



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:30 PM UTC

PDB ID : 4YVW / pdb_00004yvw
Title : crystal structure of an enterovirus 71/coxsackievirus A16 chimeric virus-like particle
Authors : Chen, R.; Lyu, K.
Deposited on : 2015-03-20
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

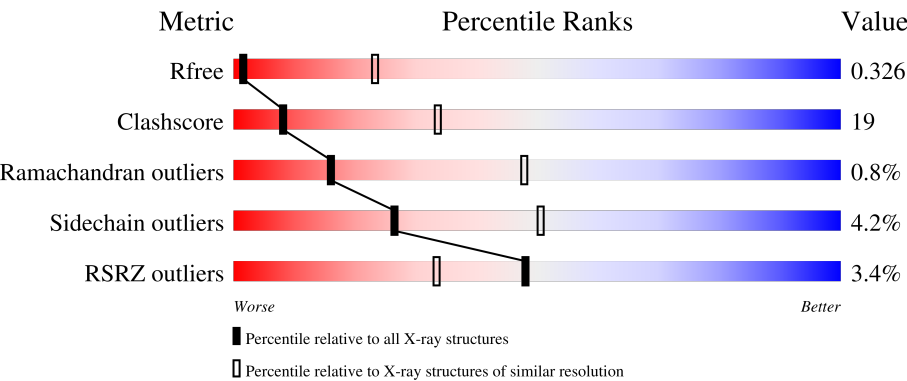
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	297	
1	D	297	
1	E	297	
1	J	297	
1	M	297	

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Mol	Chain	Length	Quality of chain
2	B	242	
2	F	242	
2	H	242	
2	K	242	
2	N	242	
3	C	323	
3	G	323	
3	I	323	
3	L	323	
3	O	323	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26525 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	225	Total	C	N	O	S	0	0	0
			1773	1134	299	329	11			
1	A	225	Total	C	N	O	S	0	0	0
			1773	1134	299	329	11			
1	D	225	Total	C	N	O	S	0	0	0
			1773	1134	299	329	11			
1	J	225	Total	C	N	O	S	0	0	0
			1773	1134	299	329	11			
1	M	225	Total	C	N	O	S	0	0	0
			1773	1134	299	329	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	215	LEU	LYS	engineered mutation	UNP F6KTB0
E	217	ALA	GLU	engineered mutation	UNP F6KTB0
E	218	ASN	LYS	engineered mutation	UNP F6KTB0
E	221	ASP	GLU	engineered mutation	UNP F6KTB0
A	215	LEU	LYS	engineered mutation	UNP F6KTB0
A	217	ALA	GLU	engineered mutation	UNP F6KTB0
A	218	ASN	LYS	engineered mutation	UNP F6KTB0
A	221	ASP	GLU	engineered mutation	UNP F6KTB0
D	215	LEU	LYS	engineered mutation	UNP F6KTB0
D	217	ALA	GLU	engineered mutation	UNP F6KTB0
D	218	ASN	LYS	engineered mutation	UNP F6KTB0
D	221	ASP	GLU	engineered mutation	UNP F6KTB0
J	215	LEU	LYS	engineered mutation	UNP F6KTB0
J	217	ALA	GLU	engineered mutation	UNP F6KTB0
J	218	ASN	LYS	engineered mutation	UNP F6KTB0
J	221	ASP	GLU	engineered mutation	UNP F6KTB0
M	215	LEU	LYS	engineered mutation	UNP F6KTB0
M	217	ALA	GLU	engineered mutation	UNP F6KTB0
M	218	ASN	LYS	engineered mutation	UNP F6KTB0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	221	ASP	GLU	engineered mutation	UNP F6KTB0

- Molecule 2 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	224	Total	C	N	O	S	0	0	0
			1712	1103	281	317	11			
2	B	224	Total	C	N	O	S	0	0	0
			1712	1103	281	317	11			
2	H	224	Total	C	N	O	S	0	0	0
			1712	1103	281	317	11			
2	K	224	Total	C	N	O	S	0	0	0
			1712	1103	281	317	11			
2	N	224	Total	C	N	O	S	0	0	0
			1712	1103	281	317	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	227	GLN	LYS	engineered mutation	UNP F6KTB0
B	227	GLN	LYS	engineered mutation	UNP F6KTB0
H	227	GLN	LYS	engineered mutation	UNP F6KTB0
K	227	GLN	LYS	engineered mutation	UNP F6KTB0
N	227	GLN	LYS	engineered mutation	UNP F6KTB0

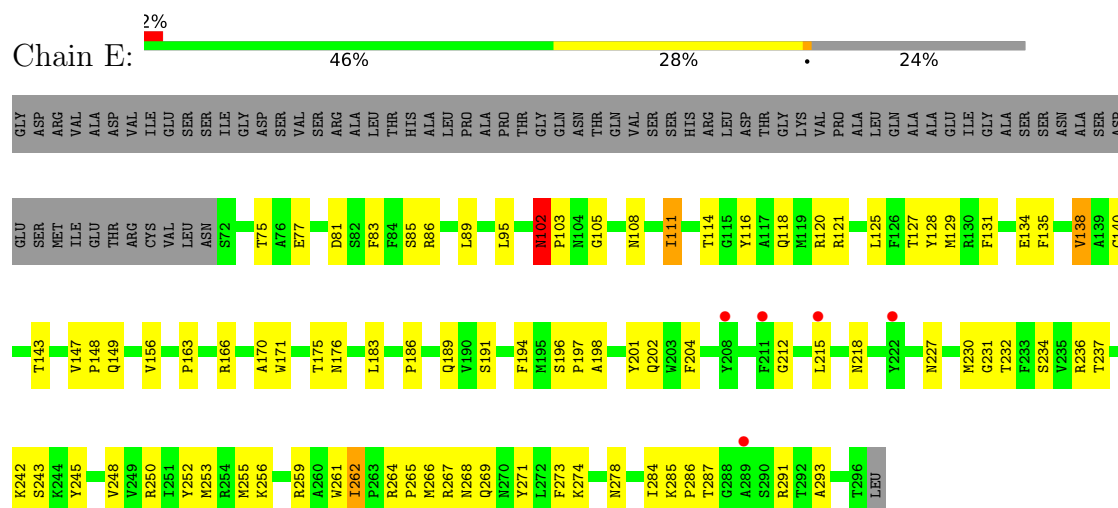
- Molecule 3 is a protein called Capsid protein VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	235	Total	C	N	O	S	0	0	0
			1820	1170	299	343	8			
3	C	235	Total	C	N	O	S	0	0	0
			1820	1170	299	343	8			
3	I	235	Total	C	N	O	S	0	0	0
			1820	1170	299	343	8			
3	L	235	Total	C	N	O	S	0	0	0
			1820	1170	299	343	8			
3	O	235	Total	C	N	O	S	0	0	0
			1820	1170	299	343	8			

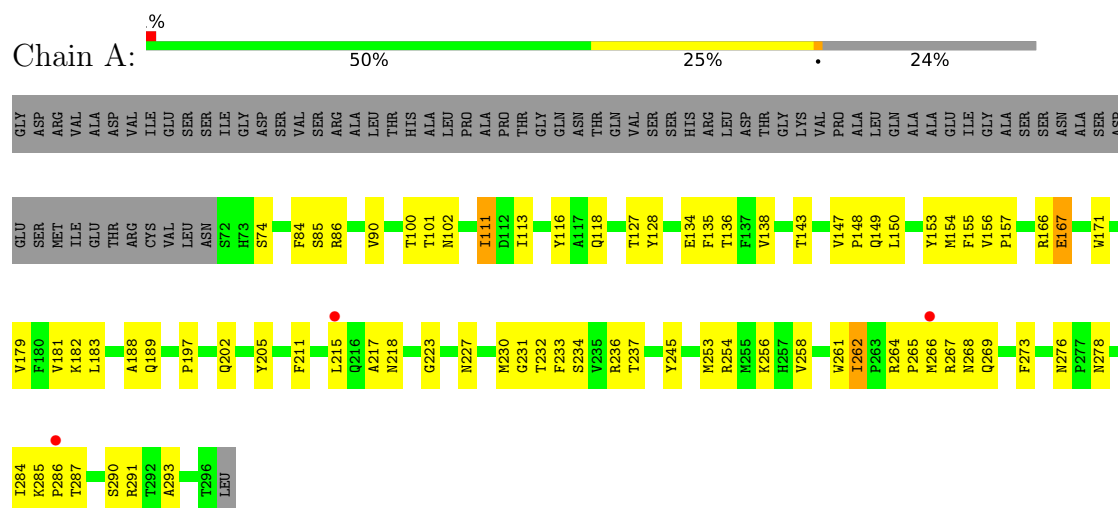
3 Residue-property plots [i](#)

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.

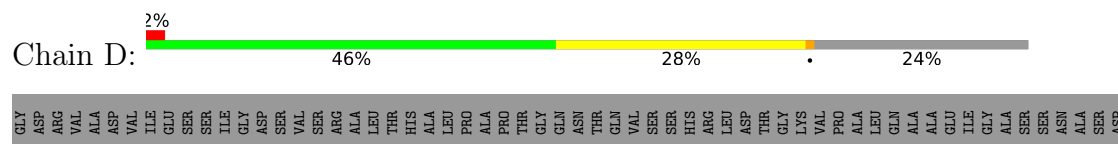
• Molecule 1: Capsid protein VP1

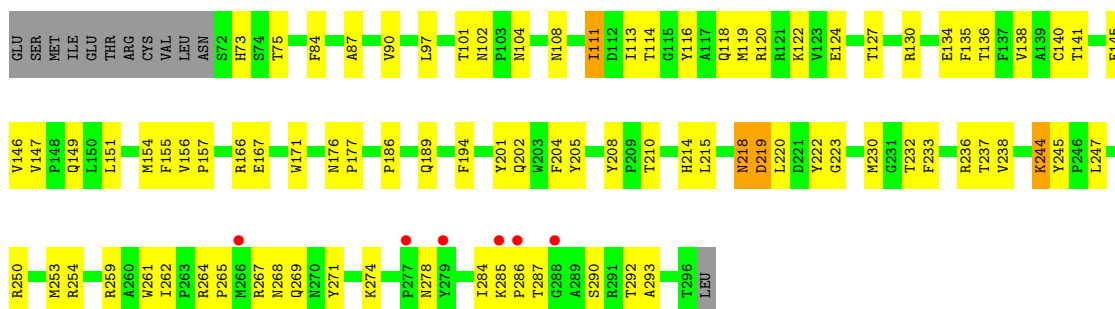


• Molecule 1: Capsid protein VP1

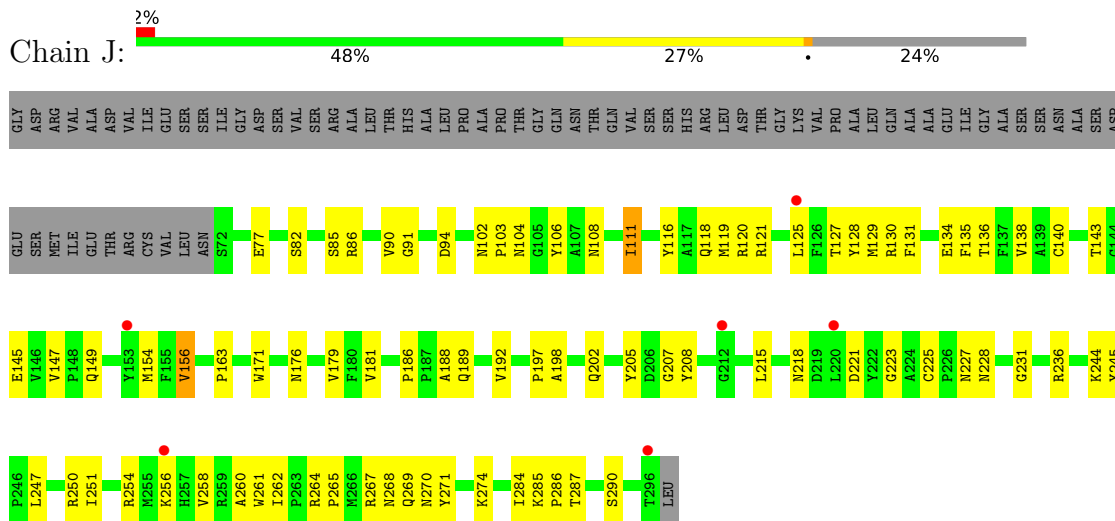


• Molecule 1: Capsid protein VP1

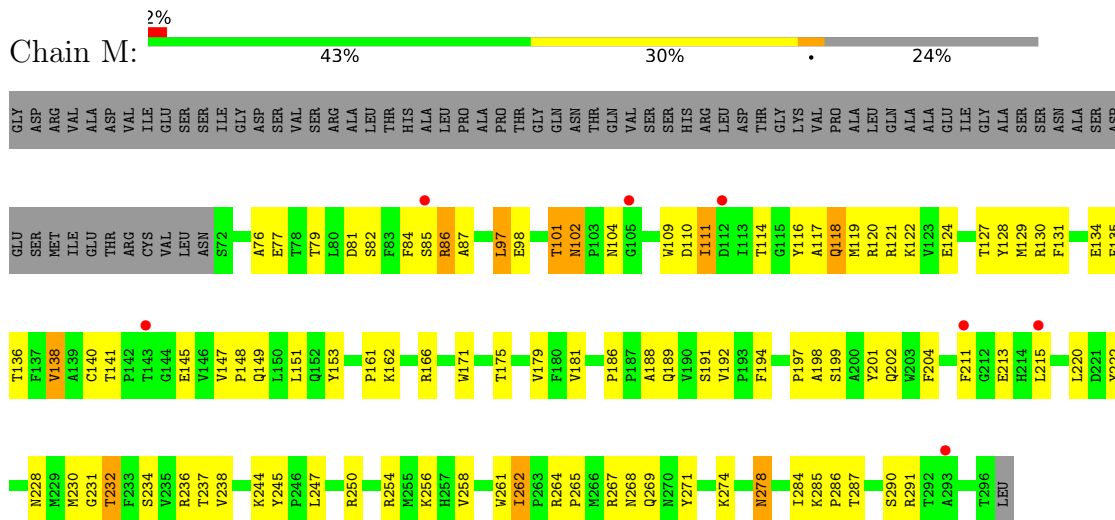




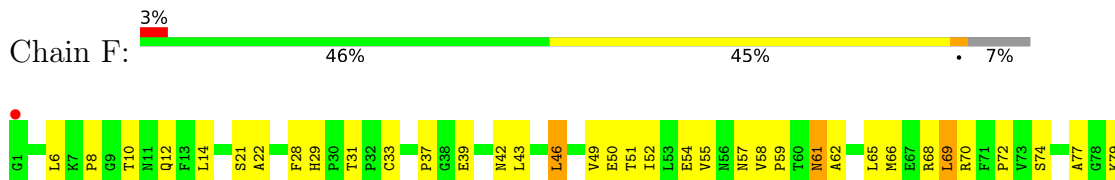
• Molecule 1: Capsid protein VP1

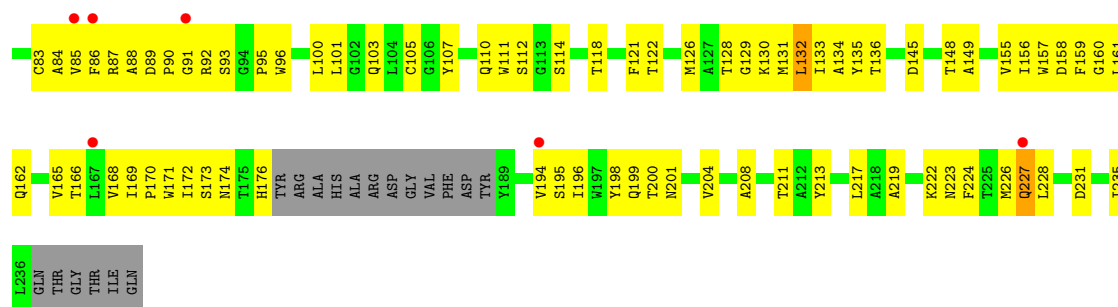


• Molecule 1: Capsid protein VP1

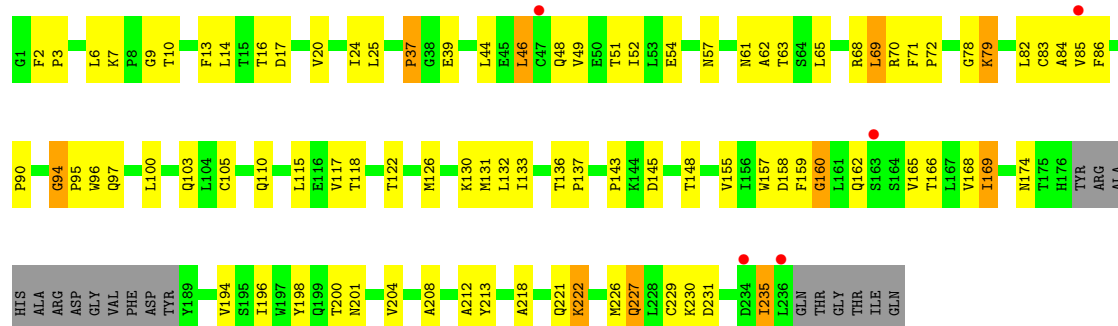


• Molecule 2: Capsid protein VP3

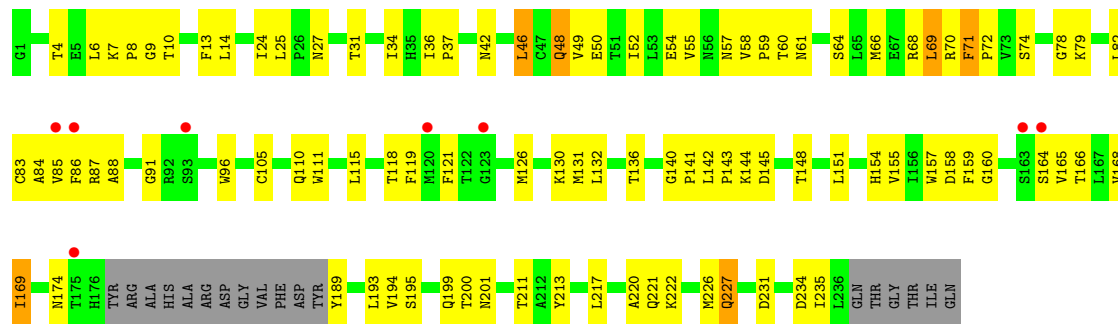




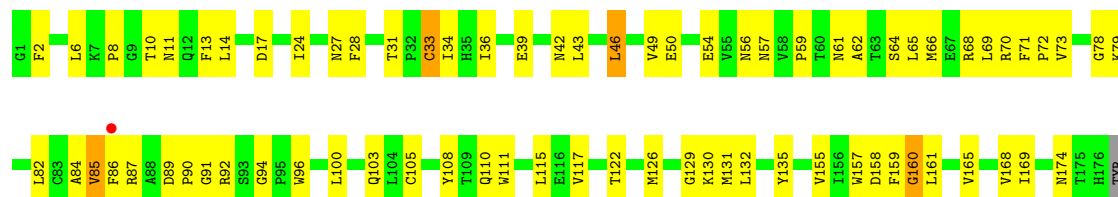
• Molecule 2: Capsid protein VP3

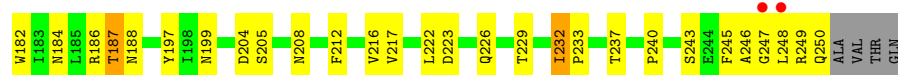


• Molecule 2: Capsid protein VP3

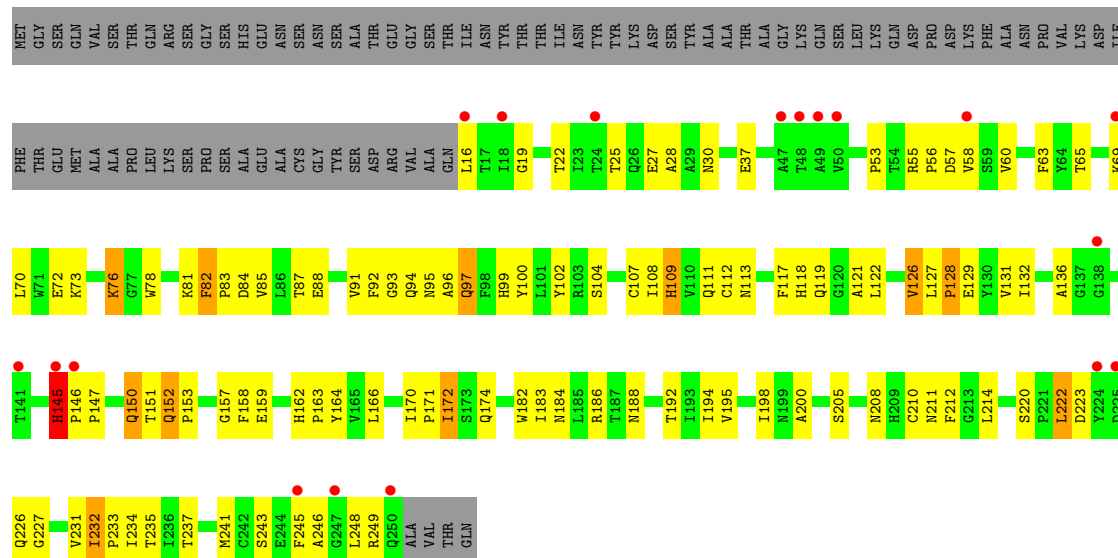


• Molecule 2: Capsid protein VP3

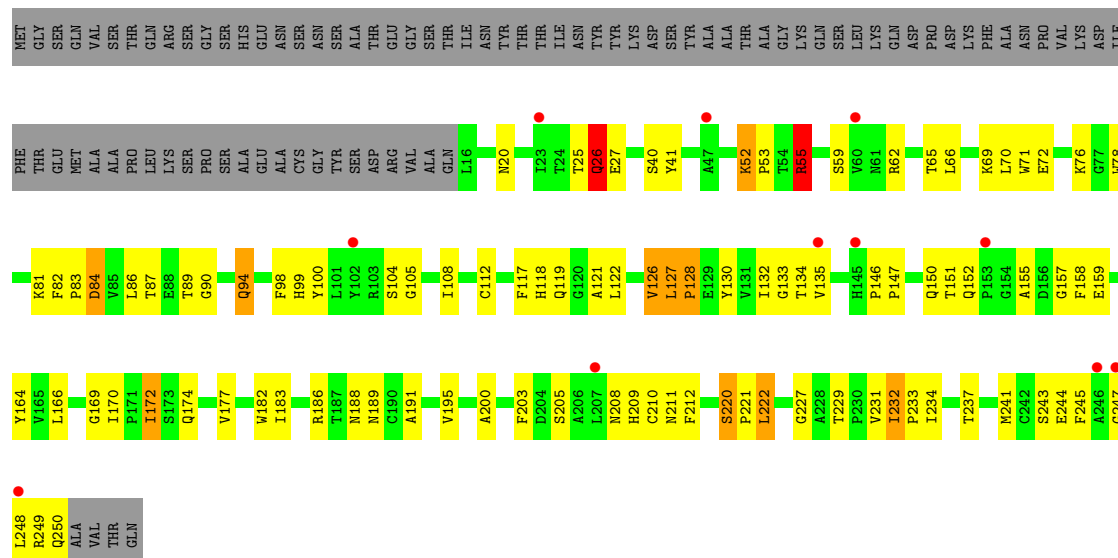




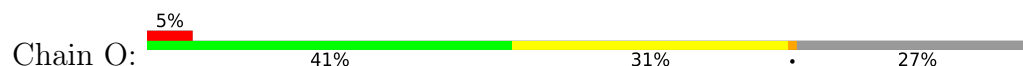
• Molecule 3: Capsid protein VP0

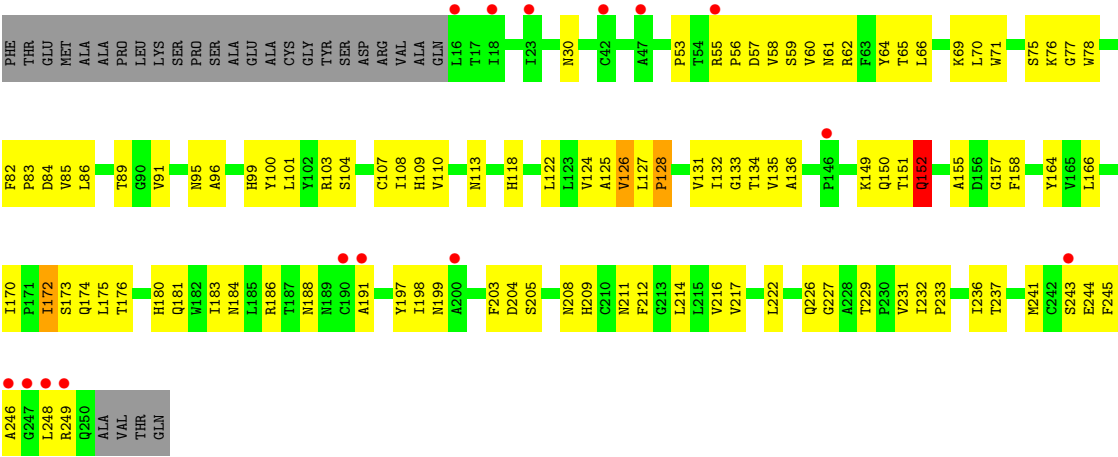


• Molecule 3: Capsid protein VP0



• Molecule 3: Capsid protein VP0





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 3 2	Depositor
Cell constants a, b, c, α , β , γ	349.15Å 349.15Å 349.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.96 – 3.80 47.96 – 3.80	Depositor EDS
% Data completeness (in resolution range)	78.7 (47.96-3.80) 61.3 (47.96-3.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.286 , 0.324 0.289 , 0.326	Depositor DCC
R_{free} test set	2000 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å ²)	94.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	26525	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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	0.39	0/1828	0.90	3/2495 (0.1%)
1	D	0.36	0/1828	0.89	2/2495 (0.1%)
1	E	0.34	0/1828	0.94	7/2495 (0.3%)
1	J	0.34	0/1828	0.87	3/2495 (0.1%)
1	M	0.36	0/1828	0.90	5/2495 (0.2%)
2	B	0.35	0/1759	0.93	8/2408 (0.3%)
2	F	0.35	0/1759	0.94	5/2408 (0.2%)
2	H	0.35	0/1759	0.94	8/2408 (0.3%)
2	K	0.34	0/1759	0.92	2/2408 (0.1%)
2	N	0.35	0/1759	0.90	8/2408 (0.3%)
3	C	0.34	0/1875	1.00	10/2573 (0.4%)
3	G	0.36	0/1875	0.94	9/2573 (0.3%)
3	I	0.39	0/1875	0.99	15/2573 (0.6%)
3	L	0.37	0/1875	1.02	19/2573 (0.7%)
3	O	0.38	0/1875	0.95	5/2573 (0.2%)
All	All	0.36	0/27310	0.94	109/37380 (0.3%)

There are no bond length outliers.

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	220	LEU	N-CA-C	-8.63	102.51	113.72
2	F	169	ILE	CA-C-N	8.53	127.84	118.97
2	F	169	ILE	C-N-CA	8.53	127.84	118.97
3	C	88	GLU	N-CA-C	-7.97	104.01	112.93
3	C	232	ILE	CA-C-N	7.75	128.04	119.90
3	C	232	ILE	C-N-CA	7.75	128.04	119.90
2	B	169	ILE	CA-C-N	7.65	126.92	118.97
2	B	169	ILE	C-N-CA	7.65	126.92	118.97
3	G	88	GLU	N-CA-C	-7.51	104.15	112.72
1	E	102	ASN	CA-C-N	7.39	129.07	119.84
1	E	102	ASN	C-N-CA	7.39	129.07	119.84
3	I	162	HIS	CA-C-N	7.34	127.35	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	162	HIS	C-N-CA	7.34	127.35	119.28
3	I	232	ILE	CA-C-N	7.22	127.48	119.90
3	I	232	ILE	C-N-CA	7.22	127.48	119.90
2	K	160	GLY	N-CA-C	-7.04	103.76	112.77
3	O	152	GLN	CA-C-N	-6.99	112.56	119.90
3	O	152	GLN	C-N-CA	-6.99	112.56	119.90
3	L	84	ASP	N-CA-C	6.93	118.63	111.14
3	L	55	ARG	CA-C-N	6.88	126.84	120.03
3	L	55	ARG	C-N-CA	6.88	126.84	120.03
2	H	71	PHE	CA-C-N	6.83	127.00	120.31
2	H	71	PHE	C-N-CA	6.83	127.00	120.31
2	B	160	GLY	N-CA-C	-6.64	104.46	112.49
1	E	212	GLY	N-CA-C	-6.58	104.37	112.33
1	J	156	VAL	CA-C-N	6.52	127.09	120.38
1	J	156	VAL	C-N-CA	6.52	127.09	120.38
3	L	26	GLN	N-CA-C	-6.45	105.28	113.02
1	D	111	ILE	N-CA-C	6.37	113.03	106.21
2	H	169	ILE	CA-C-N	6.37	127.80	119.84
2	H	169	ILE	C-N-CA	6.37	127.80	119.84
1	E	111	ILE	N-CA-C	6.34	113.00	106.21
1	A	111	ILE	N-CA-C	6.32	112.98	106.21
3	I	152	GLN	CA-C-N	-6.31	113.00	120.13
3	I	152	GLN	C-N-CA	-6.31	113.00	120.13
2	H	199	GLN	N-CA-C	-6.27	104.52	111.36
2	B	9	GLY	N-CA-C	-6.24	106.81	114.92
3	I	19	GLY	N-CA-C	6.17	118.76	110.43
3	I	57	ASP	N-CA-C	6.14	120.50	112.89
2	N	169	ILE	CA-C-N	6.13	127.50	119.84
2	N	169	ILE	C-N-CA	6.13	127.50	119.84
3	C	151	THR	N-CA-C	-6.11	101.73	110.59
2	F	199	GLN	N-CA-C	-6.09	104.73	111.36
3	I	88	GLU	N-CA-C	-6.07	106.13	112.93
1	M	111	ILE	N-CA-C	6.06	112.70	106.21
3	C	132	ILE	N-CA-C	6.04	117.29	111.91
3	L	146	PRO	CA-C-N	-6.00	113.51	119.99
3	L	146	PRO	C-N-CA	-6.00	113.51	119.99
2	B	71	PHE	CA-C-N	6.00	126.19	120.31
2	B	71	PHE	C-N-CA	6.00	126.19	120.31
2	F	29	HIS	CA-C-N	5.95	125.92	120.03
2	F	29	HIS	C-N-CA	5.95	125.92	120.03
3	L	59	SER	N-CA-C	5.86	118.17	111.02
3	O	227	GLY	N-CA-C	-5.86	107.23	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	116	LYS	N-CA-C	-5.85	106.19	113.15
3	L	220	SER	CA-C-N	5.81	127.11	119.84
3	L	220	SER	C-N-CA	5.81	127.11	119.84
3	G	232	ILE	CA-C-N	5.80	127.36	120.23
3	G	232	ILE	C-N-CA	5.80	127.36	120.23
2	N	160	GLY	N-CA-C	-5.79	105.36	112.77
1	E	262	ILE	CA-C-N	5.78	125.54	119.76
1	E	262	ILE	C-N-CA	5.78	125.54	119.76
3	G	150	GLN	N-CA-C	-5.76	104.91	111.07
3	L	52	LYS	CA-C-N	5.75	125.68	119.76
3	L	52	LYS	C-N-CA	5.75	125.68	119.76
1	M	228	ASN	N-CA-C	-5.74	106.32	113.38
3	L	229	THR	CA-C-N	5.72	126.22	120.04
3	L	229	THR	C-N-CA	5.72	126.22	120.04
1	M	262	ILE	CA-C-N	5.72	125.48	119.76
1	M	262	ILE	C-N-CA	5.72	125.48	119.76
3	I	109	HIS	CA-C-N	-5.71	115.24	122.37
3	I	109	HIS	C-N-CA	-5.71	115.24	122.37
2	N	106	GLY	N-CA-C	-5.69	107.27	114.16
2	N	136	THR	CA-C-N	5.66	126.21	120.38
2	N	136	THR	C-N-CA	5.66	126.21	120.38
1	A	262	ILE	CA-C-N	5.65	125.41	119.76
1	A	262	ILE	C-N-CA	5.65	125.41	119.76
2	H	9	GLY	N-CA-C	-5.57	107.68	114.92
1	D	244	LYS	N-CA-C	-5.56	106.62	113.41
3	L	227	GLY	N-CA-C	-5.52	107.49	115.27
3	C	45	SER	N-CA-C	-5.44	103.52	111.30
3	G	57	ASP	N-CA-C	5.41	119.73	113.18
3	C	93	GLY	N-CA-C	-5.40	106.14	113.37
1	E	186	PRO	O-C-N	5.35	123.77	121.31
3	C	229	THR	CA-C-N	5.32	125.79	120.04
3	C	229	THR	C-N-CA	5.32	125.79	120.04
3	G	227	GLY	N-CA-C	-5.32	107.98	115.32
3	I	82	PHE	CA-C-N	-5.32	113.15	119.05
3	I	82	PHE	C-N-CA	-5.32	113.15	119.05
3	L	232	ILE	N-CA-C	5.31	113.78	107.73
3	L	232	ILE	CA-C-N	5.25	126.69	120.23
3	L	232	ILE	C-N-CA	5.25	126.69	120.23
2	H	142	LEU	CA-C-N	5.25	125.50	119.83
2	H	142	LEU	C-N-CA	5.25	125.50	119.83
1	J	111	ILE	N-CA-C	5.24	111.82	106.21
3	I	227	GLY	N-CA-C	-5.21	108.13	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	229	THR	CA-C-N	5.21	125.67	120.04
3	O	229	THR	C-N-CA	5.21	125.67	120.04
3	C	217	VAL	N-CA-C	5.20	113.56	107.89
2	K	204	VAL	N-CA-C	5.16	113.42	109.19
3	I	58	VAL	N-CA-C	5.08	118.08	113.20
3	L	127	LEU	CA-C-N	5.08	126.19	119.84
3	L	127	LEU	C-N-CA	5.08	126.19	119.84
3	G	82	PHE	CA-C-N	-5.05	113.73	119.28
3	G	82	PHE	C-N-CA	-5.05	113.73	119.28
2	N	71	PHE	CA-C-N	5.04	125.25	120.31
2	N	71	PHE	C-N-CA	5.04	125.25	120.31
2	B	94	GLY	CA-C-N	5.02	124.80	119.28
2	B	94	GLY	C-N-CA	5.02	124.80	119.28

There are no chirality outliers.

There are no planarity outliers.

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	1773	0	1712	72	0
1	D	1773	0	1712	82	0
1	E	1773	0	1712	85	0
1	J	1773	0	1712	84	0
1	M	1773	0	1712	94	0
2	B	1712	0	1699	71	0
2	F	1712	0	1699	93	0
2	H	1712	0	1699	79	2
2	K	1712	0	1699	67	0
2	N	1712	0	1699	75	0
3	C	1820	0	1758	67	0
3	G	1820	0	1758	82	0
3	I	1820	0	1758	95	1
3	L	1820	0	1758	83	0
3	O	1820	0	1758	94	0
All	All	26525	0	25845	1014	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1014) 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:M:189:GLN:HE21	2:N:21:SER:HB3	1.28	0.95
3:L:26:GLN:HE21	3:L:26:GLN:HA	1.33	0.93
1:J:262:ILE:HG21	3:L:128:PRO:HG2	1.52	0.90
3:G:132:ILE:HG12	3:G:150:GLN:HE21	1.40	0.87
1:E:262:ILE:HG21	3:G:128:PRO:HG2	1.57	0.87
3:I:248:LEU:HD23	3:I:249:ARG:H	1.40	0.86
3:I:147:PRO:HG2	3:I:150:GLN:HB2	1.58	0.86
3:G:248:LEU:HD23	3:G:249:ARG:H	1.42	0.85
3:G:83:PRO:HG2	3:G:211:ASN:H	1.42	0.85
3:I:182:TRP:O	3:I:188:ASN:ND2	2.10	0.84
1:A:262:ILE:HG21	3:C:128:PRO:HG2	1.59	0.84
1:D:262:ILE:HG21	3:I:128:PRO:HG2	1.59	0.84
1:D:285:LYS:NZ	3:I:164:TYR:OH	2.11	0.83
1:A:269:GLN:HE22	1:A:284:ILE:HB	1.42	0.83
1:M:166:ARG:NH2	1:M:237:THR:O	2.12	0.82
1:A:287:THR:O	2:B:68:ARG:NH1	2.12	0.82
2:N:159:PHE:O	3:O:186:ARG:NH2	2.13	0.81
1:A:166:ARG:NH2	1:A:237:THR:O	2.14	0.81
3:L:53:PRO:HB3	3:L:55:ARG:HH21	1.46	0.80
1:A:217:ALA:O	1:A:218:ASN:ND2	2.11	0.80
3:C:86:LEU:HA	3:C:89:THR:HB	1.64	0.80
1:D:166:ARG:NH2	1:D:237:THR:O	2.15	0.79
1:M:262:ILE:HG21	3:O:128:PRO:HG2	1.65	0.79
1:J:108:ASN:HD21	1:J:163:PRO:HG2	1.47	0.79
3:I:53:PRO:HA	3:I:246:ALA:HB2	1.65	0.79
2:H:159:PHE:O	3:I:186:ARG:NH2	2.16	0.79
3:I:55:ARG:NH2	3:I:60:VAL:H	1.82	0.78
1:M:161:PRO:HD2	2:B:230:LYS:HZ1	1.49	0.78
3:L:166:LEU:HD11	3:L:172:ILE:HG23	1.65	0.78
3:L:147:PRO:HG2	3:L:150:GLN:HB2	1.64	0.77
1:E:103:PRO:O	1:E:242:LYS:NZ	2.18	0.77
2:B:14:LEU:HB3	2:B:17:ASP:HB2	1.67	0.77
1:A:118:GLN:NE2	2:B:231:ASP:HB3	1.99	0.77
1:J:202:GLN:O	1:J:228:ASN:ND2	2.18	0.76
3:L:26:GLN:HA	3:L:26:GLN:NE2	1.96	0.76
3:C:53:PRO:HA	3:C:246:ALA:HB2	1.66	0.76
3:G:69:LYS:HZ1	3:G:78:TRP:CG	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:LYS:HE3	1:M:287:THR:H	1.49	0.76
3:C:166:LEU:HD11	3:C:172:ILE:HG23	1.67	0.76
3:L:55:ARG:HH12	3:L:245:PHE:H	1.35	0.75
1:M:287:THR:O	2:N:68:ARG:NH1	2.20	0.74
2:F:87:ARG:HH12	2:F:93:SER:C	1.95	0.74
3:G:86:LEU:HA	3:G:89:THR:HB	1.69	0.74
3:G:249:ARG:NH2	2:N:135:TYR:O	2.20	0.74
1:J:181:VAL:HG11	1:J:188:ALA:HB2	1.68	0.74
3:G:166:LEU:HD11	3:G:172:ILE:HG23	1.69	0.74
1:M:285:LYS:NZ	3:O:164:TYR:OH	2.19	0.74
1:D:265:PRO:HB3	3:I:174:GLN:HB2	1.68	0.73
1:M:254:ARG:NH1	2:N:17:ASP:O	2.22	0.73
3:I:55:ARG:NH1	3:I:56:PRO:O	2.22	0.73
3:I:109:HIS:CD2	3:I:192:THR:OG1	2.42	0.72
1:D:290:SER:OG	2:H:57:ASN:O	2.07	0.72
1:J:269:GLN:HE22	1:J:284:ILE:H	1.35	0.72
2:K:87:ARG:NH1	2:K:189:TYR:O	2.22	0.72
2:H:158:ASP:OD1	2:H:160:GLY:N	2.23	0.72
2:F:110:GLN:O	2:F:227:GLN:HB2	1.89	0.72
2:B:159:PHE:HB3	3:C:186:ARG:HH21	1.55	0.72
3:L:203:PHE:HE2	3:L:244:GLU:HG2	1.52	0.71
2:F:87:ARG:HG3	2:F:89:ASP:H	1.54	0.71
1:D:287:THR:O	2:H:68:ARG:NH1	2.24	0.71
1:E:166:ARG:NH2	1:E:237:THR:O	2.24	0.71
2:H:126:MET:HG3	3:I:117:PHE:HE1	1.56	0.71
3:L:83:PRO:HG2	3:L:211:ASN:H	1.56	0.71
1:A:267:ARG:NH2	1:A:278:ASN:O	2.25	0.70
1:M:140:CYS:SG	1:M:250:ARG:NH1	2.64	0.70
3:I:60:VAL:HG13	3:I:91:VAL:HG13	1.74	0.70
3:G:126:VAL:HG13	3:G:212:PHE:HE1	1.56	0.70
3:O:69:LYS:HZ1	3:O:78:TRP:CG	2.10	0.70
1:M:111:ILE:HD13	1:M:230:MET:HG3	1.74	0.70
2:B:110:GLN:O	2:B:227:GLN:HB2	1.92	0.70
1:A:217:ALA:C	1:A:218:ASN:HD22	1.98	0.69
1:D:75:THR:HB	2:H:42:ASN:HD21	1.55	0.69
3:G:55:ARG:NH2	3:G:61:ASN:OD1	2.24	0.69
2:H:132:LEU:HD11	2:H:154:HIS:HB2	1.75	0.69
3:L:84:ASP:CG	3:L:152:GLN:HA	2.18	0.69
1:A:171:TRP:CD2	1:A:236:ARG:HD2	2.28	0.69
3:G:162:HIS:N	3:G:167:ASP:OD1	2.22	0.69
1:J:287:THR:O	2:K:68:ARG:NH1	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:ASP:N	1:D:219:ASP:OD1	2.25	0.69
2:N:159:PHE:HB3	3:O:186:ARG:HH21	1.58	0.69
3:O:104:SER:HB2	3:O:243:SER:HA	1.75	0.68
1:E:265:PRO:HB3	3:G:174:GLN:HB2	1.75	0.68
3:L:81:LYS:HE2	3:L:130:TYR:HB3	1.74	0.68
3:L:182:TRP:O	3:L:188:ASN:ND2	2.26	0.68
2:F:126:MET:HG3	3:G:117:PHE:HE1	1.59	0.68
3:O:166:LEU:HD11	3:O:172:ILE:HG23	1.74	0.68
2:F:159:PHE:O	3:G:186:ARG:NH2	2.27	0.68
3:G:57:ASP:O	3:G:61:ASN:ND2	2.26	0.68
2:F:87:ARG:HD3	2:F:92:ARG:HD3	1.76	0.68
3:G:248:LEU:HD23	3:G:249:ARG:HG2	1.74	0.68
1:M:181:VAL:HG11	1:M:188:ALA:HB2	1.75	0.68
3:G:248:LEU:HD11	2:N:137:PRO:HG3	1.74	0.68
1:J:285:LYS:NZ	3:L:164:TYR:OH	2.24	0.68
1:E:287:THR:O	2:F:68:ARG:NH2	2.26	0.68
2:F:6:LEU:HB2	2:K:10:THR:HG23	1.76	0.67
2:K:56:ASN:HB2	2:K:71:PHE:HB3	1.77	0.67
3:O:126:VAL:HG13	3:O:212:PHE:HE1	1.59	0.67
3:L:55:ARG:NH2	3:L:245:PHE:O	2.27	0.67
1:A:285:LYS:NZ	3:C:164:TYR:OH	2.27	0.67
2:F:131:MET:O	2:F:157:TRP:N	2.24	0.67
1:J:127:THR:HG22	1:J:264:ARG:HD2	1.76	0.67
2:K:159:PHE:HB3	3:L:186:ARG:HH21	1.58	0.67
2:F:10:THR:HG23	2:N:6:LEU:HB2	1.76	0.67
1:M:127:THR:HG22	1:M:264:ARG:HD2	1.77	0.66
1:M:120:ARG:HH12	1:M:274:LYS:HA	1.60	0.66
1:E:134:GLU:HB2	1:E:256:LYS:HE3	1.76	0.66
1:E:171:TRP:CE2	1:E:236:ARG:HD3	2.29	0.66
1:M:285:LYS:HZ3	2:N:54:GLU:CD	2.04	0.66
2:N:121:PHE:O	3:O:184:ASN:ND2	2.29	0.66
1:E:285:LYS:NZ	2:F:54:GLU:OE1	2.28	0.66
1:D:186:PRO:HG2	2:K:10:THR:HB	1.75	0.66
2:K:126:MET:HG3	3:L:117:PHE:HE1	1.59	0.66
1:E:285:LYS:HE3	1:E:287:THR:H	1.61	0.66
3:C:99:HIS:HA	3:C:248:LEU:HD13	1.76	0.66
3:I:55:ARG:HH11	3:I:56:PRO:HD2	1.61	0.65
3:O:132:ILE:HD11	3:O:150:GLN:HG2	1.78	0.65
3:O:83:PRO:HG2	3:O:211:ASN:H	1.62	0.65
1:M:79:THR:HG23	1:M:82:SER:H	1.62	0.65
1:M:138:VAL:HG13	1:M:250:ARG:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:151:THR:OG1	3:I:210:CYS:SG	2.54	0.65
3:L:126:VAL:HG13	3:L:212:PHE:HE1	1.61	0.65
2:H:48:GLN:HE22	2:H:222:LYS:HG2	1.61	0.64
1:A:118:GLN:HE22	2:B:231:ASP:HB3	1.61	0.64
2:F:135:TYR:O	3:L:249:ARG:NH2	2.31	0.64
1:D:269:GLN:NE2	1:D:284:ILE:H	1.95	0.64
3:I:248:LEU:HD23	3:I:249:ARG:HG2	1.78	0.64
1:J:171:TRP:CE2	1:J:236:ARG:HD3	2.33	0.64
3:O:126:VAL:HG13	3:O:212:PHE:CE1	2.33	0.64
3:L:55:ARG:NH1	3:L:245:PHE:H	1.95	0.64
3:O:205:SER:HB2	3:O:208:ASN:HD21	1.62	0.63
1:J:265:PRO:HB3	3:L:174:GLN:HB2	1.80	0.63
3:I:112:CYS:HB3	3:I:234:ILE:HG22	1.80	0.63
3:O:82:PHE:HE2	3:O:108:ILE:HG21	1.63	0.63
3:O:86:LEU:HA	3:O:89:THR:HB	1.79	0.63
1:J:134:GLU:HB3	1:J:254:ARG:HB3	1.80	0.63
2:B:137:PRO:HD2	3:O:249:ARG:HH12	1.63	0.63
1:E:127:THR:HG22	1:E:264:ARG:HD2	1.80	0.63
1:D:101:THR:OG1	1:D:102:ASN:N	2.30	0.63
2:N:118:THR:HG22	2:N:166:THR:HG23	1.81	0.63
3:O:109:HIS:HB3	3:O:237:THR:HB	1.81	0.63
1:E:285:LYS:NZ	3:G:164:TYR:OH	2.30	0.62
1:E:267:ARG:NH2	1:E:278:ASN:O	2.32	0.62
1:D:204:PHE:HB2	3:I:131:VAL:HG21	1.82	0.62
2:H:126:MET:HG3	3:I:117:PHE:CE1	2.34	0.62
1:A:197:PRO:HG2	1:A:227:ASN:HD22	1.65	0.62
2:H:87:ARG:NH1	2:H:189:TYR:O	2.33	0.62
2:B:51:THR:HG21	2:B:100:LEU:H	1.65	0.62
2:K:105:CYS:HA	2:K:226:MET:HE1	1.81	0.62
2:B:158:ASP:OD1	2:B:160:GLY:N	2.32	0.62
3:O:199:ASN:ND2	3:O:204:ASP:OD2	2.33	0.62
1:E:75:THR:HB	2:F:42:ASN:HD21	1.65	0.62
1:A:171:TRP:CE2	1:A:236:ARG:HD2	2.34	0.62
3:C:124:VAL:HG22	3:C:216:VAL:HG22	1.81	0.62
1:E:108:ASN:HD21	1:E:163:PRO:HG2	1.64	0.62
3:I:122:LEU:HB2	3:I:183:ILE:HB	1.81	0.62
3:L:100:TYR:HD2	3:L:248:LEU:HD21	1.65	0.61
3:I:16:LEU:HD21	3:I:241:MET:HE2	1.82	0.61
3:L:132:ILE:HG12	3:L:150:GLN:HE21	1.63	0.61
3:L:134:THR:HG22	3:L:135:VAL:H	1.64	0.61
3:C:54:THR:N	3:C:245:PHE:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:GLN:NE2	2:H:231:ASP:OD2	2.33	0.61
3:I:126:VAL:HG11	3:I:195:VAL:HG11	1.83	0.61
3:C:132:ILE:HG12	3:C:150:GLN:HE21	1.66	0.61
1:E:259:ARG:NH2	2:F:39:GLU:OE2	2.34	0.61
1:A:101:THR:OG1	1:A:102:ASN:N	2.33	0.61
2:B:110:GLN:HB2	2:B:174:ASN:HB3	1.82	0.61
3:G:84:ASP:OD1	3:G:152:GLN:HA	2.01	0.61
1:A:269:GLN:NE2	1:A:284:ILE:HB	2.15	0.61
1:D:116:TYR:OH	1:D:118:GLN:NE2	2.33	0.60
1:J:218:ASN:ND2	1:J:221:ASP:OD2	2.34	0.60
2:K:110:GLN:O	2:K:227:GLN:HB2	2.00	0.60
3:O:132:ILE:HG12	3:O:150:GLN:HE21	1.66	0.60
1:D:134:GLU:HB3	1:D:254:ARG:HB3	1.82	0.60
1:M:134:GLU:HB2	1:M:256:LYS:HE3	1.82	0.60
2:F:46:LEU:O	2:F:49:VAL:HG12	2.02	0.60
2:F:85:VAL:HG12	2:F:194:VAL:HB	1.82	0.60
3:L:82:PHE:CE2	3:L:108:ILE:HG21	2.36	0.60
1:D:134:GLU:CD	1:D:189:GLN:HE21	2.08	0.60
1:J:225:CYS:HB3	1:J:228:ASN:HB2	1.84	0.60
3:C:118:HIS:HD1	3:C:232:ILE:HD11	1.67	0.60
3:O:53:PRO:HA	3:O:246:ALA:HB2	1.83	0.60
1:E:140:CYS:SG	1:E:250:ARG:NH1	2.74	0.60
3:I:84:ASP:OD1	3:I:85:VAL:N	2.35	0.60
2:F:121:PHE:O	3:G:184:ASN:ND2	2.34	0.60
3:G:203:PHE:HE2	3:G:244:GLU:HG2	1.67	0.60
1:J:116:TYR:OH	1:J:118:GLN:NE2	2.35	0.60
1:M:222:TYR:OH	3:O:150:GLN:NE2	2.34	0.60
3:C:134:THR:HG22	3:C:135:VAL:H	1.67	0.60
1:D:171:TRP:CD2	1:D:236:ARG:HD3	2.37	0.60
2:B:85:VAL:HG12	2:B:194:VAL:HB	1.83	0.60
1:E:116:TYR:OH	1:E:118:GLN:NE2	2.35	0.59
1:J:82:SER:O	1:J:86:ARG:NH2	2.34	0.59
2:K:135:TYR:O	3:I:249:ARG:NH2	2.34	0.59
3:I:69:LYS:HZ1	3:I:78:TRP:CD1	2.20	0.59
2:H:227:GLN:HA	2:H:227:GLN:HE21	1.67	0.59
1:A:285:LYS:HE3	1:A:287:THR:H	1.66	0.59
1:J:90:VAL:HG12	1:J:116:TYR:HB2	1.83	0.59
2:F:158:ASP:OD1	2:F:160:GLY:N	2.32	0.59
1:A:264:ARG:HH12	3:C:127:LEU:HD21	1.66	0.59
2:K:158:ASP:OD1	2:K:160:GLY:N	2.30	0.59
3:C:205:SER:HB2	3:C:208:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:84:ASP:O	3:I:87:THR:HG23	2.02	0.59
1:M:204:PHE:HB2	3:O:131:VAL:HG21	1.84	0.59
2:N:56:ASN:ND2	2:N:67:GLU:O	2.36	0.59
3:G:28:ALA:O	3:G:30:ASN:N	2.34	0.59
2:B:122:THR:HA	3:C:184:ASN:HD21	1.66	0.59
1:D:284:ILE:HG22	1:D:285:LYS:H	1.67	0.59
2:B:10:THR:HG23	2:H:6:LEU:HB2	1.85	0.59
3:C:132:ILE:HD11	3:C:150:GLN:HG2	1.84	0.59
2:F:8:PRO:HB2	1:J:189:GLN:HB2	1.83	0.59
1:M:149:GLN:HG2	1:M:247:LEU:HD11	1.84	0.59
2:B:37:PRO:HB3	3:C:37:GLU:CD	2.28	0.59
2:H:24:ILE:HD12	2:K:14:LEU:HD21	1.84	0.59
3:I:118:HIS:HD1	3:I:232:ILE:HD11	1.67	0.59
1:E:121:ARG:HG3	1:E:267:ARG:HB3	1.84	0.59
1:D:135:PHE:HE1	1:D:253:MET:HB2	1.67	0.59
3:I:121:ALA:HB3	3:I:220:SER:H	1.68	0.59
3:L:83:PRO:HG2	3:L:211:ASN:N	2.18	0.59
3:G:70:LEU:HB3	3:G:231:VAL:HG13	1.85	0.58
1:J:269:GLN:NE2	1:J:284:ILE:H	2.01	0.58
1:J:130:ARG:NH1	2:K:33:CYS:SG	2.76	0.58
1:A:111:ILE:HD13	1:A:230:MET:HG3	1.85	0.58
1:J:285:LYS:HZ1	1:J:286:PRO:HG2	1.68	0.58
1:M:118:GLN:OE1	2:N:231:ASP:HB3	2.03	0.58
3:O:65:THR:HG22	3:O:237:THR:HG23	1.85	0.58
2:H:48:GLN:NE2	2:H:222:LYS:HG2	2.17	0.58
3:L:205:SER:HB2	3:L:208:ASN:HD21	1.68	0.58
3:O:82:PHE:CE2	3:O:108:ILE:HG21	2.38	0.58
3:O:126:VAL:HG22	3:O:212:PHE:HZ	1.68	0.58
3:O:134:THR:HG22	3:O:135:VAL:H	1.69	0.58
1:J:285:LYS:HD2	1:J:286:PRO:HD2	1.84	0.58
3:O:118:HIS:ND1	3:O:232:ILE:HD11	2.19	0.58
3:L:69:LYS:HZ1	3:L:78:TRP:CD1	2.21	0.58
1:J:149:GLN:HG2	1:J:247:LEU:HD11	1.84	0.58
2:B:6:LEU:HB2	2:N:10:THR:HG23	1.84	0.58
3:O:99:HIS:CE1	3:O:245:PHE:HA	2.38	0.58
3:O:107:CYS:HB2	3:O:241:MET:HE2	1.85	0.58
2:H:4:THR:HG22	2:K:2:PHE:HB3	1.85	0.58
3:L:157:GLY:HA3	3:L:158:PHE:CD1	2.39	0.58
2:N:84:ALA:HA	2:N:195:SER:HA	1.86	0.58
3:L:82:PHE:HE2	3:L:108:ILE:HG21	1.69	0.57
2:F:114:SER:N	2:F:223:ASN:OD1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:126:VAL:HG13	3:G:212:PHE:CE1	2.39	0.57
1:D:210:THR:HG21	1:D:214:HIS:HB3	1.86	0.57
1:D:292:THR:HA	2:H:58:VAL:HG22	1.86	0.57
3:O:172:ILE:HG22	3:O:175:LEU:HD22	1.86	0.57
1:M:284:ILE:HG22	1:M:285:LYS:H	1.69	0.57
1:M:285:LYS:HD2	1:M:286:PRO:HD2	1.86	0.57
2:F:51:THR:HG21	2:F:100:LEU:H	1.69	0.57
1:D:127:THR:HG22	1:D:264:ARG:HD2	1.86	0.57
1:M:171:TRP:CE2	1:M:236:ARG:HD3	2.40	0.57
2:B:62:ALA:HA	2:B:65:LEU:HB2	1.84	0.57
1:J:111:ILE:HD11	1:J:135:PHE:CZ	2.40	0.57
1:A:127:THR:HG22	1:A:264:ARG:HD2	1.85	0.57
2:B:52:ILE:HG21	2:B:69:LEU:HB3	1.86	0.57
1:E:81:ASP:O	1:E:85:SER:N	2.35	0.57
2:N:14:LEU:HB3	2:N:17:ASP:HB2	1.84	0.57
2:F:228:LEU:HB3	2:K:28:PHE:CD1	2.40	0.57
1:D:285:LYS:HE3	1:D:287:THR:H	1.70	0.57
2:H:227:GLN:HA	2:H:227:GLN:NE2	2.20	0.57
3:I:136:ALA:HB2	3:I:145:HIS:HB2	1.85	0.57
1:D:149:GLN:HG2	1:D:247:LEU:HD11	1.86	0.57
1:M:130:ARG:NH1	1:M:199:SER:O	2.38	0.57
2:H:10:THR:HG23	2:K:6:LEU:HB2	1.87	0.57
1:A:135:PHE:HE1	1:A:253:MET:HB2	1.70	0.57
1:A:189:GLN:HB2	2:H:8:PRO:HB2	1.87	0.57
3:O:172:ILE:HA	3:O:175:LEU:HB2	1.87	0.57
2:H:46:LEU:O	2:H:49:VAL:HG12	2.05	0.56
3:O:99:HIS:HD2	3:O:100:TYR:H	1.53	0.56
1:E:189:GLN:NE2	2:F:21:SER:HB3	2.21	0.56
2:F:130:LYS:HB2	2:F:200:THR:HG22	1.87	0.56
3:G:41:TYR:OH	3:G:57:ASP:OD1	2.22	0.56
3:L:151:THR:OG1	3:L:210:CYS:SG	2.64	0.56
2:H:200:THR:OG1	2:H:201:ASN:N	2.39	0.56
3:C:84:ASP:CG	3:C:152:GLN:HA	2.31	0.56
1:E:204:PHE:HB2	3:G:131:VAL:HG21	1.87	0.56
2:B:24:ILE:HD12	2:H:14:LEU:HD21	1.87	0.56
2:H:110:GLN:O	2:H:227:GLN:HB2	2.05	0.56
1:E:171:TRP:CD2	1:E:236:ARG:HD3	2.41	0.56
1:E:111:ILE:HD13	1:E:230:MET:HG3	1.87	0.56
2:F:171:TRP:NE1	2:F:173:SER:OG	2.39	0.56
1:D:244:LYS:HB2	1:J:143:THR:HG21	1.88	0.56
1:M:285:LYS:HE3	1:M:287:THR:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ARG:NH1	1:E:273:PHE:O	2.22	0.56
2:B:46:LEU:O	2:B:49:VAL:HG12	2.05	0.56
3:I:100:TYR:HD2	3:I:248:LEU:HD12	1.70	0.56
1:J:197:PRO:HA	2:K:31:THR:HG21	1.88	0.55
1:E:215:LEU:O	1:E:218:ASN:ND2	2.39	0.55
1:J:261:TRP:HA	2:K:39:GLU:HA	1.89	0.55
1:M:111:ILE:HD11	1:M:135:PHE:CZ	2.41	0.55
2:B:162:GLN:OE1	3:C:186:ARG:NH1	2.38	0.55
2:N:158:ASP:OD1	2:N:160:GLY:N	2.34	0.55
3:L:53:PRO:HB3	3:L:55:ARG:NH2	2.21	0.55
1:E:102:ASN:N	1:E:102:ASN:HD22	2.03	0.55
1:M:147:VAL:HG11	1:M:245:TYR:CG	2.42	0.55
2:N:85:VAL:HG12	2:N:194:VAL:HB	1.89	0.55
1:E:285:LYS:HD2	1:E:286:PRO:HD2	1.88	0.55
2:H:59:PRO:HD2	2:H:68:ARG:HG2	1.88	0.55
1:D:73:HIS:CE1	3:C:47:ALA:HB3	2.41	0.55
2:N:200:THR:OG1	2:N:201:ASN:N	2.40	0.55
2:F:84:ALA:HA	2:F:195:SER:HA	1.88	0.55
1:M:102:ASN:OD1	1:M:102:ASN:N	2.40	0.55
1:M:136:THR:HG21	2:N:13:PHE:CE1	2.41	0.55
2:K:110:GLN:NE2	2:K:227:GLN:HG2	2.21	0.55
2:K:131:MET:O	2:K:157:TRP:N	2.31	0.55
3:L:122:LEU:HB2	3:L:183:ILE:HB	1.88	0.55
2:H:131:MET:N	2:H:157:TRP:O	2.35	0.55
1:J:208:TYR:HE2	3:L:151:THR:HG21	1.72	0.55
1:J:285:LYS:NZ	2:K:54:GLU:OE1	2.22	0.55
2:H:84:ALA:C	2:H:86:PHE:H	2.13	0.55
3:G:132:ILE:HD11	3:G:150:GLN:HG2	1.89	0.55
2:K:62:ALA:HA	2:K:65:LEU:HB2	1.88	0.55
2:F:10:THR:HB	1:J:186:PRO:HG2	1.89	0.54
3:G:182:TRP:O	3:G:188:ASN:ND2	2.38	0.54
1:E:265:PRO:HB2	3:G:170:ILE:HG23	1.88	0.54
2:F:204:VAL:HB	2:F:208:ALA:HB3	1.88	0.54
1:J:265:PRO:HB2	3:L:170:ILE:HG23	1.89	0.54
1:M:116:TYR:CD2	1:M:119:MET:HB2	2.42	0.54
1:M:265:PRO:HB3	3:O:174:GLN:HB2	1.89	0.54
3:L:99:HIS:CE1	3:L:245:PHE:HA	2.42	0.54
3:L:104:SER:HB2	3:L:243:SER:HA	1.88	0.54
1:D:285:LYS:HD2	1:D:286:PRO:HD2	1.89	0.54
1:M:101:THR:HG23	1:M:102:ASN:H	1.71	0.54
3:L:25:THR:C	3:L:27:GLU:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:LEU:HA	2:H:220:ALA:HA	1.90	0.54
3:I:95:ASN:O	3:I:99:HIS:HB2	2.07	0.54
1:D:151:LEU:HA	1:D:238:VAL:HG23	1.89	0.54
3:G:118:HIS:ND1	3:G:232:ILE:HD11	2.23	0.54
3:L:121:ALA:HB3	3:L:220:SER:H	1.73	0.54
2:B:70:ARG:HD2	2:B:213:TYR:CD2	2.41	0.54
3:C:73:LYS:NZ	3:C:223:ASP:OD1	2.37	0.54
1:D:138:VAL:HG13	1:D:250:ARG:HB2	1.89	0.54
1:M:116:TYR:HD2	1:M:119:MET:HB2	1.73	0.54
3:C:182:TRP:O	3:C:188:ASN:ND2	2.41	0.54
3:I:73:LYS:NZ	3:I:223:ASP:OD1	2.40	0.54
2:F:84:ALA:C	2:F:86:PHE:H	2.16	0.54
1:M:265:PRO:HB2	3:O:170:ILE:HG23	1.90	0.54
1:M:285:LYS:HZ1	1:M:286:PRO:HG2	1.73	0.54
2:N:110:GLN:HB2	2:N:174:ASN:O	2.08	0.54
3:O:203:PHE:HE2	3:O:244:GLU:HG2	1.72	0.54
2:H:70:ARG:HD2	2:H:213:TYR:CD2	2.43	0.54
3:C:84:ASP:O	3:C:87:THR:HG23	2.08	0.54
2:F:136:THR:OG1	3:L:249:ARG:NH1	2.41	0.53
2:B:130:LYS:HB2	2:B:200:THR:HG22	1.90	0.53
3:O:55:ARG:HH12	3:O:60:VAL:HG23	1.73	0.53
2:F:59:PRO:O	2:F:68:ARG:NH1	2.41	0.53
3:G:122:LEU:HB2	3:G:183:ILE:HB	1.90	0.53
3:C:104:SER:HB2	3:C:243:SER:HA	1.90	0.53
3:L:70:LEU:HB3	3:L:231:VAL:HG13	1.89	0.53
1:E:189:GLN:HB2	2:N:8:PRO:HB2	1.89	0.53
2:F:50:GLU:HA	2:F:219:ALA:HB2	1.90	0.53
1:A:113:ILE:HA	1:A:253:MET:HE1	1.90	0.53
1:J:120:ARG:NH1	1:J:274:LYS:HA	2.23	0.53
3:O:103:ARG:HG3	3:O:197:TYR:CG	2.43	0.53
1:D:90:VAL:HG12	1:D:116:TYR:H	1.73	0.53
1:D:265:PRO:HB2	3:I:170:ILE:HG23	1.89	0.53
1:J:285:LYS:HE3	1:J:287:THR:H	1.73	0.53
2:B:70:ARG:HD2	2:B:213:TYR:CG	2.43	0.53
1:D:285:LYS:HZ2	1:D:286:PRO:HG2	1.74	0.53
1:D:114:THR:HG23	1:D:120:ARG:HB2	1.89	0.53
2:H:119:PHE:O	2:H:164:SER:OG	2.17	0.53
1:A:166:ARG:NH2	1:A:237:THR:OG1	2.38	0.53
3:O:30:ASN:O	3:O:181:GLN:NE2	2.42	0.53
1:A:84:PHE:HD2	1:A:258:VAL:HG11	1.74	0.53
3:I:99:HIS:HE1	3:I:245:PHE:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:99:HIS:HA	3:L:248:LEU:HD13	1.90	0.53
1:E:118:GLN:NE2	2:F:231:ASP:OD2	2.42	0.53
2:N:50:GLU:HA	2:N:219:ALA:HB2	1.91	0.53
1:A:153:TYR:HB2	1:A:179:VAL:HB	1.91	0.52
1:D:141:THR:HG1	1:D:145:GLU:N	2.07	0.52
1:D:268:ASN:OD1	1:D:269:GLN:HG2	2.09	0.52
2:H:110:GLN:NE2	2:H:227:GLN:HG2	2.24	0.52
3:I:83:PRO:HG2	3:I:211:ASN:H	1.74	0.52
3:O:69:LYS:HZ1	3:O:78:TRP:CD1	2.27	0.52
2:H:7:LYS:O	2:H:10:THR:OG1	2.24	0.52
2:K:72:PRO:HB3	2:K:213:TYR:CE1	2.45	0.52
1:A:154:MET:HE1	1:A:171:TRP:HA	1.91	0.52
1:M:97:LEU:HD12	1:M:98:GLU:H	1.75	0.52
3:G:83:PRO:HG2	3:G:211:ASN:N	2.19	0.52
3:C:28:ALA:O	3:C:30:ASN:N	2.38	0.52
1:A:266:MET:HE2	2:B:103:GLN:HB3	1.91	0.52
1:D:118:GLN:HA	2:H:235:ILE:HD11	1.90	0.52
2:B:105:CYS:HA	2:B:226:MET:HE1	1.91	0.52
3:C:151:THR:HG22	3:C:152:GLN:H	1.75	0.52
3:O:66:LEU:HB3	3:O:155:ALA:HB1	1.91	0.52
3:O:181:GLN:HG2	3:O:191:ALA:HB1	1.90	0.52
1:E:102:ASN:HD22	1:E:102:ASN:H	1.55	0.52
2:N:70:ARG:HD2	2:N:213:TYR:CD2	2.44	0.52
3:I:81:LYS:NZ	3:I:150:GLN:OE1	2.43	0.52
2:N:72:PRO:HB3	2:N:213:TYR:CE1	2.45	0.52
3:L:90:GLY:O	3:L:94:GLN:HG2	2.10	0.52
3:O:124:VAL:HG22	3:O:216:VAL:HG22	1.91	0.52
1:E:118:GLN:HA	2:F:235:ILE:HD11	1.91	0.52
1:A:285:LYS:NZ	2:B:54:GLU:OE2	2.41	0.52
1:J:271:TYR:HD1	2:K:235:ILE:HG21	1.73	0.52
1:M:211:PHE:HA	3:O:208:ASN:HD22	1.75	0.52
2:B:126:MET:HG3	3:C:117:PHE:HE1	1.74	0.52
2:H:66:MET:SD	3:I:172:ILE:HD11	2.50	0.52
1:A:215:LEU:HG	1:A:217:ALA:H	1.74	0.51
1:J:285:LYS:HG2	2:K:68:ARG:CZ	2.40	0.51
1:M:284:ILE:HG22	1:M:285:LYS:N	2.26	0.51
2:N:90:PRO:HA	2:N:96:TRP:CG	2.46	0.51
3:C:166:LEU:HD13	3:C:170:ILE:O	2.09	0.51
3:L:84:ASP:OD1	3:L:152:GLN:HA	2.09	0.51
2:F:57:ASN:ND2	2:F:95:PRO:HG3	2.26	0.51
2:F:74:SER:HA	2:F:211:THR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:126:MET:HG3	3:L:117:PHE:CE1	2.41	0.51
3:C:247:GLY:C	3:C:248:LEU:HD12	2.34	0.51
2:F:91:GLY:HA3	2:F:111:TRP:CH2	2.45	0.51
2:B:44:LEU:O	2:B:48:GLN:HG3	2.09	0.51
2:B:61:ASN:ND2	2:B:63:THR:OG1	2.43	0.51
2:N:110:GLN:O	2:N:227:GLN:HB2	2.11	0.51
3:O:95:ASN:OD1	3:O:96:ALA:N	2.43	0.51
1:E:175:THR:HG22	1:M:86:ARG:HH11	1.76	0.51
3:G:65:THR:HG22	3:G:237:THR:HG23	1.93	0.51
1:M:271:TYR:HD1	2:N:235:ILE:HG21	1.76	0.51
2:K:49:VAL:HG11	3:L:177:VAL:HG23	1.93	0.51
1:J:91:GLY:HA3	1:J:251:ILE:HB	1.93	0.51
1:M:131:PHE:HB3	1:M:258:VAL:HG22	1.93	0.51
2:K:59:PRO:HD2	2:K:68:ARG:HG2	1.92	0.51
2:F:61:ASN:O	2:F:65:LEU:N	2.44	0.51
1:J:156:VAL:HG12	1:J:176:ASN:HB3	1.91	0.51
1:J:267:ARG:HG2	1:J:271:TYR:CE1	2.46	0.51
1:M:198:ALA:O	2:N:31:THR:OG1	2.23	0.51
2:F:122:THR:O	3:G:119:GLN:HB2	2.10	0.51
1:A:134:GLU:CD	1:A:189:GLN:HE21	2.18	0.51
3:I:104:SER:HB2	3:I:243:SER:HA	1.92	0.51
3:I:119:GLN:O	3:I:222:LEU:HA	2.11	0.51
3:I:243:SER:HB3	3:I:245:PHE:CE2	2.46	0.51
3:G:82:PHE:CZ	3:G:108:ILE:HG21	2.45	0.51
1:A:86:ARG:HH12	2:B:229:CYS:HB2	1.75	0.51
3:L:86:LEU:HA	3:L:89:THR:HB	1.92	0.51
2:F:105:CYS:HA	2:F:226:MET:HE1	1.93	0.51
1:M:122:LYS:HG3	2:N:107:TYR:HE2	1.75	0.51
2:H:151:LEU:HD23	3:C:250:GLN:HB3	1.92	0.51
3:C:187:THR:HG23	3:C:188:ASN:H	1.74	0.51
1:M:285:LYS:NZ	1:M:286:PRO:HG2	2.26	0.51
2:H:50:GLU:HB3	2:H:217:LEU:HD13	1.93	0.51
3:G:76:LYS:O	3:G:163:PRO:HB3	2.11	0.50
2:H:72:PRO:O	2:H:82:LEU:HD11	2.11	0.50
2:K:129:GLY:N	2:K:159:PHE:HD2	2.09	0.50
2:N:51:THR:OG1	3:O:173:SER:O	2.29	0.50
2:F:87:ARG:NH1	2:F:92:ARG:HG2	2.26	0.50
1:A:264:ARG:NH1	3:C:127:LEU:HD21	2.25	0.50
1:D:269:GLN:HE22	1:D:284:ILE:H	1.59	0.50
1:J:140:CYS:SG	1:J:250:ARG:NH1	2.83	0.50
1:J:269:GLN:HE22	1:J:284:ILE:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:ILE:HG23	2:H:25:LEU:HG	1.93	0.50
3:O:110:VAL:HG22	3:O:236:ILE:HG23	1.92	0.50
2:H:72:PRO:HB3	2:H:213:TYR:HE1	1.76	0.50
3:I:111:GLN:O	3:I:235:THR:N	2.45	0.50
1:E:111:ILE:HD11	1:E:135:PHE:CZ	2.47	0.50
1:E:120:ARG:NH1	1:E:274:LYS:HA	2.27	0.50
1:J:85:SER:OG	1:J:254:ARG:NH1	2.44	0.50
2:B:7:LYS:O	2:B:10:THR:OG1	2.22	0.50
2:H:61:ASN:OD1	2:H:64:SER:HB3	2.11	0.50
2:H:130:LYS:HB2	2:H:200:THR:HG22	1.94	0.50
3:C:147:PRO:HB2	3:C:150:GLN:HB2	1.93	0.50
1:A:86:ARG:HH11	1:M:175:THR:HG22	1.77	0.50
1:A:149:GLN:HB3	1:A:183:LEU:HD13	1.94	0.50
1:J:102:ASN:C	1:J:104:ASN:H	2.19	0.50
2:H:52:ILE:HG21	2:H:69:LEU:HB3	1.93	0.50
1:E:267:ARG:HG2	1:E:271:TYR:CE1	2.47	0.50
1:D:113:ILE:HG22	1:D:119:MET:HG2	1.94	0.50
1:M:76:ALA:O	1:M:79:THR:HG22	2.11	0.50
3:I:195:VAL:HG21	3:I:212:PHE:CE2	2.46	0.50
2:H:105:CYS:HA	2:H:226:MET:HE1	1.94	0.50
2:F:110:GLN:HB2	2:F:174:ASN:HB3	1.93	0.50
1:J:268:ASN:OD1	1:J:269:GLN:HG2	2.12	0.50
2:K:46:LEU:O	2:K:49:VAL:HG12	2.12	0.50
3:G:132:ILE:O	3:G:134:THR:HG22	2.12	0.49
3:G:248:LEU:CD2	3:G:249:ARG:H	2.20	0.49
1:J:147:VAL:HG11	1:J:245:TYR:CG	2.47	0.49
1:M:153:TYR:HB2	1:M:179:VAL:HB	1.94	0.49
3:C:199:ASN:ND2	3:C:204:ASP:OD2	2.45	0.49
3:G:121:ALA:HB3	3:G:220:SER:H	1.76	0.49
1:A:261:TRP:HA	2:B:39:GLU:HA	1.94	0.49
3:O:75:SER:HB3	3:O:78:TRP:CZ2	2.47	0.49
2:F:72:PRO:HB3	2:F:213:TYR:HE1	1.77	0.49
3:G:166:LEU:HD13	3:G:170:ILE:O	2.12	0.49
1:J:106:TYR:OH	1:J:163:PRO:O	2.29	0.49
3:L:166:LEU:HD13	3:L:170:ILE:O	2.11	0.49
1:E:163:PRO:HB3	1:E:170:ALA:HB3	1.93	0.49
1:A:205:TYR:O	1:A:223:GLY:HA2	2.12	0.49
1:M:77:GLU:O	2:N:108:TYR:OH	2.27	0.49
3:L:208:ASN:OD1	3:L:208:ASN:N	2.44	0.49
2:N:133:ILE:HG12	2:N:196:ILE:HG23	1.95	0.49
3:C:100:TYR:HD1	3:C:101:LEU:N	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:102:TYR:HD1	3:I:245:PHE:CZ	2.30	0.49
2:H:159:PHE:HB3	3:I:186:ARG:HH21	1.77	0.49
2:K:72:PRO:HB3	2:K:213:TYR:HE1	1.77	0.49
2:N:24:ILE:HG23	2:N:25:LEU:HG	1.94	0.49
2:N:62:ALA:HA	2:N:65:LEU:HB2	1.94	0.49
3:I:65:THR:HG22	3:I:237:THR:HG23	1.95	0.49
3:L:112:CYS:O	3:L:189:ASN:HB2	2.12	0.49
3:O:109:HIS:O	3:O:237:THR:N	2.41	0.49
2:B:145:ASP:OD1	2:B:148:THR:N	2.46	0.49
2:K:14:LEU:HB3	2:K:17:ASP:HB2	1.95	0.49
3:C:118:HIS:ND1	3:C:232:ILE:HD11	2.27	0.49
3:O:103:ARG:HG3	3:O:197:TYR:CD2	2.48	0.49
2:F:77:ALA:HB3	2:F:198:TYR:HE2	1.76	0.49
1:A:265:PRO:HB3	3:C:174:GLN:HB2	1.94	0.49
2:H:110:GLN:HB2	2:H:174:ASN:HB3	1.95	0.49
2:H:145:ASP:OD1	2:H:148:THR:N	2.43	0.49
3:O:60:VAL:HG13	3:O:91:VAL:HG13	1.95	0.49
1:D:84:PHE:HE1	1:D:122:LYS:HG2	1.78	0.49
1:M:111:ILE:HG22	1:M:231:GLY:O	2.13	0.49
2:N:230:LYS:HE3	2:N:232:ALA:HB2	1.95	0.49
3:I:84:ASP:HB2	3:I:152:GLN:HA	1.94	0.49
3:I:99:HIS:ND1	3:I:245:PHE:HD1	2.11	0.49
3:I:166:LEU:HD11	3:I:172:ILE:HG23	1.94	0.49
3:O:56:PRO:HG2	3:O:59:SER:OG	2.12	0.49
1:M:87:ALA:N	1:M:254:ARG:HG3	2.27	0.49
3:O:71:TRP:HB3	3:O:232:ILE:HB	1.94	0.49
3:O:122:LEU:HB2	3:O:183:ILE:HB	1.95	0.49
1:M:267:ARG:NH2	1:M:278:ASN:O	2.46	0.48
2:N:114:SER:OG	2:N:170:PRO:O	2.31	0.48
1:E:156:VAL:HG12	1:E:176:ASN:HB3	1.95	0.48
1:E:198:ALA:HB1	3:G:200:ALA:HB1	1.95	0.48
1:M:120:ARG:NH1	1:M:274:LYS:HA	2.26	0.48
1:M:171:TRP:CD2	1:M:236:ARG:HD3	2.49	0.48
2:K:84:ALA:C	2:K:86:PHE:H	2.20	0.48
2:N:72:PRO:HB3	2:N:213:TYR:HE1	1.78	0.48
3:O:166:LEU:HD13	3:O:170:ILE:O	2.13	0.48
1:D:267:ARG:HG2	1:D:271:TYR:CE1	2.48	0.48
1:D:285:LYS:NZ	1:D:286:PRO:HG2	2.27	0.48
2:N:51:THR:HG21	2:N:100:LEU:H	1.78	0.48
3:O:128:PRO:O	3:O:212:PHE:HA	2.12	0.48
2:F:200:THR:OG1	2:F:201:ASN:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:LYS:HG2	2:H:68:ARG:CZ	2.44	0.48
1:M:261:TRP:HA	2:N:39:GLU:HA	1.95	0.48
3:O:203:PHE:CE2	3:O:244:GLU:HG2	2.48	0.48
1:E:108:ASN:OD1	1:E:234:SER:OG	2.29	0.48
2:F:118:THR:HG22	2:F:166:THR:HG22	1.95	0.48
1:A:86:ARG:NH1	1:M:175:THR:HG22	2.28	0.48
1:A:284:ILE:HG22	1:A:285:LYS:N	2.28	0.48
2:F:110:GLN:HB2	2:F:174:ASN:O	2.13	0.48
3:G:55:ARG:NE	3:G:243:SER:HB2	2.28	0.48
3:G:99:HIS:HD2	3:G:101:LEU:O	1.96	0.48
1:D:102:ASN:C	1:D:104:ASN:H	2.20	0.48
2:K:78:GLY:O	2:K:79:LYS:HG2	2.14	0.48
2:K:130:LYS:HB2	2:K:200:THR:HG22	1.95	0.48
1:D:218:ASN:ND2	1:D:220:LEU:H	2.12	0.48
3:L:247:GLY:C	3:L:248:LEU:HD12	2.39	0.48
1:J:131:PHE:HB3	1:J:258:VAL:HG22	1.96	0.48
1:M:191:SER:HB2	2:N:21:SER:OG	2.14	0.48
1:E:114:THR:HG23	1:E:120:ARG:HB2	1.96	0.48
3:G:205:SER:HB2	3:G:208:ASN:HD21	1.77	0.48
1:J:154:MET:HE1	1:J:171:TRP:HA	1.96	0.48
1:M:121:ARG:HG3	1:M:267:ARG:HB3	1.96	0.48
2:H:70:ARG:HD2	2:H:213:TYR:CG	2.49	0.48
2:H:121:PHE:O	3:I:184:ASN:ND2	2.47	0.48
2:F:70:ARG:HD2	2:F:213:TYR:CD2	2.49	0.48
3:G:208:ASN:OD1	3:G:208:ASN:N	2.42	0.48
1:D:264:ARG:NH1	3:I:127:LEU:HD21	2.28	0.48
2:N:70:ARG:HD2	2:N:213:TYR:CG	2.49	0.48
3:I:84:ASP:CG	3:I:153:PRO:HD2	2.39	0.48
3:O:232:ILE:HA	3:O:233:PRO:HD3	1.71	0.48
1:E:268:ASN:OD1	1:E:269:GLN:HG2	2.14	0.47
1:E:293:ALA:HB1	2:F:83:CYS:SG	2.53	0.47
3:G:203:PHE:CE2	3:G:244:GLU:HG2	2.47	0.47
1:A:155:PHE:HB2	1:A:233:PHE:CE1	2.49	0.47
1:A:181:VAL:HG11	1:A:188:ALA:HB2	1.95	0.47
1:J:120:ARG:HH12	1:J:274:LYS:HA	1.79	0.47
1:M:186:PRO:HG2	2:B:10:THR:HB	1.96	0.47
3:I:76:LYS:O	3:I:163:PRO:HB3	2.14	0.47
3:O:69:LYS:NZ	3:O:78:TRP:CG	2.82	0.47
2:B:24:ILE:HG23	2:B:25:LEU:HG	1.96	0.47
2:B:126:MET:HG3	3:C:117:PHE:CE1	2.49	0.47
3:I:232:ILE:HD13	3:I:232:ILE:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:112:SER:HB2	2:F:171:TRP:CZ2	2.49	0.47
3:G:81:LYS:HB3	3:G:210:CYS:HB3	1.96	0.47
1:M:285:LYS:HG2	2:N:68:ARG:CZ	2.44	0.47
2:H:37:PRO:HB3	3:I:37:GLU:CD	2.39	0.47
3:C:82:PHE:O	3:C:85:VAL:HG12	2.14	0.47
3:G:25:THR:C	3:G:27:GLU:H	2.22	0.47
1:A:90:VAL:HG21	1:A:253:MET:HE2	1.96	0.47
3:O:101:LEU:HD13	3:O:203:PHE:HB3	1.96	0.47
1:A:287:THR:HB	2:B:97:GLN:OE1	2.14	0.47
1:A:293:ALA:HB1	2:B:83:CYS:SG	2.54	0.47
1:J:129:MET:HA	1:J:260:ALA:HA	1.97	0.47
1:J:197:PRO:HG2	1:J:227:ASN:HD22	1.79	0.47
1:M:124:GLU:OE2	1:M:271:TYR:OH	2.31	0.47
1:M:192:VAL:HG22	2:N:24:ILE:HG21	1.96	0.47
3:C:208:ASN:OD1	3:C:208:ASN:N	2.40	0.47
3:I:83:PRO:HG2	3:I:210:CYS:HA	1.96	0.47
1:A:136:THR:HG21	2:B:13:PHE:CD1	2.50	0.47
1:E:227:ASN:HB3	2:N:176:HIS:O	2.15	0.47
2:F:14:LEU:HG	1:J:179:VAL:HG22	1.97	0.47
3:G:59:SER:OG	3:G:60:VAL:HG23	2.15	0.47
3:G:103:ARG:HD2	3:G:202:PRO:O	2.14	0.47
1:D:166:ARG:NH2	1:D:237:THR:OG1	2.36	0.47
1:J:171:TRP:CD2	1:J:236:ARG:HD3	2.49	0.47
1:M:110:ASP:CG	1:M:162:LYS:HZ3	2.22	0.47
2:B:131:MET:O	2:B:157:TRP:N	2.33	0.47
3:C:65:THR:HG22	3:C:237:THR:HG23	1.95	0.47
3:I:132:ILE:HD11	3:I:150:GLN:HG2	1.97	0.47
3:L:152:GLN:O	3:L:152:GLN:HG3	2.13	0.47
2:F:114:SER:HB2	2:F:223:ASN:HD21	1.79	0.47
1:A:143:THR:HG21	1:M:244:LYS:HB2	1.97	0.47
1:M:147:VAL:O	1:M:149:GLN:N	2.45	0.47
2:H:72:PRO:HB3	2:H:213:TYR:CE1	2.49	0.47
2:H:143:PRO:HD3	3:C:249:ARG:HH12	1.79	0.47
2:K:50:GLU:HA	2:K:219:ALA:HB2	1.97	0.47
2:N:204:VAL:HB	2:N:208:ALA:HB3	1.97	0.47
3:I:91:VAL:HA	3:I:94:GLN:HB3	1.97	0.47
3:L:98:PHE:O	3:L:248:LEU:HD22	2.15	0.47
3:L:203:PHE:CE2	3:L:244:GLU:HG2	2.42	0.47
3:L:205:SER:HB2	3:L:208:ASN:ND2	2.30	0.47
1:E:285:LYS:HE3	1:E:287:THR:N	2.27	0.47
2:F:50:GLU:HB3	2:F:217:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:VAL:HG11	1:D:245:TYR:CG	2.50	0.47
1:J:269:GLN:NE2	1:J:284:ILE:HG22	2.30	0.47
1:M:116:TYR:HD2	1:M:119:MET:HE2	1.80	0.47
3:O:84:ASP:OD2	3:O:152:GLN:HA	2.15	0.47
3:O:124:VAL:O	3:O:181:GLN:N	2.42	0.47
1:E:83:PHE:CG	2:F:43:LEU:HD11	2.49	0.47
1:E:237:THR:HG21	1:E:243:SER:HB2	1.97	0.47
1:A:285:LYS:HD2	1:A:286:PRO:HD2	1.96	0.47
1:J:290:SER:OG	2:K:57:ASN:O	2.25	0.47
1:M:117:ALA:HB1	2:N:235:ILE:HD11	1.97	0.47
3:I:87:THR:O	3:I:93:GLY:HA3	2.15	0.47
3:L:183:ILE:HG13	3:L:191:ALA:HB2	1.96	0.47
2:F:28:PHE:HE1	2:N:227:GLN:HE21	1.62	0.46
2:F:62:ALA:HA	2:F:65:LEU:HB2	1.96	0.46
2:K:159:PHE:O	3:L:186:ARG:NH2	2.48	0.46
3:C:55:ARG:HH11	3:C:60:VAL:HG23	1.80	0.46
3:I:84:ASP:OD2	3:I:153:PRO:HD2	2.16	0.46
2:B:85:VAL:CG1	2:B:194:VAL:HB	2.44	0.46
2:H:84:ALA:HA	2:H:195:SER:HA	1.96	0.46
2:H:144:LYS:HB3	2:H:148:THR:HG21	1.97	0.46
2:K:161:LEU:HD23	2:K:161:LEU:O	2.15	0.46
3:I:128:PRO:O	3:I:212:PHE:HA	2.15	0.46
1:E:267:ARG:HD2	3:G:169:GLY:O	2.15	0.46
1:A:90:VAL:HG12	1:A:116:TYR:H	1.79	0.46
1:A:147:VAL:HG11	1:A:245:TYR:CG	2.50	0.46
2:N:84:ALA:C	2:N:86:PHE:H	2.24	0.46
3:G:55:ARG:CZ	3:G:243:SER:H	2.27	0.46
1:J:121:ARG:HH22	2:K:103:GLN:CD	2.22	0.46
3:I:69:LYS:HZ1	3:I:78:TRP:CG	2.32	0.46
3:I:157:GLY:HA3	3:I:158:PHE:CD1	2.50	0.46
1:E:135:PHE:HE1	1:E:253:MET:HB2	1.80	0.46
1:A:290:SER:OG	2:B:57:ASN:O	2.25	0.46
1:D:202:GLN:NE2	3:I:129:GLU:OE2	2.47	0.46
1:D:245:TYR:HE2	1:J:145:GLU:HG2	1.80	0.46
1:M:111:ILE:HD11	1:M:135:PHE:HZ	1.79	0.46
1:M:290:SER:OG	2:N:57:ASN:O	2.23	0.46
3:O:109:HIS:N	3:O:237:THR:O	2.37	0.46
1:D:154:MET:HE1	1:D:171:TRP:HA	1.97	0.46
2:K:70:ARG:HH11	3:L:221:PRO:HD3	1.80	0.46
2:N:78:GLY:O	2:N:79:LYS:HG2	2.16	0.46
3:O:62:ARG:HB3	3:O:64:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:99:HIS:CD2	3:O:100:TYR:H	2.32	0.46
1:E:166:ARG:NH2	1:E:237:THR:OG1	2.39	0.46
2:F:126:MET:HG3	3:G:117:PHE:CE1	2.47	0.46
1:J:270:ASN:HA	2:K:235:ILE:HG22	1.97	0.46
3:I:87:THR:HG21	3:I:152:GLN:HE22	1.79	0.46
2:F:12:GLN:HB2	1:J:181:VAL:HG12	1.98	0.46
1:J:130:ARG:O	1:J:258:VAL:HA	2.15	0.46
1:M:285:LYS:NZ	2:N:54:GLU:OE1	2.31	0.46
3:C:126:VAL:HB	3:C:212:PHE:CZ	2.51	0.46
3:C:164:TYR:O	3:C:171:PRO:HA	2.16	0.46
3:L:71:TRP:HB3	3:L:232:ILE:HB	1.98	0.46
3:O:55:ARG:NH1	3:O:60:VAL:HG23	2.30	0.46
3:O:125:ALA:HA	3:O:180:HIS:HA	1.98	0.46
1:D:285:LYS:NZ	2:H:54:GLU:OE1	2.49	0.46
1:M:86:ARG:NH1	2:N:229:CYS:HB2	2.29	0.46
2:K:110:GLN:HB2	2:K:174:ASN:O	2.16	0.46
3:C:147:PRO:HG2	3:C:150:GLN:HB2	1.98	0.46
3:G:60:VAL:HG13	3:G:91:VAL:HG13	1.97	0.46
3:G:85:VAL:HG13	3:G:86:LEU:HG	1.97	0.46
1:A:149:GLN:HG3	1:A:150:LEU:N	2.31	0.46
1:D:120:ARG:NH1	1:D:274:LYS:HA	2.31	0.46
1:M:151:LEU:HA	1:M:238:VAL:HG23	1.97	0.46
2:B:212:ALA:HA	3:C:119:GLN:HE22	1.80	0.46
3:I:109:HIS:HD2	3:I:192:THR:OG1	1.94	0.46
3:G:195:VAL:HG21	3:G:212:PHE:CE2	2.51	0.45
1:A:156:VAL:HA	1:A:157:PRO:HD3	1.85	0.45
1:J:127:THR:OG1	1:J:128:TYR:N	2.50	0.45
1:J:285:LYS:NZ	1:J:286:PRO:HG2	2.31	0.45
1:M:171:TRP:CH2	1:M:234:SER:HB3	2.51	0.45
1:E:111:ILE:HG22	1:E:231:GLY:O	2.16	0.45
1:E:191:SER:N	2:F:22:ALA:O	2.47	0.45
1:E:285:LYS:NZ	1:E:286:PRO:HG2	2.32	0.45
3:I:55:ARG:HD2	3:I:56:PRO:HD2	1.97	0.45
1:E:118:GLN:OE1	2:F:231:ASP:HB3	2.16	0.45
3:G:166:LEU:CD1	3:G:172:ILE:HG23	2.40	0.45
1:A:284:ILE:HG22	1:A:285:LYS:H	1.81	0.45
2:B:235:ILE:H	2:B:235:ILE:HG13	1.59	0.45
2:K:100:LEU:N	3:L:174:GLN:HG2	2.32	0.45
3:C:32:ILE:HD13	3:C:180:HIS:O	2.16	0.45
3:C:135:VAL:HG22	3:C:136:ALA:H	1.80	0.45
3:I:205:SER:HB2	3:I:208:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:99:HIS:HD2	3:L:100:TYR:H	1.64	0.45
2:F:52:ILE:HG21	2:F:69:LEU:HB3	1.98	0.45
1:D:293:ALA:HB1	2:H:83:CYS:SG	2.57	0.45
1:J:205:TYR:O	1:J:223:GLY:HA2	2.17	0.45
1:M:128:TYR:CE1	1:M:202:GLN:HG3	2.51	0.45
1:M:141:THR:OG1	1:M:145:GLU:N	2.50	0.45
2:B:204:VAL:HB	2:B:208:ALA:HB3	1.99	0.45
2:N:85:VAL:CG1	2:N:194:VAL:HB	2.46	0.45
3:I:82:PHE:O	3:I:85:VAL:HG12	2.17	0.45
1:E:138:VAL:HG13	1:E:250:ARG:HB2	1.99	0.45
1:E:198:ALA:O	2:F:31:THR:OG1	2.28	0.45
2:F:133:ILE:HG23	2:F:196:ILE:HG12	1.99	0.45
1:J:269:GLN:HE22	1:J:284:ILE:N	2.11	0.45
2:B:54:GLU:O	2:B:95:PRO:HB3	2.16	0.45
1:A:273:PHE:HB2	1:A:276:ASN:OD1	2.16	0.45
2:H:78:GLY:O	2:H:79:LYS:HG2	2.16	0.45
3:C:205:SER:HB2	3:C:208:ASN:ND2	2.32	0.45
3:I:25:THR:C	3:I:27:GLU:H	2.24	0.45
1:E:134:GLU:CD	1:E:189:GLN:HE21	2.25	0.45
1:D:171:TRP:CE2	1:D:236:ARG:HD3	2.52	0.45
1:A:268:ASN:OD1	1:A:269:GLN:N	2.50	0.45
1:D:120:ARG:NE	1:D:124:GLU:OE1	2.37	0.45
1:M:127:THR:OG1	1:M:128:TYR:N	2.50	0.45
2:K:73:VAL:HG12	2:K:82:LEU:HD13	1.99	0.45
1:E:77:GLU:OE2	2:F:228:LEU:HA	2.17	0.45
1:E:147:VAL:O	1:E:149:GLN:N	2.48	0.45
1:E:266:MET:HE1	2:F:107:TYR:CE1	2.52	0.45
3:G:119:GLN:O	3:G:222:LEU:HA	2.17	0.45
1:D:111:ILE:HD13	1:D:230:MET:HG3	1.99	0.45
1:J:128:TYR:CD1	1:J:202:GLN:HG3	2.52	0.45
1:M:197:PRO:O	2:N:31:THR:HG21	2.16	0.45
2:B:137:PRO:HG3	3:O:248:LEU:HD11	1.99	0.45
3:C:98:PHE:O	3:C:248:LEU:HD22	2.17	0.45
3:C:119:GLN:O	3:C:222:LEU:HA	2.17	0.45
2:F:66:MET:SD	3:G:172:ILE:HD11	2.57	0.44
1:A:167:GLU:H	1:A:167:GLU:HG2	1.61	0.44
1:D:156:VAL:HA	1:D:157:PRO:HD3	1.86	0.44
1:D:205:TYR:O	1:D:223:GLY:HA2	2.17	0.44
1:D:208:TYR:C	1:D:210:THR:H	2.24	0.44
1:J:116:TYR:CD2	1:J:119:MET:HB2	2.51	0.44
2:B:110:GLN:CD	2:B:227:GLN:HG2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:40:SER:OG	3:L:41:TYR:N	2.50	0.44
3:L:84:ASP:O	3:L:87:THR:HG23	2.17	0.44
3:G:95:ASN:O	3:G:99:HIS:HB2	2.18	0.44
2:B:84:ALA:C	2:B:86:PHE:H	2.25	0.44
2:B:90:PRO:HA	2:B:96:TRP:CG	2.52	0.44
2:B:131:MET:SD	2:B:198:TYR:HD1	2.40	0.44
2:H:88:ALA:HA	2:H:96:TRP:HE1	1.82	0.44
3:C:100:TYR:CD2	3:C:248:LEU:HD11	2.53	0.44
3:C:232:ILE:HA	3:C:233:PRO:HD3	1.61	0.44
3:O:70:LEU:HD22	3:O:231:VAL:HG11	2.00	0.44
3:G:105:GLY:N	3:G:241:MET:O	2.45	0.44
1:A:85:SER:OG	1:A:254:ARG:NH2	2.50	0.44
3:O:77:GLY:HA3	3:O:217:VAL:HG22	1.99	0.44
3:O:99:HIS:ND1	3:O:245:PHE:HD1	2.16	0.44
3:G:164:TYR:O	3:G:171:PRO:HA	2.18	0.44
1:M:84:PHE:CD2	1:M:258:VAL:HG11	2.51	0.44
1:M:110:ASP:HA	1:M:232:THR:HB	1.98	0.44
2:B:133:ILE:HG23	2:B:196:ILE:HG12	1.99	0.44
3:C:82:PHE:CE2	3:C:108:ILE:HG21	2.52	0.44
3:L:26:GLN:NE2	3:L:26:GLN:CA	2.74	0.44
3:G:232:ILE:HA	3:G:233:PRO:HD3	1.64	0.44
1:D:141:THR:OG1	1:D:145:GLU:N	2.50	0.44
1:J:125:LEU:O	1:J:264:ARG:N	2.35	0.44
1:J:287:THR:HG21	2:K:94:GLY:O	2.17	0.44
3:I:126:VAL:HG13	3:I:212:PHE:HE1	1.81	0.44
1:A:182:LYS:HD3	1:D:146:VAL:HG21	1.99	0.44
3:I:232:ILE:HA	3:I:233:PRO:HD3	1.61	0.44
3:L:105:GLY:N	3:L:241:MET:O	2.43	0.44
3:O:157:GLY:HA2	3:O:158:PHE:HA	1.80	0.44
1:E:147:VAL:HG11	1:E:245:TYR:CG	2.53	0.44
2:B:61:ASN:O	2:B:65:LEU:N	2.50	0.44
3:O:69:LYS:HE2	3:O:69:LYS:HB3	1.47	0.44
1:M:129:MET:O	1:M:201:TYR:HB2	2.17	0.44
1:M:268:ASN:OD1	1:M:269:GLN:HG2	2.18	0.44
1:E:95:LEU:HD23	1:E:105:GLY:HA2	1.99	0.44
2:K:200:THR:OG1	2:K:201:ASN:N	2.50	0.44
3:C:148:TYR:CE2	3:C:149:LYS:HD3	2.53	0.44
3:I:107:CYS:HA	3:I:194:ILE:HG12	1.99	0.44
3:I:118:HIS:ND1	3:I:232:ILE:HD11	2.30	0.44
3:O:55:ARG:HD3	3:O:56:PRO:O	2.17	0.44
3:O:108:ILE:HD12	3:O:214:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:132:LEU:HA	2:F:156:ILE:HA	2.00	0.43
3:G:98:PHE:CZ	3:G:250:GLN:HG3	2.53	0.43
3:G:118:HIS:CD2	3:G:224:TYR:HB3	2.53	0.43
2:B:200:THR:OG1	2:B:201:ASN:N	2.51	0.43
2:H:118:THR:HG22	2:H:166:THR:HG23	1.99	0.43
3:O:209:HIS:CE1	3:O:211:ASN:HD22	2.36	0.43
2:F:66:MET:HE3	2:F:66:MET:HB3	1.80	0.43
2:F:87:ARG:NH1	2:F:92:ARG:O	2.51	0.43
1:A:111:ILE:HD11	1:A:135:PHE:CZ	2.53	0.43
1:A:285:LYS:NZ	1:A:286:PRO:HG2	2.33	0.43
1:A:287:THR:HG21	2:B:94:GLY:O	2.18	0.43
1:D:111:ILE:HD11	1:D:135:PHE:HZ	1.83	0.43
1:J:82:SER:HA	2:H:27:ASN:ND2	2.34	0.43
3:C:126:VAL:HB	3:C:212:PHE:CE1	2.53	0.43
1:E:121:ARG:HD3	2:F:107:TYR:OH	2.17	0.43
2:F:79:LYS:HB3	2:F:79:LYS:HE2	1.75	0.43
1:J:111:ILE:HG22	1:J:231:GLY:O	2.19	0.43
1:M:77:GLU:OE2	2:N:228:LEU:HA	2.18	0.43
1:M:122:LYS:NZ	2:N:231:ASP:OD2	2.48	0.43
3:C:116:LYS:HD2	3:C:116:LYS:N	2.33	0.43
3:L:195:VAL:HG21	3:L:212:PHE:CE2	2.53	0.43
1:E:197:PRO:O	2:F:31:THR:HG21	2.18	0.43
2:F:145:ASP:O	2:F:148:THR:OG1	2.37	0.43
2:F:162:GLN:OE1	3:G:186:ARG:NH1	2.51	0.43
1:D:189:GLN:HB2	2:K:8:PRO:HB2	2.00	0.43
1:J:267:ARG:HD2	3:L:169:GLY:O	2.19	0.43
2:H:85:VAL:CG1	2:H:194:VAL:HB	2.48	0.43
2:K:90:PRO:HA	2:K:96:TRP:CB	2.48	0.43
3:C:103:ARG:HG3	3:C:197:TYR:CG	2.53	0.43
1:E:143:THR:CG2	1:J:244:LYS:HB2	2.49	0.43
3:G:249:ARG:NH1	2:N:136:THR:OG1	2.51	0.43
1:J:261:TRP:CD1	2:K:36:ILE:HB	2.53	0.43
2:N:136:THR:O	2:N:193:LEU:N	2.41	0.43
1:E:197:PRO:HB3	2:N:110:GLN:NE2	2.33	0.43
1:E:269:GLN:OE1	1:E:284:ILE:HG22	2.18	0.43
1:A:128:TYR:CD1	1:A:202:GLN:HG3	2.54	0.43
1:D:268:ASN:HD22	3:I:171:PRO:HB3	1.84	0.43
1:M:81:ASP:O	1:M:85:SER:N	2.40	0.43
2:K:84:ALA:HA	2:K:195:SER:HA	2.00	0.43
2:K:122:THR:O	3:L:119:GLN:HB2	2.18	0.43
2:F:79:LYS:HA	2:F:198:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:134:GLU:CD	1:J:189:GLN:HE21	2.26	0.43
2:B:51:THR:OG1	3:C:173:SER:O	2.37	0.43
2:N:46:LEU:O	2:N:49:VAL:HG12	2.18	0.43
3:I:108:ILE:HD12	3:I:214:LEU:HD22	2.01	0.43
3:O:127:LEU:HA	3:O:128:PRO:HD3	1.84	0.43
3:O:166:LEU:CD1	3:O:172:ILE:HG23	2.46	0.43
1:A:127:THR:OG1	1:A:128:TYR:N	2.51	0.43
2:B:115:LEU:HD12	2:B:169:ILE:HD11	2.00	0.43
3:I:93:GLY:O	3:I:97:GLN:HB2	2.19	0.43
1:E:261:TRP:HA	2:F:39:GLU:HA	1.99	0.43
1:A:217:ALA:C	1:A:218:ASN:ND2	2.72	0.43
2:B:226:MET:HE2	2:B:226:MET:HB3	1.93	0.43
2:H:136:THR:OG1	3:C:249:ARG:NH2	2.51	0.43
2:H:136:THR:HB	2:H:193:LEU:HB2	2.01	0.43
2:K:87:ARG:HB3	2:K:191:THR:OG1	2.18	0.43
3:O:205:SER:HB2	3:O:208:ASN:ND2	2.30	0.43
1:M:114:THR:HG23	1:M:120:ARG:HD2	2.00	0.43
2:B:78:GLY:O	2:B:79:LYS:HG2	2.18	0.43
2:N:107:TYR:HA	2:N:230:LYS:O	2.18	0.43
3:L:52:LYS:HA	3:L:53:PRO:HD2	1.89	0.43
3:O:113:ASN:O	3:O:233:PRO:HD2	2.19	0.43
3:G:92:PHE:HZ	3:G:102:TYR:HE1	1.67	0.42
3:G:157:GLY:HA3	3:G:158:PHE:CG	2.54	0.42
2:N:115:LEU:HD11	2:N:172:ILE:HD11	2.01	0.42
3:I:70:LEU:HB3	3:I:231:VAL:HG13	2.01	0.42
3:L:20:ASN:OD1	3:L:62:ARG:NH1	2.52	0.42
2:F:235:ILE:H	2:F:235:ILE:HG13	1.48	0.42
1:A:171:TRP:CH2	1:A:234:SER:HB3	2.54	0.42
1:D:87:ALA:HA	1:D:253:MET:O	2.19	0.42
1:D:201:TYR:CZ	1:D:230:MET:HE2	2.54	0.42
1:M:116:TYR:CD2	1:M:119:MET:HE2	2.54	0.42
3:O:57:ASP:O	3:O:61:ASN:ND2	2.52	0.42
3:O:85:VAL:HG13	3:O:86:LEU:HG	2.00	0.42
1:A:166:ARG:HG2	1:A:236:ARG:HH21	1.83	0.42
2:N:56:ASN:O	2:N:68:ARG:HA	2.19	0.42
3:I:157:GLY:HA2	3:I:158:PHE:HA	1.80	0.42
3:O:248:LEU:HG	3:O:249:ARG:H	1.84	0.42
1:E:149:GLN:HB3	1:E:183:LEU:HD13	2.01	0.42
3:G:109:HIS:NE2	3:G:190:CYS:HB2	2.34	0.42
3:G:133:GLY:HA3	3:G:134:THR:HA	1.75	0.42
1:D:136:THR:HG21	2:H:13:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:PRO:HB2	3:I:170:ILE:CG2	2.49	0.42
1:M:261:TRP:NE1	2:N:36:ILE:HB	2.34	0.42
2:K:115:LEU:HB2	2:K:169:ILE:HD11	2.01	0.42
3:C:106:PHE:CE2	3:C:240:PRO:HB3	2.55	0.42
2:F:65:LEU:HD22	3:G:164:TYR:CG	2.54	0.42
1:A:127:THR:OG1	1:A:262:ILE:HB	2.20	0.42
1:A:171:TRP:HH2	1:A:234:SER:HB3	1.84	0.42
1:D:97:LEU:HD12	1:D:97:LEU:HA	1.86	0.42
1:D:237:THR:HG22	1:D:247:LEU:HD12	2.00	0.42
1:D:259:ARG:HH21	1:D:261:TRP:HZ2	1.68	0.42
1:J:171:TRP:CZ2	1:J:236:ARG:HD3	2.55	0.42
2:B:136:THR:HG23	3:O:249:ARG:NH1	2.34	0.42
2:B:221:GLN:HB2	2:B:222:LYS:H	1.62	0.42
2:N:157:TRP:CD2	2:N:165:VAL:HG11	2.55	0.42
3:I:128:PRO:HB3	3:I:198:ILE:HD12	2.00	0.42
3:L:84:ASP:O	3:L:86:LEU:N	2.53	0.42
3:O:126:VAL:HG22	3:O:212:PHE:CZ	2.52	0.42
1:E:125:LEU:O	1:E:264:ARG:N	2.43	0.42
2:F:90:PRO:HA	2:F:96:TRP:CB	2.50	0.42
1:J:111:ILE:HD11	1:J:135:PHE:CE2	2.54	0.42
2:H:66:MET:HB3	2:H:66:MET:HE3	1.68	0.42
3:I:99:HIS:HD2	3:I:100:TYR:H	1.66	0.42
3:G:82:PHE:HZ	3:G:108:ILE:HG21	1.85	0.42
1:D:130:ARG:NH2	2:H:31:THR:O	2.53	0.42
1:J:118:GLN:HB2	2:K:233:SER:OG	2.19	0.42
1:J:186:PRO:HG3	2:K:11:ASN:OD1	2.20	0.42
2:K:85:VAL:O	2:K:85:VAL:HG13	2.20	0.42
2:K:117:VAL:HG13	2:K:218:ALA:HB2	2.01	0.42
3:C:128:PRO:O	3:C:212:PHE:HA	2.20	0.42
2:F:59:PRO:HD2	2:F:68:ARG:HG2	2.01	0.42
2:F:61:ASN:OD1	2:F:61:ASN:N	2.53	0.42
1:A:256:LYS:O	1:A:258:VAL:HG23	2.19	0.42
1:J:198:ALA:HB1	3:L:200:ALA:HB1	2.01	0.42
2:H:136:THR:N	2:H:193:LEU:O	2.33	0.42
1:E:128:TYR:CE1	1:E:202:GLN:HG3	2.55	0.42
1:D:111:ILE:HD11	1:D:135:PHE:CZ	2.55	0.42
1:J:125:LEU:HD12	1:J:264:ARG:O	2.19	0.42
3:I:126:VAL:HG13	3:I:212:PHE:CE1	2.55	0.42
2:B:117:VAL:HG13	2:B:218:ALA:HB2	2.01	0.42
2:K:42:ASN:OD1	2:K:43:LEU:N	2.53	0.42
2:K:91:GLY:HA3	2:K:111:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:119:GLN:O	3:L:222:LEU:HA	2.19	0.42
1:E:227:ASN:OD1	1:E:227:ASN:N	2.53	0.41
1:D:177:PRO:HB2	2:H:24:ILE:HD11	2.02	0.41
2:B:72:PRO:O	2:B:82:LEU:HD11	2.20	0.41
2:K:108:TYR:HB2	2:K:226:MET:HE2	2.02	0.41
3:L:232:ILE:HA	3:L:233:PRO:HD3	1.66	0.41
1:E:194:PHE:CZ	1:E:196:SER:HB3	2.55	0.41
1:E:264:ARG:NH1	3:G:127:LEU:HD21	2.35	0.41
2:F:72:PRO:HB3	2:F:213:TYR:CE1	2.54	0.41
2:F:134:ALA:CB	2:F:149:ALA:HB1	2.50	0.41
3:I:146:PRO:HA	3:I:147:PRO:HD3	1.92	0.41
3:I:166:LEU:CD1	3:I:172:ILE:HG23	2.50	0.41
1:E:127:THR:OG1	1:E:262:ILE:HB	2.20	0.41
3:I:81:LYS:O	3:I:85:VAL:HB	2.20	0.41
3:I:195:VAL:HG21	3:I:212:PHE:CZ	2.56	0.41
3:O:99:HIS:CD2	3:O:100:TYR:N	2.88	0.41
3:O:157:GLY:HA3	3:O:158:PHE:CD1	2.55	0.41
3:O:176:THR:HB	3:O:180:HIS:CE1	2.54	0.41
1:D:222:TYR:OH	3:I:150:GLN:NE2	2.47	0.41
1:J:207:GLY:HA3	3:L:209:HIS:HA	2.02	0.41
1:M:161:PRO:HD2	2:B:230:LYS:NZ	2.27	0.41
2:H:36:ILE:HD11	3:I:200:ALA:HA	2.02	0.41
2:H:140:GLY:HA2	2:H:141:PRO:HD3	1.90	0.41
2:K:61:ASN:OD1	2:K:64:SER:HB3	2.20	0.41
3:C:84:ASP:O	3:C:86:LEU:N	2.54	0.41
3:I:81:LYS:HB2	3:I:84:ASP:OD2	2.20	0.41
3:O:133:GLY:HA3	3:O:134:THR:HA	1.76	0.41
1:E:89:LEU:HB2	1:E:252:TYR:CE2	2.55	0.41
2:F:101:LEU:HD11	2:F:224:PHE:CZ	2.56	0.41
2:F:114:SER:OG	2:F:170:PRO:O	2.22	0.41
1:D:135:PHE:CE1	1:D:253:MET:HB2	2.51	0.41
1:D:140:CYS:SG	1:D:250:ARG:NH1	2.92	0.41
1:D:285:LYS:HA	1:D:286:PRO:HD2	1.96	0.41
1:J:136:THR:HG21	2:K:13:PHE:CD1	2.56	0.41
2:H:91:GLY:HA3	2:H:111:TRP:CH2	2.54	0.41
2:H:115:LEU:HD12	2:H:169:ILE:HD11	2.02	0.41
2:N:100:LEU:N	3:O:174:GLN:HG2	2.34	0.41
1:E:102:ASN:N	1:E:102:ASN:ND2	2.69	0.41
2:F:88:ALA:O	2:F:172:ILE:HG21	2.21	0.41
3:G:128:PRO:O	3:G:212:PHE:HA	2.21	0.41
1:A:211:PHE:HA	3:C:208:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:109:TRP:CZ3	1:M:111:ILE:HA	2.55	0.41
2:B:57:ASN:OD1	2:B:57:ASN:N	2.54	0.41
2:H:234:ASP:OD1	2:H:235:ILE:HG23	2.20	0.41
2:K:66:MET:HE3	2:K:66:MET:HB3	1.80	0.41
3:O:135:VAL:HG22	3:O:136:ALA:H	1.86	0.41
1:E:127:THR:OG1	1:E:128:TYR:N	2.53	0.41
1:E:131:PHE:CZ	1:E:255:MET:HE3	2.56	0.41
1:J:264:ARG:NH1	3:L:127:LEU:HD21	2.36	0.41
2:K:89:ASP:O	2:K:92:ARG:HB3	2.21	0.41
3:I:22:THR:HG22	3:I:63:PHE:HE2	1.85	0.41
3:L:65:THR:HG22	3:L:237:THR:HG23	2.02	0.41
3:O:83:PRO:HG2	3:O:211:ASN:N	2.32	0.41
1:E:264:ARG:HH12	3:G:127:LEU:HD21	1.85	0.41
1:E:266:MET:HE2	2:F:103:GLN:HB3	2.01	0.41
1:D:210:THR:HG21	1:D:214:HIS:CB	2.50	0.41
2:H:57:ASN:OD1	2:H:57:ASN:N	2.46	0.41
2:N:113:GLY:HA3	2:N:224:PHE:HA	2.02	0.41
1:E:129:MET:O	1:E:201:TYR:HB2	2.21	0.41
1:E:140:CYS:O	1:E:248:VAL:N	2.49	0.41
2:F:57:ASN:HB2	2:F:68:ARG:HH21	1.86	0.41
2:F:128:THR:HG22	2:F:129:GLY:N	2.35	0.41
1:A:285:LYS:HZ2	1:A:286:PRO:HG2	1.86	0.41
1:D:194:PHE:HE1	1:D:201:TYR:CD1	2.38	0.41
1:J:77:GLU:HG3	2:H:27:ASN:O	2.20	0.41
1:M:271:TYR:CD1	2:N:235:ILE:HG21	2.54	0.41
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.90	0.41
2:B:136:THR:OG1	2:B:143:PRO:HD3	2.21	0.41
2:H:69:LEU:H	2:H:69:LEU:HG	1.60	0.41
2:H:74:SER:HA	2:H:211:THR:HA	2.03	0.41
2:N:66:MET:SD	3:O:172:ILE:HD11	2.61	0.41
3:C:157:GLY:HA2	3:C:158:PHE:HA	1.76	0.41
3:I:69:LYS:NZ	3:I:78:TRP:CG	2.89	0.41
3:I:92:PHE:O	3:I:96:ALA:N	2.40	0.41
3:L:99:HIS:CD2	3:L:248:LEU:HD11	2.55	0.41
3:L:134:THR:HG22	3:L:135:VAL:N	2.35	0.41
3:O:128:PRO:HB3	3:O:198:ILE:HD12	2.03	0.41
1:E:77:GLU:HG3	2:K:27:ASN:O	2.20	0.41
2:F:70:ARG:HD2	2:F:213:TYR:CG	2.55	0.41
1:D:155:PHE:HB2	1:D:233:PHE:CE1	2.56	0.41
1:M:194:PHE:O	2:N:30:PRO:HB3	2.21	0.41
3:I:69:LYS:HE2	3:I:69:LYS:HB3	1.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:248:LEU:CD2	3:I:249:ARG:H	2.21	0.41
3:L:248:LEU:HB3	3:L:249:ARG:H	1.52	0.41
3:G:22:THR:HG22	3:G:63:PHE:CE2	2.56	0.40
3:G:70:LEU:HD22	3:G:231:VAL:HG11	2.03	0.40
3:L:112:CYS:HB3	3:L:234:ILE:HG22	2.02	0.40
3:O:149:LYS:HD2	3:O:149:LYS:HA	1.81	0.40
2:F:226:MET:HE2	2:F:226:MET:HB3	2.00	0.40
3:G:127:LEU:HA	3:G:128:PRO:HD3	1.90	0.40
3:G:232:ILE:HA	3:G:232:ILE:HD13	1.86	0.40
1:D:176:ASN:HA	1:D:177:PRO:HD2	1.91	0.40
1:M:285:LYS:HA	1:M:286:PRO:HD2	1.96	0.40
2:B:2:PHE:HA	2:B:3:PRO:HD3	1.84	0.40
2:N:119:PHE:HB2	2:N:165:VAL:HG13	2.03	0.40
2:N:145:ASP:O	2:N:148:THR:OG1	2.36	0.40
1:E:135:PHE:CE1	1:E:253:MET:HB2	2.55	0.40
2:F:161:LEU:HD23	2:F:161:LEU:O	2.20	0.40
3:G:126:VAL:HG22	3:G:212:PHE:HZ	1.86	0.40
1:J:192:VAL:HG22	2:K:24:ILE:HG21	2.03	0.40
1:M:102:ASN:C	1:M:104:ASN:H	2.29	0.40
2:B:14:LEU:HD23	2:B:16:THR:H	1.86	0.40
2:B:118:THR:HG22	2:B:166:THR:HG22	2.03	0.40
2:H:71:PHE:HA	2:H:72:PRO:HD3	1.90	0.40
2:N:66:MET:HE3	2:N:66:MET:HB3	1.91	0.40
3:L:133:GLY:HA3	3:L:134:THR:HA	1.81	0.40
1:A:111:ILE:HG22	1:A:231:GLY:O	2.21	0.40
1:M:254:ARG:HH12	2:N:18:ASP:HA	1.86	0.40
2:H:84:ALA:C	2:H:86:PHE:N	2.78	0.40
3:I:28:ALA:O	3:I:30:ASN:N	2.46	0.40
3:L:66:LEU:HB3	3:L:155:ALA:HB1	2.04	0.40
2:F:174:ASN:HD21	2:F:176:HIS:CE1	2.39	0.40
3:G:157:GLY:HA2	3:G:158:PHE:HA	1.86	0.40
1:J:256:LYS:O	1:J:258:VAL:HG23	2.21	0.40
3:C:100:TYR:CD1	3:C:101:LEU:N	2.88	0.40
3:L:118:HIS:ND1	3:L:232:ILE:HD11	2.36	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:THR:OG1	2:H:60:THR:OG1[14_777]	2.02	0.18
2:H:158:ASP:OD2	3:I:113:ASN:ND2[5_636]	2.19	0.01

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	223/297 (75%)	199 (89%)	22 (10%)	2 (1%)	14	45
1	D	223/297 (75%)	202 (91%)	21 (9%)	0	100	100
1	E	223/297 (75%)	198 (89%)	23 (10%)	2 (1%)	14	45
1	J	223/297 (75%)	199 (89%)	23 (10%)	1 (0%)	30	62
1	M	223/297 (75%)	199 (89%)	22 (10%)	2 (1%)	14	45
2	B	220/242 (91%)	198 (90%)	20 (9%)	2 (1%)	14	45
2	F	220/242 (91%)	201 (91%)	17 (8%)	2 (1%)	14	45
2	H	220/242 (91%)	200 (91%)	20 (9%)	0	100	100
2	K	220/242 (91%)	201 (91%)	19 (9%)	0	100	100
2	N	220/242 (91%)	199 (90%)	20 (9%)	1 (0%)	24	57
3	C	233/323 (72%)	196 (84%)	34 (15%)	3 (1%)	9	38
3	G	233/323 (72%)	197 (84%)	32 (14%)	4 (2%)	7	34
3	I	233/323 (72%)	198 (85%)	32 (14%)	3 (1%)	9	38
3	L	233/323 (72%)	195 (84%)	36 (16%)	2 (1%)	14	45
3	O	233/323 (72%)	196 (84%)	34 (15%)	3 (1%)	9	38
All	All	3380/4310 (78%)	2978 (88%)	375 (11%)	27 (1%)	16	48

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	128	PRO
3	I	145	HIS
3	G	27	GLU
3	G	128	PRO
3	I	128	PRO
3	L	128	PRO
3	O	128	PRO
1	A	291	ARG

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Mol	Chain	Res	Type
3	C	20	ASN
3	G	29	ALA
2	B	79	LYS
3	C	226	GLN
3	L	222	LEU
3	O	222	LEU
3	O	226	GLN
1	E	291	ARG
3	G	222	LEU
1	M	291	ARG
3	I	222	LEU
2	B	37	PRO
1	M	148	PRO
2	N	37	PRO
2	F	37	PRO
1	E	148	PRO
1	A	148	PRO
2	F	58	VAL
1	J	103	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	192/250 (77%)	187 (97%)	5 (3%)	40	60
1	D	192/250 (77%)	185 (96%)	7 (4%)	31	54
1	E	192/250 (77%)	188 (98%)	4 (2%)	47	64
1	J	192/250 (77%)	189 (98%)	3 (2%)	55	68
1	M	192/250 (77%)	182 (95%)	10 (5%)	21	46
2	B	188/202 (93%)	178 (95%)	10 (5%)	20	45
2	F	188/202 (93%)	177 (94%)	11 (6%)	18	43
2	H	188/202 (93%)	178 (95%)	10 (5%)	20	45
2	K	188/202 (93%)	178 (95%)	10 (5%)	20	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	188/202 (93%)	173 (92%)	15 (8%)	11	36
3	C	200/272 (74%)	193 (96%)	7 (4%)	32	54
3	G	200/272 (74%)	194 (97%)	6 (3%)	36	57
3	I	200/272 (74%)	191 (96%)	9 (4%)	24	48
3	L	200/272 (74%)	191 (96%)	9 (4%)	24	48
3	O	200/272 (74%)	193 (96%)	7 (4%)	32	54
All	All	2900/3620 (80%)	2777 (96%)	123 (4%)	26	50

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	86	ARG
1	E	102	ASN
1	E	138	VAL
1	E	232	THR
2	F	33	CYS
2	F	46	LEU
2	F	55	VAL
2	F	61	ASN
2	F	69	LEU
2	F	132	LEU
2	F	155	VAL
2	F	165	VAL
2	F	168	VAL
2	F	222	LYS
2	F	227	GLN
3	G	27	GLU
3	G	72	GLU
3	G	126	VAL
3	G	135	VAL
3	G	151	THR
3	G	172	ILE
1	A	74	SER
1	A	100	THR
1	A	138	VAL
1	A	167	GLU
1	A	232	THR
1	D	108	ASN
1	D	167	GLU
1	D	215	LEU

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Mol	Chain	Res	Type
1	D	218	ASN
1	D	219	ASP
1	D	232	THR
1	D	278	ASN
1	J	94	ASP
1	J	138	VAL
1	J	215	LEU
1	M	86	ARG
1	M	97	LEU
1	M	101	THR
1	M	102	ASN
1	M	118	GLN
1	M	138	VAL
1	M	213	GLU
1	M	215	LEU
1	M	232	THR
1	M	278	ASN
2	B	20	VAL
2	B	46	LEU
2	B	69	LEU
2	B	132	LEU
2	B	155	VAL
2	B	165	VAL
2	B	168	VAL
2	B	222	LYS
2	B	227	GLN
2	B	235	ILE
2	H	34	ILE
2	H	46	LEU
2	H	48	GLN
2	H	55	VAL
2	H	69	LEU
2	H	155	VAL
2	H	165	VAL
2	H	168	VAL
2	H	221	GLN
2	H	227	GLN
2	K	33	CYS
2	K	34	ILE
2	K	46	LEU
2	K	69	LEU
2	K	85	VAL

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Mol	Chain	Res	Type
2	K	132	LEU
2	K	155	VAL
2	K	165	VAL
2	K	168	VAL
2	K	221	GLN
2	N	33	CYS
2	N	34	ILE
2	N	35	HIS
2	N	46	LEU
2	N	55	VAL
2	N	61	ASN
2	N	64	SER
2	N	69	LEU
2	N	76	GLN
2	N	93	SER
2	N	132	LEU
2	N	155	VAL
2	N	165	VAL
2	N	168	VAL
2	N	222	LYS
3	C	44	ASP
3	C	55	ARG
3	C	72	GLU
3	C	76	LYS
3	C	159	GLU
3	C	172	ILE
3	C	187	THR
3	I	72	GLU
3	I	76	LYS
3	I	97	GLN
3	I	126	VAL
3	I	145	HIS
3	I	150	GLN
3	I	159	GLU
3	I	172	ILE
3	I	226	GLN
3	L	26	GLN
3	L	55	ARG
3	L	72	GLU
3	L	76	LYS
3	L	94	GLN
3	L	126	VAL

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Mol	Chain	Res	Type
3	L	159	GLU
3	L	172	ILE
3	L	250	GLN
3	O	58	VAL
3	O	76	LYS
3	O	126	VAL
3	O	151	THR
3	O	152	GLN
3	O	172	ILE
3	O	188	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	102	ASN
1	E	118	GLN
1	E	149	GLN
1	E	189	GLN
1	E	218	ASN
1	E	270	ASN
1	E	278	ASN
2	F	176	HIS
3	G	161	GLN
1	A	104	ASN
1	A	269	GLN
1	D	102	ASN
1	D	118	GLN
1	D	189	GLN
1	D	216	GLN
1	J	118	GLN
1	J	218	ASN
1	J	228	ASN
1	J	269	GLN
1	J	270	ASN
1	M	149	GLN
1	M	189	GLN
1	M	202	GLN
1	M	214	HIS
2	B	61	ASN
2	B	221	GLN
2	H	110	GLN
2	H	227	GLN

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Mol	Chain	Res	Type
2	K	162	GLN
2	N	48	GLN
2	N	76	GLN
2	N	110	GLN
2	N	221	GLN
3	C	99	HIS
3	C	111	GLN
3	C	119	GLN
3	C	152	GLN
3	C	161	GLN
3	I	109	HIS
3	I	161	GLN
3	I	180	HIS
3	L	26	GLN
3	L	99	HIS
3	O	30	ASN
3	O	109	HIS
3	O	150	GLN
3	O	181	GLN
3	O	209	HIS

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	225/297 (75%)	0.31	3 (1%)	75 53	75, 100, 167, 219	0
1	D	225/297 (75%)	0.33	6 (2%)	56 38	74, 96, 172, 219	0
1	E	225/297 (75%)	0.27	5 (2%)	62 44	77, 98, 163, 222	0
1	J	225/297 (75%)	0.34	6 (2%)	56 38	76, 99, 170, 212	0
1	M	225/297 (75%)	0.37	7 (3%)	51 35	75, 100, 172, 220	0
2	B	224/242 (92%)	0.36	5 (2%)	62 44	77, 101, 128, 163	0
2	F	224/242 (92%)	0.38	7 (3%)	51 35	78, 96, 124, 153	0
2	H	224/242 (92%)	0.41	8 (3%)	46 32	76, 96, 122, 156	0
2	K	224/242 (92%)	0.32	3 (1%)	75 53	78, 101, 127, 168	0
2	N	224/242 (92%)	0.31	7 (3%)	51 35	79, 103, 127, 161	0
3	C	235/323 (72%)	0.55	8 (3%)	48 33	76, 121, 195, 213	0
3	G	235/323 (72%)	0.46	8 (3%)	48 33	75, 116, 191, 212	0
3	I	235/323 (72%)	0.65	18 (7%)	19 18	74, 117, 200, 223	0
3	L	235/323 (72%)	0.49	11 (4%)	36 27	78, 122, 201, 226	0
3	O	235/323 (72%)	0.62	15 (6%)	25 21	79, 124, 193, 222	0
All	All	3420/4310 (79%)	0.41	117 (3%)	48 33	74, 102, 183, 226	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	247	GLY	5.2
3	O	16	LEU	5.0
3	O	247	GLY	5.0
3	L	246	ALA	4.4
2	N	235	ILE	4.3
3	O	248	LEU	4.1
2	F	85	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
3	I	18	ILE	3.9
2	K	235	ILE	3.8
3	L	23	ILE	3.7
1	E	211	PHE	3.5
2	N	128	THR	3.5
3	I	48	THR	3.5
1	M	85	SER	3.4
3	I	49	ALA	3.4
3	O	246	ALA	3.3
3	L	247	GLY	3.3
2	H	93	SER	3.2
3	I	16	LEU	3.2
3	I	146	PRO	3.1
1	M	215	LEU	3.1
2	H	85	VAL	3.1
3	O	191	ALA	3.1
3	C	135	VAL	3.1
3	O	23	ILE	3.1
2	H	175	THR	3.1
2	F	227	GLN	3.0
3	G	248	LEU	3.0
3	O	249	ARG	3.0
1	J	153	TYR	3.0
1	M	211	PHE	2.9
3	O	18	ILE	2.9
2	F	194	VAL	2.8
3	L	248	LEU	2.8
2	N	163	SER	2.8
1	D	266	MET	2.7
3	L	102	TYR	2.7
2	H	123	GLY	2.7
1	E	208	TYR	2.7
1	D	277	PRO	2.7
1	D	288	GLY	2.7
2	K	206	ILE	2.7
3	O	146	PRO	2.6
1	J	256	LYS	2.6
2	N	1	GLY	2.6
3	O	47	ALA	2.6
1	M	293	ALA	2.6
1	D	286	PRO	2.6
2	N	190	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	50	VAL	2.6
2	H	120	MET	2.6
3	C	248	LEU	2.6
2	N	170	PRO	2.5
3	G	48	THR	2.5
1	E	215	LEU	2.5
3	G	63	PHE	2.5
3	L	145	HIS	2.5
2	B	163	SER	2.5
3	G	49	ALA	2.5
1	J	220	LEU	2.5
3	O	42	CYS	2.5
1	E	222	TYR	2.4
3	I	145	HIS	2.4
1	J	212	GLY	2.4
3	I	47	ALA	2.4
3	O	55	ARG	2.4
3	I	24	THR	2.4
3	C	133	GLY	2.4
3	I	138	GLY	2.4
3	C	99	HIS	2.4
2	F	91	GLY	2.3
3	L	135	VAL	2.3
2	H	86	PHE	2.3
3	G	18	ILE	2.3
3	C	85	VAL	2.3
1	M	143	THR	2.3
2	H	164	SER	2.3
3	G	19	GLY	2.3
2	B	85	VAL	2.3
1	A	286	PRO	2.3
3	I	141	THR	2.3
2	F	167	LEU	2.2
3	C	146	PRO	2.2
3	L	207	LEU	2.2
3	O	190	CYS	2.2
3	O	243	SER	2.2
2	F	1	GLY	2.2
1	A	215	LEU	2.2
3	I	58	VAL	2.2
2	K	86	PHE	2.1
1	J	296	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	236	LEU	2.1
3	C	49	ALA	2.1
3	I	69	LYS	2.1
3	I	225	ASP	2.1
3	C	247	GLY	2.1
2	F	86	PHE	2.1
3	I	245	PHE	2.1
3	I	224	TYR	2.1
2	N	173	SER	2.1
3	G	225	ASP	2.1
3	O	200	ALA	2.1
1	A	266	MET	2.1
1	D	279	TYR	2.0
2	B	234	ASP	2.0
3	G	47	ALA	2.0
2	B	47	CYS	2.0
3	L	60	VAL	2.0
1	D	285	LYS	2.0
3	L	153	PRO	2.0
1	E	289	ALA	2.0
2	H	163	SER	2.0
3	L	47	ALA	2.0
3	I	250	GLN	2.0
1	M	105	GLY	2.0
1	J	125	LEU	2.0
1	M	112	ASP	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 [i](#)

There are no such residues in this entry.