



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 PM UTC

PDB ID : 4MJI / pdb_00004mji
Title : T cell response to a HIV reverse transcriptase epitope presented by the protective allele HLA-B*51:01
Authors : Rizkallah, P.J.; Cole, D.K.; Sewell, A.K.; Motozono, C.; Takiguchi, M.
Deposited on : 2013-09-03
Resolution : 2.99 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

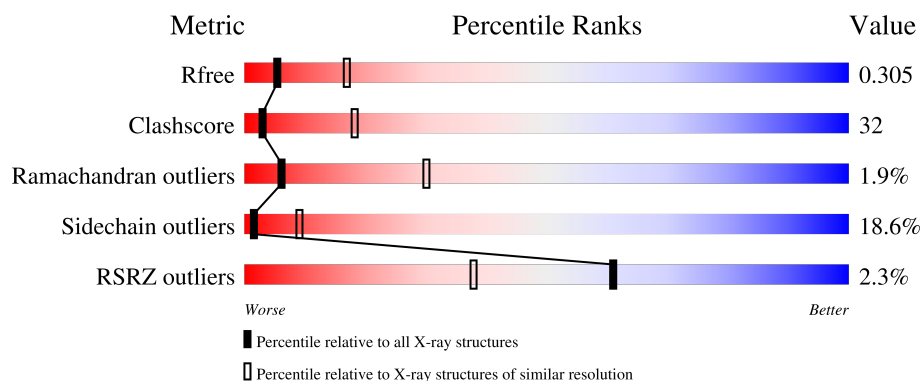
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	276	2% 50% 39% 11%
1	F	276	% 46% 41% 11%
2	B	99	61% 36%
2	G	99	55% 35% 9%
3	C	8	38% 50% 12%

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Mol	Chain	Length	Quality of chain
3	H	8	12%38%38%25%
4	D	195	6%37%41%18%••
4	I	195	4%42%37%16%••
5	E	242	2%43%45%10%••
5	J	242	2%48%42%9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13067 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 HLA class I histocompatibility antigen, B-51 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2263	1412	412	432	7			
1	F	275	Total	C	N	O	S	0	0	0
			2255	1407	411	430	7			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called HIV Reverse Transcriptase peptide Marker.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			60	40	8	12			
3	H	8	Total	C	N	O	0	0	0
			60	40	8	12			

- Molecule 4 is a protein called T-Cell Receptor Chain alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	192	Total	C	N	O	S	0	0	0
			1492	912	261	311	8			
4	I	194	Total	C	N	O	S	0	0	0
			1502	915	263	316	8			

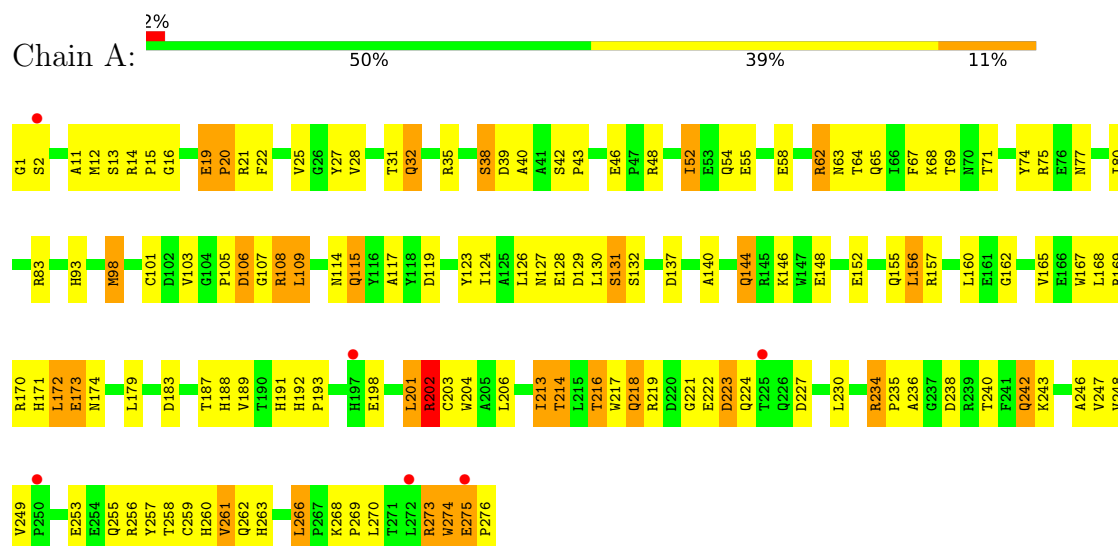
- Molecule 5 is a protein called T-cell Receptor Beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1884	1189	327	363	5			
5	J	241	Total	C	N	O	S	0	0	0
			1893	1193	328	367	5			

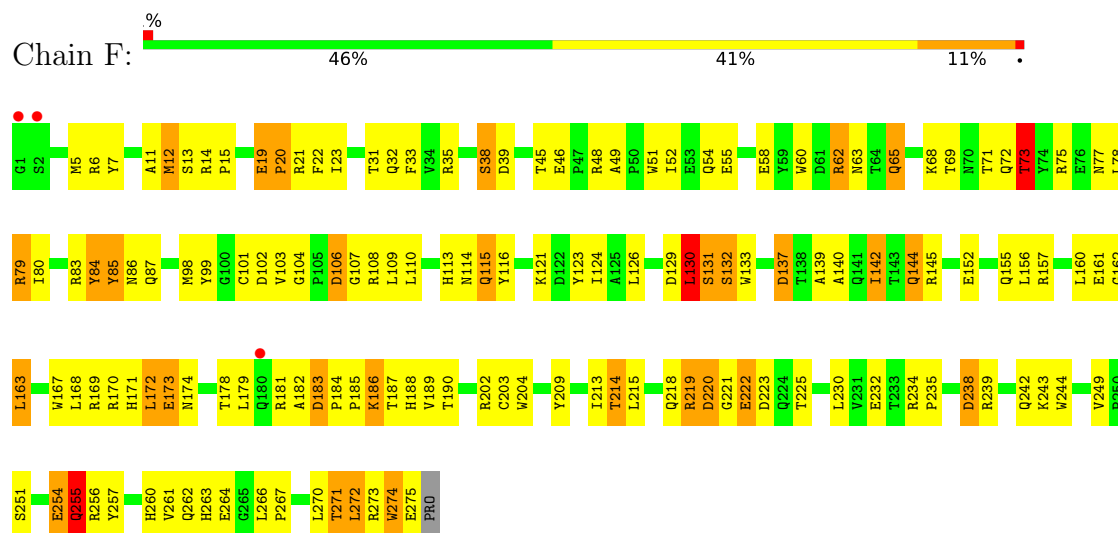
3 Residue-property plots

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

- Molecule 1: HLA class I histocompatibility antigen, B-51 alpha chain



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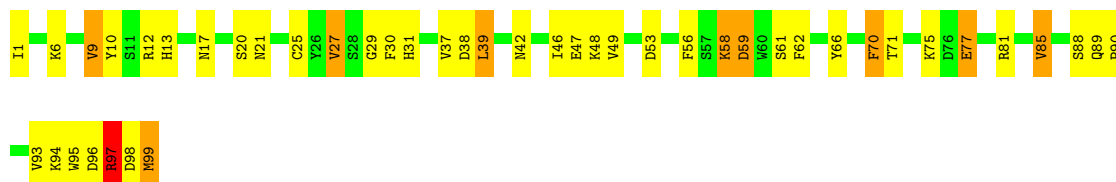


- Molecule 2: Beta-2-microglobulin





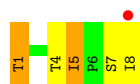
• Molecule 2: Beta-2-microglobulin



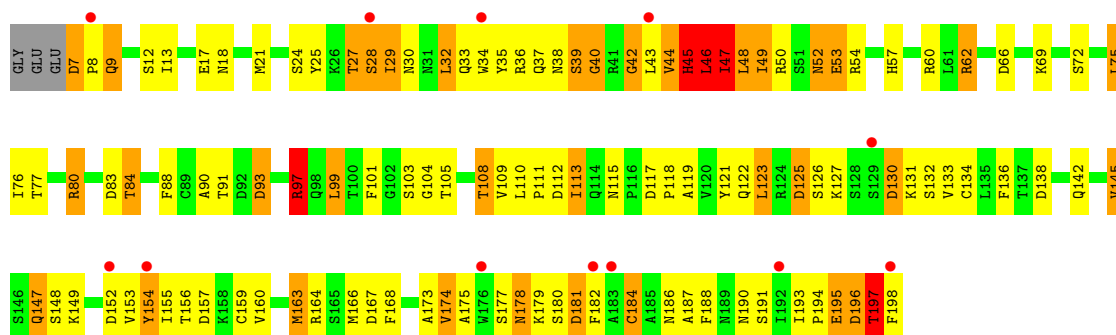
• Molecule 3: HIV Reverse Transcriptase peptide Marker



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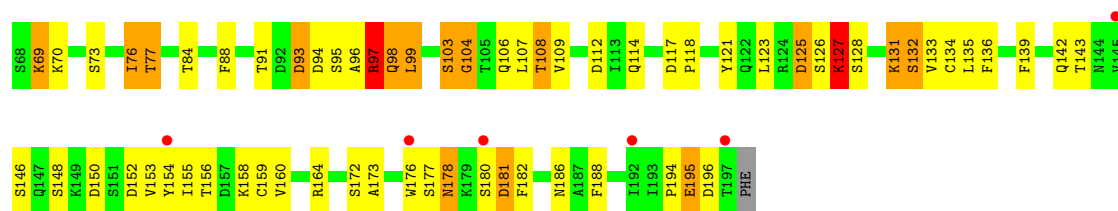


• Molecule 4: T-Cell Receptor Chain alpha

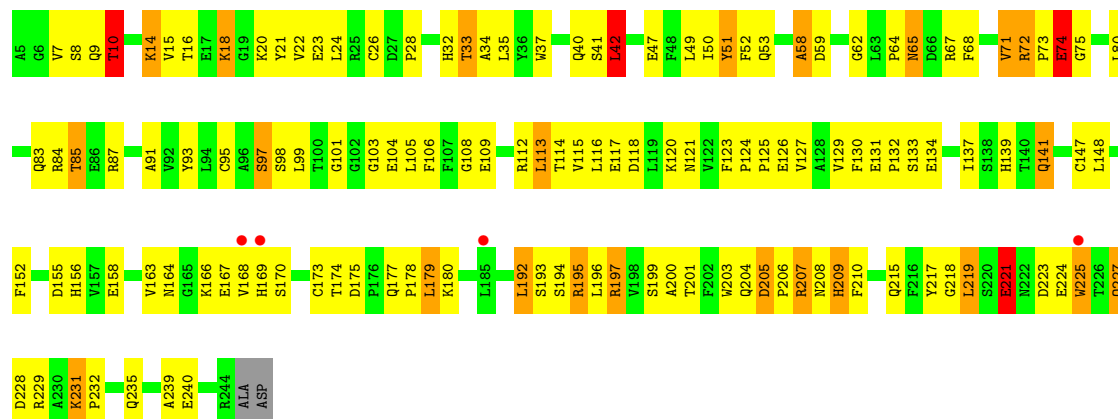


• Molecule 4: T-Cell Receptor Chain alpha

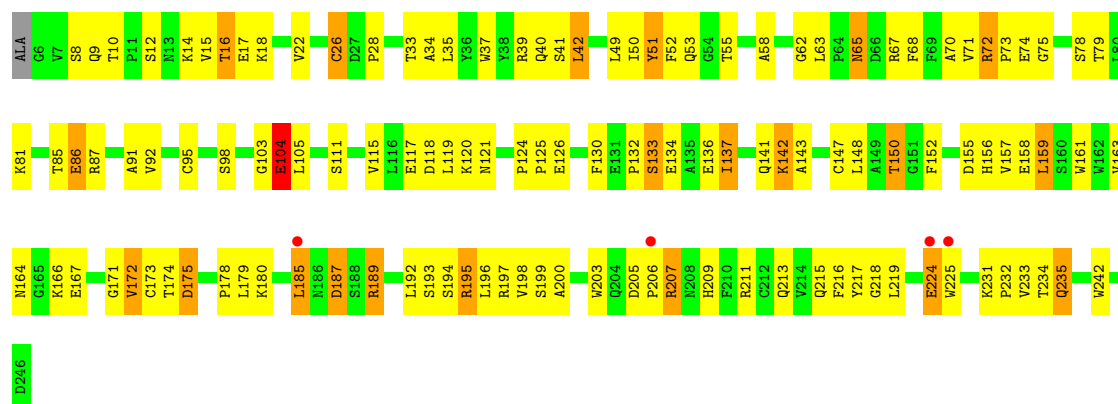




• Molecule 5: T-cell Receptor Beta chain



• Molecule 5: T-cell Receptor Beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.51Å 88.87Å 129.27Å 102.91° 95.92° 90.09°	Depositor
Resolution (Å)	64.75 – 2.99 64.75 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.7 (64.75-2.99) 98.6 (64.75-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.304 0.242 , 0.305	Depositor DCC
R_{free} test set	1965 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.885	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13067	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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	0.73	0/2329	1.08	3/3170 (0.1%)
1	F	0.75	0/2320	1.11	12/3158 (0.4%)
2	B	0.78	1/852 (0.1%)	1.00	0/1152
2	G	0.72	1/852 (0.1%)	1.12	4/1152 (0.3%)
3	C	0.76	0/61	1.53	2/82 (2.4%)
3	H	0.85	0/61	1.53	2/82 (2.4%)
4	D	0.96	4/1515 (0.3%)	1.31	16/2049 (0.8%)
4	I	0.89	5/1524 (0.3%)	1.21	16/2062 (0.8%)
5	E	0.72	0/1934	1.08	13/2631 (0.5%)
5	J	0.73	0/1943	1.04	5/2643 (0.2%)
All	All	0.78	11/13391 (0.1%)	1.13	73/18181 (0.4%)

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	F	0	1
4	D	0	2
4	I	0	8
5	E	0	1
All	All	0	12

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	47	ILE	N-CA	11.20	1.58	1.46
4	D	47	ILE	CA-C	7.54	1.61	1.52
4	D	48	LEU	N-CA	7.46	1.55	1.46
4	I	53	GLU	C-O	-7.16	1.15	1.24
4	I	47	ILE	N-CA	6.15	1.54	1.46
4	D	93	ASP	C-O	-6.14	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	48	LEU	N-CA	5.87	1.53	1.46
4	I	93	ASP	C-O	-5.81	1.17	1.24
2	G	59	ASP	C-O	-5.71	1.16	1.24
2	B	59	ASP	C-O	-5.55	1.16	1.24
4	I	45	HIS	N-CA	5.30	1.53	1.46

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	46	LEU	N-CA-C	11.25	128.02	109.24
4	D	93	ASP	N-CA-C	10.57	122.80	111.28
2	G	59	ASP	CA-C-N	-9.51	107.75	122.49
2	G	59	ASP	C-N-CA	-9.51	107.75	122.49
5	E	72	ARG	CA-C-N	9.21	128.82	119.24
5	E	72	ARG	C-N-CA	9.21	128.82	119.24
4	I	53	GLU	N-CA-C	9.09	126.75	114.12
4	I	46	LEU	N-CA-C	9.08	123.48	110.14
1	F	73	THR	CB-CA-C	7.64	125.95	109.99
1	F	222	GLU	N-CA-C	7.46	121.70	110.14
4	D	45	HIS	N-CA-C	7.45	119.47	108.14
4	D	48	LEU	N-CA-C	7.27	120.26	108.34
4	I	132	SER	N-CA-C	7.11	120.05	109.59
2	G	97	ARG	N-CA-C	-6.98	104.64	113.01
4	D	42	GLY	N-CA-C	6.91	129.55	113.18
4	D	47	ILE	N-CA-C	6.80	118.98	108.44
4	I	48	LEU	N-CA-C	6.75	120.40	109.40
4	I	34	TRP	N-CA-C	6.53	117.20	108.38
3	H	5	ILE	CA-C-N	6.52	127.99	119.84
3	H	5	ILE	C-N-CA	6.52	127.99	119.84
4	D	184	CYS	N-CA-C	6.51	118.26	111.03
4	D	196	ASP	N-CA-C	6.50	118.39	108.52
5	J	72	ARG	CA-C-N	6.40	125.90	119.24
5	J	72	ARG	C-N-CA	6.40	125.90	119.24
1	F	183	ASP	CA-C-N	6.21	126.78	120.38
1	F	183	ASP	C-N-CA	6.21	126.78	120.38
4	I	18	ASN	N-CA-C	6.16	118.75	108.96
5	E	205	ASP	CA-C-N	6.14	125.83	119.56
5	E	205	ASP	C-N-CA	6.14	125.83	119.56
1	A	223	ASP	N-CA-C	6.11	118.72	111.33
4	I	150	ASP	N-CA-C	6.06	118.39	109.24
3	C	5	ILE	CA-C-N	6.00	125.97	120.03
3	C	5	ILE	C-N-CA	6.00	125.97	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	238	ASP	N-CA-C	-5.98	102.10	110.35
4	D	49	ILE	N-CA-C	5.87	116.93	108.48
1	F	202	ARG	N-CA-C	5.82	117.86	107.80
5	E	97	SER	CB-CA-C	-5.77	99.56	109.65
2	G	59	ASP	O-C-N	-5.74	114.95	122.59
1	F	84	TYR	N-CA-C	5.74	118.28	111.33
4	D	119	ALA	N-CA-C	5.72	116.76	107.32
4	D	97	ARG	N-CA-C	5.72	122.98	110.80
4	I	97	ARG	N-CA-C	5.65	122.83	110.80
4	I	43	LEU	N-CA-C	5.64	117.61	110.33
4	I	55	GLU	N-CA-C	5.63	118.62	108.48
5	E	74	GLU	N-CA-C	-5.62	106.00	112.92
1	F	254	GLU	N-CA-C	5.54	117.13	111.14
1	F	272	LEU	N-CA-C	5.48	117.35	108.26
4	I	46	LEU	CA-C-N	5.47	131.82	121.97
4	I	46	LEU	C-N-CA	5.47	131.82	121.97
5	E	58	ALA	N-CA-C	-5.45	106.63	113.72
1	F	255	GLN	N-CA-C	5.44	119.09	112.23
5	J	171	GLY	N-CA-C	-5.43	108.23	114.69
5	J	58	ALA	N-CA-C	-5.40	107.06	113.97
5	J	104	GLU	N-CA-C	5.38	117.47	109.25
1	F	213	ILE	N-CA-C	5.36	114.24	107.70
4	D	18	ASN	N-CA-C	5.34	117.45	108.96
4	D	93	ASP	CA-C-N	-5.33	111.47	121.81
4	D	93	ASP	C-N-CA	-5.33	111.47	121.81
4	I	45	HIS	N-CA-C	5.29	122.07	110.80
1	A	202	ARG	N-CA-C	5.27	117.41	108.02
4	I	93	ASP	N-CA-C	5.24	116.69	109.15
5	E	231	LYS	CA-C-N	5.22	126.37	119.84
5	E	231	LYS	C-N-CA	5.22	126.37	119.84
5	E	65	ASN	N-CA-C	5.22	116.07	108.14
5	E	179	LEU	N-CA-C	5.20	117.72	109.50
4	I	28	SER	CA-C-N	-5.20	112.61	121.97
4	I	28	SER	C-N-CA	-5.20	112.61	121.97
1	A	155	GLN	N-CA-C	-5.15	105.58	111.14
4	D	29	ILE	CB-CA-C	5.13	119.70	111.29
5	E	10	THR	CB-CA-C	5.06	116.80	109.92
4	D	154	TYR	N-CA-C	5.03	117.03	109.23
1	F	85	TYR	N-CA-C	-5.03	100.98	109.07
5	E	215	GLN	N-CA-C	5.00	117.06	107.75

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	45	HIS	Peptide
4	D	46	LEU	Peptide
5	E	208	ASN	Peptide
1	F	221	GLY	Peptide
4	I	104	GLY	Peptide
4	I	127	LYS	Peptide
4	I	131	LYS	Peptide
4	I	43	LEU	Peptide
4	I	45	HIS	Peptide
4	I	46	LEU	Peptide
4	I	7	ASP	Peptide
4	I	8	PRO	Peptide

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	2263	0	2113	146	0
1	F	2255	0	2106	143	0
2	B	829	0	794	31	0
2	G	829	0	794	37	0
3	C	60	0	64	19	0
3	H	60	0	64	11	0
4	D	1492	0	1429	126	0
4	I	1502	0	1433	158	0
5	E	1884	0	1794	122	0
5	J	1893	0	1798	113	0
All	All	13067	0	12389	812	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 32.

All (812) 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)
4:D:36:ARG:HA	4:D:45:HIS:O	1.31	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:VAL:HG11	1:F:257:TYR:CE1	1.76	1.19
1:F:189:VAL:O	1:F:274:TRP:HE3	1.24	1.17
4:I:29:ILE:HD12	4:I:29:ILE:N	1.57	1.16
4:I:36:ARG:HA	4:I:45:HIS:O	1.44	1.14
1:A:129:ASP:OD1	1:A:129:ASP:O	1.67	1.13
1:A:32:GLN:HE21	1:A:48:ARG:HG3	1.08	1.09
4:D:62:ARG:HG2	4:D:62:ARG:HH11	1.18	1.09
4:I:29:ILE:H	4:I:29:ILE:CD1	1.63	1.09
4:D:125:ASP:OD2	4:D:130:ASP:HB3	1.51	1.08
1:A:275:GLU:HG3	1:A:276:PRO:HD3	1.31	1.07
1:F:114:ASN:HD22	1:F:156:LEU:CD2	1.69	1.06
1:F:6:ARG:HD3	1:F:113:HIS:HE2	1.17	1.05
4:I:34:TRP:HH2	5:J:103:GLY:C	1.64	1.03
1:F:215:LEU:HG	1:F:261:VAL:HG12	1.37	1.03
4:I:34:TRP:HH2	5:J:103:GLY:O	1.39	1.01
1:F:249:VAL:HG11	1:F:257:TYR:HE1	1.18	1.01
4:I:47:ILE:HD11	4:I:63:VAL:HG21	1.40	1.00
4:D:36:ARG:CA	4:D:45:HIS:O	2.09	1.00
4:D:138:ASP:OD1	5:E:197:ARG:NH2	1.96	0.99
1:A:275:GLU:CG	1:A:276:PRO:HD3	1.92	0.99
1:A:77:ASN:ND2	3:C:8:ILE:H	1.60	0.99
4:I:34:TRP:CZ3	4:I:48:LEU:HD12	1.97	0.99
4:I:46:LEU:HD13	4:I:47:ILE:HA	1.45	0.99
1:F:129:ASP:OD1	1:F:129:ASP:O	1.82	0.98
1:F:189:VAL:O	1:F:274:TRP:CE3	2.16	0.97
1:A:77:ASN:HD21	3:C:8:ILE:H	1.12	0.97
4:I:34:TRP:CH2	5:J:103:GLY:O	2.18	0.97
4:D:123:LEU:HD12	5:E:131:GLU:O	1.64	0.96
4:I:62:ARG:HG2	4:I:62:ARG:HH21	1.30	0.96
4:I:30:ASN:ND2	4:I:91:THR:HB	1.80	0.96
4:D:52:ASN:N	4:D:52:ASN:HD22	1.63	0.96
4:D:52:ASN:HD22	4:D:52:ASN:H	1.06	0.95
4:I:29:ILE:HD12	4:I:29:ILE:H	0.80	0.94
1:A:146:LYS:HD2	3:C:8:ILE:CD1	1.97	0.94
4:I:7:ASP:HB3	4:I:103:SER:HB3	1.48	0.93
4:I:146:SER:O	4:I:155:ILE:HD11	1.68	0.93
4:I:34:TRP:CH2	5:J:103:GLY:C	2.46	0.93
1:F:77:ASN:HD21	3:H:8:ILE:H	1.01	0.93
4:I:47:ILE:HD11	4:I:63:VAL:CG2	1.98	0.92
1:F:114:ASN:HD22	1:F:156:LEU:HD22	1.31	0.91
1:A:114:ASN:ND2	1:A:156:LEU:HD21	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:30:ASN:HD22	4:I:91:THR:HB	1.34	0.91
1:F:77:ASN:ND2	3:H:8:ILE:H	1.67	0.91
2:G:9:VAL:HG22	2:G:95:TRP:HB3	1.50	0.90
4:D:27:THR:HG21	4:D:93:ASP:OD1	1.71	0.90
1:A:106:ASP:OD1	1:A:108:ARG:HG2	1.71	0.89
4:I:41:ARG:HH12	5:J:12:SER:HB2	1.35	0.89
4:I:125:ASP:HA	5:J:130:PHE:HA	1.54	0.89
4:I:8:PRO:HB2	4:I:9:GLN:C	1.97	0.89
1:A:109:LEU:HD12	1:A:109:LEU:O	1.73	0.88
2:G:21:ASN:HB3	2:G:70:PHE:CE2	2.09	0.87
1:F:130:LEU:HD12	1:F:130:LEU:H	1.39	0.87
4:I:36:ARG:HH12	5:J:105:LEU:H	1.23	0.86
5:J:174:THR:HG23	5:J:194:SER:HB2	1.54	0.86
1:A:14:ARG:NH1	1:A:21:ARG:HB2	1.91	0.86
2:B:17:ASN:ND2	2:B:97:ARG:HH12	1.74	0.86
1:F:219:ARG:HG3	1:F:219:ARG:HH11	1.42	0.85
4:D:52:ASN:H	4:D:52:ASN:ND2	1.73	0.85
1:F:163:LEU:HD23	4:I:29:ILE:HD11	1.58	0.84
1:F:155:GLN:NE2	4:I:50:ARG:HH12	1.75	0.84
4:I:34:TRP:HZ3	4:I:48:LEU:HD12	1.40	0.83
5:E:227:GLN:HA	5:E:227:GLN:NE2	1.93	0.83
4:I:27:THR:O	4:I:28:SER:O	1.96	0.83
1:A:146:LYS:HD2	3:C:8:ILE:CG1	2.08	0.83
1:A:32:GLN:NE2	1:A:48:ARG:HG3	1.91	0.82
1:F:249:VAL:CG1	1:F:257:TYR:HE1	1.93	0.82
1:A:146:LYS:HD2	3:C:8:ILE:HD13	1.59	0.82
5:E:227:GLN:HB2	5:E:231:LYS:HD3	1.61	0.82
1:F:32:GLN:HE21	1:F:48:ARG:HG3	1.44	0.81
5:E:87:ARG:HD2	5:E:117:GLU:HG2	1.62	0.81
1:F:80:ILE:HD12	3:H:8:ILE:HA	1.61	0.81
5:J:225:TRP:CB	5:J:231:LYS:HG3	2.10	0.81
5:E:174:THR:HG23	5:E:194:SER:HB2	1.63	0.81
1:F:189:VAL:HB	1:F:274:TRP:HB2	1.62	0.81
1:F:114:ASN:HD22	1:F:156:LEU:HD21	1.45	0.81
1:A:216:THR:HG23	1:A:260:HIS:HB3	1.61	0.80
4:D:159:CYS:HB3	5:E:195:ARG:HH21	1.45	0.80
1:A:146:LYS:HD2	3:C:8:ILE:HG12	1.63	0.80
4:D:99:LEU:CD2	5:E:105:LEU:HD13	2.11	0.80
4:D:60:ARG:NH2	4:D:83:ASP:OD2	2.14	0.79
4:D:32:LEU:HG	4:D:48:LEU:HD11	1.64	0.79
1:A:130:LEU:HB2	1:A:157:ARG:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:LEU:HG	1:F:261:VAL:CG1	2.13	0.79
4:D:34:TRP:CZ3	4:D:46:LEU:HB2	2.18	0.79
4:D:62:ARG:HG2	4:D:62:ARG:NH1	1.91	0.79
1:A:13:SER:HB3	1:A:15:PRO:HD3	1.64	0.78
4:I:46:LEU:HD22	4:I:47:ILE:N	1.98	0.78
4:I:14:GLN:O	4:I:17:GLU:HG2	1.82	0.78
4:I:27:THR:HG21	4:I:93:ASP:OD1	1.84	0.78
2:G:21:ASN:HB3	2:G:70:PHE:HE2	1.46	0.78
4:I:34:TRP:CE3	4:I:48:LEU:HD12	2.18	0.78
1:A:146:LYS:CD	3:C:8:ILE:CD1	2.61	0.77
1:A:274:TRP:HE3	1:A:275:GLU:H	1.29	0.77
4:D:152:ASP:CG	4:D:179:LYS:HG3	2.09	0.77
5:J:225:TRP:HB3	5:J:231:LYS:HG3	1.66	0.77
4:D:84:THR:CG2	4:D:109:VAL:H	1.97	0.77
5:E:112:ARG:HG3	5:E:156:HIS:CE1	2.20	0.77
1:A:146:LYS:CD	3:C:8:ILE:HD13	2.15	0.76
4:D:84:THR:HG22	4:D:109:VAL:H	1.49	0.76
2:B:34:ASP:O	2:B:84:HIS:HD2	1.69	0.76
4:D:33:GLN:HE22	4:D:72:SER:HB3	1.49	0.76
1:F:6:ARG:HD3	1:F:113:HIS:NE2	1.98	0.76
4:I:96:ALA:O	4:I:98:GLN:N	2.18	0.75
4:I:34:TRP:HB2	4:I:47:ILE:O	1.86	0.75
4:D:156:THR:HB	4:D:174:VAL:H	1.49	0.75
1:F:114:ASN:ND2	1:F:156:LEU:HD22	2.01	0.75
1:F:129:ASP:O	1:F:131:SER:N	2.19	0.75
4:I:195:GLU:CD	4:I:195:GLU:H	1.95	0.75
5:E:207:ARG:O	5:E:207:ARG:HG2	1.86	0.75
4:D:195:GLU:CD	4:D:195:GLU:H	1.95	0.75
1:F:63:ASN:HD21	3:H:1:THR:HG22	1.52	0.74
4:D:145:VAL:HA	4:D:191:SER:HB2	1.70	0.74
1:A:106:ASP:CG	1:A:108:ARG:HG2	2.12	0.74
5:E:164:ASN:HB2	5:E:209:HIS:ND1	2.03	0.74
5:E:84:ARG:O	5:E:84:ARG:HG2	1.87	0.74
1:F:214:THR:O	1:F:261:VAL:HA	1.88	0.74
5:E:164:ASN:HB2	5:E:209:HIS:CE1	2.23	0.74
4:D:43:LEU:CD1	4:D:45:HIS:HD2	2.00	0.73
5:E:33:THR:HB	5:E:53:GLN:HE21	1.54	0.73
1:F:55:GLU:O	1:F:60:TRP:HZ3	1.70	0.73
1:F:218:GLN:OE1	1:F:260:HIS:CE1	2.41	0.73
4:I:133:VAL:HG21	5:J:130:PHE:CE2	2.23	0.73
4:I:139:PHE:HD1	4:I:143:THR:HB	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:33:THR:HB	5:E:53:GLN:NE2	2.02	0.73
1:A:273:ARG:HG2	1:A:273:ARG:HH21	1.52	0.73
5:E:219:LEU:HD22	5:E:232:PRO:O	1.89	0.73
4:I:46:LEU:O	4:I:47:ILE:HG23	1.88	0.73
5:E:71:VAL:CG1	5:E:73:PRO:HD3	2.18	0.73
4:I:46:LEU:CD1	4:I:47:ILE:HA	2.18	0.73
1:A:16:GLY:O	4:I:60:ARG:HA	1.89	0.72
1:A:129:ASP:O	1:A:131:SER:N	2.22	0.72
1:A:129:ASP:O	1:A:129:ASP:CG	2.32	0.72
4:I:34:TRP:CZ2	4:I:99:LEU:HD21	2.24	0.72
1:F:62:ARG:O	1:F:65:GLN:HG3	1.90	0.72
1:A:77:ASN:ND2	3:C:8:ILE:N	2.38	0.71
4:I:52:ASN:HD22	4:I:52:ASN:C	1.97	0.71
4:I:36:ARG:CA	4:I:45:HIS:O	2.34	0.71
1:A:14:ARG:NH1	1:A:21:ARG:HD2	2.06	0.70
4:I:5:GLU:HG3	4:I:6:GLU:H	1.56	0.70
5:J:189:ARG:HG2	5:J:189:ARG:HH11	1.55	0.70
1:F:152:GLU:O	1:F:152:GLU:HG3	1.92	0.70
4:I:41:ARG:HG3	4:I:42:GLY:N	2.06	0.70
1:F:249:VAL:CG1	1:F:257:TYR:CE1	2.66	0.69
4:I:84:THR:HG22	4:I:109:VAL:H	1.56	0.69
1:A:214:THR:O	1:A:261:VAL:HA	1.92	0.69
4:D:43:LEU:CD1	4:D:45:HIS:CD2	2.76	0.69
5:E:225:TRP:CG	5:E:225:TRP:O	2.45	0.69
4:I:146:SER:O	4:I:155:ILE:CD1	2.39	0.69
1:F:188:HIS:HB2	1:F:274:TRP:CZ3	2.28	0.69
1:A:77:ASN:HD21	3:C:8:ILE:N	1.88	0.69
5:J:28:PRO:HG3	5:J:35:LEU:HD12	1.75	0.69
4:I:46:LEU:HD13	4:I:47:ILE:CA	2.23	0.68
2:G:9:VAL:CG2	2:G:95:TRP:HB3	2.21	0.68
4:D:33:GLN:HE22	4:D:72:SER:CB	2.06	0.68
5:J:141:GLN:O	5:J:200:ALA:HB2	1.93	0.68
5:E:9:GLN:NE2	5:E:93:TYR:O	2.26	0.68
2:B:11:SER:HB2	2:B:21:ASN:ND2	2.07	0.68
4:I:34:TRP:HZ2	4:I:99:LEU:HD21	1.58	0.68
4:I:99:LEU:HD22	5:J:105:LEU:HD13	1.74	0.68
4:D:118:PRO:O	4:D:196:ASP:HB3	1.94	0.68
4:D:25:TYR:CB	4:D:91:THR:HG21	2.24	0.68
4:D:57:HIS:NE2	4:D:62:ARG:HD3	2.09	0.68
5:J:124:PRO:HD3	5:J:232:PRO:HB3	1.76	0.68
1:A:275:GLU:OE1	1:A:275:GLU:HA	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ASN:HD21	2:B:97:ARG:HH12	1.40	0.67
1:F:219:ARG:HG3	1:F:219:ARG:NH1	2.08	0.67
4:I:159:CYS:HB3	5:J:195:ARG:HH22	1.59	0.67
1:A:202:ARG:HG3	1:A:246:ALA:HB2	1.75	0.67
1:F:22:PHE:H	1:F:38:SER:HB3	1.58	0.67
1:F:6:ARG:CD	1:F:113:HIS:HE2	2.01	0.67
1:F:114:ASN:ND2	1:F:156:LEU:CD2	2.51	0.67
1:F:129:ASP:O	1:F:129:ASP:CG	2.37	0.67
1:F:130:LEU:HB2	1:F:157:ARG:HD2	1.76	0.67
1:F:255:GLN:HG3	1:F:273:ARG:HD2	1.76	0.67
5:E:163:VAL:O	5:E:164:ASN:HB3	1.94	0.67
4:I:62:ARG:HG2	4:I:62:ARG:NH2	2.01	0.67
4:I:123:LEU:HD21	4:I:135:LEU:HB2	1.76	0.67
4:D:62:ARG:HH11	4:D:62:ARG:CG	2.02	0.67
2:G:29:GLY:HA2	2:G:61:SER:HB2	1.76	0.67
4:I:29:ILE:N	4:I:29:ILE:CD1	2.35	0.67
1:F:163:LEU:CD2	4:I:29:ILE:HD11	2.25	0.66
1:A:103:VAL:CG1	1:A:168:LEU:HD23	2.24	0.66
5:E:28:PRO:HG3	5:E:35:LEU:HD12	1.76	0.66
5:E:227:GLN:HE21	5:E:228:ASP:H	1.44	0.66
2:G:20:SER:HA	2:G:71:THR:HG22	1.78	0.66
1:F:52:ILE:C	1:F:54:GLN:H	2.03	0.66
2:B:2:GLN:HG2	2:B:32:PRO:HD2	1.77	0.65
1:F:21:ARG:HG3	1:F:39:ASP:OD1	1.94	0.65
5:E:71:VAL:HG12	5:E:73:PRO:HD3	1.77	0.65
1:A:80:ILE:O	1:A:83:ARG:HB2	1.97	0.65
1:A:167:TRP:CD1	3:C:1:THR:N	2.65	0.65
5:J:156:HIS:HB3	5:J:217:TYR:HB2	1.78	0.65
4:I:34:TRP:HE1	4:I:36:ARG:HE	1.44	0.65
4:I:41:ARG:NH1	5:J:12:SER:HB2	2.09	0.65
5:J:40:GLN:O	5:J:91:ALA:HB1	1.97	0.65
1:A:218:GLN:HG3	1:A:258:THR:O	1.96	0.64
1:F:62:ARG:HE	1:F:65:GLN:NE2	1.95	0.64
5:J:85:THR:CG2	5:J:115:VAL:HG21	2.28	0.64
5:J:51:TYR:OH	5:J:53:GLN:NE2	2.31	0.64
1:A:201:LEU:HD13	1:A:217:TRP:CZ2	2.32	0.64
4:D:148:SER:HB2	4:D:153:VAL:HG13	1.80	0.64
4:D:156:THR:HG22	4:D:157:ASP:O	1.97	0.64
5:J:198:VAL:HG22	5:J:199:SER:H	1.63	0.64
5:J:224:GLU:OE1	5:J:224:GLU:HA	1.97	0.63
4:D:125:ASP:HA	5:E:130:PHE:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:THR:HG22	4:D:108:THR:HA	1.81	0.63
5:E:227:GLN:HA	5:E:227:GLN:HE21	1.63	0.63
4:I:152:ASP:OD1	4:I:177:SER:HB3	1.99	0.63
1:F:137:ASP:OD1	1:F:137:ASP:C	2.41	0.63
4:I:93:ASP:O	4:I:94:ASP:HB2	1.99	0.63
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.34	0.63
5:E:134:GLU:HA	5:E:137:ILE:HG13	1.81	0.63
5:J:85:THR:HG22	5:J:115:VAL:HG21	1.81	0.63
4:D:34:TRP:CZ3	4:D:46:LEU:CB	2.81	0.62
5:E:32:HIS:HE1	5:E:106:PHE:HD2	1.47	0.62
5:E:118:ASP:HB2	5:E:120:LYS:HG3	1.78	0.62
2:G:39:LEU:HB3	2:G:46:ILE:HD12	1.81	0.62
5:E:134:GLU:HA	5:E:137:ILE:CG1	2.29	0.62
4:I:139:PHE:CD1	4:I:143:THR:HB	2.32	0.62
4:I:25:TYR:HB3	4:I:91:THR:HG21	1.82	0.62
1:A:69:THR:HA	5:E:58:ALA:HB1	1.82	0.62
4:I:9:GLN:OE1	4:I:9:GLN:HA	1.99	0.62
4:D:36:ARG:CB	4:D:45:HIS:O	2.48	0.62
4:I:99:LEU:CD2	5:J:105:LEU:HD13	2.30	0.62
4:D:43:LEU:HD23	5:E:109:GLU:OE2	2.00	0.61
4:I:159:CYS:HB3	5:J:195:ARG:NH2	2.15	0.61
1:A:13:SER:HB3	1:A:15:PRO:CD	2.29	0.61
1:F:204:TRP:HH2	2:G:99:MET:HA	1.64	0.61
4:I:34:TRP:HE3	4:I:48:LEU:HB2	1.64	0.61
5:J:159:LEU:HD11	5:J:194:SER:HB3	1.81	0.61
4:I:133:VAL:CG2	5:J:130:PHE:CE2	2.83	0.61
5:J:50:ILE:HD13	5:J:70:ALA:HB3	1.83	0.61
4:D:25:TYR:HB3	4:D:91:THR:HG21	1.82	0.61
4:I:34:TRP:HB3	4:I:48:LEU:HA	1.83	0.61
1:F:139:ALA:O	1:F:142:ILE:HG23	2.01	0.60
2:B:34:ASP:O	2:B:84:HIS:CD2	2.54	0.60
5:E:121:ASN:O	5:E:123:PHE:HD1	1.84	0.60
3:C:5:ILE:HB	3:C:6:PRO:HD2	1.82	0.60
5:E:209:HIS:ND1	5:E:209:HIS:N	2.50	0.60
5:E:227:GLN:HE21	5:E:227:GLN:CA	2.15	0.60
4:D:99:LEU:HD22	5:E:105:LEU:HD13	1.82	0.60
1:A:22:PHE:H	1:A:38:SER:HB3	1.66	0.60
4:D:113:ILE:HD12	4:D:115:ASN:H	1.66	0.60
1:F:98:MET:HG2	2:G:56:PHE:HE1	1.67	0.60
1:A:103:VAL:HG13	1:A:168:LEU:HD23	1.84	0.59
5:J:189:ARG:HG2	5:J:189:ARG:NH1	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:72:ARG:N	5:E:73:PRO:HD3	2.17	0.59
1:A:171:HIS:O	1:A:174:ASN:N	2.35	0.59
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.37	0.59
4:D:125:ASP:OD2	4:D:130:ASP:CB	2.38	0.59
5:E:67:ARG:HD3	5:E:84:ARG:HE	1.68	0.59
1:A:273:ARG:HG2	1:A:273:ARG:NH2	2.14	0.59
5:E:152:PHE:HE1	5:E:155:ASP:HA	1.66	0.59
1:A:219:ARG:HG2	1:A:224:GLN:HB2	1.82	0.59
1:F:214:THR:C	1:F:215:LEU:HD12	2.27	0.59
4:I:84:THR:CG2	4:I:109:VAL:H	2.14	0.59
2:G:89:GLN:HG3	2:G:90:PRO:HD2	1.85	0.59
5:J:16:THR:CG2	5:J:17:GLU:N	2.65	0.59
4:D:37:GLN:O	4:D:45:HIS:HB2	2.02	0.59
4:D:122:GLN:HG2	4:D:184:CYS:SG	2.43	0.59
1:F:84:TYR:OH	3:H:8:ILE:HG23	2.03	0.59
2:B:21:ASN:HB3	2:B:70:PHE:CE2	2.38	0.58
4:D:32:LEU:HG	4:D:48:LEU:CD1	2.33	0.58
1:F:48:ARG:O	1:F:239:ARG:NH2	2.35	0.58
4:I:125:ASP:OD1	4:I:125:ASP:N	2.21	0.58
5:J:225:TRP:HB2	5:J:231:LYS:HG3	1.82	0.58
5:E:219:LEU:HB3	5:E:223:ASP:OD1	2.04	0.58
2:G:27:VAL:HG13	2:G:30:PHE:CE2	2.39	0.58
4:I:126:SER:C	4:I:127:LYS:HG2	2.28	0.58
1:A:216:THR:CG2	1:A:260:HIS:HB3	2.31	0.58
1:F:218:GLN:HA	1:F:222:GLU:O	2.03	0.58
1:F:234:ARG:NH1	1:F:242:GLN:OE1	2.37	0.58
4:D:34:TRP:CZ3	4:D:47:ILE:HA	2.39	0.58
4:D:130:ASP:OD2	4:D:131:LYS:N	2.36	0.58
1:F:223:ASP:HB3	1:F:225:THR:HG23	1.84	0.58
1:F:189:VAL:HB	1:F:274:TRP:CB	2.31	0.58
2:B:19:LYS:HD3	2:B:20:SER:O	2.04	0.58
4:D:38:ASN:HD22	4:D:88:PHE:HE2	1.50	0.58
2:G:98:ASP:C	2:G:99:MET:HG2	2.29	0.58
4:I:47:ILE:HD12	4:I:47:ILE:C	2.29	0.58
5:J:124:PRO:HB3	5:J:235:GLN:NE2	2.19	0.58
4:I:176:TRP:CD2	5:J:148:LEU:HD21	2.38	0.58
1:A:65:GLN:NE2	5:E:59:ASP:OD2	2.37	0.57
4:I:50:ARG:O	4:I:53:GLU:HB2	2.02	0.57
1:F:133:TRP:HB2	1:F:144:GLN:NE2	2.18	0.57
4:I:34:TRP:CE3	4:I:48:LEU:HB2	2.38	0.57
5:J:225:TRP:HB2	5:J:231:LYS:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.87	0.57
2:G:9:VAL:CG1	2:G:93:VAL:HG12	2.35	0.57
4:I:118:PRO:O	4:I:196:ASP:CB	2.52	0.57
5:E:71:VAL:HG13	5:E:73:PRO:HD3	1.86	0.57
5:J:211:ARG:NH1	5:J:213:GLN:OE1	2.38	0.57
4:D:62:ARG:HB3	4:D:75:LEU:HD23	1.86	0.57
4:D:181:ASP:OD2	4:D:181:ASP:N	2.33	0.57
1:F:12:MET:HE3	1:F:21:ARG:HB3	1.87	0.57
5:J:18:LYS:HD3	5:J:117:GLU:OE1	2.03	0.57
5:E:32:HIS:HE1	5:E:106:PHE:CD2	2.23	0.57
2:G:9:VAL:HG22	2:G:95:TRP:CB	2.30	0.57
1:A:98:MET:HE1	2:B:58:LYS:HA	1.87	0.57
4:I:62:ARG:HH21	4:I:62:ARG:CG	2.13	0.57
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.40	0.57
4:D:126:SER:O	4:D:127:LYS:HB2	2.05	0.57
1:A:114:ASN:HD22	1:A:156:LEU:HD21	1.69	0.57
4:I:48:LEU:HD23	4:I:48:LEU:C	2.30	0.57
5:J:49:LEU:HA	5:J:62:GLY:HA3	1.86	0.56
1:A:64:THR:O	1:A:68:LYS:HG3	2.05	0.56
1:F:49:ALA:O	1:F:52:ILE:HG22	2.05	0.56
4:D:121:TYR:O	4:D:134:CYS:HA	2.04	0.56
4:D:164:ARG:HH22	5:E:169:HIS:CD2	2.23	0.56
2:G:27:VAL:HG13	2:G:30:PHE:HE2	1.70	0.56
3:H:4:THR:OG1	4:I:96:ALA:HA	2.05	0.56
1:A:14:ARG:HH11	1:A:21:ARG:HB2	1.71	0.56
1:A:106:ASP:OD2	1:A:108:ARG:HG2	2.04	0.56
5:E:37:TRP:HB2	5:E:50:ILE:HG22	1.88	0.56
1:A:189:VAL:HB	1:A:274:TRP:HB2	1.88	0.56
1:A:275:GLU:HG3	1:A:276:PRO:CD	2.21	0.56
5:E:130:PHE:HE1	5:E:148:LEU:HB2	1.70	0.56
1:F:14:ARG:NH1	1:F:21:ARG:HB2	2.20	0.56
1:A:167:TRP:CD1	3:C:1:THR:H1	2.22	0.56
5:E:121:ASN:O	5:E:123:PHE:CD1	2.59	0.56
5:J:142:LYS:HD3	5:J:197:ARG:HE	1.71	0.56
4:D:8:PRO:O	4:D:9:GLN:O	2.24	0.56
4:D:125:ASP:N	4:D:125:ASP:OD1	2.38	0.56
4:I:47:ILE:HD12	4:I:48:LEU:N	2.21	0.56
4:I:46:LEU:O	4:I:47:ILE:CG2	2.54	0.55
1:F:123:TYR:CZ	1:F:140:ALA:HA	2.41	0.55
4:D:46:LEU:O	4:D:47:ILE:HG23	2.06	0.55
1:F:35:ARG:HD3	2:G:53:ASP:OD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:163:VAL:HG13	5:J:163:VAL:O	2.05	0.55
4:D:123:LEU:HB2	4:D:133:VAL:HG23	1.88	0.55
5:E:20:LYS:O	5:E:85:THR:HB	2.06	0.55
5:E:127:VAL:HG12	5:E:239:ALA:HB2	1.88	0.55
4:I:133:VAL:HG21	5:J:130:PHE:CD2	2.41	0.55
4:I:8:PRO:HB3	4:I:106:GLN:H	1.72	0.55
5:J:179:LEU:HG	5:J:180:LYS:H	1.72	0.55
5:J:205:ASP:HB3	5:J:207:ARG:HH11	1.71	0.54
4:D:152:ASP:OD1	4:D:177:SER:HB3	2.07	0.54
4:I:36:ARG:NH1	5:J:105:LEU:HB2	2.21	0.54
4:D:34:TRP:HZ3	4:D:46:LEU:HB2	1.72	0.54
4:D:159:CYS:CB	5:E:195:ARG:HH21	2.19	0.54
4:I:46:LEU:HG	5:J:104:GLU:HB2	1.89	0.54
2:B:20:SER:HA	2:B:71:THR:HG22	1.90	0.54
4:I:34:TRP:HZ2	4:I:99:LEU:CD2	2.21	0.54
5:J:189:ARG:HH11	5:J:189:ARG:CG	2.20	0.54
5:E:168:VAL:HG22	5:E:170:SER:H	1.72	0.54
4:I:32:LEU:HD13	4:I:34:TRP:CE3	2.42	0.54
4:I:180:SER:C	4:I:182:PHE:H	2.14	0.54
2:B:21:ASN:HB3	2:B:70:PHE:HE2	1.73	0.54
1:A:160:LEU:O	1:A:165:VAL:HG13	2.07	0.54
1:A:187:THR:HA	1:A:204:TRP:O	2.08	0.54
5:E:34:ALA:HB3	5:E:98:SER:HB3	1.90	0.54
1:F:35:ARG:HD3	2:G:53:ASP:CG	2.32	0.54
4:I:36:ARG:NH2	4:I:46:LEU:HB2	2.23	0.54
1:F:234:ARG:HD2	2:G:10:TYR:CZ	2.43	0.53
4:D:156:THR:O	4:D:173:ALA:HB1	2.08	0.53
1:F:103:VAL:HG13	1:F:168:LEU:HD23	1.90	0.53
1:A:103:VAL:HG13	1:A:168:LEU:CD2	2.39	0.53
1:A:103:VAL:HG11	1:A:168:LEU:HD23	1.89	0.53
1:A:191:HIS:CG	1:A:191:HIS:O	2.61	0.53
5:E:32:HIS:ND1	5:E:97:SER:HB3	2.24	0.53
5:E:224:GLU:OE1	5:E:224:GLU:HA	2.09	0.53
4:I:8:PRO:HA	4:I:104:GLY:O	2.08	0.53
4:I:11:LEU:HD11	4:I:13:ILE:HG23	1.89	0.53
4:I:46:LEU:HD22	4:I:47:ILE:H	1.70	0.53
1:F:220:ASP:HB2	1:F:256:ARG:NH1	2.23	0.53
4:I:118:PRO:O	4:I:196:ASP:HB3	2.09	0.53
2:G:17:ASN:HD21	2:G:97:ARG:HH22	1.55	0.53
4:I:126:SER:O	4:I:127:LYS:HG2	2.08	0.53
5:J:72:ARG:NE	5:J:75:GLY:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:THR:O	1:F:73:THR:CG2	2.57	0.53
5:E:18:LYS:HD2	5:E:117:GLU:OE1	2.09	0.53
4:I:34:TRP:NE1	4:I:36:ARG:HE	2.06	0.53
4:I:43:LEU:O	4:I:44:VAL:HG22	2.09	0.53
5:J:51:TYR:C	5:J:51:TYR:CD1	2.87	0.53
1:A:219:ARG:O	1:A:219:ARG:HG3	2.08	0.52
5:E:114:THR:HG22	5:E:116:LEU:HD21	1.91	0.52
5:E:156:HIS:HB3	5:E:217:TYR:HB2	1.91	0.52
1:F:52:ILE:C	1:F:54:GLN:N	2.67	0.52
5:J:35:LEU:HD13	5:J:72:ARG:HD2	1.91	0.52
5:J:72:ARG:CZ	5:J:75:GLY:O	2.57	0.52
4:D:180:SER:C	4:D:182:PHE:H	2.16	0.52
1:A:52:ILE:CD1	1:A:55:GLU:HG3	2.39	0.52
1:A:109:LEU:O	1:A:109:LEU:CD1	2.52	0.52
1:F:230:LEU:CD2	1:F:243:LYS:HE3	2.39	0.52
1:A:222:GLU:HG3	1:A:223:ASP:H	1.75	0.52
5:E:178:PRO:HB3	5:E:192:LEU:HB2	1.91	0.52
1:F:109:LEU:HD22	1:F:161:GLU:HG2	1.92	0.52
4:D:34:TRP:HZ3	4:D:47:ILE:HA	1.74	0.52
4:I:172:SER:O	5:J:195:ARG:NH2	2.42	0.52
1:A:263:HIS:O	1:A:266:LEU:HB2	2.10	0.52
1:F:171:HIS:O	1:F:174:ASN:N	2.42	0.52
5:J:71:VAL:O	5:J:78:SER:HA	2.10	0.52
5:J:164:ASN:HD22	5:J:209:HIS:H	1.58	0.52
1:A:152:GLU:OE2	4:D:97:ARG:NH2	2.30	0.52
1:F:167:TRP:O	1:F:168:LEU:C	2.53	0.52
5:J:178:PRO:HB3	5:J:192:LEU:HB2	1.92	0.52
4:D:47:ILE:HD12	4:D:47:ILE:C	2.35	0.51
4:D:97:ARG:HG2	5:E:101:GLY:C	2.35	0.51
5:E:163:VAL:O	5:E:163:VAL:HG23	2.10	0.51
1:F:188:HIS:HB2	1:F:274:TRP:CH2	2.45	0.51
1:A:35:ARG:HD3	2:B:53:ASP:OD2	2.11	0.51
1:F:189:VAL:CB	1:F:274:TRP:HB2	2.37	0.51
4:I:53:GLU:O	4:I:55:GLU:N	2.42	0.51
2:B:45:ARG:HH22	4:I:164:ARG:HG3	1.76	0.51
5:J:118:ASP:HB2	5:J:120:LYS:HG2	1.90	0.51
1:A:14:ARG:NH1	1:A:21:ARG:CB	2.70	0.51
5:E:227:GLN:HE21	5:E:228:ASP:N	2.08	0.51
1:F:234:ARG:HD2	2:G:10:TYR:CE1	2.45	0.51
1:F:98:MET:O	1:F:114:ASN:HA	2.11	0.51
4:I:76:ILE:HD12	4:I:76:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:LEU:HD12	1:F:132:SER:O	2.10	0.51
1:A:144:GLN:NE2	1:A:148:GLU:OE2	2.43	0.51
1:A:213:ILE:HG13	1:A:263:HIS:HB2	1.92	0.51
4:D:57:HIS:CD2	4:D:62:ARG:HB2	2.46	0.51
1:F:182:ALA:O	1:F:184:PRO:HD3	2.10	0.51
4:I:32:LEU:C	4:I:32:LEU:HD12	2.36	0.51
5:J:215:GLN:NE2	5:J:216:PHE:O	2.43	0.51
5:E:164:ASN:CG	5:E:164:ASN:O	2.53	0.51
5:E:200:ALA:O	5:E:204:GLN:HB2	2.11	0.51
1:F:69:THR:O	1:F:73:THR:HG22	2.11	0.51
4:I:33:GLN:HE21	4:I:34:TRP:N	2.09	0.51
4:D:43:LEU:CD2	5:E:109:GLU:OE2	2.59	0.50
1:A:106:ASP:OD2	1:A:108:ARG:HD3	2.11	0.50
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.45	0.50
4:I:38:ASN:CB	4:I:88:PHE:HE2	2.25	0.50
4:I:178:ASN:OD1	4:I:178:ASN:N	2.45	0.50
5:J:65:ASN:HB3	5:J:67:ARG:H	1.76	0.50
5:J:132:PRO:HG3	5:J:143:ALA:HB1	1.93	0.50
5:J:233:VAL:HG12	5:J:234:THR:N	2.27	0.50
1:A:168:LEU:O	1:A:172:LEU:HD12	2.12	0.50
5:J:134:GLU:HA	5:J:137:ILE:HG22	1.93	0.50
2:B:12:ARG:HD2	2:B:13:HIS:CE1	2.47	0.50
5:E:50:ILE:HG12	5:E:51:TYR:H	1.77	0.50
5:J:14:LYS:HE3	5:J:16:THR:OG1	2.12	0.50
1:A:52:ILE:C	1:A:54:GLN:H	2.19	0.50
1:A:198:GLU:HG2	1:A:248:VAL:HG22	1.94	0.50
5:E:209:HIS:C	5:E:210:PHE:CD1	2.90	0.50
1:F:63:ASN:ND2	3:H:1:THR:HG22	2.23	0.50
3:H:7:SER:O	3:H:8:ILE:HB	2.12	0.50
5:J:65:ASN:HB2	5:J:68:PHE:HD2	1.77	0.50
1:A:40:ALA:HB3	1:A:43:PRO:HA	1.93	0.50
1:A:58:GLU:O	1:A:62:ARG:HB2	2.11	0.50
4:D:33:GLN:NE2	4:D:72:SER:CB	2.74	0.50
1:F:62:ARG:HH21	1:F:65:GLN:NE2	2.10	0.50
4:I:52:ASN:C	4:I:52:ASN:ND2	2.69	0.50
5:E:40:GLN:O	5:E:91:ALA:HB1	2.12	0.50
1:F:186:LYS:O	1:F:186:LYS:HG3	2.11	0.50
4:I:34:TRP:NE1	4:I:36:ARG:NE	2.59	0.50
4:I:37:GLN:O	4:I:44:VAL:HA	2.12	0.50
5:J:34:ALA:HA	5:J:52:PHE:O	2.12	0.50
1:A:146:LYS:HD3	3:C:8:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:SER:HB3	4:D:110:LEU:HD11	1.92	0.49
4:I:33:GLN:O	4:I:34:TRP:HB3	2.12	0.49
4:I:118:PRO:O	4:I:196:ASP:HB2	2.11	0.49
4:I:176:TRP:CH2	5:J:150:THR:HG21	2.47	0.49
5:J:9:GLN:HG2	5:J:95:CYS:HB3	1.94	0.49
5:J:159:LEU:C	5:J:159:LEU:HD23	2.38	0.49
4:D:47:ILE:HD12	4:D:48:LEU:N	2.26	0.49
4:D:178:ASN:OD1	4:D:178:ASN:N	2.45	0.49
5:E:64:PRO:HG2	5:E:68:PHE:CD2	2.48	0.49
5:E:72:ARG:CZ	5:E:75:GLY:O	2.60	0.49
4:I:8:PRO:HB2	4:I:10:ALA:N	2.27	0.49
5:J:172:VAL:HG22	5:J:196:LEU:HD13	1.94	0.49
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.30	0.49
5:E:124:PRO:HB3	5:E:235:GLN:NE2	2.28	0.49
1:F:20:PRO:HG2	1:F:75:ARG:HG2	1.92	0.49
5:J:65:ASN:HB2	5:J:68:PHE:CD2	2.48	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.46	0.49
5:E:114:THR:HG22	5:E:116:LEU:CD2	2.42	0.49
1:F:14:ARG:N	1:F:15:PRO:CD	2.76	0.49
1:F:55:GLU:O	1:F:60:TRP:CZ3	2.58	0.49
1:F:77:ASN:HD21	3:H:8:ILE:N	1.87	0.49
2:G:17:ASN:HD21	2:G:97:ARG:NH2	2.11	0.49
1:A:171:HIS:O	1:A:172:LEU:C	2.56	0.49
1:A:234:ARG:NH1	1:A:242:GLN:OE1	2.41	0.49
4:D:50:ARG:HB3	4:D:52:ASN:HD21	1.78	0.49
4:D:195:GLU:CD	4:D:195:GLU:N	2.68	0.49
1:A:14:ARG:HH11	1:A:21:ARG:CB	2.25	0.49
1:A:52:ILE:HD12	1:A:55:GLU:CG	2.43	0.49
1:A:253:GLU:OE1	1:A:256:ARG:HD3	2.12	0.49
5:E:9:GLN:C	5:E:10:THR:HG22	2.37	0.49
4:I:18:ASN:CG	4:I:77:THR:HG22	2.38	0.49
1:A:224:GLN:HG3	1:A:227:ASP:HB2	1.94	0.49
1:A:249:VAL:HG11	1:A:257:TYR:CZ	2.48	0.49
4:D:43:LEU:HD13	4:D:45:HIS:CD2	2.47	0.49
1:F:58:GLU:H	1:F:58:GLU:CD	2.19	0.49
4:I:69:LYS:O	4:I:70:LYS:C	2.55	0.49
1:A:52:ILE:O	1:A:52:ILE:HG13	2.12	0.49
5:E:14:LYS:NZ	5:E:22:VAL:HG13	2.28	0.49
1:A:25:VAL:HG21	2:B:54:LEU:O	2.13	0.48
4:D:34:TRP:CZ2	5:E:104:GLU:HA	2.48	0.48
4:I:34:TRP:HE3	4:I:48:LEU:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:152:ASP:OD1	4:I:177:SER:CB	2.61	0.48
1:A:19:GLU:C	1:A:20:PRO:O	2.55	0.48
1:F:33:PHE:C	1:F:48:ARG:HB2	2.38	0.48
1:A:249:VAL:HG11	1:A:257:TYR:CE2	2.49	0.48
2:B:40:LEU:HD21	2:B:81:ARG:NH1	2.28	0.48
2:B:92:ILE:O	2:B:92:ILE:HG13	2.14	0.48
5:E:71:VAL:O	5:E:72:ARG:HB2	2.12	0.48
4:D:38:ASN:HB2	4:D:44:VAL:HG13	1.94	0.48
1:F:104:GLY:HA2	1:F:110:LEU:HD22	1.95	0.48
4:I:123:LEU:HD21	4:I:135:LEU:CB	2.42	0.48
5:J:70:ALA:HA	5:J:79:THR:O	2.14	0.48
4:D:60:ARG:HH22	4:D:83:ASP:CG	2.21	0.48
4:D:145:VAL:HA	4:D:191:SER:CB	2.40	0.48
1:F:234:ARG:HD3	2:G:10:TYR:CE2	2.49	0.48
4:I:46:LEU:HD22	4:I:47:ILE:CA	2.42	0.48
1:A:52:ILE:HD12	1:A:55:GLU:HG3	1.94	0.48
1:A:227:ASP:O	1:A:247:VAL:HG23	2.14	0.48
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.96	0.48
4:D:27:THR:OG1	4:D:28:SER:N	2.46	0.48
4:D:111:PRO:HG3	4:D:160:VAL:HG21	1.96	0.48
5:E:83:GLN:O	5:E:84:ARG:C	2.57	0.48
4:I:5:GLU:CG	4:I:6:GLU:H	2.25	0.48
1:A:106:ASP:OD1	1:A:107:GLY:N	2.47	0.48
4:D:46:LEU:O	4:D:47:ILE:CG2	2.62	0.48
4:I:41:ARG:CG	4:I:42:GLY:N	2.76	0.48
1:A:126:LEU:HD11	1:A:130:LEU:HA	1.96	0.48
4:D:34:TRP:CZ3	4:D:47:ILE:CA	2.97	0.48
5:E:74:GLU:O	5:E:74:GLU:OE2	2.31	0.48
3:C:5:ILE:CB	3:C:6:PRO:HD2	2.44	0.47
2:G:9:VAL:HG11	2:G:93:VAL:HG12	1.96	0.47
4:D:48:LEU:HD23	4:D:48:LEU:C	2.39	0.47
5:E:209:HIS:C	5:E:210:PHE:HD1	2.22	0.47
1:F:80:ILE:CD1	3:H:8:ILE:HA	2.39	0.47
1:F:22:PHE:HB3	1:F:71:THR:HG23	1.96	0.47
1:F:85:TYR:O	1:F:87:GLN:N	2.47	0.47
4:D:36:ARG:HB3	4:D:44:VAL:HG12	1.97	0.47
1:F:106:ASP:OD1	1:F:108:ARG:N	2.35	0.47
4:D:8:PRO:HD2	4:D:104:GLY:O	2.14	0.47
4:D:43:LEU:HD13	4:D:45:HIS:HD2	1.77	0.47
1:F:106:ASP:OD1	1:F:107:GLY:N	2.47	0.47
5:J:39:ARG:HB3	5:J:49:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TRP:CZ3	1:A:259:CYS:HB2	2.49	0.47
5:E:51:TYR:C	5:E:51:TYR:CD1	2.93	0.47
5:E:179:LEU:HG	5:E:180:LYS:H	1.80	0.47
1:F:58:GLU:OE1	1:F:58:GLU:N	2.30	0.47
1:F:219:ARG:O	1:F:222:GLU:N	2.46	0.47
4:I:5:GLU:HG3	4:I:6:GLU:N	2.28	0.47
4:I:5:GLU:CG	4:I:6:GLU:N	2.77	0.47
5:J:141:GLN:O	5:J:200:ALA:CB	2.60	0.47
1:A:19:GLU:O	1:A:20:PRO:C	2.58	0.47
5:E:28:PRO:HB2	5:E:97:SER:OG	2.14	0.47
1:F:130:LEU:HD12	1:F:130:LEU:N	2.19	0.47
1:F:230:LEU:HD21	1:F:243:LYS:HE3	1.97	0.47
4:I:7:ASP:HB3	4:I:103:SER:CB	2.34	0.47
4:I:64:THR:HB	4:I:73:SER:HB2	1.97	0.47
1:A:275:GLU:CB	1:A:276:PRO:HD3	2.45	0.47
4:D:133:VAL:HA	4:D:175:ALA:O	2.15	0.47
5:E:21:TYR:OH	5:E:23:GLU:OE2	2.24	0.47
5:E:41:SER:O	5:E:42:LEU:C	2.58	0.47
4:D:43:LEU:HD11	4:D:45:HIS:CD2	2.49	0.47
5:E:134:GLU:HA	5:E:137:ILE:HG12	1.95	0.46
1:A:103:VAL:HA	1:A:108:ARG:O	2.15	0.46
5:E:141:GLN:O	5:E:200:ALA:CB	2.63	0.46
1:F:129:ASP:OD1	1:F:132:SER:OG	2.33	0.46
1:A:146:LYS:HE3	1:A:146:LYS:HB2	1.74	0.46
1:A:38:SER:O	1:A:43:PRO:HG3	2.15	0.46
4:I:47:ILE:CD1	4:I:63:VAL:HG21	2.29	0.46
4:I:123:LEU:CD2	4:I:135:LEU:HB2	2.45	0.46
5:J:72:ARG:N	5:J:73:PRO:HD3	2.30	0.46
1:A:109:LEU:CD1	1:A:109:LEU:C	2.89	0.46
4:I:125:ASP:HB2	4:I:128:SER:HB3	1.97	0.46
5:E:50:ILE:HD13	5:E:52:PHE:CE2	2.50	0.46
1:F:114:ASN:ND2	1:F:156:LEU:HD21	2.20	0.46
1:F:169:ARG:HH11	1:F:169:ARG:HB3	1.80	0.46
5:J:16:THR:HG22	5:J:17:GLU:N	2.30	0.46
5:J:141:GLN:O	5:J:141:GLN:CG	2.63	0.46
5:E:49:LEU:HA	5:E:62:GLY:HA3	1.98	0.46
5:E:225:TRP:O	5:E:225:TRP:CD2	2.69	0.46
1:F:80:ILE:O	1:F:83:ARG:HB2	2.16	0.46
5:J:85:THR:CG2	5:J:115:VAL:CG2	2.94	0.46
4:D:9:GLN:OE1	4:D:9:GLN:HA	2.15	0.46
1:F:11:ALA:HA	1:F:21:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:TRP:CH2	2:G:99:MET:HA	2.49	0.46
5:J:14:LYS:HE3	5:J:16:THR:HG1	1.80	0.46
5:E:85:THR:HG23	5:E:115:VAL:HG11	1.97	0.46
5:E:163:VAL:O	5:E:163:VAL:CG2	2.64	0.46
5:J:62:GLY:O	5:J:63:LEU:C	2.59	0.46
1:F:84:TYR:OH	3:H:8:ILE:CG2	2.63	0.45
4:D:39:SER:O	4:D:40:GLY:C	2.59	0.45
4:D:159:CYS:HB3	5:E:195:ARG:NH2	2.23	0.45
5:J:15:VAL:HB	5:J:218:GLY:O	2.16	0.45
1:A:235:PRO:O	2:B:10:TYR:OH	2.27	0.45
4:D:90:ALA:HB2	4:D:101:PHE:CE1	2.51	0.45
4:I:34:TRP:HE3	4:I:48:LEU:CG	2.29	0.45
4:I:121:TYR:O	4:I:134:CYS:HA	2.16	0.45
5:J:87:ARG:HA	5:J:115:VAL:HB	1.98	0.45
1:A:183:ASP:O	1:A:263:HIS:CE1	2.70	0.45
4:D:99:LEU:HD12	4:D:99:LEU:HA	1.85	0.45
4:D:182:PHE:HE1	4:D:187:ALA:HA	1.81	0.45
1:F:72:GLN:OE1	1:F:75:ARG:NH1	2.49	0.45
1:A:273:ARG:H	1:A:273:ARG:HD3	1.80	0.45
1:F:113:HIS:ND1	1:F:115:GLN:NE2	2.64	0.45
2:G:20:SER:CA	2:G:71:THR:HG22	2.44	0.45
4:I:99:LEU:HD22	5:J:105:LEU:CD1	2.44	0.45
4:I:159:CYS:SG	4:I:160:VAL:N	2.89	0.45
1:A:1:GLY:HA2	1:A:105:PRO:HA	1.98	0.45
4:D:25:TYR:HB2	4:D:91:THR:HG21	1.99	0.45
4:I:76:ILE:N	4:I:76:ILE:CD1	2.80	0.45
1:A:13:SER:HB2	1:A:93:HIS:H	1.81	0.45
1:A:167:TRP:O	1:A:168:LEU:C	2.58	0.45
4:D:166:MET:O	4:D:167:ASP:C	2.59	0.45
5:E:125:PRO:HB3	5:E:152:PHE:HB3	1.99	0.45
5:E:139:HIS:CD2	5:E:139:HIS:O	2.70	0.45
5:E:147:CYS:O	5:E:193:SER:HA	2.17	0.45
5:J:124:PRO:CG	5:J:235:GLN:HE22	2.29	0.45
4:I:34:TRP:CB	4:I:48:LEU:HA	2.46	0.45
4:I:58:SER:O	4:I:59:GLY:C	2.58	0.45
4:I:136:PHE:HB2	4:I:188:PHE:CZ	2.52	0.45
4:I:195:GLU:CD	4:I:195:GLU:N	2.70	0.45
1:A:63:ASN:OD1	3:C:1:THR:HB	2.16	0.45
1:F:14:ARG:NH1	1:F:21:ARG:HD2	2.32	0.45
1:F:85:TYR:OH	1:F:137:ASP:OD2	2.30	0.45
5:J:119:LEU:HD12	5:J:119:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:209:HIS:CD2	5:J:242:TRP:CD1	3.05	0.45
2:B:45:ARG:NH2	4:I:164:ARG:HG3	2.32	0.45
4:D:21:MET:HG2	4:D:105:THR:HG21	1.98	0.45
4:D:134:CYS:HB2	4:D:175:ALA:HB3	1.98	0.45
5:E:127:VAL:HG12	5:E:239:ALA:CB	2.47	0.45
5:E:210:PHE:CD1	5:E:210:PHE:N	2.85	0.45
5:J:85:THR:HG22	5:J:86:GLU:N	2.31	0.45
5:E:137:ILE:O	5:E:141:GLN:HA	2.17	0.44
1:F:13:SER:HB3	1:F:78:LEU:HD13	2.00	0.44
4:I:49:ILE:HD13	4:I:65:LEU:HB2	1.98	0.44
2:B:30:PHE:H	2:B:30:PHE:HD2	1.65	0.44
1:F:254:GLU:O	1:F:257:TYR:HB2	2.17	0.44
2:G:37:VAL:HG11	2:G:66:TYR:CD2	2.53	0.44
5:J:159:LEU:HD21	5:J:161:TRP:CD1	2.52	0.44
1:A:11:ALA:HA	1:A:21:ARG:O	2.17	0.44
5:E:225:TRP:HE3	5:E:225:TRP:H	1.66	0.44
2:G:58:LYS:C	2:G:59:ASP:O	2.58	0.44
4:I:36:ARG:HG3	4:I:45:HIS:O	2.17	0.44
4:D:35:TYR:O	4:D:46:LEU:HA	2.18	0.44
4:D:197:THR:O	4:D:197:THR:CG2	2.65	0.44
5:E:205:ASP:HA	5:E:206:PRO:HD3	1.74	0.44
4:D:43:LEU:HG	5:E:109:GLU:OE2	2.17	0.44
5:E:139:HIS:O	5:E:139:HIS:HD2	2.01	0.44
1:F:19:GLU:O	1:F:20:PRO:C	2.59	0.44
4:I:112:ASP:OD1	4:I:112:ASP:C	2.60	0.44
5:J:133:SER:HB3	5:J:136:GLU:H	1.83	0.44
1:A:19:GLU:O	1:A:20:PRO:O	2.36	0.44
4:D:118:PRO:O	4:D:196:ASP:CB	2.65	0.44
5:E:50:ILE:HG12	5:E:51:TYR:N	2.32	0.44
5:J:87:ARG:HG2	5:J:115:VAL:O	2.17	0.44
5:E:225:TRP:HB2	5:E:231:LYS:HG3	2.00	0.44
5:J:37:TRP:HB2	5:J:50:ILE:HG22	1.99	0.44
1:A:1:GLY:HA2	1:A:105:PRO:CA	2.48	0.44
5:E:72:ARG:NE	5:E:75:GLY:O	2.51	0.44
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.99	0.44
1:F:130:LEU:H	1:F:130:LEU:CD1	2.11	0.44
5:J:163:VAL:O	5:J:163:VAL:CG1	2.66	0.44
5:J:185:LEU:HD13	5:J:187:ASP:O	2.17	0.44
1:A:93:HIS:CD2	1:A:119:ASP:OD2	2.69	0.44
1:F:187:THR:HA	1:F:204:TRP:O	2.17	0.44
1:A:48:ARG:HD2	1:A:48:ARG:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:GLN:HB2	1:A:221:GLY:HA2	2.00	0.43
5:E:24:LEU:HB2	5:E:80:LEU:HB3	2.00	0.43
1:F:263:HIS:HB3	1:F:266:LEU:HG	2.00	0.43
2:G:38:ASP:HB2	2:G:81:ARG:HB3	1.98	0.43
4:I:48:LEU:HD23	4:I:49:ILE:N	2.32	0.43
1:A:14:ARG:HH12	1:A:21:ARG:HD2	1.82	0.43
1:A:275:GLU:CD	1:A:276:PRO:HD3	2.42	0.43
1:A:67:PHE:O	1:A:71:THR:N	2.44	0.43
4:D:90:ALA:HB2	4:D:101:PHE:CD1	2.53	0.43
5:E:64:PRO:HG2	5:E:68:PHE:CE2	2.53	0.43
5:E:124:PRO:HB3	5:E:235:GLN:HE21	1.83	0.43
5:E:218:GLY:C	5:E:219:LEU:HD13	2.43	0.43
4:D:156:THR:HG21	5:E:195:ARG:NH2	2.33	0.43
5:E:129:VAL:HG11	5:E:240:GLU:O	2.19	0.43
2:G:25:CYS:HB2	2:G:39:LEU:HD11	2.01	0.43
4:I:27:THR:HG21	4:I:93:ASP:CG	2.42	0.43
4:I:34:TRP:CD1	4:I:34:TRP:C	2.95	0.43
4:I:181:ASP:OD2	4:I:181:ASP:N	2.31	0.43
1:A:236:ALA:HB1	2:B:12:ARG:HG3	2.00	0.43
5:E:132:PRO:HD2	5:E:203:TRP:CZ2	2.54	0.43
1:F:45:THR:HG22	1:F:60:TRP:HD1	1.82	0.43
4:I:180:SER:C	4:I:182:PHE:N	2.77	0.43
5:J:205:ASP:HA	5:J:206:PRO:HD3	1.93	0.43
1:A:171:HIS:O	1:A:173:GLU:N	2.52	0.43
4:D:32:LEU:C	4:D:32:LEU:HD22	2.43	0.43
5:E:118:ASP:OD2	5:E:120:LYS:HE2	2.18	0.43
1:F:183:ASP:HB2	1:F:209:TYR:HB3	2.00	0.43
1:F:185:PRO:HD2	1:F:266:LEU:HD21	2.00	0.43
4:I:36:ARG:NH1	5:J:105:LEU:H	2.04	0.43
4:I:84:THR:HG22	4:I:108:THR:HA	2.00	0.43
1:A:188:HIS:O	1:A:204:TRP:HB2	2.19	0.43
4:D:60:ARG:NH2	4:D:83:ASP:CG	2.74	0.43
4:I:21:MET:HE1	4:I:107:LEU:HD13	1.99	0.43
5:J:35:LEU:C	5:J:35:LEU:HD23	2.43	0.43
1:A:52:ILE:C	1:A:54:GLN:N	2.77	0.43
4:D:147:GLN:O	4:D:190:ASN:ND2	2.52	0.43
1:F:33:PHE:HD1	1:F:52:ILE:HD13	1.84	0.43
5:J:218:GLY:O	5:J:219:LEU:HD23	2.18	0.43
1:A:218:GLN:HA	1:A:222:GLU:O	2.19	0.43
4:D:66:ASP:OD2	4:D:69:LYS:HD2	2.18	0.43
4:D:118:PRO:CG	4:D:194:PRO:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:ARG:HH11	5:E:117:GLU:HG2	1.84	0.43
5:J:74:GLU:CA	5:J:74:GLU:OE2	2.67	0.43
5:J:124:PRO:CB	5:J:235:GLN:NE2	2.81	0.43
5:J:152:PHE:HE1	5:J:155:ASP:HA	1.83	0.43
1:A:192:HIS:HA	1:A:193:PRO:HD2	1.85	0.43
4:D:7:ASP:HA	4:D:103:SER:HB3	2.01	0.43
5:E:87:ARG:HG2	5:E:115:VAL:O	2.19	0.43
5:E:134:GLU:O	5:E:137:ILE:HG13	2.19	0.43
4:I:34:TRP:HH2	5:J:103:GLY:CA	2.29	0.43
4:D:34:TRP:HE1	5:E:103:GLY:C	2.26	0.42
4:D:39:SER:O	4:D:40:GLY:O	2.37	0.42
4:I:36:ARG:HG3	4:I:45:HIS:C	2.44	0.42
1:A:222:GLU:HG3	1:A:223:ASP:N	2.33	0.42
4:D:32:LEU:HD12	4:D:50:ARG:NH1	2.34	0.42
4:D:177:SER:HB2	4:D:182:PHE:CD2	2.54	0.42
5:J:92:VAL:HG23	5:J:111:SER:C	2.43	0.42
4:D:117:ASP:O	4:D:118:PRO:C	2.62	0.42
1:F:171:HIS:O	1:F:172:LEU:C	2.61	0.42
1:F:235:PRO:O	2:G:10:TYR:OH	2.28	0.42
1:A:219:ARG:C	1:A:221:GLY:N	2.77	0.42
5:E:7:VAL:O	5:E:108:GLY:HA2	2.19	0.42
1:F:51:TRP:CE2	1:F:179:LEU:HD11	2.55	0.42
1:F:62:ARG:HH21	1:F:65:GLN:CD	2.27	0.42
2:G:31:HIS:CD2	2:G:62:PHE:CE2	3.08	0.42
4:I:136:PHE:HB2	4:I:188:PHE:CE2	2.55	0.42
4:I:46:LEU:HD13	4:I:47:ILE:N	2.34	0.42
5:E:67:ARG:CD	5:E:84:ARG:HE	2.31	0.42
5:E:221:GLU:H	5:E:221:GLU:HG3	1.53	0.42
4:I:8:PRO:HB2	4:I:9:GLN:O	2.16	0.42
4:I:34:TRP:CZ2	4:I:99:LEU:CD2	2.99	0.42
5:J:175:ASP:OD1	5:J:195:ARG:NH1	2.53	0.42
1:A:248:VAL:O	1:A:249:VAL:HG13	2.20	0.42
4:D:25:TYR:HB3	4:D:91:THR:CG2	2.47	0.42
1:F:45:THR:HG22	1:F:60:TRP:CD1	2.55	0.42
1:F:51:TRP:CZ3	1:F:52:ILE:HB	2.54	0.42
2:B:20:SER:CA	2:B:71:THR:HG22	2.49	0.42
4:D:163:MET:HE3	4:D:168:PHE:HB3	2.02	0.42
4:I:34:TRP:CE3	4:I:48:LEU:CD1	2.99	0.42
1:F:126:LEU:HD22	1:F:156:LEU:HD23	2.02	0.42
1:F:219:ARG:O	1:F:220:ASP:C	2.62	0.42
1:A:27:TYR:HA	1:A:32:GLN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:TYR:O	1:A:75:ARG:C	2.63	0.41
1:A:217:TRP:CE3	1:A:217:TRP:HA	2.54	0.41
4:D:166:MET:HE2	4:D:166:MET:HB3	1.94	0.41
1:F:79:ARG:O	1:F:80:ILE:C	2.63	0.41
5:J:41:SER:O	5:J:42:LEU:C	2.63	0.41
4:D:46:LEU:H	4:D:46:LEU:HG	1.39	0.41
5:E:9:GLN:HG3	5:E:95:CYS:HB3	2.02	0.41
5:E:34:ALA:HA	5:E:52:PHE:O	2.20	0.41
1:F:219:ARG:HH11	1:F:219:ARG:CG	2.22	0.41
5:J:9:GLN:HA	5:J:26:CYS:HA	2.02	0.41
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.03	0.41
1:A:126:LEU:HD12	1:A:127:ASN:H	1.85	0.41
4:D:60:ARG:HD2	4:D:80:ARG:NH2	2.35	0.41
4:D:152:ASP:HB2	4:D:179:LYS:HE3	2.02	0.41
1:F:133:TRP:HB2	1:F:144:GLN:HE22	1.83	0.41
1:F:187:THR:O	1:F:188:HIS:HB3	2.20	0.41
5:J:142:LYS:HD2	5:J:197:ARG:HH21	1.85	0.41
1:A:77:ASN:HD22	1:A:80:ILE:HD12	1.85	0.41
1:F:173:GLU:HG2	1:F:174:ASN:OD1	2.19	0.41
3:C:7:SER:O	3:C:8:ILE:HB	2.20	0.41
1:F:129:ASP:OD1	1:F:129:ASP:C	2.57	0.41
4:I:148:SER:OG	4:I:154:TYR:HA	2.20	0.41
5:E:32:HIS:CE1	5:E:106:PHE:HD2	2.32	0.41
1:F:260:HIS:CE1	1:F:271:THR:HB	2.56	0.41
5:J:159:LEU:HD23	5:J:159:LEU:O	2.20	0.41
1:A:106:ASP:OD2	1:A:108:ARG:CG	2.68	0.41
2:B:42:ASN:OD1	2:B:77:GLU:HG3	2.21	0.41
1:F:14:ARG:N	1:F:15:PRO:HD3	2.36	0.41
1:F:114:ASN:CB	1:F:156:LEU:HD21	2.50	0.41
2:G:17:ASN:ND2	2:G:97:ARG:HH12	2.18	0.41
2:G:97:ARG:H	2:G:97:ARG:HG3	1.62	0.41
5:J:203:TRP:CD1	5:J:203:TRP:C	2.99	0.41
1:A:21:ARG:HG3	1:A:39:ASP:OD1	2.21	0.41
1:A:25:VAL:CG1	1:A:32:GLN:OE1	2.69	0.41
1:A:167:TRP:NE1	3:C:1:THR:HG23	2.36	0.41
4:D:34:TRP:CH2	4:D:46:LEU:HB2	2.54	0.41
5:E:14:LYS:O	5:E:113:LEU:HA	2.21	0.41
4:I:36:ARG:HB3	4:I:44:VAL:HG12	2.02	0.41
5:J:85:THR:HG21	5:J:115:VAL:CG2	2.51	0.41
5:J:124:PRO:CB	5:J:235:GLN:HE22	2.33	0.41
5:J:179:LEU:HG	5:J:180:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:TRP:CG	3:C:1:THR:H1	2.38	0.41
2:B:70:PHE:O	2:B:70:PHE:CD2	2.74	0.41
4:D:136:PHE:HB2	4:D:188:PHE:CZ	2.56	0.41
4:D:154:TYR:CG	4:D:155:ILE:N	2.88	0.41
4:D:155:ILE:HG22	4:D:156:THR:O	2.21	0.41
5:J:125:PRO:HB3	5:J:152:PHE:HB3	2.03	0.41
1:A:42:SER:O	1:A:43:PRO:C	2.64	0.41
1:A:137:ASP:OD1	1:A:137:ASP:C	2.64	0.41
1:F:7:TYR:HB2	1:F:99:TYR:CZ	2.55	0.41
2:G:12:ARG:HD2	2:G:13:HIS:NE2	2.36	0.41
4:I:33:GLN:HE21	4:I:34:TRP:H	1.67	0.41
4:I:52:ASN:ND2	4:I:53:GLU:HG3	2.35	0.41
2:B:11:SER:HB2	2:B:21:ASN:HD21	1.82	0.40
1:F:19:GLU:C	1:F:20:PRO:O	2.64	0.40
4:I:118:PRO:HG2	4:I:194:PRO:HB2	2.03	0.40
1:A:98:MET:HG2	1:A:115:GLN:HB3	2.03	0.40
1:F:72:GLN:HA	1:F:75:ARG:NH1	2.36	0.40
1:F:232:GLU:OE2	2:G:6:LYS:HD2	2.21	0.40
4:I:88:PHE:HD1	4:I:103:SER:O	2.04	0.40
5:J:147:CYS:O	5:J:193:SER:HA	2.20	0.40
5:J:231:LYS:HA	5:J:232:PRO:HD3	1.78	0.40
1:A:234:ARG:HE	2:B:8:GLN:NE2	2.20	0.40
1:F:116:TYR:HB2	1:F:124:ILE:HG22	2.03	0.40
2:G:94:LYS:H	2:G:94:LYS:HG2	1.52	0.40
4:I:156:THR:O	4:I:173:ALA:HB1	2.21	0.40
4:D:49:ILE:HD11	4:D:53:GLU:O	2.21	0.40
1:F:266:LEU:HD13	1:F:270:LEU:HD23	2.04	0.40
4:I:123:LEU:HD12	5:J:132:PRO:HA	2.03	0.40
1:A:13:SER:O	1:A:14:ARG:HG3	2.21	0.40
2:B:31:HIS:CD2	2:B:62:PHE:CE2	3.08	0.40
1:F:52:ILE:O	1:F:54:GLN:N	2.54	0.40
2:G:42:ASN:OD1	2:G:77:GLU:HG3	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	245 (89%)	25 (9%)	4 (2%)	8	35
1	F	273/276 (99%)	239 (88%)	26 (10%)	8 (3%)	3	20
2	B	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
2	G	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	12	45
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	H	6/8 (75%)	6 (100%)	0	0	100	100
4	D	190/195 (97%)	166 (87%)	17 (9%)	7 (4%)	2	15
4	I	192/195 (98%)	163 (85%)	23 (12%)	6 (3%)	3	19
5	E	238/242 (98%)	213 (90%)	22 (9%)	3 (1%)	9	38
5	J	239/242 (99%)	219 (92%)	19 (8%)	1 (0%)	30	65
All	All	1612/1640 (98%)	1436 (89%)	146 (9%)	30 (2%)	6	30

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	9	GLN
4	D	28	SER
4	D	42	GLY
4	D	197	THR
1	F	130	LEU
4	I	28	SER
4	I	97	ARG
4	D	40	GLY
4	D	130	ASP
5	E	221	GLU
1	F	220	ASP
1	F	264	GLU
4	I	54	ARG
4	I	131	LYS
5	E	42	LEU
1	F	172	LEU
4	I	42	GLY
1	F	86	ASN
1	F	267	PRO
4	I	103	SER

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Mol	Chain	Res	Type
5	J	42	LEU
1	A	172	LEU
1	A	269	PRO
5	E	18	LYS
1	F	20	PRO
2	G	85	VAL
4	D	97	ARG
1	A	20	PRO
1	F	162	GLY
1	A	162	GLY

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	234/234 (100%)	190 (81%)	44 (19%)	1	9
1	F	233/234 (100%)	190 (82%)	43 (18%)	1	9
2	B	94/94 (100%)	84 (89%)	10 (11%)	6	27
2	G	94/94 (100%)	78 (83%)	16 (17%)	2	11
3	C	7/7 (100%)	7 (100%)	0	100	100
3	H	7/7 (100%)	5 (71%)	2 (29%)	0	2
4	D	172/174 (99%)	130 (76%)	42 (24%)	1	4
4	I	173/174 (99%)	137 (79%)	36 (21%)	1	7
5	E	203/204 (100%)	165 (81%)	38 (19%)	1	9
5	J	204/204 (100%)	170 (83%)	34 (17%)	2	12
All	All	1421/1426 (100%)	1156 (81%)	265 (19%)	1	9

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	12	MET
1	A	19	GLU

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Mol	Chain	Res	Type
1	A	31	THR
1	A	32	GLN
1	A	38	SER
1	A	46	GLU
1	A	52	ILE
1	A	62	ARG
1	A	98	MET
1	A	101	CYS
1	A	106	ASP
1	A	108	ARG
1	A	109	LEU
1	A	115	GLN
1	A	124	ILE
1	A	128	GLU
1	A	131	SER
1	A	132	SER
1	A	144	GLN
1	A	156	LEU
1	A	169	ARG
1	A	173	GLU
1	A	201	LEU
1	A	202	ARG
1	A	203	CYS
1	A	206	LEU
1	A	213	ILE
1	A	214	THR
1	A	216	THR
1	A	218	GLN
1	A	230	LEU
1	A	234	ARG
1	A	242	GLN
1	A	243	LYS
1	A	255	GLN
1	A	261	VAL
1	A	262	GLN
1	A	266	LEU
1	A	268	LYS
1	A	270	LEU
1	A	273	ARG
1	A	274	TRP
1	A	275	GLU
2	B	3	ARG

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Mol	Chain	Res	Type
2	B	9	VAL
2	B	17	ASN
2	B	39	LEU
2	B	44	GLU
2	B	49	VAL
2	B	70	PHE
2	B	77	GLU
2	B	85	VAL
2	B	99	MET
4	D	7	ASP
4	D	13	ILE
4	D	17	GLU
4	D	24	SER
4	D	27	THR
4	D	29	ILE
4	D	30	ASN
4	D	32	LEU
4	D	39	SER
4	D	44	VAL
4	D	45	HIS
4	D	46	LEU
4	D	47	ILE
4	D	52	ASN
4	D	53	GLU
4	D	54	ARG
4	D	62	ARG
4	D	75	LEU
4	D	76	ILE
4	D	77	THR
4	D	80	ARG
4	D	84	THR
4	D	99	LEU
4	D	108	THR
4	D	112	ASP
4	D	113	ILE
4	D	123	LEU
4	D	125	ASP
4	D	132	SER
4	D	142	GLN
4	D	145	VAL
4	D	147	GLN
4	D	149	LYS

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Mol	Chain	Res	Type
4	D	163	MET
4	D	174	VAL
4	D	178	ASN
4	D	181	ASP
4	D	186	ASN
4	D	193	ILE
4	D	195	GLU
4	D	197	THR
4	D	198	PHE
5	E	8	SER
5	E	10	THR
5	E	14	LYS
5	E	15	VAL
5	E	16	THR
5	E	26	CYS
5	E	33	THR
5	E	42	LEU
5	E	47	GLU
5	E	51	TYR
5	E	65	ASN
5	E	71	VAL
5	E	74	GLU
5	E	85	THR
5	E	99	LEU
5	E	113	LEU
5	E	126	GLU
5	E	133	SER
5	E	141	GLN
5	E	158	GLU
5	E	166	LYS
5	E	167	GLU
5	E	173	CYS
5	E	175	ASP
5	E	177	GLN
5	E	192	LEU
5	E	195	ARG
5	E	196	LEU
5	E	197	ARG
5	E	199	SER
5	E	201	THR
5	E	207	ARG
5	E	209	HIS

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Mol	Chain	Res	Type
5	E	219	LEU
5	E	221	GLU
5	E	225	TRP
5	E	227	GLN
5	E	229	ARG
1	F	12	MET
1	F	19	GLU
1	F	23	ILE
1	F	31	THR
1	F	38	SER
1	F	46	GLU
1	F	62	ARG
1	F	65	GLN
1	F	68	LYS
1	F	73	THR
1	F	79	ARG
1	F	101	CYS
1	F	102	ASP
1	F	106	ASP
1	F	115	GLN
1	F	121	LYS
1	F	130	LEU
1	F	131	SER
1	F	132	SER
1	F	137	ASP
1	F	142	ILE
1	F	144	GLN
1	F	145	ARG
1	F	160	LEU
1	F	163	LEU
1	F	170	ARG
1	F	173	GLU
1	F	178	THR
1	F	181	ARG
1	F	186	LYS
1	F	190	THR
1	F	203	CYS
1	F	214	THR
1	F	219	ARG
1	F	238	ASP
1	F	244	TRP
1	F	251	SER

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Mol	Chain	Res	Type
1	F	255	GLN
1	F	262	GLN
1	F	271	THR
1	F	272	LEU
1	F	274	TRP
1	F	275	GLU
2	G	1	ILE
2	G	9	VAL
2	G	27	VAL
2	G	39	LEU
2	G	47	GLU
2	G	48	LYS
2	G	49	VAL
2	G	58	LYS
2	G	70	PHE
2	G	75	LYS
2	G	77	GLU
2	G	85	VAL
2	G	88	SER
2	G	96	ASP
2	G	97	ARG
2	G	99	MET
3	H	1	THR
3	H	5	ILE
4	I	5	GLU
4	I	21	MET
4	I	22	ASN
4	I	24	SER
4	I	27	THR
4	I	29	ILE
4	I	30	ASN
4	I	43	LEU
4	I	44	VAL
4	I	46	LEU
4	I	47	ILE
4	I	48	LEU
4	I	52	ASN
4	I	62	ARG
4	I	63	VAL
4	I	67	THR
4	I	69	LYS
4	I	76	ILE

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Mol	Chain	Res	Type
4	I	77	THR
4	I	95	SER
4	I	97	ARG
4	I	98	GLN
4	I	99	LEU
4	I	108	THR
4	I	114	GLN
4	I	117	ASP
4	I	125	ASP
4	I	127	LYS
4	I	132	SER
4	I	142	GLN
4	I	153	VAL
4	I	158	LYS
4	I	178	ASN
4	I	181	ASP
4	I	186	ASN
4	I	195	GLU
5	J	8	SER
5	J	10	THR
5	J	16	THR
5	J	22	VAL
5	J	26	CYS
5	J	33	THR
5	J	51	TYR
5	J	55	THR
5	J	65	ASN
5	J	81	LYS
5	J	86	GLU
5	J	98	SER
5	J	104	GLU
5	J	121	ASN
5	J	126	GLU
5	J	133	SER
5	J	137	ILE
5	J	142	LYS
5	J	150	THR
5	J	157	VAL
5	J	158	GLU
5	J	159	LEU
5	J	166	LYS
5	J	167	GLU

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Mol	Chain	Res	Type
5	J	172	VAL
5	J	173	CYS
5	J	175	ASP
5	J	185	LEU
5	J	187	ASP
5	J	189	ARG
5	J	195	ARG
5	J	207	ARG
5	J	224	GLU
5	J	235	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	93	HIS
1	A	114	ASN
1	A	180	GLN
1	A	188	HIS
1	A	262	GLN
2	B	13	HIS
2	B	17	ASN
2	B	31	HIS
4	D	14	GLN
4	D	30	ASN
4	D	33	GLN
4	D	38	ASN
4	D	45	HIS
4	D	52	ASN
4	D	147	GLN
4	D	189	ASN
5	E	53	GLN
5	E	83	GLN
5	E	139	HIS
5	E	169	HIS
5	E	215	GLN
5	E	227	GLN
5	E	235	GLN
1	F	32	GLN
1	F	65	GLN
1	F	77	ASN
1	F	114	ASN

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Mol	Chain	Res	Type
1	F	115	GLN
1	F	144	GLN
1	F	155	GLN
1	F	171	HIS
1	F	180	GLN
1	F	191	HIS
1	F	192	HIS
1	F	226	GLN
1	F	260	HIS
1	F	262	GLN
2	G	8	GLN
2	G	17	ASN
2	G	24	ASN
4	I	30	ASN
4	I	33	GLN
4	I	52	ASN
4	I	98	GLN
4	I	171	ASN
4	I	186	ASN
4	I	189	ASN
5	J	32	HIS
5	J	53	GLN
5	J	164	ASN
5	J	182	GLN
5	J	209	HIS
5	J	227	GLN
5	J	235	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	0.36	6 (2%) 62 39	35, 59, 113, 130	0
1	F	275/276 (99%)	0.28	3 (1%) 78 57	37, 59, 103, 124	0
2	B	99/99 (100%)	-0.05	0 100 100	45, 57, 76, 82	0
2	G	99/99 (100%)	0.02	0 100 100	49, 59, 79, 82	0
3	C	8/8 (100%)	0.63	0 100 100	48, 50, 58, 58	0
3	H	8/8 (100%)	1.00	1 (12%) 8 5	45, 46, 53, 53	0
4	D	192/195 (98%)	0.52	12 (6%) 26 13	39, 63, 112, 124	0
4	I	194/195 (99%)	0.70	8 (4%) 41 23	39, 65, 113, 122	0
5	E	240/242 (99%)	0.26	4 (1%) 69 45	37, 69, 100, 129	0
5	J	241/242 (99%)	0.26	4 (1%) 69 45	37, 65, 95, 122	0
All	All	1632/1640 (99%)	0.34	38 (2%) 61 38	35, 61, 107, 130	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	154	TYR	3.9
4	I	197	THR	3.9
4	D	154	TYR	3.9
5	E	185	LEU	3.3
4	D	192	ILE	3.2
5	J	224	GLU	3.1
4	I	176	TRP	3.0
5	E	168	VAL	3.0
5	J	225	TRP	2.9
1	F	2	SER	2.9
4	D	34	TRP	2.7
3	H	8	ILE	2.7
1	F	1	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
4	D	176	TRP	2.7
4	D	43	LEU	2.5
4	I	192	ILE	2.5
5	J	206	PRO	2.5
4	D	183	ALA	2.5
5	E	169	HIS	2.5
5	J	185	LEU	2.4
5	E	225	TRP	2.4
1	A	225	THR	2.4
1	A	197	HIS	2.4
1	A	250	PRO	2.4
4	I	28	SER	2.3
1	F	180	GLN	2.3
4	D	28	SER	2.3
4	I	145	VAL	2.3
4	D	8	PRO	2.3
1	A	275	GLU	2.2
4	I	180	SER	2.2
4	D	152	ASP	2.2
1	A	2	SER	2.1
4	D	198	PHE	2.1
4	D	129	SER	2.1
4	D	182	PHE	2.1
4	I	7	ASP	2.1
1	A	272	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.