PHE:CD2	2.94	0.51
1:2:10:ARG:NH1	1:2:76:GLU:HG2	2.25	0.51
1:3:116:LYS:CG	1:3:117:ALA:N	2.74	0.51
1:4:133:ASP:CB	2:F:118:LYS:NZ	2.73	0.51
2:F:178:GLU:C	2:F:179:LEU:HD23	2.36	0.51
2:F:242:LEU:HD21	2:F:268:TYR:HB2	1.93	0.51
1:2:107:ILE:HG12	1:2:112:GLU:HG2	1.92	0.51
2:F:8:GLU:HA	4:B:100:ARG:CZ	2.41	0.51
1:1:134:VAL:HG13	1:1:138:ALA:HB3	1.93	0.51
1:2:7:GLN:HE22	1:2:126:ARG:NH2	2.08	0.51
2:F:179:LEU:HD21	2:F:344:LYS:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:35:ASP:O	1:4:36:PHE:C	2.54	0.51
2:F:406:VAL:C	2:F:407:LYS:CG	2.83	0.51
1:3:29:LEU:HD21	1:3:54:CYS:HA	1.93	0.50
2:F:23:GLN:HE22	2:F:24:ILE:HG22	1.75	0.50
3:G:3:GLN:HE21	3:G:4:THR:N	2.08	0.50
4:B:102:GLN:O	4:B:105:GLU:HB2	2.11	0.50
1:4:151:VAL:C	1:4:152:MET:CG	2.76	0.50
1:1:106:ASN:HD21	1:1:113:ARG:HD3	1.77	0.50
1:4:87:HIS:CE1	1:4:88:PRO:HG2	2.47	0.50
1:1:26:VAL:HG11	1:1:65:PHE:HB2	1.94	0.50
1:4:68:TYR:O	1:4:69:PRO:C	2.53	0.50
1:4:62:THR:O	1:4:65:PHE:HB3	2.12	0.50
1:4:68:TYR:HH	1:4:139:GLU:CD	2.16	0.50
1:4:90:ASN:O	1:4:91:ILE:C	2.54	0.50
2:F:60:ILE:HD11	2:F:370:PHE:CE1	2.46	0.50
2:F:241:ASN:C	2:F:241:ASN:OD1	2.54	0.50
3:G:62:MET:SD	3:G:131:VAL:HG12	2.51	0.50
1:4:87:HIS:CE1	1:4:89:VAL:HG23	2.46	0.50
2:F:173:LEU:HD12	2:F:325:PRO:CG	2.41	0.50
1:1:42:VAL:HG12	1:1:43:TRP:N	2.26	0.50
2:F:8:GLU:CA	4:B:100:ARG:CZ	2.90	0.50
2:F:152:ASN:O	2:F:153:GLN:C	2.54	0.50
3:G:18:LEU:HD22	3:G:20:LEU:H	1.77	0.50
2:F:167:ASN:OD1	2:F:167:ASN:C	2.54	0.50
1:3:35:ASP:O	1:3:39:SER:N	2.45	0.49
1:4:121:PHE:CZ	1:4:125:LEU:HD11	2.47	0.49
2:F:247:TYR:CD1	2:F:248:ASP:N	2.77	0.49
2:F:299:ILE:HG22	2:F:300:GLN:N	2.27	0.49
2:F:7:ALA:O	4:B:100:ARG:CD	2.55	0.49
2:F:8:GLU:N	4:B:100:ARG:CZ	2.76	0.49
3:G:48:THR:HG22	3:G:154:LYS:HG2	1.94	0.49
3:G:75:VAL:O	3:G:75:VAL:HG13	2.12	0.49
1:4:140:GLU:O	1:4:141:ASN:C	2.55	0.49
2:F:23:GLN:NE2	2:F:401:GLN:NE2	2.59	0.49
2:F:157:ARG:CZ	2:F:158:TYR:OH	2.57	0.49
2:F:320:TYR:OH	2:F:350:TRP:HZ3	1.96	0.49
4:B:93:ARG:O	4:B:94:PHE:HB2	2.10	0.49
4:B:94:PHE:CE1	4:B:104:ALA:HB3	2.48	0.49
1:2:7:GLN:O	1:2:7:GLN:HG2	2.12	0.49
2:F:8:GLU:CG	2:F:8:GLU:O	2.57	0.49
1:2:71:PHE:CD1	1:2:71:PHE:C	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:191:ASP:O	2:F:194:GLY:N	2.43	0.49
1:3:127:VAL:O	1:3:131:ASN:ND2	2.46	0.49
2:F:172:PRO:HG2	2:F:379:LEU:HD13	1.95	0.49
1:3:125:LEU:O	1:3:128:ARG:HB3	2.13	0.49
4:B:4:LEU:HB3	4:B:108:ARG:HB3	1.95	0.49
1:3:75:VAL:HG23	1:3:102:GLU:O	2.13	0.48
2:F:333:VAL:O	2:F:333:VAL:HG12	2.12	0.48
1:3:87:HIS:CE1	1:3:89:VAL:HG23	2.47	0.48
1:3:127:VAL:HG12	1:3:131:ASN:HD21	1.77	0.48
1:4:133:ASP:HA	1:4:136:THR:OG1	2.13	0.48
2:F:239:ARG:O	2:F:239:ARG:CG	2.59	0.48
3:G:62:MET:HG3	3:G:131:VAL:HG12	1.95	0.48
1:1:60:TYR:CD2	1:1:70:ARG:HD3	2.48	0.48
2:F:24:ILE:O	2:F:24:ILE:HG23	2.12	0.48
3:G:87:PHE:CB	3:G:148:SER:HB2	2.43	0.48
1:3:48:ARG:O	1:3:51:ALA:HB3	2.14	0.48
2:F:104:ASP:O	2:F:105:HIS:CB	2.59	0.48
2:F:378:ASP:O	2:F:380:GLN:N	2.47	0.48
3:G:62:MET:SD	3:G:131:VAL:CG1	3.02	0.48
1:2:106:ASN:HD22	1:2:113:ARG:HH21	1.60	0.48
1:2:110:GLY:O	1:2:111:VAL:C	2.56	0.48
1:1:52:ARG:O	1:1:56:GLU:HB2	2.14	0.48
1:2:124:THR:C	1:2:126:ARG:H	2.21	0.48
1:2:113:ARG:NH2	1:2:119:GLU:OE1	2.45	0.48
1:1:44:ILE:HG22	1:1:45:ALA:N	2.28	0.48
2:F:191:ASP:O	2:F:192:ILE:C	2.57	0.48
2:F:296:THR:HB	2:F:363:HIS:HB2	1.95	0.48
3:G:12:ASN:ND2	3:G:13:PHE:N	2.58	0.48
1:2:43:TRP:H	1:2:90:ASN:HD21	1.62	0.47
1:2:52:ARG:O	1:2:53:ARG:C	2.57	0.47
1:4:27:LEU:CD1	1:4:58:CYS:SG	3.02	0.47
2:F:72:PRO:HD2	2:F:75:HIS:CE1	2.47	0.47
1:1:116:LYS:HZ3	1:1:119:GLU:HB2	1.79	0.47
1:4:52:ARG:O	1:4:53:ARG:C	2.56	0.47
2:F:397:VAL:O	2:F:397:VAL:CG1	2.62	0.47
4:B:94:PHE:HA	4:B:102:GLN:OE1	2.14	0.47
4:B:105:GLU:O	4:B:106:PHE:CB	2.59	0.47
3:G:131:VAL:O	3:G:140:VAL:HG11	2.15	0.47
1:3:116:LYS:O	1:3:117:ALA:C	2.57	0.47
2:F:305:LYS:NZ	2:F:312:ASP:CG	2.73	0.47
3:G:9:HIS:HB2	3:G:74:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:38:THR:O	3:G:38:THR:HG22	2.13	0.47
1:1:75:VAL:HG11	1:1:103:PHE:HE1	1.78	0.47
1:2:7:GLN:C	1:2:9:VAL:N	2.72	0.47
1:2:75:VAL:HG12	1:2:123:PHE:CD2	2.50	0.47
2:F:185:THR:HG22	2:F:186:SER:O	2.14	0.47
2:F:386:ARG:O	2:F:388:HIS:N	2.48	0.47
1:2:135:LEU:HD13	1:2:136:THR:N	2.30	0.47
1:4:98:MET:HB2	1:4:120:LEU:HD13	1.95	0.47
2:F:20:LEU:HD22	2:F:30:ILE:HG23	1.97	0.47
2:F:29:THR:HG22	2:F:286:LEU:CD2	2.45	0.47
2:F:169:TRP:HZ3	2:F:375:PRO:HG3	1.77	0.47
4:B:94:PHE:O	4:B:95:ASP:HB2	2.14	0.47
1:1:134:VAL:HG12	1:1:135:LEU:N	2.30	0.47
1:3:60:TYR:N	1:3:60:TYR:CD1	2.79	0.47
2:F:11:PRO:O	2:F:11:PRO:HG2	2.13	0.47
2:F:284:PHE:N	2:F:284:PHE:CD1	2.82	0.47
2:F:372:GLN:O	2:F:373:GLU:HB2	2.15	0.47
2:F:128:LEU:HD23	2:F:160:PHE:HZ	1.79	0.47
2:F:202:LEU:O	2:F:205:ASP:N	2.48	0.47
2:F:380:GLN:H	2:F:382:ARG:H	1.62	0.47
1:1:87:HIS:ND1	1:1:89:VAL:HB	2.30	0.47
1:1:116:LYS:HZ1	1:1:119:GLU:CD	2.23	0.47
1:3:21:ILE:O	1:3:22:GLN:C	2.57	0.47
2:F:135:PHE:O	2:F:136:LYS:CB	2.55	0.47
3:G:73:VAL:HG11	3:G:142:VAL:HG11	1.97	0.47
3:G:161:LEU:N	3:G:161:LEU:HD12	2.29	0.46
1:2:106:ASN:ND2	1:2:119:GLU:OE1	2.48	0.46
1:3:116:LYS:CG	1:3:117:ALA:H	2.28	0.46
2:F:338:ASP:OD1	2:F:338:ASP:C	2.58	0.46
1:2:95:CYS:SG	1:2:121:PHE:HA	2.56	0.46
2:F:263:ARG:HH21	2:F:265:GLN:HE22	1.63	0.46
2:F:273:PRO:O	2:F:274:ARG:C	2.58	0.46
2:F:82:ILE:HD12	2:F:82:ILE:H	1.76	0.46
2:F:247:TYR:HD1	2:F:248:ASP:N	2.03	0.46
2:F:418:THR:HG21	2:F:420:ARG:HD3	1.97	0.46
1:2:79:ALA:HA	1:2:124:THR:HG22	1.97	0.46
1:2:116:LYS:HB2	1:2:119:GLU:OE2	2.16	0.46
1:3:47:ASP:O	1:3:48:ARG:C	2.58	0.46
1:4:44:ILE:CG2	1:4:45:ALA:N	2.78	0.46
2:F:390:TYR:O	2:F:394:PHE:CD2	2.69	0.46
1:3:30:THR:O	1:3:31:GLU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:320:TYR:CE2	2:F:348:GLY:HA2	2.51	0.46
2:F:403:ASN:HB3	2:F:405:GLN:HE22	1.81	0.46
1:2:68:TYR:N	1:2:68:TYR:CD1	2.83	0.46
1:2:71:PHE:CB	1:2:72:PRO:CD	2.93	0.46
2:F:92:THR:HA	2:F:93:PRO:HD2	1.49	0.46
2:F:98:ASN:HB2	2:F:149:ASN:HD21	1.80	0.46
2:F:100:THR:HG23	2:F:149:ASN:HA	1.98	0.46
2:F:183:MET:HE1	2:F:194:GLY:C	2.40	0.46
3:G:20:LEU:HG	3:G:21:THR:N	2.31	0.46
1:4:151:VAL:O	1:4:152:MET:SD	2.74	0.46
2:F:78:GLY:C	2:F:80:GLN:H	2.23	0.46
2:F:170:THR:C	2:F:172:PRO:HD3	2.41	0.46
2:F:319:LEU:C	2:F:321:GLY:N	2.72	0.46
2:F:15:SER:HB3	2:F:409:ASN:HA	1.99	0.45
2:F:390:TYR:O	2:F:394:PHE:HD2	2.00	0.45
3:G:87:PHE:HB3	3:G:148:SER:HB2	1.97	0.45
1:2:8:SER:C	1:2:10:ARG:N	2.69	0.45
1:2:97:ILE:HG13	1:2:97:ILE:H	1.57	0.45
2:F:41:PHE:CA	2:F:412:VAL:HG13	2.45	0.45
2:F:63:THR:HG23	2:F:243:TRP:CE2	2.51	0.45
2:F:128:LEU:CD2	2:F:160:PHE:HZ	2.29	0.45
3:G:13:PHE:H	3:G:13:PHE:HD1	1.65	0.45
2:F:152:ASN:HB2	2:F:155:ASP:H	1.81	0.45
2:F:334:PHE:CD2	2:F:374:PRO:HB3	2.51	0.45
2:F:418:THR:CG2	2:F:419:THR:N	2.79	0.45
4:B:82:THR:OG1	4:B:91:TYR:CD2	2.59	0.45
1:2:68:TYR:N	1:2:68:TYR:HD1	2.13	0.45
2:F:39:ASP:OD2	2:F:414:ARG:NH2	2.50	0.45
2:F:229:ASP:O	2:F:231:ASP:N	2.50	0.45
3:G:160:SER:C	3:G:161:LEU:HD12	2.42	0.45
2:F:30:ILE:HG21	2:F:408:PHE:HZ	1.79	0.45
3:G:4:THR:HG22	3:G:6:ILE:H	1.82	0.45
3:G:164:VAL:O	3:G:164:VAL:HG12	2.16	0.45
1:3:104:THR:O	1:3:108:ILE:HG13	2.17	0.45
1:1:33:ASP:O	1:1:36:PHE:HB3	2.17	0.45
1:4:60:TYR:HD1	1:4:63:LEU:HD12	1.81	0.45
2:F:20:LEU:O	2:F:21:ALA:HB2	2.17	0.45
1:3:24:SER:HA	1:4:89:VAL:HG22	1.99	0.45
1:4:135:LEU:O	1:4:136:THR:C	2.59	0.45
2:F:183:MET:HG3	2:F:184:THR:N	2.32	0.45
2:F:172:PRO:HG2	2:F:379:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:PRO:HD2	2:F:177:THR:CG2	2.47	0.45
2:F:183:MET:HE1	2:F:195:LEU:N	2.32	0.44
1:3:62:THR:HG21	1:4:89:VAL:O	2.16	0.44
1:4:52:ARG:NH1	1:4:102:GLU:CD	2.75	0.44
2:F:295:ALA:HA	2:F:371:ILE:CG2	2.44	0.44
3:G:29:ALA:O	3:G:102:THR:HA	2.17	0.44
4:B:94:PHE:HA	4:B:102:GLN:CD	2.42	0.44
1:1:90:ASN:ND2	1:1:90:ASN:O	2.49	0.44
2:F:388:HIS:C	2:F:390:TYR:H	2.25	0.44
1:1:79:ALA:HB1	1:1:124:THR:HG22	1.98	0.44
1:2:35:ASP:HB3	1:2:41:LYS:HZ1	1.81	0.44
1:3:92:GLN:HG3	1:3:121:PHE:CD2	2.52	0.44
1:3:104:THR:CB	1:4:126:ARG:HH12	2.30	0.44
1:4:98:MET:HB2	1:4:120:LEU:CD1	2.48	0.44
2:F:329:SER:HB2	2:F:339:SER:HA	2.00	0.44
1:3:91:ILE:O	1:3:94:ALA:HB3	2.18	0.44
2:F:363:HIS:O	2:F:364:LEU:CB	2.66	0.44
4:B:102:GLN:HB3	4:B:103:PRO:HD2	1.99	0.44
1:4:123:PHE:CD2	1:4:134:VAL:HG11	2.53	0.44
4:B:3:GLN:HE22	4:B:90:ILE:CG2	2.30	0.44
2:F:60:ILE:HG22	2:F:61:ASP:H	1.82	0.44
2:F:236:LEU:O	2:F:237:VAL:C	2.58	0.44
2:F:326:ARG:HH21	2:F:347:GLU:CD	2.24	0.44
2:F:329:SER:O	2:F:330:MET:C	2.58	0.44
1:1:93:THR:O	1:1:97:ILE:HG23	2.17	0.44
1:2:8:SER:C	1:2:10:ARG:H	2.26	0.44
1:2:20:LEU:HB3	1:2:65:PHE:CZ	2.52	0.44
1:2:121:PHE:CE2	1:2:125:LEU:HD22	2.53	0.44
1:4:10:ARG:CZ	1:4:139:GLU:CD	2.91	0.44
1:4:50:ARG:HH11	1:4:53:ARG:HH11	1.66	0.44
1:4:123:PHE:CE2	1:4:134:VAL:CG1	3.01	0.44
2:F:245:SER:OG	2:F:246:GLY:N	2.48	0.44
2:F:399:LEU:HD13	2:F:403:ASN:OD1	2.17	0.44
1:1:37:LEU:HG	1:1:54:CYS:HB3	1.99	0.44
1:4:105:GLU:CG	1:4:106:ASN:N	2.79	0.44
2:F:69:PHE:CD2	2:F:130:ILE:HD13	2.53	0.44
4:B:6:LYS:CE	4:B:83:CYS:SG	2.99	0.44
2:F:388:HIS:O	2:F:390:TYR:N	2.51	0.43
1:3:131:ASN:O	1:3:135:LEU:N	2.50	0.43
2:F:74:ARG:NH2	2:F:229:ASP:HB2	2.33	0.43
1:1:103:PHE:O	1:1:104:THR:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:132:THR:C	1:2:133:ASP:OD1	2.62	0.43
2:F:79:GLU:CA	2:F:82:ILE:HD13	2.46	0.43
2:F:122:HIS:CD2	2:F:282:THR:HG21	2.54	0.43
1:2:9:VAL:HG13	1:3:88:PRO:HB3	2.00	0.43
1:2:18:ILE:O	1:2:19:LYS:C	2.62	0.43
1:3:115:VAL:HG13	1:3:119:GLU:CB	2.45	0.43
1:4:71:PHE:CE2	1:4:72:PRO:O	2.71	0.43
4:B:87:SER:O	4:B:91:TYR:CD2	2.71	0.43
1:3:95:CYS:C	1:3:97:ILE:N	2.75	0.43
1:3:121:PHE:HE1	1:3:125:LEU:HD21	1.84	0.43
2:F:88:GLY:O	2:F:90:ASN:N	2.51	0.43
1:1:120:LEU:O	1:1:124:THR:HG23	2.19	0.43
1:2:125:LEU:HD12	1:2:125:LEU:HA	1.84	0.43
1:4:30:THR:C	1:4:32:ASP:N	2.76	0.43
2:F:7:ALA:C	4:B:100:ARG:CZ	2.92	0.43
2:F:195:LEU:HD23	2:F:195:LEU:HA	1.76	0.43
2:F:273:PRO:CD	4:B:107:TYR:OH	2.63	0.43
3:G:75:VAL:HA	3:G:160:SER:O	2.18	0.43
1:1:113:ARG:NH2	3:G:136:PRO:CG	2.82	0.43
1:2:55:VAL:O	1:2:59:VAL:HG23	2.19	0.43
2:F:146:ALA:HB3	2:F:150:GLU:OE2	2.18	0.43
2:F:202:LEU:O	2:F:203:HIS:C	2.62	0.43
2:F:418:THR:CG2	2:F:419:THR:H	2.29	0.43
3:G:19:VAL:HG13	3:G:20:LEU:N	2.33	0.43
1:1:31:GLU:H	1:1:147:ARG:HE	1.65	0.43
1:2:48:ARG:HG2	1:2:97:ILE:HG23	2.00	0.43
1:2:78:ILE:HD12	1:2:104:THR:HG21	2.00	0.43
1:1:117:ALA:O	1:1:118:ALA:C	2.60	0.43
2:F:46:VAL:HG12	2:F:47:GLY:N	2.33	0.43
2:F:73:HIS:CE1	2:F:281:GLY:HA2	2.53	0.43
2:F:239:ARG:NH1	4:B:120:PHE:HD1	2.16	0.43
2:F:293:PRO:O	2:F:294:THR:HG23	2.19	0.43
1:1:87:HIS:ND1	1:1:89:VAL:N	2.61	0.42
1:2:36:PHE:HB2	1:2:50:ARG:NH1	2.34	0.42
1:2:108:ILE:O	1:2:111:VAL:HG13	2.19	0.42
1:3:29:LEU:HD22	1:3:33:ASP:CB	2.49	0.42
1:4:23:ALA:HB1	1:4:26:VAL:HG23	2.01	0.42
2:F:60:ILE:HG22	2:F:61:ASP:N	2.34	0.42
2:F:261:SER:OG	2:F:262:GLY:N	2.48	0.42
3:G:149:ASN:C	3:G:149:ASN:HD22	2.27	0.42
1:1:11:PHE:CE1	1:1:15:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:43:TRP:H	1:2:90:ASN:ND2	2.17	0.42
1:4:87:HIS:CG	1:4:88:PRO:HD2	2.54	0.42
2:F:168:ILE:HD13	2:F:168:ILE:HG21	1.63	0.42
2:F:173:LEU:HD12	2:F:325:PRO:HG2	1.99	0.42
2:F:216:ARG:HH21	2:F:229:ASP:HA	1.84	0.42
1:3:48:ARG:O	1:3:51:ALA:N	2.52	0.42
1:4:15:LEU:HD23	1:4:62:THR:HG21	2.01	0.42
1:4:44:ILE:HG22	1:4:45:ALA:H	1.84	0.42
2:F:405:GLN:CD	2:F:405:GLN:N	2.76	0.42
3:G:123:VAL:HG22	3:G:124:LYS:N	2.34	0.42
1:1:34:PHE:C	1:1:36:PHE:N	2.76	0.42
1:4:40:ASN:OD1	1:4:40:ASN:O	2.36	0.42
2:F:79:GLU:H	2:F:82:ILE:HD13	1.84	0.42
3:G:52:GLY:O	3:G:150:PHE:N	2.52	0.42
2:F:328:ILE:CG2	2:F:332:ASP:HB2	2.47	0.42
1:4:62:THR:HA	1:4:65:PHE:HB3	2.01	0.42
1:4:65:PHE:HD2	1:4:66:VAL:HG23	1.83	0.42
1:2:108:ILE:HG22	1:2:109:ASN:ND2	2.35	0.42
1:2:135:LEU:HA	1:2:135:LEU:HD22	1.78	0.42
1:4:64:ASP:CG	1:4:70:ARG:NH2	2.78	0.42
2:F:209:ASP:O	2:F:213:GLN:NE2	2.53	0.42
3:G:62:MET:HE3	3:G:142:VAL:HB	2.02	0.42
1:1:113:ARG:NH2	3:G:136:PRO:HG2	2.34	0.42
1:2:18:ILE:HA	1:2:21:ILE:HD12	2.01	0.42
1:3:87:HIS:HE1	1:3:89:VAL:HG23	1.85	0.42
1:4:30:THR:O	1:4:31:GLU:C	2.62	0.42
1:4:52:ARG:HH12	1:4:102:GLU:CD	2.28	0.42
2:F:100:THR:OG1	2:F:105:HIS:CD2	2.73	0.42
2:F:323:LEU:HA	2:F:324:PRO:HD2	1.90	0.42
2:F:379:LEU:HD12	2:F:383:VAL:CG2	2.50	0.42
1:1:25:ALA:HB3	1:1:62:THR:HG22	2.02	0.42
4:B:3:GLN:CD	4:B:90:ILE:HB	2.44	0.42
1:1:60:TYR:O	1:1:63:LEU:HB2	2.18	0.42
1:2:120:LEU:HD23	1:2:120:LEU:HA	1.67	0.42
2:F:71:VAL:HG22	2:F:234:PRO:HB3	2.02	0.42
2:F:324:PRO:O	2:F:325:PRO:C	2.62	0.42
1:2:33:ASP:O	1:2:36:PHE:HB3	2.19	0.41
1:2:113:ARG:NH2	1:2:119:GLU:OE2	2.53	0.41
3:G:84:ASP:OD1	3:G:84:ASP:C	2.62	0.41
1:1:131:ASN:OD1	1:1:131:ASN:C	2.63	0.41
1:4:133:ASP:CB	2:F:118:LYS:HZ2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:69:PHE:HE1	2:F:134:TYR:CD2	2.36	0.41
2:F:362:TYR:CD1	2:F:368:PHE:CZ	3.08	0.41
3:G:158:LEU:N	3:G:158:LEU:CD2	2.82	0.41
4:B:83:CYS:O	4:B:84:ASP:HB2	2.21	0.41
1:2:18:ILE:HG21	1:2:84:TYR:CE2	2.56	0.41
1:3:87:HIS:ND1	1:3:89:VAL:HB	2.35	0.41
2:F:24:ILE:CD1	2:F:291:PHE:HD2	2.34	0.41
2:F:171:ALA:N	2:F:172:PRO:HD3	2.36	0.41
4:B:93:ARG:H	4:B:93:ARG:HD2	1.85	0.41
1:1:134:VAL:CG1	1:1:135:LEU:N	2.83	0.41
1:3:135:LEU:O	1:3:135:LEU:HD22	2.21	0.41
2:F:22:GLY:HA3	2:F:28:ILE:HD12	2.03	0.41
3:G:30:PRO:O	3:G:57:LEU:HD23	2.20	0.41
1:3:20:LEU:HD21	1:4:91:ILE:HD12	2.03	0.41
1:3:51:ALA:O	1:3:52:ARG:C	2.63	0.41
2:F:161:ARG:HD2	2:F:385:ILE:O	2.21	0.41
4:B:95:ASP:O	4:B:96:LYS:C	2.63	0.41
1:2:36:PHE:CZ	1:2:50:ARG:HD2	2.55	0.41
1:2:121:PHE:O	1:2:125:LEU:HB2	2.21	0.41
1:4:10:ARG:O	1:4:11:PHE:C	2.63	0.41
2:F:279:GLU:O	2:F:280:HIS:C	2.63	0.41
2:F:399:LEU:HD23	2:F:399:LEU:HA	1.89	0.41
1:1:27:LEU:HD22	1:1:29:LEU:CD1	2.51	0.41
1:3:15:LEU:CD2	1:3:131:ASN:OD1	2.69	0.41
1:4:128:ARG:HG2	1:4:128:ARG:NH1	2.27	0.41
2:F:275:PHE:CD2	2:F:283:MET:HE1	2.55	0.41
1:1:25:ALA:HB3	1:1:62:THR:HG21	2.02	0.41
1:1:29:LEU:H	1:1:29:LEU:HG	1.24	0.41
1:1:108:ILE:HG23	1:2:123:PHE:CZ	2.56	0.41
2:F:93:PRO:O	2:F:94:LEU:HB2	2.21	0.41
2:F:316:ASP:HA	2:F:317:PRO:HD2	1.84	0.41
3:G:26:ALA:C	3:G:54:GLY:HA3	2.46	0.41
3:G:29:ALA:CB	3:G:55:GLY:O	2.69	0.41
4:B:93:ARG:O	4:B:94:PHE:CB	2.69	0.41
1:2:10:ARG:CG	1:2:10:ARG:NH1	2.70	0.41
1:3:44:ILE:CG2	1:3:45:ALA:H	2.29	0.41
1:3:136:THR:C	1:3:138:ALA:H	2.29	0.41
1:4:74:PRO:O	1:4:75:VAL:C	2.63	0.41
1:1:114:PRO:O	1:1:114:PRO:HG2	2.21	0.40
1:3:20:LEU:CD2	1:4:91:ILE:HD12	2.51	0.40
1:3:131:ASN:O	1:3:132:THR:C	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:128:ARG:CG	1:4:128:ARG:NH1	2.65	0.40
2:F:99:THR:HB	2:F:113:ASN:HD21	1.84	0.40
3:G:60:ILE:HG22	3:G:62:MET:HE2	2.02	0.40
1:1:30:THR:O	1:1:33:ASP:N	2.54	0.40
1:1:135:LEU:HD23	1:1:135:LEU:HA	1.84	0.40
1:2:124:THR:C	1:2:126:ARG:N	2.79	0.40
1:4:18:ILE:CD1	1:4:26:VAL:HG11	2.51	0.40
2:F:101:GLY:HA2	2:F:117:ASN:OD1	2.21	0.40
2:F:132:ASN:HA	2:F:136:LYS:HD2	2.03	0.40
3:G:9:HIS:HD2	3:G:74:SER:CB	2.35	0.40
3:G:19:VAL:CG1	3:G:20:LEU:N	2.85	0.40
2:F:16:HIS:O	2:F:16:HIS:CG	2.74	0.40
2:F:40:SER:O	2:F:41:PHE:O	2.39	0.40
2:F:82:ILE:N	2:F:82:ILE:CD1	2.80	0.40
2:F:174:PRO:HD2	2:F:177:THR:HG21	2.02	0.40
2:F:165:LEU:HD23	2:F:165:LEU:HA	1.90	0.40
1:3:85:TYR:N	1:3:85:TYR:CD1	2.89	0.40
1:4:33:ASP:O	1:4:34:PHE:C	2.65	0.40
1:4:71:PHE:HB2	1:4:72:PRO:HD2	2.03	0.40
1:4:79:ALA:O	1:4:80:ALA:C	2.64	0.40
1:4:135:LEU:HD23	1:4:135:LEU:HA	1.83	0.40
2:F:61:ASP:CG	2:F:245:SER:HB2	2.47	0.40
2:F:83:LYS:O	2:F:84:PHE:C	2.65	0.40
4:B:104:ALA:C	4:B:105:GLU:O	2.62	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	1	141/152 (93%)	125 (89%)	14 (10%)	2 (1%)	9 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	131/152 (86%)	103 (79%)	20 (15%)	8 (6%)	1	12
1	3	138/152 (91%)	114 (83%)	13 (9%)	11 (8%)	1	8
1	4	144/152 (95%)	112 (78%)	26 (18%)	6 (4%)	2	19
2	F	416/426 (98%)	331 (80%)	47 (11%)	38 (9%)	0	7
3	G	173/175 (99%)	152 (88%)	18 (10%)	3 (2%)	7	35
4	B	45/120 (38%)	25 (56%)	9 (20%)	11 (24%)	0	0
All	All	1188/1329 (89%)	962 (81%)	147 (12%)	79 (7%)	1	11

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	111	VAL
1	3	9	VAL
1	3	61	GLY
1	3	117	ALA
1	4	8	SER
1	4	22	GLN
1	4	70	ARG
2	F	5	THR
2	F	41	PHE
2	F	93	PRO
2	F	105	HIS
2	F	168	ILE
2	F	185	THR
2	F	212	MET
2	F	230	ALA
2	F	237	VAL
2	F	316	ASP
2	F	355	PRO
2	F	356	SER
2	F	364	LEU
2	F	379	LEU
3	G	37	ALA
4	B	81	ALA
4	B	84	ASP
4	B	94	PHE
4	B	95	ASP
4	B	114	VAL
1	1	61	GLY
1	1	136	THR

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Mol	Chain	Res	Type
1	2	137	ASP
1	3	6	GLU
1	4	105	GLU
2	F	101	GLY
2	F	213	GLN
2	F	380	GLN
3	G	75	VAL
4	B	2	GLU
4	B	96	LYS
4	B	106	PHE
4	B	108	ARG
1	2	8	SER
1	2	28	ASP
1	2	118	ALA
1	2	134	VAL
1	3	7	GLN
1	3	31	GLU
1	3	99	GLU
1	3	136	THR
1	3	138	ALA
2	F	94	LEU
2	F	266	GLN
2	F	371	ILE
2	F	372	GLN
2	F	373	GLU
2	F	389	ASP
4	B	117	PHE
1	3	132	THR
1	4	71	PHE
2	F	57	GLY
2	F	68	THR
2	F	79	GLU
2	F	136	LYS
2	F	239	ARG
2	F	248	ASP
2	F	257	LEU
2	F	325	PRO
2	F	370	PHE
1	2	102	GLU
1	3	45	ALA
2	F	167	ASN
2	F	286	LEU

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Mol	Chain	Res	Type
2	F	400	LEU
3	G	136	PRO
4	B	107	TYR
1	2	7	GLN
1	4	67	GLY
2	F	262	GLY
2	F	249	VAL
2	F	317	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	1	119/127 (94%)	106 (89%)	13 (11%)	6	26
1	2	110/127 (87%)	93 (84%)	17 (16%)	2	15
1	3	117/127 (92%)	104 (89%)	13 (11%)	6	25
1	4	121/127 (95%)	106 (88%)	15 (12%)	4	22
2	F	364/372 (98%)	310 (85%)	54 (15%)	3	17
3	G	153/153 (100%)	134 (88%)	19 (12%)	4	22
4	B	42/101 (42%)	36 (86%)	6 (14%)	3	18
All	All	1026/1134 (90%)	889 (87%)	137 (13%)	4	20

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	7	GLN
1	1	17	SER
1	1	26	VAL
1	1	27	LEU
1	1	29	LEU
1	1	37	LEU
1	1	89	VAL
1	1	90	ASN
1	1	105	GLU

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Mol	Chain	Res	Type
1	1	116	LYS
1	1	126	ARG
1	1	136	THR
1	1	147	ARG
1	2	10	ARG
1	2	13	THR
1	2	27	LEU
1	2	35	ASP
1	2	37	LEU
1	2	44	ILE
1	2	50	ARG
1	2	89	VAL
1	2	93	THR
1	2	96	LEU
1	2	102	GLU
1	2	109	ASN
1	2	111	VAL
1	2	113	ARG
1	2	119	GLU
1	2	126	ARG
1	2	135	LEU
1	3	9	VAL
1	3	17	SER
1	3	40	ASN
1	3	43	TRP
1	3	58	CYS
1	3	65	PHE
1	3	71	PHE
1	3	85	TYR
1	3	99	GLU
1	3	104	THR
1	3	113	ARG
1	3	134	VAL
1	3	135	LEU
1	4	21	ILE
1	4	52	ARG
1	4	70	ARG
1	4	76	GLU
1	4	93	THR
1	4	96	LEU
1	4	103	PHE
1	4	105	GLU

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Mol	Chain	Res	Type
1	4	111	VAL
1	4	119	GLU
1	4	126	ARG
1	4	128	ARG
1	4	132	THR
1	4	133	ASP
1	4	145	LYS
2	F	4	GLN
2	F	9	ARG
2	F	10	MET
2	F	23	GLN
2	F	31	SER
2	F	52	SER
2	F	58	LEU
2	F	60	ILE
2	F	62	SER
2	F	63	THR
2	F	68	THR
2	F	89	VAL
2	F	97	VAL
2	F	104	ASP
2	F	105	HIS
2	F	115	ASP
2	F	136	LYS
2	F	144	THR
2	F	148	PRO
2	F	158	TYR
2	F	164	HIS
2	F	168	ILE
2	F	179	LEU
2	F	183	MET
2	F	188	THR
2	F	202	LEU
2	F	212	MET
2	F	213	GLN
2	F	226	THR
2	F	229	ASP
2	F	233	ARG
2	F	235	LEU
2	F	237	VAL
2	F	238	MET
2	F	239	ARG

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Mol	Chain	Res	Type
2	F	242	LEU
2	F	247	TYR
2	F	248	ASP
2	F	259	GLN
2	F	279	GLU
2	F	282	THR
2	F	297	LYS
2	F	333	VAL
2	F	335	ARG
2	F	349	GLN
2	F	350	TRP
2	F	353	TYR
2	F	359	SER
2	F	364	LEU
2	F	372	GLN
2	F	389	ASP
2	F	393	CYS
2	F	413	TYR
2	F	414	ARG
3	G	13	PHE
3	G	18	LEU
3	G	22	SER
3	G	23	VAL
3	G	24	THR
3	G	41	THR
3	G	60	ILE
3	G	91	LEU
3	G	92	VAL
3	G	109	VAL
3	G	115	ARG
3	G	126	CYS
3	G	128	THR
3	G	136	PRO
3	G	140	VAL
3	G	159	VAL
3	G	165	ILE
3	G	169	ILE
3	G	174	LEU
4	B	3	GLN
4	B	4	LEU
4	B	84	ASP
4	B	85	ASP

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Mol	Chain	Res	Type
4	B	94	PHE
4	B	114	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	90	ASN
1	1	106	ASN
1	2	7	GLN
1	2	22	GLN
1	2	87	HIS
1	2	90	ASN
1	2	106	ASN
1	2	109	ASN
1	3	131	ASN
1	3	144	GLN
2	F	23	GLN
2	F	75	HIS
2	F	80	GLN
2	F	105	HIS
2	F	149	ASN
2	F	206	GLN
2	F	232	ASN
2	F	265	GLN
2	F	270	HIS
2	F	405	GLN
2	F	415	ASN
3	G	3	GLN
3	G	9	HIS
3	G	10	ASN
3	G	12	ASN
3	G	70	ASN
3	G	138	ASN
3	G	149	ASN
3	G	162	ASN
3	G	163	GLN
4	B	3	GLN
4	B	110	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	1	143/152 (94%)	4.10	87 (60%) 0 0	20, 20, 20, 20	0
1	2	133/152 (87%)	3.13	74 (55%) 0 0	20, 20, 20, 20	0
1	3	140/152 (92%)	1.66	40 (28%) 1 1	20, 20, 20, 20	0
1	4	146/152 (96%)	2.32	59 (40%) 0 1	20, 20, 20, 20	0
2	F	418/426 (98%)	3.75	237 (56%) 0 0	20, 20, 20, 20	0
3	G	175/175 (100%)	2.89	92 (52%) 0 0	20, 20, 20, 20	0
4	B	49/120 (40%)	4.05	34 (69%) 0 0	20, 20, 20, 20	0
All	All	1204/1329 (90%)	3.20	623 (51%) 0 1	20, 20, 20, 20	0

All (623) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	381	GLU	23.4
1	2	130	GLY	21.0
2	F	376	SER	19.4
2	F	378	ASP	19.2
1	1	100	GLY	19.2
1	1	112	GLU	18.6
2	F	219	ILE	18.1
1	1	72	PRO	17.9
3	G	70	ASN	17.7
2	F	377	GLY	17.3
2	F	153	GLN	16.3
1	4	40	ASN	15.9
2	F	189	SER	15.8
2	F	176	GLU	15.6
1	1	110	GLY	15.5
1	1	109	ASN	15.3
1	1	99	GLU	15.1

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Mol	Chain	Res	Type	RSRZ
2	F	241	ASN	14.9
2	F	348	GLY	14.8
1	1	142	VAL	14.2
2	F	191	ASP	14.2
1	1	56	GLU	14.1
1	2	6	GLU	13.9
4	B	8	GLN	13.9
3	G	167	GLU	13.8
3	G	128	THR	13.8
2	F	185	THR	13.6
2	F	110	GLY	13.5
2	F	340	SER	13.5
2	F	197	ALA	13.4
2	F	380	GLN	13.3
2	F	308	LEU	13.3
1	2	99	GLU	13.1
1	1	113	ARG	13.1
2	F	347	GLU	13.0
2	F	391	ASP	13.0
2	F	320	TYR	12.9
1	1	106	ASN	12.5
2	F	142	ASP	12.3
2	F	373	GLU	12.0
2	F	388	HIS	11.8
1	1	6	GLU	11.7
4	B	108	ARG	11.6
2	F	389	ASP	11.6
3	G	65	SER	11.3
3	G	113	ASN	11.2
2	F	258	GLY	11.2
2	F	248	ASP	11.2
2	F	256	SER	11.1
1	2	29	LEU	11.1
2	F	338	ASP	10.9
2	F	312	ASP	10.6
3	G	67	ASN	10.4
2	F	194	GLY	10.4
2	F	350	TRP	10.3
3	G	78	ASP	10.3
2	F	311	THR	10.1
1	1	114	PRO	10.1
1	2	116	LYS	10.1

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Mol	Chain	Res	Type	RSRZ
2	F	154	ASP	10.1
4	B	116	THR	10.1
2	F	190	ILE	10.1
1	4	130	GLY	10.1
4	B	99	TRP	10.0
2	F	316	ASP	10.0
1	1	117	ALA	9.9
1	3	100	GLY	9.9
3	G	130	ASP	9.9
3	G	136	PRO	9.9
1	1	107	ILE	9.9
1	4	116	LYS	9.8
1	1	101	ALA	9.8
2	F	301	TYR	9.7
2	F	314	ALA	9.7
2	F	152	ASN	9.5
2	F	346	ALA	9.4
1	2	104	THR	9.4
2	F	386	ARG	9.3
2	F	339	SER	9.2
2	F	195	LEU	9.2
2	F	202	LEU	9.2
1	2	72	PRO	9.2
2	F	395	GLN	9.1
2	F	259	GLN	9.1
1	1	102	GLU	9.1
1	3	126	ARG	9.0
1	4	128	ARG	8.9
3	G	173	PRO	8.9
1	4	68	TYR	8.9
3	G	21	THR	8.6
2	F	218	VAL	8.6
2	F	375	PRO	8.4
2	F	198	ALA	8.4
1	1	34	PHE	8.3
4	B	7	ASN	8.3
1	1	47	ASP	8.3
1	2	118	ALA	8.2
1	4	29	LEU	8.2
3	G	5	PHE	8.2
2	F	265	GLN	8.2
2	F	315	GLY	8.2

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Mol	Chain	Res	Type	RSRZ
2	F	319	LEU	8.2
1	1	39	SER	8.1
1	3	5	THR	8.1
3	G	45	ASP	8.1
1	2	132	THR	8.1
2	F	313	ILE	8.1
1	1	111	VAL	8.0
2	F	345	ILE	8.0
2	F	199	TYR	8.0
1	1	146	LEU	7.9
1	2	57	ALA	7.9
2	F	138	PRO	7.9
3	G	69	ALA	7.9
1	2	109	ASN	7.8
4	B	2	GLU	7.8
4	B	93	ARG	7.8
2	F	141	PRO	7.8
2	F	302	LEU	7.7
2	F	183	MET	7.7
1	1	136	THR	7.7
1	2	131	ASN	7.7
2	F	125	GLN	7.7
2	F	392	GLN	7.6
2	F	351	TYR	7.6
2	F	226	THR	7.6
1	4	144	GLN	7.5
2	F	310	TYR	7.4
2	F	264	VAL	7.4
1	3	31	GLU	7.4
2	F	254	GLN	7.3
1	4	113	ARG	7.3
1	2	7	GLN	7.2
1	3	140	GLU	7.2
1	3	110	GLY	7.2
3	G	132	LEU	7.2
2	F	366	GLU	7.2
3	G	172	GLN	7.2
1	1	84	TYR	7.1
1	3	34	PHE	7.1
2	F	333	VAL	7.1
2	F	323	LEU	7.0
2	F	161	ARG	7.0

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Mol	Chain	Res	Type	RSRZ
1	3	70	ARG	7.0
1	4	107	ILE	7.0
2	F	398	GLN	6.9
2	F	168	ILE	6.9
1	1	105	GLU	6.9
1	1	69	PRO	6.9
2	F	115	ASP	6.8
1	1	140	GLU	6.8
4	B	115	ASN	6.8
4	B	81	ALA	6.8
3	G	108	ASP	6.8
2	F	215	TYR	6.8
1	1	70	ARG	6.8
1	2	37	LEU	6.8
2	F	251	GLY	6.7
2	F	34	PRO	6.7
1	3	142	VAL	6.7
2	F	341	LYS	6.7
1	4	119	GLU	6.7
1	2	103	PHE	6.6
2	F	336	SER	6.6
2	F	326	ARG	6.6
2	F	342	LYS	6.6
1	2	34	PHE	6.5
1	1	33	ASP	6.5
2	F	405	GLN	6.5
2	F	145	GLU	6.4
1	1	92	GLN	6.4
4	B	117	PHE	6.4
2	F	250	ASP	6.4
4	B	80	GLY	6.4
2	F	157	ARG	6.4
1	4	36	PHE	6.4
1	3	143	ARG	6.4
1	4	18	ILE	6.3
2	F	192	ILE	6.3
2	F	216	ARG	6.3
1	3	109	ASN	6.3
2	F	54	LEU	6.3
1	1	104	THR	6.3
1	2	108	ILE	6.3
4	B	89	GLN	6.3

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Mol	Chain	Res	Type	RSRZ
1	2	110	GLY	6.3
1	1	90	ASN	6.2
2	F	7	ALA	6.2
1	1	41	LYS	6.2
2	F	271	SER	6.2
1	4	27	LEU	6.1
3	G	97	SER	6.1
1	3	32	ASP	6.1
3	G	3	GLN	6.1
2	F	260	PHE	6.0
2	F	262	GLY	6.0
1	1	73	ALA	6.0
1	3	72	PRO	6.0
1	1	43	TRP	6.0
1	1	134	VAL	6.0
1	1	52	ARG	5.9
3	G	82	ASP	5.9
2	F	129	ASN	5.9
1	2	117	ALA	5.9
3	G	137	GLY	5.9
2	F	144	THR	5.9
2	F	328	ILE	5.9
3	G	120	TYR	5.8
2	F	257	LEU	5.8
4	B	1	MET	5.8
3	G	47	LEU	5.8
2	F	309	THR	5.8
2	F	207	GLU	5.7
2	F	196	GLN	5.7
2	F	9	ARG	5.7
1	3	112	GLU	5.7
1	4	99	GLU	5.6
2	F	166	LYS	5.6
3	G	166	LYS	5.6
2	F	263	ARG	5.6
2	F	59	ALA	5.5
1	1	27	LEU	5.5
1	1	116	LYS	5.5
2	F	372	GLN	5.5
2	F	193	MET	5.5
1	1	36	PHE	5.5
1	2	136	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	2	48	ARG	5.4
2	F	253	ASP	5.4
2	F	335	ARG	5.4
4	B	87	SER	5.4
2	F	379	LEU	5.4
3	G	171	LEU	5.4
3	G	134	ARG	5.4
1	4	141	ASN	5.4
3	G	105	THR	5.4
4	B	88	ALA	5.3
2	F	8	GLU	5.3
3	G	8	ARG	5.3
2	F	146	ALA	5.3
2	F	233	ARG	5.3
2	F	349	GLN	5.3
1	2	53	ARG	5.3
1	2	33	ASP	5.2
1	3	144	GLN	5.2
3	G	117	ASP	5.2
1	4	34	PHE	5.2
2	F	205	ASP	5.2
1	1	29	LEU	5.2
2	F	132	ASN	5.2
1	4	31	GLU	5.2
1	2	52	ARG	5.2
2	F	238	MET	5.2
1	3	40	ASN	5.2
2	F	150	GLU	5.2
1	1	37	LEU	5.2
4	B	104	ALA	5.2
1	1	32	ASP	5.2
2	F	249	VAL	5.1
3	G	149	ASN	5.1
1	4	9	VAL	5.1
2	F	113	ASN	5.1
2	F	201	ASN	5.1
1	2	38	THR	5.1
1	4	22	GLN	5.1
1	2	10	ARG	5.1
1	4	28	ASP	5.1
1	4	106	ASN	5.1
2	F	327	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	2	28	ASP	5.1
2	F	300	GLN	5.0
2	F	155	ASP	5.0
2	F	387	HIS	5.0
1	3	134	VAL	5.0
1	4	10	ARG	5.0
1	1	96	LEU	5.0
1	1	42	VAL	5.0
1	1	67	GLY	5.0
1	1	75	VAL	4.9
4	B	118	GLY	4.9
1	2	50	ARG	4.9
1	1	115	VAL	4.9
1	2	36	PHE	4.9
2	F	322	ASN	4.9
2	F	217	ASP	4.8
1	1	119	GLU	4.8
1	2	31	GLU	4.8
2	F	186	SER	4.8
1	2	43	TRP	4.8
1	2	27	LEU	4.8
1	4	146	LEU	4.8
1	1	26	VAL	4.8
1	1	71	PHE	4.8
1	1	53	ARG	4.8
2	F	240	SER	4.8
2	F	325	PRO	4.8
4	B	96	LYS	4.8
1	4	114	PRO	4.8
1	1	89	VAL	4.7
1	2	85	TYR	4.7
2	F	44	ASP	4.7
3	G	124	LYS	4.7
2	F	261	SER	4.7
4	B	91	TYR	4.7
1	2	113	ARG	4.7
1	2	114	PRO	4.7
2	F	420	ARG	4.7
2	F	188	THR	4.7
1	4	137	ASP	4.7
1	1	40	ASN	4.7
1	4	109	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	2	102	GLU	4.6
2	F	413	TYR	4.6
3	G	7	SER	4.6
1	1	133	ASP	4.6
1	4	70	ARG	4.6
2	F	214	ARG	4.6
1	2	55	VAL	4.6
1	2	138	ALA	4.6
2	F	278	PRO	4.5
2	F	305	LYS	4.5
2	F	282	THR	4.5
2	F	359	SER	4.5
2	F	58	LEU	4.5
1	2	40	ASN	4.5
2	F	399	LEU	4.5
2	F	358	VAL	4.5
2	F	306	GLY	4.5
1	1	91	ILE	4.5
1	1	98	MET	4.5
1	1	131	ASN	4.5
2	F	32	THR	4.4
1	3	133	ASP	4.4
2	F	415	ASN	4.4
1	2	56	GLU	4.4
1	2	96	LEU	4.4
3	G	11	SER	4.4
3	G	64	THR	4.4
1	1	85	TYR	4.4
2	F	252	THR	4.4
3	G	55	GLY	4.4
3	G	87	PHE	4.3
3	G	111	PRO	4.3
3	G	133	PRO	4.3
2	F	228	TYR	4.3
1	1	118	ALA	4.3
1	1	108	ILE	4.2
2	F	244	ALA	4.2
3	G	135	THR	4.2
1	3	28	ASP	4.2
2	F	55	ARG	4.1
3	G	32	LEU	4.1
1	4	132	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	3	67	GLY	4.1
3	G	58	HIS	4.1
1	3	24	SER	4.1
2	F	382	ARG	4.1
2	F	239	ARG	4.1
1	1	35	ASP	4.1
1	3	22	GLN	4.1
3	G	68	ALA	4.0
1	2	35	ASP	4.0
4	B	113	GLU	4.0
2	F	90	ASN	4.0
3	G	146	VAL	4.0
2	F	92	THR	4.0
1	2	47	ASP	4.0
1	2	112	GLU	4.0
1	3	15	LEU	4.0
3	G	53	ASN	4.0
3	G	49	VAL	3.9
2	F	409	ASN	3.9
1	3	27	LEU	3.9
2	F	269	LYS	3.9
3	G	81	PHE	3.9
2	F	384	LEU	3.9
1	4	33	ASP	3.9
1	4	147	ARG	3.9
1	1	60	TYR	3.8
3	G	43	TYR	3.8
2	F	182	GLN	3.8
3	G	139	ASN	3.8
2	F	419	THR	3.8
2	F	13	ASP	3.8
1	1	38	THR	3.8
3	G	119	GLY	3.8
2	F	247	TYR	3.8
2	F	151	LEU	3.8
4	B	82	THR	3.8
3	G	110	TYR	3.8
3	G	2	PHE	3.8
1	1	130	GLY	3.8
1	4	110	GLY	3.8
2	F	51	LEU	3.7
1	1	128	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	74	ARG	3.7
1	4	63	LEU	3.7
1	3	47	ASP	3.7
2	F	68	THR	3.7
1	2	66	VAL	3.7
1	4	35	ASP	3.7
1	4	23	ALA	3.6
4	B	94	PHE	3.6
2	F	242	LEU	3.6
1	2	23	ALA	3.6
2	F	15	SER	3.6
1	3	18	ILE	3.6
1	4	14	ALA	3.6
1	4	118	ALA	3.6
2	F	200	ALA	3.6
2	F	104	ASP	3.6
2	F	149	ASN	3.5
1	3	29	LEU	3.5
1	4	151	VAL	3.5
2	F	177	THR	3.5
1	3	45	ALA	3.5
1	1	86	VAL	3.5
2	F	136	LYS	3.5
1	1	143	ARG	3.5
2	F	164	HIS	3.5
3	G	15	SER	3.5
3	G	52	GLY	3.5
1	1	141	ASN	3.5
2	F	93	PRO	3.5
4	B	85	ASP	3.4
1	1	83	ALA	3.4
3	G	59	CYS	3.4
1	1	68	TYR	3.4
1	1	31	GLU	3.4
1	4	32	ASP	3.4
1	4	75	VAL	3.4
3	G	109	VAL	3.4
2	F	360	PRO	3.4
1	4	140	GLU	3.4
1	2	32	ASP	3.4
1	2	121	PHE	3.4
3	G	118	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	162	CYS	3.3
1	1	59	VAL	3.3
1	4	76	GLU	3.3
2	F	418	THR	3.3
4	B	3	GLN	3.3
2	F	243	TRP	3.3
1	2	134	VAL	3.3
1	1	135	LEU	3.3
4	B	102	GLN	3.3
1	4	117	ALA	3.3
2	F	295	ALA	3.3
2	F	203	HIS	3.3
1	2	51	ALA	3.3
2	F	371	ILE	3.3
4	B	100	ARG	3.2
3	G	1	MET	3.2
2	F	332	ASP	3.2
1	4	51	ALA	3.2
1	2	54	CYS	3.2
2	F	220	SER	3.2
2	F	96	THR	3.1
1	4	112	GLU	3.1
4	B	110	HIS	3.1
1	3	7	GLN	3.1
3	G	31	VAL	3.1
2	F	204	THR	3.1
3	G	42	LEU	3.1
3	G	40	SER	3.1
1	1	11	PHE	3.1
2	F	374	PRO	3.1
1	4	62	THR	3.1
1	1	139	GLU	3.1
1	4	102	GLU	3.1
2	F	184	THR	3.1
3	G	79	ILE	3.0
1	2	119	GLU	3.0
1	2	133	ASP	3.0
1	1	144	GLN	3.0
2	F	49	LEU	3.0
3	G	170	CYS	3.0
2	F	298	GLU	3.0
1	2	21	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	3	48	ARG	3.0
3	G	115	ARG	3.0
2	F	337	GLY	3.0
1	2	42	VAL	3.0
3	G	22	SER	3.0
2	F	229	ASP	3.0
3	G	138	ASN	2.9
1	4	88	PRO	2.9
2	F	227	SER	2.9
1	3	68	TYR	2.9
3	G	44	PHE	2.9
2	F	137	ALA	2.9
3	G	158	LEU	2.9
2	F	273	PRO	2.9
1	1	18	ILE	2.9
2	F	211	PHE	2.9
1	3	6	GLU	2.9
2	F	173	LEU	2.9
3	G	13	PHE	2.9
1	4	149	GLU	2.9
1	2	111	VAL	2.8
2	F	354	ALA	2.8
2	F	206	GLN	2.8
2	F	208	ARG	2.8
1	1	74	PRO	2.8
1	4	7	GLN	2.8
2	F	163	CYS	2.8
3	G	100	PRO	2.8
3	G	116	HIS	2.8
2	F	139	TRP	2.8
2	F	158	TYR	2.8
1	3	122	ALA	2.8
1	2	88	PRO	2.8
1	3	131	ASN	2.8
1	1	87	HIS	2.7
2	F	393	CYS	2.7
2	F	362	TYR	2.7
1	3	128	ARG	2.7
2	F	143	ARG	2.7
2	F	140	MET	2.7
1	3	130	GLY	2.7
3	G	106	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	98	ASN	2.7
2	F	10	MET	2.7
1	1	7	GLN	2.7
3	G	156	ARG	2.7
4	B	103	PRO	2.7
1	1	127	VAL	2.7
2	F	106	ALA	2.7
4	B	86	LYS	2.7
2	F	212	MET	2.7
3	G	27	SER	2.7
2	F	390	TYR	2.6
2	F	83	LYS	2.6
2	F	283	MET	2.6
2	F	47	GLY	2.6
3	G	157	GLY	2.6
2	F	65	ASP	2.6
1	2	65	PHE	2.6
1	2	24	SER	2.6
2	F	299	ILE	2.6
3	G	103	LEU	2.6
4	B	90	ILE	2.6
2	F	324	PRO	2.6
2	F	237	VAL	2.6
2	F	396	SER	2.5
3	G	37	ALA	2.5
3	G	121	TYR	2.5
1	1	147	ARG	2.5
4	B	111	ASP	2.5
1	3	139	GLU	2.5
3	G	76	GLY	2.5
1	3	10	ARG	2.5
3	G	66	VAL	2.5
2	F	50	ARG	2.5
3	G	174	LEU	2.5
2	F	303	ASN	2.4
1	4	37	LEU	2.4
1	2	30	THR	2.4
3	G	75	VAL	2.4
4	B	83	CYS	2.4
1	1	44	ILE	2.4
1	2	68	TYR	2.4
1	4	24	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	331	LYS	2.4
3	G	46	SER	2.4
4	B	98	ASP	2.4
2	F	25	GLY	2.4
2	F	133	ASN	2.4
2	F	14	LEU	2.4
1	2	25	ALA	2.4
2	F	175	PRO	2.3
2	F	385	ILE	2.3
3	G	57	LEU	2.3
1	1	46	THR	2.3
4	B	84	ASP	2.3
2	F	235	LEU	2.3
2	F	147	ASN	2.3
2	F	407	LYS	2.3
3	G	126	CYS	2.3
3	G	150	PHE	2.3
1	4	66	VAL	2.3
2	F	255	THR	2.3
2	F	35	VAL	2.3
2	F	95	PRO	2.3
1	2	60	TYR	2.3
2	F	210	TYR	2.3
3	G	72	VAL	2.3
1	1	93	THR	2.2
1	2	62	THR	2.2
1	2	63	LEU	2.2
1	4	97	ILE	2.2
1	2	95	CYS	2.2
1	1	97	ILE	2.2
1	4	82	ILE	2.2
1	4	131	ASN	2.2
1	2	122	ALA	2.2
1	2	129	ALA	2.2
1	4	83	ALA	2.2
1	2	19	LYS	2.2
2	F	37	ALA	2.2
2	F	296	THR	2.2
1	1	64	ASP	2.1
1	3	53	ARG	2.1
3	G	145	MET	2.1
1	2	73	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	163	GLN	2.1
1	2	26	VAL	2.1
2	F	57	GLY	2.1
2	F	222	PHE	2.1
1	4	50	ARG	2.1
2	F	48	ALA	2.1
3	G	28	SER	2.1
3	G	71	GLN	2.1
1	4	142	VAL	2.1
2	F	134	TYR	2.0
3	G	91	LEU	2.0
2	F	26	ARG	2.0
3	G	25	PRO	2.0
1	3	23	ALA	2.0
1	4	60	TYR	2.0
1	2	101	ALA	2.0
1	2	137	ASP	2.0
1	2	59	VAL	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.