



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:42 PM UTC

PDB ID : 3E5Q / pdb_00003e5q
Title : Unbound Oxidised CprK
Authors : Levy, C.
Deposited on : 2008-08-14
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

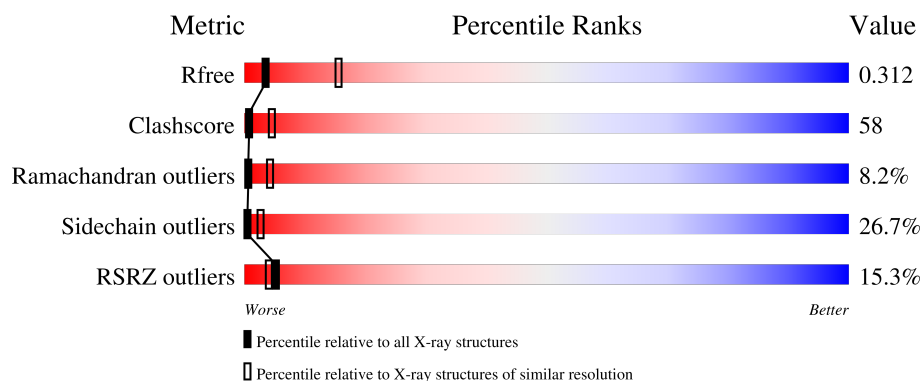
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	15% 19% 34% 22% 5% 19%
1	B	250	11% 17% 36% 22% 5% 20%
1	C	250	17% 22% 37% 19% • 19%
1	D	250	13% 18% 40% 20% • 20%
1	E	250	10% 18% 42% 19% • 19%

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Mol	Chain	Length	Quality of chain
1	F	250	8% 23% 37% 17% • 19%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9641 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 Cyclic nucleotide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1600	1034	265	293	8			
1	B	201	Total	C	N	O	S	0	0	0
			1611	1043	268	292	8			
1	C	203	Total	C	N	O	S	0	0	0
			1605	1037	266	294	8			
1	D	201	Total	C	N	O	S	0	0	0
			1605	1040	265	292	8			
1	E	203	Total	C	N	O	S	0	0	0
			1605	1037	266	294	8			
1	F	203	Total	C	N	O	S	0	0	0
			1615	1045	269	293	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	SER	-	expression tag	UNP Q18R04
A	234	ASP	-	expression tag	UNP Q18R04
A	235	PRO	-	expression tag	UNP Q18R04
A	236	ASN	-	expression tag	UNP Q18R04
A	237	SER	-	expression tag	UNP Q18R04
A	238	SER	-	expression tag	UNP Q18R04
A	239	SER	-	expression tag	UNP Q18R04
A	240	VAL	-	expression tag	UNP Q18R04
A	241	ASP	-	expression tag	UNP Q18R04
A	242	LYS	-	expression tag	UNP Q18R04
A	243	LEU	-	expression tag	UNP Q18R04
A	244	ALA	-	expression tag	UNP Q18R04
A	245	ALA	-	expression tag	UNP Q18R04
A	246	ALA	-	expression tag	UNP Q18R04
A	247	LEU	-	expression tag	UNP Q18R04
A	248	ASP	-	expression tag	UNP Q18R04
A	249	HIS	-	expression tag	UNP Q18R04

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Chain	Residue	Modelled	Actual	Comment	Reference
A	250	HIS	-	expression tag	UNP Q18R04
B	233	SER	-	expression tag	UNP Q18R04
B	234	ASP	-	expression tag	UNP Q18R04
B	235	PRO	-	expression tag	UNP Q18R04
B	236	ASN	-	expression tag	UNP Q18R04
B	237	SER	-	expression tag	UNP Q18R04
B	238	SER	-	expression tag	UNP Q18R04
B	239	SER	-	expression tag	UNP Q18R04
B	240	VAL	-	expression tag	UNP Q18R04
B	241	ASP	-	expression tag	UNP Q18R04
B	242	LYS	-	expression tag	UNP Q18R04
B	243	LEU	-	expression tag	UNP Q18R04
B	244	ALA	-	expression tag	UNP Q18R04
B	245	ALA	-	expression tag	UNP Q18R04
B	246	ALA	-	expression tag	UNP Q18R04
B	247	LEU	-	expression tag	UNP Q18R04
B	248	ASP	-	expression tag	UNP Q18R04
B	249	HIS	-	expression tag	UNP Q18R04
B	250	HIS	-	expression tag	UNP Q18R04
C	233	SER	-	expression tag	UNP Q18R04
C	234	ASP	-	expression tag	UNP Q18R04
C	235	PRO	-	expression tag	UNP Q18R04
C	236	ASN	-	expression tag	UNP Q18R04
C	237	SER	-	expression tag	UNP Q18R04
C	238	SER	-	expression tag	UNP Q18R04
C	239	SER	-	expression tag	UNP Q18R04
C	240	VAL	-	expression tag	UNP Q18R04
C	241	ASP	-	expression tag	UNP Q18R04
C	242	LYS	-	expression tag	UNP Q18R04
C	243	LEU	-	expression tag	UNP Q18R04
C	244	ALA	-	expression tag	UNP Q18R04
C	245	ALA	-	expression tag	UNP Q18R04
C	246	ALA	-	expression tag	UNP Q18R04
C	247	LEU	-	expression tag	UNP Q18R04
C	248	ASP	-	expression tag	UNP Q18R04
C	249	HIS	-	expression tag	UNP Q18R04
C	250	HIS	-	expression tag	UNP Q18R04
D	233	SER	-	expression tag	UNP Q18R04
D	234	ASP	-	expression tag	UNP Q18R04
D	235	PRO	-	expression tag	UNP Q18R04
D	236	ASN	-	expression tag	UNP Q18R04
D	237	SER	-	expression tag	UNP Q18R04

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Chain	Residue	Modelled	Actual	Comment	Reference
D	238	SER	-	expression tag	UNP Q18R04
D	239	SER	-	expression tag	UNP Q18R04
D	240	VAL	-	expression tag	UNP Q18R04
D	241	ASP	-	expression tag	UNP Q18R04
D	242	LYS	-	expression tag	UNP Q18R04
D	243	LEU	-	expression tag	UNP Q18R04
D	244	ALA	-	expression tag	UNP Q18R04
D	245	ALA	-	expression tag	UNP Q18R04
D	246	ALA	-	expression tag	UNP Q18R04
D	247	LEU	-	expression tag	UNP Q18R04
D	248	ASP	-	expression tag	UNP Q18R04
D	249	HIS	-	expression tag	UNP Q18R04
D	250	HIS	-	expression tag	UNP Q18R04
E	233	SER	-	expression tag	UNP Q18R04
E	234	ASP	-	expression tag	UNP Q18R04
E	235	PRO	-	expression tag	UNP Q18R04
E	236	ASN	-	expression tag	UNP Q18R04
E	237	SER	-	expression tag	UNP Q18R04
E	238	SER	-	expression tag	UNP Q18R04
E	239	SER	-	expression tag	UNP Q18R04
E	240	VAL	-	expression tag	UNP Q18R04
E	241	ASP	-	expression tag	UNP Q18R04
E	242	LYS	-	expression tag	UNP Q18R04
E	243	LEU	-	expression tag	UNP Q18R04
E	244	ALA	-	expression tag	UNP Q18R04
E	245	ALA	-	expression tag	UNP Q18R04
E	246	ALA	-	expression tag	UNP Q18R04
E	247	LEU	-	expression tag	UNP Q18R04
E	248	ASP	-	expression tag	UNP Q18R04
E	249	HIS	-	expression tag	UNP Q18R04
E	250	HIS	-	expression tag	UNP Q18R04
F	233	SER	-	expression tag	UNP Q18R04
F	234	ASP	-	expression tag	UNP Q18R04
F	235	PRO	-	expression tag	UNP Q18R04
F	236	ASN	-	expression tag	UNP Q18R04
F	237	SER	-	expression tag	UNP Q18R04
F	238	SER	-	expression tag	UNP Q18R04
F	239	SER	-	expression tag	UNP Q18R04
F	240	VAL	-	expression tag	UNP Q18R04
F	241	ASP	-	expression tag	UNP Q18R04
F	242	LYS	-	expression tag	UNP Q18R04
F	243	LEU	-	expression tag	UNP Q18R04

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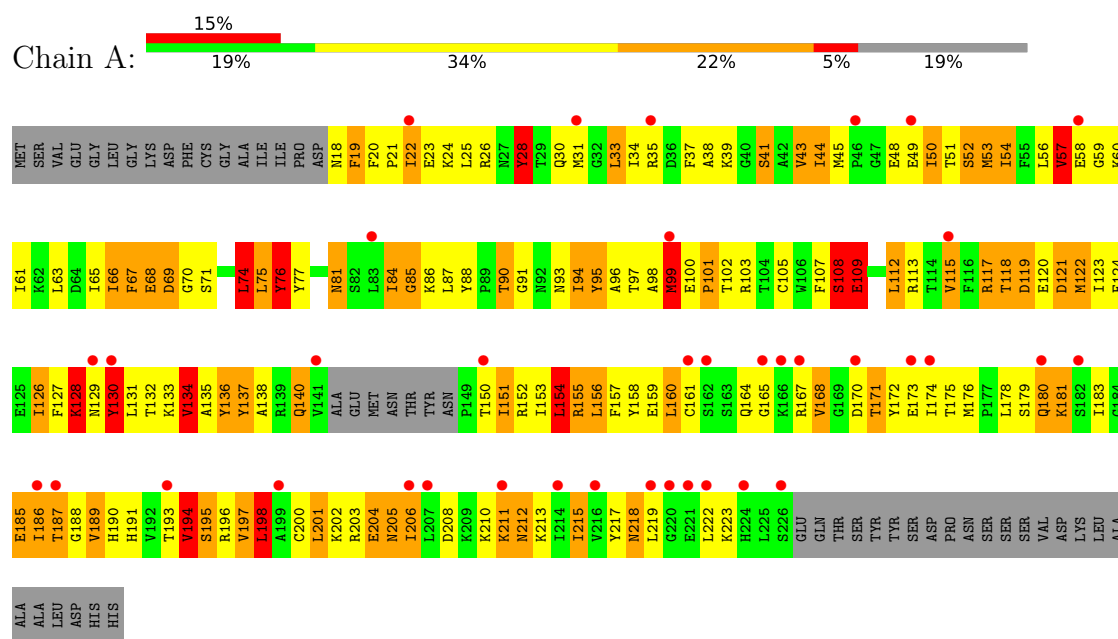
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Chain	Residue	Modelled	Actual	Comment	Reference
F	244	ALA	-	expression tag	UNP Q18R04
F	245	ALA	-	expression tag	UNP Q18R04
F	246	ALA	-	expression tag	UNP Q18R04
F	247	LEU	-	expression tag	UNP Q18R04
F	248	ASP	-	expression tag	UNP Q18R04
F	249	HIS	-	expression tag	UNP Q18R04
F	250	HIS	-	expression tag	UNP Q18R04

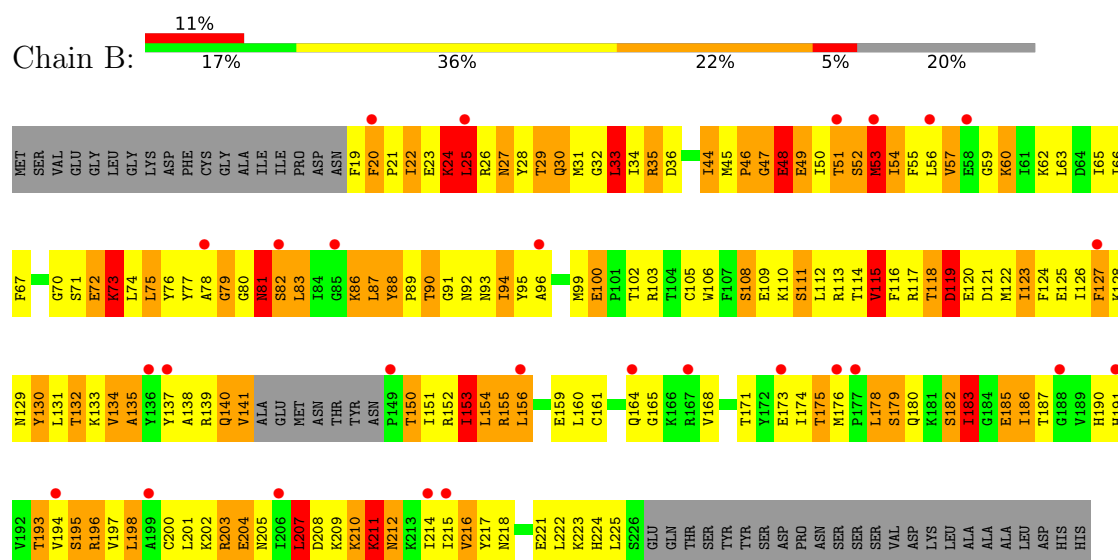
3 Residue-property plots

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.

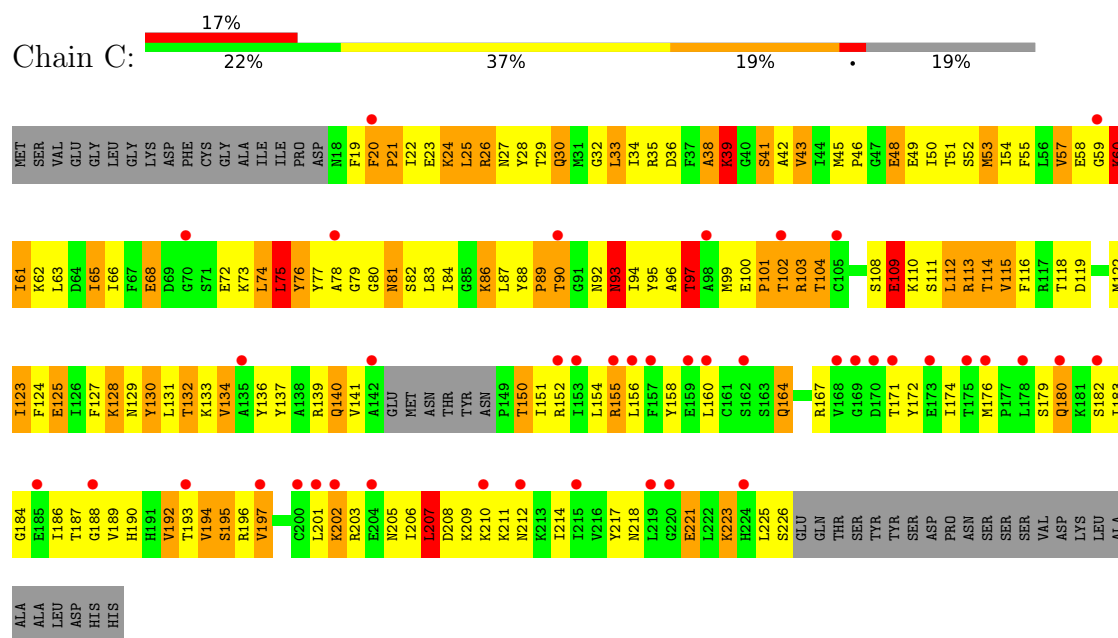
• Molecule 1: Cyclic nucleotide-binding protein

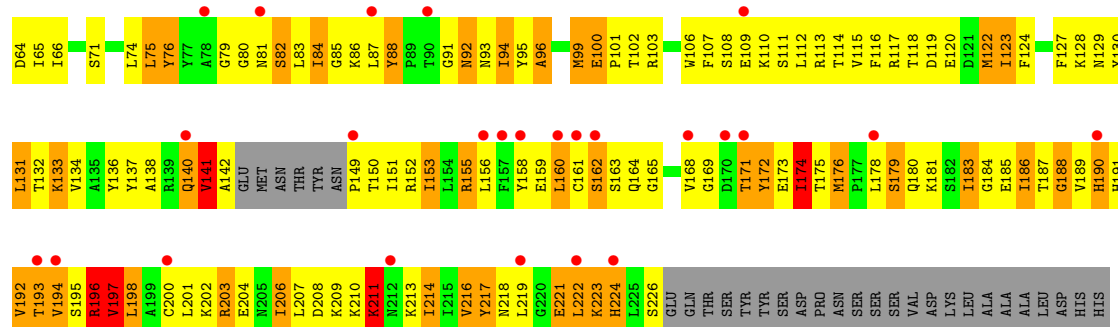


• Molecule 1: Cyclic nucleotide-binding protein

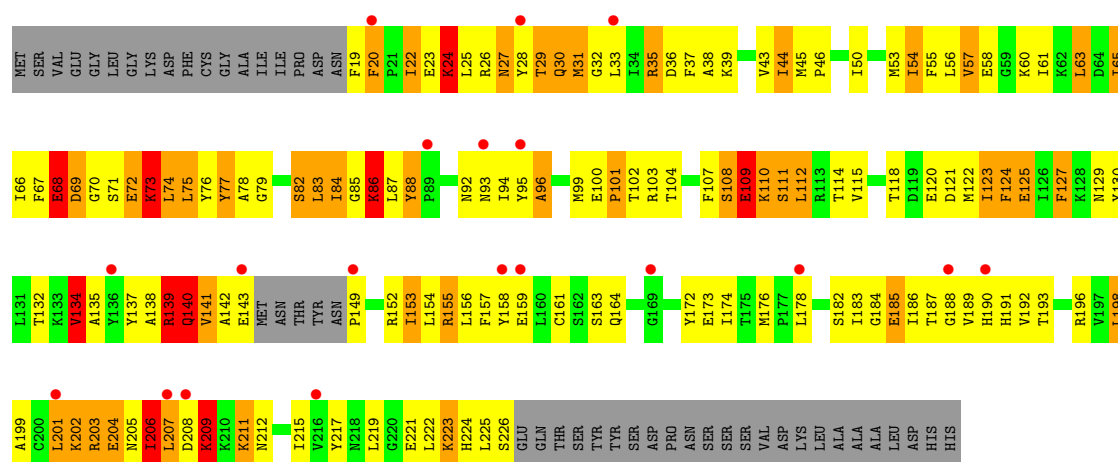
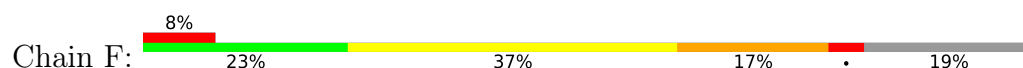


• Molecule 1: Cyclic nucleotide-binding protein





● Molecule 1: Cyclic nucleotide-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.41Å 64.71Å 148.35Å 90.00° 105.29° 90.00°	Depositor
Resolution (Å)	142.86 – 3.20 142.86 – 3.20	Depositor EDS
% Data completeness (in resolution range)	79.8 (142.86-3.20) 70.4 (142.86-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.258 , 0.318 0.319 , 0.312	Depositor DCC
R_{free} test set	1715 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	9641	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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	1.39	7/1630 (0.4%)	1.60	26/2200 (1.2%)
1	B	1.47	12/1641 (0.7%)	1.61	24/2209 (1.1%)
1	C	1.22	4/1635 (0.2%)	1.52	29/2207 (1.3%)
1	D	1.14	2/1635 (0.1%)	1.35	14/2202 (0.6%)
1	E	1.19	5/1635 (0.3%)	1.50	23/2207 (1.0%)
1	F	1.15	4/1645 (0.2%)	1.42	19/2215 (0.9%)
All	All	1.27	34/9821 (0.3%)	1.50	135/13240 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	D	0	2
1	E	0	2
1	F	0	1
All	All	0	9

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	TYR	CA-C	-8.73	1.42	1.52
1	B	90	THR	N-CA	6.88	1.54	1.46
1	F	134	VAL	CA-CB	-6.83	1.47	1.54
1	B	90	THR	CA-CB	6.63	1.62	1.53
1	B	33	LEU	CA-C	-6.34	1.44	1.52
1	A	108	SER	CA-C	-6.13	1.44	1.52
1	F	24	LYS	CA-C	6.11	1.60	1.52
1	B	132	THR	CA-CB	-5.89	1.44	1.53
1	A	57	VAL	CA-CB	5.82	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	151	ILE	CA-CB	5.67	1.61	1.54
1	A	76	TYR	N-CA	5.66	1.52	1.46
1	B	81	ASN	CA-C	-5.63	1.45	1.52
1	C	20	PHE	CA-C	-5.60	1.49	1.53
1	A	130	TYR	N-CA	-5.57	1.39	1.46
1	B	25	LEU	CA-C	5.55	1.60	1.52
1	B	132	THR	N-CA	-5.51	1.39	1.46
1	D	96	ALA	CA-CB	-5.48	1.45	1.53
1	C	134	VAL	CA-CB	-5.44	1.48	1.54
1	B	53	MET	CA-C	-5.28	1.46	1.52
1	E	96	ALA	CA-CB	-5.24	1.45	1.53
1	B	34	ILE	CA-C	-5.23	1.46	1.52
1	A	115	VAL	CA-CB	5.21	1.60	1.54
1	E	88	TYR	C-N	5.16	1.40	1.33
1	E	114	THR	CA-CB	5.15	1.61	1.53
1	C	197	VAL	CA-CB	5.15	1.61	1.54
1	F	77	TYR	CA-C	-5.13	1.46	1.52
1	B	130	TYR	N-CA	-5.12	1.40	1.46
1	C	38	ALA	CA-CB	-5.07	1.45	1.53
1	B	34	ILE	C-O	-5.05	1.18	1.24
1	B	190	HIS	CA-C	5.04	1.59	1.52
1	E	196	ARG	N-CA	5.03	1.52	1.46
1	A	137	TYR	N-CA	-5.03	1.40	1.46
1	F	127	PHE	CA-C	-5.02	1.46	1.52
1	E	61	ILE	N-CA	5.00	1.51	1.46

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	88	TYR	N-CA-C	-10.52	96.04	108.14
1	B	118	THR	N-CA-C	-9.89	100.05	113.30
1	B	20	PHE	CA-C-N	9.41	131.60	119.84
1	B	20	PHE	C-N-CA	9.41	131.60	119.84
1	F	88	TYR	CA-C-N	9.24	129.28	119.76
1	F	88	TYR	C-N-CA	9.24	129.28	119.76
1	B	54	ILE	CB-CA-C	-9.23	101.00	112.45
1	A	154	LEU	N-CA-C	-8.36	101.86	110.97
1	E	123	ILE	N-CA-C	-8.29	102.73	110.53
1	F	132	THR	N-CA-C	-8.00	102.25	110.97
1	B	130	TYR	CA-CB-CG	-7.93	99.62	113.90
1	A	194	VAL	CB-CA-C	-7.84	101.85	111.88
1	D	201	LEU	N-CA-C	-7.76	105.77	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	PHE	CB-CA-C	-7.75	104.26	111.00
1	F	138	ALA	N-CA-C	-7.62	104.13	113.50
1	D	85	GLY	N-CA-C	7.60	121.67	112.48
1	A	124	PHE	N-CA-C	-7.57	104.57	113.88
1	D	128	LYS	N-CA-C	-7.56	103.04	111.28
1	A	126	ILE	N-CA-C	-7.43	103.70	111.58
1	A	119	ASP	N-CA-C	7.34	119.49	107.23
1	E	130	TYR	N-CA-C	7.27	119.10	111.03
1	B	79	GLY	N-CA-C	-7.25	101.53	112.41
1	D	100	GLU	N-CA-C	-7.19	101.66	108.13
1	F	140	GLN	CA-C-N	7.13	134.53	121.70
1	F	140	GLN	C-N-CA	7.13	134.53	121.70
1	F	69	ASP	N-CA-C	-7.07	103.70	114.16
1	C	58	GLU	N-CA-C	7.02	122.29	108.18
1	F	118	THR	N-CA-C	-6.95	103.64	111.07
1	C	30	GLN	N-CA-C	-6.90	103.84	111.36
1	A	67	PHE	N-CA-C	-6.86	100.37	110.52
1	B	123	ILE	N-CA-C	-6.81	103.89	110.42
1	F	191	HIS	N-CA-C	6.75	119.50	111.33
1	E	92	ASN	N-CA-C	-6.73	98.44	109.40
1	A	187	THR	N-CA-C	6.72	120.79	112.59
1	C	48	GLU	N-CA-C	-6.70	100.52	110.23
1	C	150	THR	N-CA-C	-6.70	106.98	114.62
1	B	90	THR	N-CA-C	6.69	120.79	111.56
1	B	207	LEU	N-CA-C	6.68	118.95	107.93
1	E	88	TYR	CA-C-O	-6.65	114.92	120.71
1	A	136	TYR	CB-CA-C	-6.59	100.81	110.96
1	D	48	GLU	N-CA-C	-6.52	101.31	110.50
1	E	20	PHE	CA-C-N	6.52	127.05	120.14
1	E	20	PHE	C-N-CA	6.52	127.05	120.14
1	C	123	ILE	N-CA-CB	6.50	117.72	110.51
1	C	76	TYR	N-CA-C	6.42	117.98	108.60
1	A	81	ASN	N-CA-C	6.36	120.34	112.58
1	C	110	LYS	CA-C-N	6.35	129.08	120.44
1	C	110	LYS	C-N-CA	6.35	129.08	120.44
1	A	95	TYR	CA-C-N	-6.34	113.20	122.65
1	A	95	TYR	C-N-CA	-6.34	113.20	122.65
1	A	198	LEU	N-CA-C	-6.31	104.50	111.82
1	A	19	PHE	N-CA-C	-6.30	106.29	112.97
1	A	28	TYR	N-CA-C	6.28	120.57	112.41
1	D	94	ILE	N-CA-C	6.26	117.49	108.48
1	E	224	HIS	N-CA-C	6.24	120.73	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	GLY	N-CA-C	-6.22	106.51	113.79
1	F	124	PHE	N-CA-C	6.21	120.12	112.54
1	C	53	MET	CA-C-N	-6.16	114.72	123.10
1	C	53	MET	C-N-CA	-6.16	114.72	123.10
1	B	183	ILE	N-CA-C	-6.13	104.77	110.53
1	A	101	PRO	N-CA-C	-6.12	100.86	111.32
1	C	123	ILE	N-CA-C	-6.12	103.94	110.36
1	B	178	LEU	N-CA-C	-6.11	96.86	107.49
1	D	96	ALA	N-CA-C	6.11	119.20	109.24
1	E	130	TYR	CA-CB-CG	-6.11	102.91	113.90
1	F	20	PHE	CA-C-N	6.10	126.31	119.90
1	F	20	PHE	C-N-CA	6.10	126.31	119.90
1	B	186	ILE	N-CA-C	6.08	116.75	110.36
1	E	180	GLN	CA-C-N	6.07	129.22	120.79
1	E	180	GLN	C-N-CA	6.07	129.22	120.79
1	B	60	LYS	N-CA-C	5.97	118.36	108.99
1	E	224	HIS	CA-C-N	-5.96	113.11	122.65
1	E	224	HIS	C-N-CA	-5.96	113.11	122.65
1	B	48	GLU	N-CA-C	-5.93	101.87	110.24
1	C	97	THR	N-CA-C	5.89	119.11	108.69
1	E	83	LEU	CA-CB-CG	-5.89	95.70	116.30
1	F	112	LEU	N-CA-C	5.86	117.74	111.36
1	B	46	PRO	N-CA-C	-5.85	101.39	112.33
1	A	173	GLU	N-CA-C	5.76	118.97	107.62
1	A	67	PHE	CB-CA-C	5.76	119.91	109.83
1	D	130	TYR	CA-CB-CG	-5.76	103.53	113.90
1	C	26	ARG	N-CA-C	-5.76	106.21	113.18
1	E	82	SER	N-CA-C	5.69	118.26	110.24
1	F	176	MET	N-CA-C	5.68	115.44	108.11
1	C	112	LEU	N-CA-C	-5.65	104.81	110.97
1	F	201	LEU	CA-C-N	5.64	127.78	120.44
1	F	201	LEU	C-N-CA	5.64	127.78	120.44
1	C	39	LYS	N-CA-C	-5.60	102.00	110.28
1	E	57	VAL	N-CA-C	5.59	120.97	109.34
1	B	115	VAL	N-CA-CB	5.58	120.44	111.23
1	A	112	LEU	N-CA-C	-5.57	105.31	111.71
1	F	96	ALA	N-CA-C	5.56	117.79	108.73
1	A	90	THR	CB-CA-C	-5.52	98.85	110.45
1	E	174	ILE	N-CA-C	5.51	116.50	107.24
1	B	49	GLU	N-CA-C	5.46	117.64	108.96
1	A	74	LEU	N-CA-C	5.45	117.62	108.96
1	A	109	GLU	N-CA-CB	-5.45	102.08	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	THR	N-CA-C	-5.44	104.99	111.69
1	C	61	ILE	N-CA-C	5.42	115.89	107.28
1	C	207	LEU	N-CA-C	5.41	118.25	109.06
1	B	218	ASN	N-CA-C	5.38	119.12	107.49
1	D	115	VAL	CB-CA-C	-5.38	105.00	112.04
1	E	32	GLY	N-CA-C	-5.37	104.92	112.60
1	A	85	GLY	N-CA-C	5.37	125.90	113.18
1	F	92	ASN	N-CA-C	-5.37	100.57	108.99
1	B	127	PHE	N-CA-C	-5.36	105.13	110.97
1	B	78	ALA	N-CA-C	-5.36	98.53	107.80
1	B	59	GLY	N-CA-C	5.34	119.84	112.52
1	C	81	ASN	CB-CA-C	-5.34	104.37	111.63
1	C	132	THR	N-CA-C	-5.34	99.43	110.80
1	C	110	LYS	N-CA-C	-5.33	105.58	111.71
1	D	150	THR	N-CA-C	-5.33	106.48	112.87
1	F	202	LYS	N-CA-C	5.33	116.77	111.07
1	A	44	ILE	N-CA-C	5.30	115.71	107.28
1	E	172	TYR	N-CA-C	5.29	116.07	107.23
1	C	104	THR	N-CA-C	-5.29	102.64	110.46
1	E	88	TYR	O-C-N	5.24	126.00	121.54
1	A	134	VAL	N-CA-C	-5.24	105.43	110.72
1	A	99	MET	N-CA-C	-5.21	105.29	110.97
1	C	206	ILE	N-CA-C	-5.20	106.73	111.67
1	B	34	ILE	CB-CA-C	-5.19	104.68	110.96
1	E	31	MET	N-CA-C	-5.19	105.62	112.94
1	C	130	TYR	N-CA-C	5.12	119.16	113.01
1	D	137	TYR	N-CA-C	5.12	117.52	111.33
1	D	107	PHE	N-CA-C	5.10	117.11	108.02
1	B	111	SER	N-CA-C	-5.10	105.80	111.36
1	B	130	TYR	N-CA-C	-5.08	105.43	110.97
1	C	75	LEU	N-CA-C	-5.07	103.18	111.04
1	C	60	LYS	N-CA-C	5.07	116.63	108.32
1	A	121	ASP	N-CA-C	5.05	116.48	110.97
1	E	171	THR	N-CA-C	5.04	114.94	108.34
1	C	81	ASN	CA-C-N	-5.03	113.73	122.64
1	C	81	ASN	C-N-CA	-5.03	113.73	122.64
1	C	109	GLU	N-CA-C	5.02	121.50	110.80
1	D	99	MET	N-CA-C	5.01	119.02	113.01

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	THR	Peptide
1	B	47	GLY	Peptide
1	B	71	SER	Peptide
1	B	88	TYR	Peptide
1	D	87	LEU	Peptide
1	D	91	GLY	Peptide
1	E	193	THR	Peptide
1	E	91	GLY	Peptide
1	F	139	ARG	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	1600	0	1601	218	0
1	B	1611	0	1643	239	0
1	C	1605	0	1606	200	0
1	D	1605	0	1632	214	1
1	E	1605	0	1606	208	0
1	F	1615	0	1637	196	1
All	All	9641	0	9725	1133	1

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 58.

All (1133) 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:A:35:ARG:NH1	1:A:37:PHE:HZ	1.42	1.14
1:D:44:ILE:HG21	1:D:94:ILE:HG22	1.32	1.11
1:E:60:LYS:HD3	1:E:99:MET:HE3	1.13	1.10
1:C:50:ILE:HB	1:C:86:LYS:HE2	1.26	1.09
1:B:22:ILE:HG13	1:B:22:ILE:O	1.48	1.09
1:D:124:PHE:HA	1:D:127:PHE:HB2	1.30	1.09
1:F:139:ARG:O	1:F:141:VAL:CB	2.03	1.07
1:D:189:VAL:HG13	1:D:193:THR:HB	1.37	1.04
1:F:27:ASN:N	1:F:27:ASN:HD22	1.52	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ILE:CD1	1:D:123:ILE:HD13	1.89	1.03
1:A:35:ARG:HH12	1:A:37:PHE:HZ	1.02	1.02
1:C:150:THR:O	1:C:154:LEU:HG	1.58	1.01
1:A:35:ARG:NH1	1:A:37:PHE:CZ	2.28	1.01
1:F:149:PRO:HB3	1:F:152:ARG:HD2	1.38	1.01
1:B:178:LEU:O	1:B:209:LYS:HD2	1.60	1.00
1:E:198:LEU:HD13	1:E:201:LEU:HD12	1.39	1.00
1:D:120:GLU:O	1:D:123:ILE:HG13	1.60	1.00
1:B:80:GLY:O	1:B:81:ASN:HB2	1.58	1.00
1:E:193:THR:HG22	1:E:196:ARG:HG2	1.42	0.99
1:D:153:ILE:HD13	1:D:197:VAL:HG21	1.43	0.99
1:A:193:THR:O	1:A:197:VAL:HB	1.64	0.98
1:B:45:MET:HB2	1:B:48:GLU:HB3	1.45	0.98
1:A:160:LEU:HD11	1:A:176:MET:SD	2.04	0.97
1:B:54:ILE:HG22	1:B:54:ILE:O	1.60	0.97
1:D:86:LYS:HZ1	1:D:90:THR:H	1.06	0.97
1:D:110:LYS:O	1:D:112:LEU:N	1.98	0.97
1:D:189:VAL:CG1	1:D:193:THR:HB	1.94	0.97
1:D:207:LEU:HD12	1:D:216:VAL:HG22	1.47	0.97
1:F:65:ILE:O	1:F:72:GLU:O	1.82	0.97
1:A:159:GLU:HG3	1:B:186:ILE:HD11	1.47	0.96
1:A:87:LEU:HB2	1:A:88:TYR:CE1	2.00	0.96
1:D:178:LEU:HG	1:D:183:ILE:HD11	1.45	0.96
1:E:152:ARG:HD3	1:F:188:GLY:CA	1.96	0.95
1:E:161:CYS:SG	1:E:172:TYR:HB3	2.07	0.94
1:A:130:TYR:HE2	1:B:131:LEU:HD23	1.32	0.94
1:A:185:GLU:O	1:B:152:ARG:HG2	1.66	0.94
1:D:65:ILE:O	1:D:72:GLU:O	1.86	0.93
1:D:151:ILE:O	1:D:155:ARG:HG3	1.67	0.93
1:B:30:GLN:H	1:B:30:GLN:NE2	1.64	0.93
1:D:132:THR:O	1:D:135:ALA:HB3	1.68	0.93
1:A:127:PHE:HE1	1:B:130:TYR:CD1	1.87	0.93
1:F:206:ILE:O	1:F:217:TYR:HD1	1.51	0.93
1:F:67:PHE:O	1:F:69:ASP:N	2.01	0.93
1:A:155:ARG:HH11	1:B:185:GLU:HB3	1.34	0.92
1:C:46:PRO:HB3	1:C:93:ASN:HD21	1.32	0.92
1:B:44:ILE:HD13	1:B:50:ILE:HG13	1.49	0.92
1:F:153:ILE:HG13	1:F:187:THR:HG21	1.50	0.92
1:C:152:ARG:HH21	1:C:189:VAL:HG22	1.31	0.91
1:D:86:LYS:HZ1	1:D:90:THR:N	1.68	0.91
1:E:123:ILE:HG23	1:F:123:ILE:HG23	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:HD11	1:B:77:TYR:HE1	1.34	0.90
1:F:73:LYS:HZ2	1:F:74:LEU:H	1.13	0.90
1:E:60:LYS:HD3	1:E:99:MET:CE	2.02	0.90
1:E:209:LYS:HG3	1:E:214:ILE:HG23	1.52	0.89
1:C:155:ARG:HD3	1:D:185:GLU:OE1	1.72	0.88
1:D:156:LEU:O	1:D:160:LEU:HB2	1.71	0.88
1:E:64:ASP:OD1	1:E:74:LEU:HA	1.73	0.88
1:B:221:GLU:O	1:B:225:LEU:HD12	1.74	0.88
1:A:127:PHE:CZ	1:B:53:MET:HE2	2.09	0.88
1:A:155:ARG:NH1	1:B:185:GLU:HB3	1.89	0.88
1:C:123:ILE:HD13	1:D:123:ILE:HD13	1.56	0.87
1:C:202:LYS:HA	1:C:207:LEU:O	1.73	0.87
1:C:186:ILE:HG12	1:D:156:LEU:HA	1.54	0.87
1:F:63:LEU:N	1:F:63:LEU:HD12	1.87	0.87
1:C:123:ILE:HD11	1:D:123:ILE:HD13	1.53	0.87
1:E:155:ARG:HB3	1:F:186:ILE:HG13	1.53	0.87
1:E:159:GLU:HG3	1:F:186:ILE:HD11	1.57	0.87
1:F:183:ILE:O	1:F:187:THR:HG23	1.75	0.87
1:B:154:LEU:HD23	1:B:201:LEU:HD21	1.57	0.86
1:D:62:LYS:HG2	1:D:64:ASP:OD2	1.75	0.86
1:B:46:PRO:C	1:B:93:ASN:OD1	2.18	0.86
1:B:66:ILE:CD1	1:B:95:TYR:HB2	2.05	0.86
1:F:199:ALA:O	1:F:202:LYS:HB3	1.74	0.86
1:F:30:GLN:H	1:F:30:GLN:CD	1.83	0.86
1:F:205:ASN:O	1:F:217:TYR:HB2	1.75	0.86
1:B:86:LYS:NZ	1:B:88:TYR:O	2.08	0.86
1:B:175:THR:HG22	1:B:175:THR:O	1.76	0.86
1:E:186:ILE:HD11	1:F:159:GLU:HG3	1.57	0.86
1:F:157:PHE:CD2	1:F:207:LEU:HD11	2.11	0.85
1:A:164:GLN:HG2	1:B:164:GLN:CD	2.01	0.85
1:D:92:ASN:O	1:D:94:ILE:HG12	1.77	0.85
1:A:217:TYR:O	1:A:218:ASN:HB2	1.77	0.85
1:D:172:TYR:CE1	1:D:219:LEU:HB2	2.11	0.85
1:E:142:ALA:HB1	1:F:73:LYS:HD3	1.60	0.84
1:A:75:LEU:C	1:A:76:TYR:HD1	1.85	0.84
1:F:73:LYS:HZ2	1:F:74:LEU:N	1.74	0.84
1:A:131:LEU:HD21	1:B:53:MET:CE	2.07	0.84
1:E:60:LYS:CD	1:E:99:MET:HE3	2.04	0.84
1:B:30:GLN:H	1:B:30:GLN:HE21	1.22	0.84
1:B:35:ARG:HH11	1:B:35:ARG:HB3	1.42	0.84
1:C:50:ILE:HB	1:C:86:LYS:CE	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:SER:O	1:D:115:VAL:HG23	1.78	0.83
1:F:30:GLN:N	1:F:30:GLN:OE1	2.12	0.83
1:B:45:MET:HB2	1:B:48:GLU:CB	2.08	0.83
1:C:22:ILE:HG23	1:C:22:ILE:O	1.78	0.83
1:C:108:SER:O	1:C:111:SER:OG	1.96	0.83
1:B:74:LEU:HD23	1:B:75:LEU:N	1.94	0.83
1:E:174:ILE:N	1:E:214:ILE:O	2.11	0.83
1:B:175:THR:O	1:B:175:THR:CG2	2.26	0.82
1:F:73:LYS:NZ	1:F:74:LEU:H	1.76	0.82
1:D:167:ARG:HA	1:D:171:THR:O	1.78	0.82
1:E:57:VAL:CG2	1:E:57:VAL:O	2.27	0.82
1:B:22:ILE:O	1:B:22:ILE:CG1	2.28	0.82
1:E:63:LEU:HD11	1:E:84:ILE:HG21	1.62	0.82
1:F:27:ASN:HD22	1:F:27:ASN:H	1.22	0.81
1:E:198:LEU:HD13	1:E:201:LEU:CD1	2.10	0.81
1:F:149:PRO:CB	1:F:152:ARG:HD2	2.10	0.81
1:B:122:MET:HA	1:B:125:GLU:HB2	1.59	0.81
1:F:149:PRO:HB3	1:F:152:ARG:CD	2.11	0.81
1:E:44:ILE:HG12	1:E:50:ILE:HD12	1.62	0.81
1:E:188:GLY:HA3	1:F:152:ARG:NE	1.95	0.81
1:F:55:PHE:CB	1:F:107:PHE:HE1	1.93	0.81
1:A:23:GLU:HG3	1:A:81:ASN:ND2	1.96	0.81
1:E:152:ARG:HD3	1:F:188:GLY:HA2	1.63	0.80
1:B:60:LYS:HG2	1:B:99:MET:HB2	1.64	0.80
1:F:140:GLN:C	1:F:142:ALA:HB3	2.07	0.80
1:E:155:ARG:HB3	1:F:186:ILE:CG1	2.12	0.80
1:D:149:PRO:N	1:D:151:ILE:CG1	2.45	0.79
1:E:211:LYS:HE3	1:E:211:LYS:N	1.97	0.79
1:A:113:ARG:HD3	1:B:120:GLU:OE1	1.82	0.79
1:B:26:ARG:NH2	1:B:57:VAL:HG23	1.97	0.79
1:A:38:ALA:O	1:A:41:SER:HB2	1.83	0.79
1:E:150:THR:HG23	1:E:197:VAL:HG22	1.64	0.79
1:B:203:ARG:NH1	1:B:204:GLU:OE2	2.15	0.79
1:C:155:ARG:NH1	1:C:158:TYR:HD2	1.82	0.78
1:B:131:LEU:O	1:B:134:VAL:HG23	1.83	0.78
1:A:128:LYS:HG3	1:B:88:TYR:CE1	2.17	0.78
1:B:74:LEU:HD11	1:B:77:TYR:CE1	2.19	0.78
1:E:152:ARG:HD3	1:F:188:GLY:N	1.99	0.78
1:F:27:ASN:N	1:F:27:ASN:ND2	2.26	0.78
1:F:87:LEU:HD23	1:F:109:GLU:HG2	1.65	0.78
1:C:60:LYS:HG2	1:C:99:MET:HE3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:NH2	1:B:57:VAL:O	2.16	0.77
1:D:158:TYR:O	1:D:162:SER:OG	2.01	0.77
1:F:63:LEU:HD12	1:F:63:LEU:H	1.47	0.77
1:D:111:SER:O	1:D:114:THR:HB	1.84	0.77
1:B:79:GLY:O	1:B:82:SER:OG	2.03	0.77
1:A:67:PHE:C	1:A:69:ASP:H	1.91	0.77
1:C:28:TYR:CD2	1:C:115:VAL:HG13	2.20	0.77
1:D:198:LEU:O	1:D:202:LYS:HB2	1.85	0.77
1:F:60:LYS:N	1:F:100:GLU:OE2	2.17	0.77
1:A:130:TYR:CE2	1:B:131:LEU:HD23	2.18	0.76
1:A:202:LYS:HE2	1:A:208:ASP:OD2	1.85	0.76
1:B:66:ILE:HD11	1:B:95:TYR:HB2	1.66	0.76
1:B:179:SER:HA	1:B:209:LYS:NZ	2.00	0.76
1:D:55:PHE:HB2	1:D:83:LEU:HD13	1.66	0.76
1:D:193:THR:O	1:D:197:VAL:HB	1.85	0.76
1:D:63:LEU:HD21	1:D:84:ILE:CD1	2.16	0.76
1:F:55:PHE:HB3	1:F:107:PHE:HE1	1.50	0.76
1:F:63:LEU:O	1:F:74:LEU:HD23	1.85	0.76
1:A:75:LEU:HD22	1:A:76:TYR:CE1	2.21	0.75
1:C:50:ILE:CB	1:C:86:LYS:HE2	2.13	0.75
1:C:46:PRO:CB	1:C:93:ASN:HD21	1.98	0.75
1:C:55:PHE:C	1:C:55:PHE:CD2	2.64	0.75
1:D:172:TYR:CZ	1:D:219:LEU:HD22	2.21	0.75
1:A:200:CYS:O	1:A:204:GLU:HG2	1.87	0.75
1:E:191:HIS:O	1:E:195:SER:OG	2.05	0.75
1:A:74:LEU:HD23	1:A:74:LEU:O	1.87	0.75
1:E:140:GLN:O	1:E:142:ALA:N	2.17	0.75
1:A:189:VAL:HG12	1:A:194:VAL:HG22	1.69	0.74
1:A:35:ARG:HH21	1:E:35:ARG:CZ	2.00	0.74
1:A:131:LEU:HD21	1:B:53:MET:HE1	1.68	0.74
1:D:86:LYS:NZ	1:D:90:THR:H	1.84	0.74
1:E:161:CYS:O	1:E:165:GLY:HA3	1.87	0.74
1:D:45:MET:HB2	1:D:48:GLU:HB2	1.70	0.74
1:C:42:ALA:HA	1:C:97:THR:HG22	1.70	0.74
1:D:191:HIS:HA	1:D:194:VAL:CG2	2.17	0.74
1:E:56:LEU:HD13	1:E:79:GLY:O	1.88	0.74
1:E:192:VAL:O	1:E:195:SER:HB2	1.88	0.74
1:C:100:GLU:O	1:C:101:PRO:C	2.28	0.74
1:D:164:GLN:HB3	1:D:174:ILE:HG21	1.70	0.73
1:A:204:GLU:O	1:A:205:ASN:HB2	1.88	0.73
1:F:141:VAL:N	1:F:142:ALA:HB3	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:GLU:O	1:D:205:ASN:HB2	1.88	0.73
1:E:54:ILE:HG22	1:E:54:ILE:O	1.88	0.73
1:A:87:LEU:HB2	1:A:88:TYR:CD1	2.23	0.73
1:A:61:ILE:HG21	1:A:96:ALA:HB1	1.71	0.73
1:B:164:GLN:HB3	1:B:174:ILE:HG23	1.69	0.73
1:A:190:HIS:HD2	1:A:191:HIS:N	1.87	0.73
1:A:87:LEU:CB	1:A:88:TYR:CE1	2.71	0.72
1:C:127:PHE:HZ	1:D:130:TYR:CE1	2.05	0.72
1:C:136:TYR:O	1:C:139:ARG:HB3	1.90	0.72
1:F:56:LEU:HD13	1:F:79:GLY:O	1.89	0.72
1:B:48:GLU:HG2	1:B:50:ILE:HD11	1.71	0.72
1:D:44:ILE:HG21	1:D:94:ILE:CG2	2.16	0.72
1:D:189:VAL:HG12	1:D:190:HIS:O	1.88	0.72
1:A:100:GLU:HB3	1:A:101:PRO:HD2	1.71	0.72
1:C:155:ARG:HH12	1:C:158:TYR:HD2	1.36	0.72
1:D:22:ILE:HD12	1:D:25:LEU:HB2	1.70	0.72
1:D:194:VAL:O	1:D:197:VAL:HG12	1.88	0.72
1:F:206:ILE:O	1:F:217:TYR:CD1	2.39	0.72
1:A:66:ILE:HA	1:A:71:SER:O	1.90	0.71
1:F:139:ARG:C	1:F:141:VAL:CB	2.62	0.71
1:C:155:ARG:HG3	1:C:155:ARG:HH11	1.55	0.71
1:F:54:ILE:HD12	1:F:84:ILE:HD12	1.71	0.71
1:E:48:GLU:HG2	1:E:49:GLU:O	1.90	0.71
1:C:23:GLU:HG3	1:C:81:ASN:ND2	2.06	0.71
1:C:164:GLN:HB3	1:C:174:ILE:HG23	1.73	0.71
1:D:44:ILE:HB	1:D:96:ALA:HB3	1.73	0.71
1:E:57:VAL:O	1:E:57:VAL:HG22	1.88	0.71
1:E:173:GLU:C	1:E:174:ILE:HD12	2.14	0.71
1:C:28:TYR:OH	1:C:119:ASP:OD2	2.07	0.71
1:E:113:ARG:O	1:E:117:ARG:HG3	1.89	0.71
1:E:186:ILE:HG13	1:F:155:ARG:HB3	1.73	0.71
1:A:75:LEU:HD22	1:A:76:TYR:HE1	1.56	0.71
1:A:127:PHE:CE2	1:B:53:MET:HE2	2.26	0.71
1:B:118:THR:O	1:B:119:ASP:CB	2.37	0.71
1:E:179:SER:HB2	1:E:181:LYS:HB3	1.71	0.71
1:C:63:LEU:HG	1:C:96:ALA:HB2	1.72	0.70
1:A:156:LEU:HB2	1:B:186:ILE:HG23	1.72	0.70
1:D:110:LYS:O	1:D:111:SER:C	2.32	0.70
1:E:188:GLY:HA3	1:F:152:ARG:CZ	2.22	0.70
1:F:134:VAL:HG12	1:F:135:ALA:N	2.05	0.70
1:B:20:PHE:O	1:B:129:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:GLN:C	1:E:142:ALA:H	1.98	0.70
1:C:55:PHE:HE2	1:C:57:VAL:HA	1.56	0.70
1:D:88:TYR:O	1:D:89:PRO:C	2.35	0.70
1:B:46:PRO:CA	1:B:93:ASN:HD21	2.05	0.70
1:C:100:GLU:O	1:C:102:THR:OG1	2.08	0.70
1:C:137:TYR:HB3	1:D:137:TYR:HB3	1.72	0.70
1:B:66:ILE:HD11	1:B:95:TYR:CB	2.22	0.70
1:C:92:ASN:O	1:C:93:ASN:C	2.35	0.70
1:A:65:ILE:CG1	1:A:66:ILE:N	2.55	0.69
1:D:63:LEU:HD21	1:D:84:ILE:HD13	1.72	0.69
1:D:124:PHE:CA	1:D:127:PHE:HB2	2.18	0.69
1:D:218:ASN:ND2	1:D:221:GLU:HB2	2.06	0.69
1:C:127:PHE:CE1	1:D:130:TYR:CD1	2.81	0.69
1:B:19:PHE:CD1	1:B:79:GLY:N	2.60	0.69
1:C:122:MET:O	1:C:123:ILE:C	2.32	0.69
1:C:127:PHE:O	1:C:131:LEU:HG	1.92	0.69
1:D:88:TYR:O	1:D:90:THR:HG23	1.93	0.69
1:E:159:GLU:HG3	1:F:186:ILE:CD1	2.22	0.69
1:A:65:ILE:HA	1:A:93:ASN:O	1.93	0.69
1:D:28:TYR:O	1:D:31:MET:HB2	1.93	0.69
1:A:128:LYS:CG	1:B:88:TYR:CD1	2.76	0.69
1:C:38:ALA:O	1:C:41:SER:HB2	1.93	0.69
1:D:86:LYS:NZ	1:D:90:THR:HG23	2.06	0.69
1:A:128:LYS:HE3	1:B:88:TYR:CD2	2.27	0.69
1:D:44:ILE:CG2	1:D:94:ILE:HG22	2.18	0.69
1:A:128:LYS:HG3	1:B:88:TYR:CD1	2.28	0.68
1:E:200:CYS:O	1:E:204:GLU:HB2	1.94	0.68
1:A:127:PHE:CE1	1:B:130:TYR:CD1	2.78	0.68
1:B:155:ARG:HG3	1:B:155:ARG:HH11	1.59	0.68
1:C:46:PRO:HB3	1:C:93:ASN:ND2	2.07	0.68
1:C:113:ARG:CG	1:D:120:GLU:OE1	2.42	0.68
1:C:113:ARG:HG2	1:D:120:GLU:OE1	1.93	0.68
1:E:65:ILE:HB	1:E:75:LEU:HG	1.74	0.68
1:F:201:LEU:HD13	1:F:207:LEU:HD13	1.76	0.68
1:D:191:HIS:HA	1:D:194:VAL:HG23	1.75	0.68
1:E:38:ALA:O	1:E:41:SER:HB2	1.94	0.68
1:A:155:ARG:NH1	1:B:185:GLU:CB	2.58	0.67
1:E:134:VAL:HG21	1:F:130:TYR:HD2	1.59	0.67
1:F:27:ASN:H	1:F:27:ASN:ND2	1.91	0.67
1:C:28:TYR:HA	1:C:30:GLN:HE22	1.59	0.67
1:D:160:LEU:HD11	1:D:176:MET:HE1	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLY:HA3	1:A:102:THR:HG23	1.76	0.67
1:C:66:ILE:HG13	1:C:72:GLU:HG3	1.77	0.67
1:B:171:THR:HG22	1:B:217:TYR:HA	1.76	0.67
1:B:151:ILE:HA	1:B:154:LEU:HD12	1.75	0.67
1:D:49:GLU:O	1:D:49:GLU:HG2	1.93	0.67
1:D:56:LEU:HD23	1:D:59:GLY:O	1.94	0.67
1:F:26:ARG:HB2	1:F:27:ASN:ND2	2.09	0.67
1:F:46:PRO:HD3	1:F:95:TYR:CD2	2.30	0.67
1:F:110:LYS:HE3	1:F:110:LYS:O	1.95	0.67
1:A:123:ILE:O	1:A:123:ILE:HG22	1.93	0.67
1:F:155:ARG:HB3	1:F:155:ARG:HH11	1.59	0.67
1:C:130:TYR:CE2	1:D:131:LEU:HG	2.29	0.66
1:E:152:ARG:CD	1:F:188:GLY:CA	2.73	0.66
1:C:174:ILE:HG22	1:C:176:MET:HG2	1.76	0.66
1:E:123:ILE:HG23	1:F:123:ILE:CG2	2.23	0.66
1:C:77:TYR:HD2	1:C:99:MET:HE1	1.60	0.66
1:C:109:GLU:HG2	1:C:113:ARG:HH21	1.60	0.66
1:E:27:ASN:HB2	1:E:28:TYR:CE1	2.30	0.66
1:C:59:GLY:O	1:C:79:GLY:HA2	1.95	0.66
1:A:61:ILE:CG2	1:A:96:ALA:HB1	2.26	0.66
1:B:44:ILE:HD11	1:B:50:ILE:HG21	1.77	0.66
1:B:151:ILE:HA	1:B:154:LEU:CD1	2.25	0.66
1:E:190:HIS:C	1:E:190:HIS:CD2	2.73	0.66
1:A:65:ILE:HG13	1:A:66:ILE:H	1.60	0.66
1:D:22:ILE:O	1:D:22:ILE:CD1	2.44	0.66
1:A:33:LEU:CD2	1:E:36:ASP:O	2.43	0.66
1:E:57:VAL:HG13	1:E:103:ARG:O	1.96	0.66
1:F:44:ILE:HB	1:F:96:ALA:HB3	1.77	0.66
1:B:161:CYS:O	1:B:165:GLY:HA3	1.96	0.65
1:C:88:TYR:CE1	1:D:128:LYS:HB2	2.31	0.65
1:C:171:THR:HG22	1:C:217:TYR:HA	1.79	0.65
1:A:33:LEU:HD21	1:E:36:ASP:O	1.97	0.65
1:C:74:LEU:HD13	1:C:77:TYR:CE1	2.32	0.65
1:C:127:PHE:CZ	1:D:130:TYR:CE1	2.84	0.65
1:C:174:ILE:HB	1:C:214:ILE:HB	1.78	0.65
1:D:130:TYR:O	1:D:134:VAL:HG23	1.96	0.65
1:A:53:MET:HB2	1:A:107:PHE:HB2	1.79	0.65
1:E:198:LEU:CD1	1:E:201:LEU:HD12	2.23	0.65
1:F:19:PHE:CE2	1:F:79:GLY:HA3	2.31	0.65
1:A:98:ALA:HB1	1:A:100:GLU:O	1.97	0.65
1:F:87:LEU:HB2	1:F:88:TYR:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:ALA:O	1:F:202:LYS:CB	2.44	0.65
1:A:74:LEU:HD11	1:A:77:TYR:CE1	2.31	0.65
1:D:20:PHE:CD1	1:D:133:LYS:HG2	2.31	0.65
1:C:179:SER:HB2	1:C:182:SER:OG	1.97	0.65
1:E:129:ASN:O	1:E:133:LYS:HG2	1.97	0.65
1:A:164:GLN:HG2	1:B:164:GLN:NE2	2.11	0.65
1:E:188:GLY:HA3	1:F:152:ARG:HE	1.62	0.65
1:D:22:ILE:C	1:D:22:ILE:HD13	2.21	0.64
1:B:45:MET:HB3	1:B:46:PRO:HD2	1.80	0.64
1:E:174:ILE:O	1:E:214:ILE:HG13	1.96	0.64
1:D:56:LEU:HD22	1:D:79:GLY:O	1.97	0.64
1:D:54:ILE:C	1:D:83:LEU:HD12	2.23	0.64
1:F:187:THR:HB	1:F:189:VAL:HG23	1.80	0.64
1:B:100:GLU:O	1:B:102:THR:OG1	2.13	0.64
1:D:112:LEU:O	1:D:113:ARG:C	2.39	0.64
1:E:30:GLN:CD	1:E:30:GLN:H	2.05	0.64
1:F:141:VAL:H	1:F:142:ALA:C	2.05	0.64
1:E:137:TYR:O	1:E:141:VAL:HG23	1.98	0.64
1:C:86:LYS:HD2	1:C:88:TYR:O	1.98	0.64
1:A:20:PHE:CD1	1:A:133:LYS:HD3	2.33	0.64
1:C:23:GLU:O	1:C:25:LEU:N	2.31	0.64
1:C:190:HIS:HD2	1:C:192:VAL:HG23	1.62	0.64
1:E:87:LEU:HD22	1:E:109:GLU:HB2	1.80	0.64
1:A:130:TYR:CE1	1:A:133:LYS:NZ	2.66	0.63
1:D:161:CYS:SG	1:D:172:TYR:HB3	2.37	0.63
1:E:202:LYS:HG3	1:E:208:ASP:OD1	1.97	0.63
1:B:154:LEU:CD2	1:B:201:LEU:HD21	2.28	0.63
1:C:30:GLN:C	1:C:32:GLY:H	2.04	0.63
1:D:206:ILE:HG23	1:D:218:ASN:HB3	1.80	0.63
1:A:134:VAL:O	1:A:135:ALA:C	2.39	0.63
1:C:127:PHE:CZ	1:C:131:LEU:HD21	2.34	0.63
1:A:117:ARG:O	1:A:118:THR:C	2.38	0.63
1:B:46:PRO:HA	1:B:94:ILE:O	1.98	0.63
1:B:168:VAL:HG12	1:B:168:VAL:O	1.97	0.63
1:A:65:ILE:CG1	1:A:66:ILE:H	2.12	0.63
1:C:74:LEU:CD1	1:C:77:TYR:CE1	2.82	0.63
1:F:108:SER:O	1:F:111:SER:N	2.32	0.63
1:B:194:VAL:O	1:B:198:LEU:HB2	1.99	0.63
1:D:64:ASP:HB2	1:D:72:GLU:OE1	1.98	0.63
1:D:180:GLN:HE22	1:D:194:VAL:HB	1.63	0.63
1:A:60:LYS:HG2	1:A:99:MET:CE	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:O	1:A:102:THR:HA	2.00	0.62
1:B:132:THR:O	1:B:135:ALA:HB3	1.99	0.62
1:F:44:ILE:HG21	1:F:94:ILE:HG22	1.79	0.62
1:B:62:LYS:O	1:B:96:ALA:HA	1.99	0.62
1:B:74:LEU:HD23	1:B:75:LEU:H	1.63	0.62
1:C:155:ARG:CD	1:D:185:GLU:OE1	2.46	0.62
1:E:46:PRO:HB3	1:E:66:ILE:CD1	2.29	0.62
1:C:26:ARG:HD2	1:C:81:ASN:OD1	1.98	0.62
1:A:21:PRO:HA	1:A:81:ASN:O	1.98	0.62
1:B:75:LEU:HD23	1:B:76:TYR:CD1	2.35	0.62
1:C:103:ARG:O	1:C:103:ARG:HG2	1.92	0.62
1:D:61:ILE:HD11	1:D:102:THR:HG21	1.82	0.62
1:D:179:SER:O	1:D:180:GLN:C	2.43	0.62
1:A:189:VAL:CG1	1:A:194:VAL:HG22	2.28	0.62
1:B:120:GLU:O	1:B:123:ILE:N	2.21	0.62
1:D:172:TYR:OH	1:D:219:LEU:HD23	1.99	0.62
1:E:219:LEU:HA	1:E:222:LEU:HB3	1.82	0.62
1:D:216:VAL:HG11	1:D:222:LEU:HD22	1.80	0.62
1:E:155:ARG:O	1:E:159:GLU:HG2	2.00	0.62
1:E:201:LEU:HD22	1:E:207:LEU:CB	2.30	0.62
1:F:22:ILE:HG13	1:F:22:ILE:O	1.99	0.62
1:B:35:ARG:HB3	1:B:35:ARG:NH1	2.14	0.62
1:B:179:SER:HA	1:B:209:LYS:HZ3	1.62	0.62
1:E:198:LEU:HA	1:E:201:LEU:HD12	1.82	0.62
1:A:185:GLU:O	1:A:186:ILE:C	2.40	0.61
1:B:150:THR:O	1:B:153:ILE:HB	1.99	0.61
1:E:127:PHE:HE1	1:F:130:TYR:CD1	2.18	0.61
1:C:61:ILE:HG22	1:C:96:ALA:HB1	1.82	0.61
1:C:186:ILE:HG23	1:D:156:LEU:HB2	1.82	0.61
1:A:131:LEU:HD21	1:B:53:MET:HE2	1.81	0.61
1:A:185:GLU:O	1:B:152:ARG:CG	2.46	0.61
1:D:190:HIS:CD2	1:D:192:VAL:HG23	2.36	0.61
1:F:53:MET:HG2	1:F:87:LEU:HD11	1.81	0.61
1:C:108:SER:C	1:C:111:SER:OG	2.44	0.61
1:E:123:ILE:CG2	1:F:123:ILE:HG23	2.28	0.61
1:E:174:ILE:N	1:E:174:ILE:HD12	2.16	0.61
1:E:211:LYS:HE3	1:E:211:LYS:H	1.66	0.61
1:C:207:LEU:HD23	1:C:208:ASP:C	2.25	0.61
1:D:63:LEU:O	1:D:75:LEU:HB2	2.01	0.61
1:A:35:ARG:HE	1:E:35:ARG:NE	1.99	0.61
1:A:190:HIS:CD2	1:A:191:HIS:N	2.68	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:TYR:CE1	1:A:223:LYS:HB2	2.35	0.61
1:A:159:GLU:CG	1:B:186:ILE:HD11	2.28	0.60
1:C:55:PHE:HD2	1:C:55:PHE:O	1.84	0.60
1:C:75:LEU:HD22	1:D:138:ALA:HB1	1.83	0.60
1:E:186:ILE:CG1	1:F:155:ARG:HB3	2.30	0.60
1:A:74:LEU:O	1:A:74:LEU:CD2	2.48	0.60
1:C:123:ILE:HD11	1:D:123:ILE:CD1	2.29	0.60
1:C:137:TYR:CB	1:D:137:TYR:HB3	2.31	0.60
1:F:26:ARG:HB2	1:F:27:ASN:HD22	1.65	0.60
1:F:223:LYS:HG3	1:F:224:HIS:N	2.16	0.60
1:D:88:TYR:O	1:D:90:THR:CG2	2.50	0.60
1:D:124:PHE:HA	1:D:127:PHE:CB	2.21	0.60
1:D:166:LYS:O	1:D:173:GLU:HB2	2.01	0.60
1:C:77:TYR:CD2	1:C:99:MET:HE1	2.36	0.60
1:F:141:VAL:H	1:F:143:GLU:N	1.97	0.60
1:C:190:HIS:O	1:C:194:VAL:HG23	2.02	0.60
1:E:63:LEU:HD11	1:E:84:ILE:CG2	2.31	0.60
1:A:161:CYS:HA	1:A:174:ILE:HD11	1.83	0.60
1:B:27:ASN:HD22	1:B:27:ASN:N	1.99	0.60
1:D:151:ILE:O	1:D:155:ARG:CG	2.48	0.60
1:A:128:LYS:HG2	1:B:88:TYR:CD1	2.35	0.60
1:C:205:ASN:O	1:C:217:TYR:HB2	2.01	0.60
1:A:24:LYS:CB	1:A:122:MET:HE1	2.31	0.60
1:C:46:PRO:HG3	1:C:95:TYR:HB2	1.84	0.60
1:B:76:TYR:CD1	1:B:137:TYR:OH	2.54	0.60
1:F:37:PHE:CE2	1:F:43:VAL:HA	2.37	0.60
1:D:44:ILE:HB	1:D:96:ALA:CB	2.32	0.59
1:F:178:LEU:O	1:F:209:LYS:NZ	2.35	0.59
1:B:156:LEU:HD22	1:B:183:ILE:HG23	1.82	0.59
1:E:63:LEU:HD23	1:E:96:ALA:HB2	1.84	0.59
1:A:65:ILE:HG12	1:A:66:ILE:N	2.17	0.59
1:F:83:LEU:HD12	1:F:84:ILE:N	2.17	0.59
1:F:157:PHE:CG	1:F:207:LEU:HD11	2.36	0.59
1:C:53:MET:HE1	1:C:130:TYR:OH	2.02	0.59
1:C:127:PHE:HE1	1:D:130:TYR:CD1	2.20	0.59
1:C:134:VAL:HG21	1:D:130:TYR:HD2	1.68	0.59
1:B:130:TYR:O	1:B:131:LEU:C	2.46	0.59
1:D:190:HIS:O	1:D:194:VAL:HG23	2.03	0.59
1:F:108:SER:O	1:F:109:GLU:C	2.44	0.59
1:A:39:LYS:HG3	1:A:99:MET:O	2.02	0.59
1:C:156:LEU:HD22	1:C:187:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PRO:CD	1:D:151:ILE:CG1	2.81	0.59
1:F:25:LEU:O	1:F:26:ARG:C	2.45	0.59
1:A:136:TYR:O	1:A:140:GLN:HG2	2.03	0.59
1:E:153:ILE:HG12	1:E:189:VAL:HG21	1.84	0.59
1:F:63:LEU:HD21	1:F:84:ILE:HG21	1.84	0.59
1:A:128:LYS:O	1:A:131:LEU:HB2	2.03	0.59
1:A:164:GLN:CG	1:B:164:GLN:CD	2.75	0.59
1:D:185:GLU:O	1:D:186:ILE:C	2.45	0.59
1:A:127:PHE:CE1	1:B:130:TYR:CE1	2.91	0.58
1:A:87:LEU:C	1:A:88:TYR:CD1	2.81	0.58
1:E:116:PHE:CE1	1:E:122:MET:HB3	2.38	0.58
1:A:100:GLU:CB	1:A:101:PRO:HD2	2.32	0.58
1:B:22:ILE:O	1:B:23:GLU:C	2.46	0.58
1:D:110:LYS:C	1:D:112:LEU:N	2.55	0.58
1:A:76:TYR:CD1	1:A:76:TYR:N	2.71	0.58
1:B:23:GLU:O	1:B:25:LEU:N	2.36	0.58
1:F:72:GLU:O	1:F:73:LYS:HB2	2.04	0.58
1:E:79:GLY:N	1:E:82:SER:OG	2.29	0.58
1:E:186:ILE:HG23	1:F:156:LEU:HB2	1.86	0.58
1:C:152:ARG:NH2	1:C:189:VAL:HG22	2.09	0.57
1:D:155:ARG:NH1	1:D:159:GLU:OE1	2.32	0.57
1:D:207:LEU:CD1	1:D:216:VAL:HG22	2.30	0.57
1:A:22:ILE:HG12	1:A:22:ILE:O	2.04	0.57
1:A:30:GLN:H	1:A:30:GLN:CD	2.12	0.57
1:A:74:LEU:CD1	1:A:77:TYR:CE1	2.87	0.57
1:B:118:THR:O	1:B:119:ASP:HB2	2.04	0.57
1:E:210:LYS:O	1:E:213:LYS:O	2.22	0.57
1:D:34:ILE:HG21	1:D:103:ARG:HD3	1.87	0.57
1:E:201:LEU:HD22	1:E:207:LEU:HB2	1.86	0.57
1:A:152:ARG:O	1:A:156:LEU:N	2.35	0.57
1:B:112:LEU:HD22	1:B:116:PHE:CZ	2.39	0.57
1:F:58:GLU:O	1:F:102:THR:HG23	2.05	0.57
1:F:74:LEU:CD2	1:F:75:LEU:H	2.17	0.57
1:E:57:VAL:O	1:E:58:GLU:HB2	2.04	0.57
1:E:168:VAL:HB	1:E:171:THR:OG1	2.05	0.57
1:F:65:ILE:HG23	1:F:67:PHE:CE1	2.39	0.57
1:A:164:GLN:NE2	1:B:176:MET:SD	2.77	0.57
1:B:152:ARG:NH1	1:B:187:THR:O	2.38	0.57
1:C:55:PHE:CD2	1:C:55:PHE:O	2.58	0.57
1:B:46:PRO:O	1:B:93:ASN:OD1	2.23	0.57
1:C:152:ARG:HH21	1:C:189:VAL:CG2	2.10	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:PRO:HA	1:D:94:ILE:O	2.05	0.57
1:D:64:ASP:HA	1:D:74:LEU:HA	1.87	0.57
1:B:46:PRO:HA	1:B:93:ASN:HD21	1.68	0.57
1:C:24:LYS:O	1:C:27:ASN:HB2	2.04	0.57
1:C:28:TYR:HA	1:C:30:GLN:NE2	2.18	0.57
1:D:53:MET:HE1	1:D:130:TYR:OH	2.05	0.57
1:A:28:TYR:HE1	1:A:122:MET:HE3	1.69	0.57
1:A:93:ASN:C	1:A:94:ILE:HD13	2.30	0.57
1:A:128:LYS:HE3	1:B:88:TYR:CE2	2.39	0.57
1:C:27:ASN:O	1:C:30:GLN:NE2	2.38	0.57
1:C:92:ASN:O	1:C:93:ASN:O	2.23	0.57
1:F:55:PHE:HB2	1:F:107:PHE:HE1	1.67	0.57
1:F:155:ARG:NH2	1:F:159:GLU:OE1	2.38	0.57
1:B:207:LEU:HD21	1:B:214:ILE:CG2	2.35	0.56
1:E:117:ARG:NH2	1:F:120:GLU:OE1	2.34	0.56
1:E:186:ILE:HD11	1:F:159:GLU:CG	2.31	0.56
1:A:151:ILE:O	1:A:155:ARG:CG	2.53	0.56
1:B:66:ILE:CD1	1:B:95:TYR:CB	2.79	0.56
1:E:216:VAL:HG11	1:E:222:LEU:HD22	1.86	0.56
1:F:28:TYR:HB3	1:F:31:MET:HG3	1.86	0.56
1:A:119:ASP:C	1:A:119:ASP:OD1	2.47	0.56
1:A:127:PHE:HE1	1:B:130:TYR:CE1	2.23	0.56
1:A:130:TYR:C	1:A:132:THR:H	2.12	0.56
1:B:179:SER:HA	1:B:209:LYS:HZ1	1.70	0.56
1:C:65:ILE:HD11	1:C:92:ASN:ND2	2.20	0.56
1:D:172:TYR:HB2	1:D:216:VAL:HB	1.86	0.56
1:D:216:VAL:HG11	1:D:222:LEU:CD2	2.34	0.56
1:A:132:THR:O	1:A:135:ALA:HB3	2.06	0.56
1:E:27:ASN:HB2	1:E:28:TYR:CD1	2.39	0.56
1:E:56:LEU:C	1:E:56:LEU:CD2	2.78	0.56
1:A:205:ASN:O	1:A:217:TYR:HB2	2.05	0.56
1:B:115:VAL:O	1:B:118:THR:N	2.33	0.56
1:D:191:HIS:HA	1:D:194:VAL:HG21	1.86	0.56
1:E:172:TYR:CD1	1:E:219:LEU:HD22	2.40	0.56
1:F:155:ARG:HH11	1:F:155:ARG:CB	2.17	0.56
1:C:127:PHE:CZ	1:D:130:TYR:CD1	2.94	0.56
1:F:100:GLU:O	1:F:102:THR:OG1	2.23	0.56
1:D:22:ILE:CD1	1:D:22:ILE:C	2.78	0.56
1:F:19:PHE:CD2	1:F:79:GLY:HA3	2.41	0.56
1:F:120:GLU:C	1:F:122:MET:H	2.11	0.56
1:B:20:PHE:N	1:B:21:PRO:CD	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:HG22	1:B:154:LEU:N	2.20	0.56
1:D:22:ILE:HD12	1:D:22:ILE:O	2.06	0.56
1:D:172:TYR:HE1	1:D:219:LEU:HB2	1.66	0.56
1:F:44:ILE:HD11	1:F:54:ILE:HD11	1.87	0.56
1:C:23:GLU:HG3	1:C:81:ASN:HD22	1.69	0.55
1:E:86:LYS:CD	1:E:88:TYR:O	2.54	0.55
1:B:32:GLY:HA3	1:B:105:CYS:SG	2.45	0.55
1:B:209:LYS:O	1:B:209:LYS:HG2	2.06	0.55
1:D:150:THR:HA	1:D:153:ILE:HD12	1.87	0.55
1:A:179:SER:O	1:A:181:LYS:N	2.39	0.55
1:E:188:GLY:HA3	1:F:152:ARG:NH2	2.21	0.55
1:B:19:PHE:CD1	1:B:79:GLY:HA3	2.41	0.55
1:B:178:LEU:O	1:B:209:LYS:CD	2.46	0.55
1:D:172:TYR:OH	1:D:219:LEU:CD2	2.55	0.55
1:E:161:CYS:SG	1:E:172:TYR:CB	2.88	0.55
1:A:26:ARG:NH2	1:A:57:VAL:HG23	2.22	0.55
1:A:74:LEU:O	1:A:74:LEU:CG	2.51	0.55
1:C:62:LYS:O	1:C:96:ALA:HA	2.07	0.55
1:B:205:ASN:O	1:B:217:TYR:HB2	2.06	0.55
1:C:209:LYS:O	1:C:211:LYS:N	2.40	0.55
1:E:23:GLU:CD	1:E:23:GLU:H	2.15	0.55
1:C:36:ASP:OD1	1:C:103:ARG:HB2	2.06	0.55
1:D:86:LYS:NZ	1:D:88:TYR:O	2.38	0.55
1:E:186:ILE:HG12	1:F:156:LEU:N	2.22	0.55
1:F:198:LEU:HD11	1:F:209:LYS:HB2	1.89	0.55
1:B:19:PHE:CD1	1:B:79:GLY:CA	2.89	0.55
1:B:45:MET:O	1:B:47:GLY:N	2.40	0.55
1:C:89:PRO:O	1:C:90:THR:HG22	2.07	0.55
1:F:141:VAL:N	1:F:143:GLU:N	2.55	0.55
1:F:183:ILE:O	1:F:187:THR:CG2	2.51	0.55
1:A:155:ARG:HB3	1:A:155:ARG:CZ	2.37	0.55
1:C:155:ARG:HD2	1:C:226:SER:HB2	1.88	0.55
1:D:172:TYR:CZ	1:D:219:LEU:CD2	2.89	0.55
1:C:130:TYR:HA	1:C:133:LYS:HB2	1.89	0.54
1:D:86:LYS:HZ3	1:D:90:THR:HG23	1.72	0.54
1:E:142:ALA:HB1	1:F:73:LYS:CD	2.35	0.54
1:B:46:PRO:CB	1:B:93:ASN:HD21	2.19	0.54
1:E:134:VAL:HG21	1:F:130:TYR:CD2	2.42	0.54
1:A:86:LYS:HG3	1:A:88:TYR:O	2.07	0.54
1:B:27:ASN:N	1:B:27:ASN:ND2	2.55	0.54
1:C:108:SER:O	1:C:111:SER:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:PHE:CG	1:E:79:GLY:HA3	2.43	0.54
1:F:65:ILE:CG2	1:F:67:PHE:CE1	2.90	0.54
1:B:52:SER:HB3	1:B:108:SER:N	2.23	0.54
1:D:56:LEU:HD13	1:D:82:SER:HB2	1.88	0.54
1:B:120:GLU:O	1:B:123:ILE:HG13	2.08	0.54
1:C:39:LYS:HB2	1:C:100:GLU:HA	1.90	0.54
1:E:203:ARG:HB3	1:E:203:ARG:CZ	2.38	0.54
1:E:203:ARG:NH1	1:E:204:GLU:HG2	2.22	0.54
1:A:128:LYS:O	1:A:131:LEU:N	2.41	0.54
1:A:197:VAL:O	1:A:201:LEU:HG	2.08	0.54
1:C:92:ASN:HD21	1:D:139:ARG:HB2	1.73	0.54
1:D:219:LEU:CD1	1:D:222:LEU:HD23	2.37	0.54
1:E:206:ILE:HG12	1:E:221:GLU:HB3	1.89	0.54
1:A:155:ARG:NH1	1:A:155:ARG:HB3	2.23	0.54
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.08	0.54
1:B:131:LEU:O	1:B:132:THR:C	2.50	0.54
1:D:191:HIS:CA	1:D:194:VAL:HG23	2.38	0.54
1:E:19:PHE:O	1:E:20:PHE:C	2.50	0.54
1:F:55:PHE:HB2	1:F:107:PHE:CE1	2.43	0.54
1:B:134:VAL:O	1:B:135:ALA:C	2.51	0.54
1:D:62:LYS:HB3	1:D:97:THR:HB	1.90	0.54
1:F:74:LEU:HD11	1:F:77:TYR:HE1	1.72	0.54
1:A:131:LEU:HD23	1:B:130:TYR:CE2	2.42	0.54
1:B:35:ARG:NH1	1:C:35:ARG:NE	2.56	0.54
1:B:54:ILE:O	1:B:54:ILE:CG2	2.29	0.53
1:D:27:ASN:N	1:D:27:ASN:ND2	2.55	0.53
1:D:204:GLU:O	1:D:205:ASN:CB	2.56	0.53
1:E:190:HIS:HD2	1:E:191:HIS:N	2.05	0.53
1:F:60:LYS:HB3	1:F:99:MET:HB2	1.91	0.53
1:A:68:GLU:CD	1:B:139:ARG:HH22	2.16	0.53
1:C:122:MET:HA	1:C:125:GLU:HB2	1.90	0.53
1:D:156:LEU:HD22	1:D:186:ILE:HG21	1.88	0.53
1:F:153:ILE:HG13	1:F:187:THR:CG2	2.31	0.53
1:B:115:VAL:O	1:B:116:PHE:C	2.51	0.53
1:C:55:PHE:HE2	1:C:57:VAL:CA	2.21	0.53
1:C:155:ARG:NH1	1:C:155:ARG:HG3	2.21	0.53
1:D:189:VAL:HG13	1:D:193:THR:CB	2.26	0.53
1:F:38:ALA:O	1:F:39:LYS:C	2.51	0.53
1:F:108:SER:H	1:F:111:SER:HB3	1.73	0.53
1:F:141:VAL:N	1:F:142:ALA:C	2.66	0.53
1:A:35:ARG:HE	1:E:35:ARG:HE	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:CD2	1:B:76:TYR:CD1	2.92	0.53
1:B:77:TYR:CD1	1:B:77:TYR:N	2.74	0.53
1:D:27:ASN:N	1:D:27:ASN:HD22	2.06	0.53
1:E:190:HIS:CD2	1:E:192:VAL:H	2.27	0.53
1:A:159:GLU:CD	1:B:182:SER:OG	2.52	0.53
1:A:33:LEU:O	1:A:105:CYS:HA	2.08	0.53
1:A:49:GLU:C	1:A:50:ILE:HD13	2.33	0.53
1:A:95:TYR:CE1	1:A:97:THR:HG23	2.44	0.53
1:D:86:LYS:NZ	1:D:90:THR:N	2.48	0.53
1:F:120:GLU:C	1:F:122:MET:N	2.66	0.53
1:A:100:GLU:O	1:A:102:THR:OG1	2.25	0.53
1:F:74:LEU:HD11	1:F:77:TYR:CE1	2.44	0.53
1:A:23:GLU:HG3	1:A:81:ASN:HD22	1.74	0.53
1:B:36:ASP:O	1:C:33:LEU:HD23	2.09	0.53
1:B:127:PHE:O	1:B:128:LYS:C	2.51	0.53
1:C:45:MET:HB2	1:C:48:GLU:HB2	1.91	0.53
1:D:156:LEU:O	1:D:160:LEU:CB	2.53	0.53
1:E:56:LEU:HD22	1:E:56:LEU:O	2.09	0.53
1:E:57:VAL:O	1:E:57:VAL:HG23	2.08	0.53
1:A:127:PHE:O	1:A:131:LEU:HB2	2.09	0.53
1:E:60:LYS:C	1:E:61:ILE:HG13	2.34	0.53
1:F:67:PHE:O	1:F:70:GLY:N	2.38	0.53
1:C:130:TYR:CD1	1:C:130:TYR:N	2.77	0.52
1:D:63:LEU:HD21	1:D:84:ILE:HD12	1.90	0.52
1:B:20:PHE:N	1:B:21:PRO:HD2	2.22	0.52
1:B:57:VAL:HG13	1:B:103:ARG:HG2	1.91	0.52
1:C:42:ALA:HA	1:C:97:THR:CG2	2.39	0.52
1:C:62:LYS:N	1:C:99:MET:HE2	2.25	0.52
1:E:184:GLY:HA2	1:E:189:VAL:O	2.08	0.52
1:F:122:MET:O	1:F:123:ILE:C	2.52	0.52
1:B:77:TYR:N	1:B:77:TYR:HD1	2.07	0.52
1:B:222:LEU:O	1:B:223:LYS:C	2.52	0.52
1:D:176:MET:N	1:D:212:ASN:O	2.43	0.52
1:E:30:GLN:H	1:E:30:GLN:NE2	2.07	0.52
1:B:30:GLN:HE21	1:B:30:GLN:N	2.01	0.52
1:E:131:LEU:O	1:E:132:THR:C	2.52	0.52
1:C:207:LEU:HD21	1:C:214:ILE:HG23	1.92	0.52
1:D:34:ILE:CG2	1:D:103:ARG:HD3	2.39	0.52
1:C:100:GLU:O	1:C:102:THR:N	2.43	0.52
1:D:110:LYS:C	1:D:112:LEU:H	2.18	0.52
1:B:208:ASP:HB2	1:B:217:TYR:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ARG:NH2	1:D:57:VAL:O	2.36	0.52
1:A:188:GLY:H	1:B:152:ARG:HD3	1.74	0.52
1:A:191:HIS:HA	1:A:194:VAL:HG23	1.91	0.52
1:B:23:GLU:O	1:B:24:LYS:C	2.52	0.52
1:C:43:VAL:HG23	1:C:97:THR:HA	1.92	0.52
1:C:50:ILE:HG12	1:C:86:LYS:NZ	2.24	0.52
1:E:59:GLY:O	1:E:60:LYS:HB2	2.10	0.52
1:A:191:HIS:O	1:A:195:SER:OG	2.17	0.52
1:B:174:ILE:HB	1:B:214:ILE:HB	1.91	0.52
1:B:202:LYS:O	1:B:204:GLU:N	2.43	0.52
1:F:55:PHE:HB3	1:F:107:PHE:CE1	2.39	0.52
1:A:19:PHE:HE1	1:A:77:TYR:HB3	1.75	0.52
1:A:44:ILE:HD13	1:A:94:ILE:HG21	1.91	0.52
1:E:183:ILE:HG22	1:E:194:VAL:HG22	1.91	0.52
1:B:122:MET:O	1:B:123:ILE:C	2.50	0.51
1:C:88:TYR:CD1	1:D:128:LYS:HB2	2.45	0.51
1:A:123:ILE:O	1:A:123:ILE:CG2	2.57	0.51
1:C:65:ILE:CD1	1:C:92:ASN:HD22	2.23	0.51
1:E:56:LEU:HG	1:E:61:ILE:HD11	1.91	0.51
1:F:120:GLU:O	1:F:122:MET:N	2.43	0.51
1:C:61:ILE:CG2	1:C:96:ALA:HB1	2.41	0.51
1:C:63:LEU:HD11	1:C:84:ILE:HG21	1.92	0.51
1:D:161:CYS:C	1:D:163:SER:H	2.18	0.51
1:A:167:ARG:HA	1:A:172:TYR:HA	1.92	0.51
1:D:19:PHE:CD1	1:D:79:GLY:N	2.79	0.51
1:F:221:GLU:O	1:F:225:LEU:HG	2.10	0.51
1:E:219:LEU:HD12	1:E:222:LEU:HD23	1.92	0.51
1:F:20:PHE:O	1:F:129:ASN:ND2	2.38	0.51
1:F:58:GLU:O	1:F:102:THR:HA	2.10	0.51
1:A:130:TYR:O	1:A:132:THR:N	2.44	0.51
1:B:67:PHE:HE1	1:B:73:LYS:HB2	1.74	0.51
1:D:219:LEU:HD13	1:D:222:LEU:HD23	1.93	0.51
1:E:201:LEU:HD22	1:E:207:LEU:HB3	1.92	0.51
1:B:32:GLY:O	1:B:33:LEU:HD23	2.10	0.51
1:E:44:ILE:HG12	1:E:50:ILE:CD1	2.35	0.51
1:A:28:TYR:CE1	1:A:122:MET:HE3	2.44	0.51
1:C:55:PHE:CE2	1:C:57:VAL:HA	2.42	0.51
1:D:150:THR:HG23	1:D:197:VAL:CG2	2.40	0.51
1:E:56:LEU:HG	1:E:61:ILE:CD1	2.41	0.51
1:F:54:ILE:HD12	1:F:84:ILE:CD1	2.39	0.51
1:A:76:TYR:HB2	1:A:77:TYR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:O	1:A:161:CYS:N	2.34	0.51
1:F:73:LYS:NZ	1:F:73:LYS:HA	2.25	0.51
1:A:76:TYR:HD1	1:A:76:TYR:N	2.05	0.51
1:A:159:GLU:CD	1:B:182:SER:HG	2.19	0.51
1:C:22:ILE:O	1:C:22:ILE:CG2	2.52	0.51
1:A:101:PRO:O	1:A:101:PRO:HG2	2.11	0.50
1:A:151:ILE:HA	1:A:154:LEU:HD12	1.92	0.50
1:C:208:ASP:HB2	1:C:217:TYR:HE1	1.77	0.50
1:D:43:VAL:HG23	1:D:96:ALA:O	2.12	0.50
1:E:52:SER:O	1:E:54:ILE:HG13	2.12	0.50
1:A:128:LYS:HG3	1:B:88:TYR:CZ	2.47	0.50
1:C:80:GLY:O	1:C:81:ASN:HB2	2.10	0.50
1:C:218:ASN:OD1	1:C:221:GLU:HB2	2.10	0.50
1:D:209:LYS:HG2	1:D:209:LYS:O	2.11	0.50
1:E:155:ARG:CB	1:F:186:ILE:HG13	2.33	0.50
1:F:25:LEU:HD23	1:F:55:PHE:CD1	2.46	0.50
1:F:68:GLU:H	1:F:68:GLU:CD	2.19	0.50
1:E:158:TYR:O	1:E:162:SER:HB3	2.10	0.50
1:B:26:ARG:HG2	1:B:55:PHE:HZ	1.77	0.50
1:B:106:TRP:CD1	1:B:106:TRP:N	2.77	0.50
1:D:29:THR:C	1:D:31:MET:H	2.19	0.50
1:E:112:LEU:HA	1:E:115:VAL:HB	1.93	0.50
1:E:136:TYR:CE2	1:E:140:GLN:NE2	2.79	0.50
1:F:55:PHE:CB	1:F:107:PHE:CE1	2.84	0.50
1:F:189:VAL:HG12	1:F:193:THR:HB	1.93	0.50
1:C:155:ARG:HH22	1:C:158:TYR:HE2	1.60	0.50
1:E:133:LYS:O	1:E:137:TYR:HD1	1.93	0.50
1:A:187:THR:OG1	1:A:189:VAL:HB	2.11	0.50
1:B:66:ILE:HD13	1:B:93:ASN:ND2	2.26	0.50
1:B:202:LYS:C	1:B:204:GLU:H	2.18	0.50
1:F:44:ILE:HG21	1:F:94:ILE:CG2	2.42	0.50
1:F:74:LEU:HD22	1:F:75:LEU:N	2.26	0.50
1:D:74:LEU:HD23	1:D:75:LEU:O	2.11	0.50
1:A:33:LEU:HD23	1:E:36:ASP:O	2.12	0.50
1:B:86:LYS:HG3	1:B:88:TYR:O	2.10	0.50
1:B:113:ARG:O	1:B:114:THR:C	2.52	0.50
1:A:44:ILE:HB	1:A:96:ALA:H	1.76	0.50
1:B:126:ILE:HG22	1:B:130:TYR:HD1	1.77	0.50
1:B:182:SER:O	1:B:186:ILE:HG13	2.12	0.49
1:C:87:LEU:HD11	1:C:112:LEU:HD12	1.93	0.49
1:D:52:SER:N	1:D:86:LYS:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:MET:HG2	1:F:87:LEU:CD1	2.42	0.49
1:B:72:GLU:O	1:B:73:LYS:O	2.30	0.49
1:C:151:ILE:HG23	1:C:154:LEU:HD12	1.94	0.49
1:D:180:GLN:O	1:D:182:SER:N	2.44	0.49
1:F:53:MET:HE3	1:F:83:LEU:CD1	2.42	0.49
1:F:85:GLY:C	1:F:86:LYS:HG2	2.35	0.49
1:A:167:ARG:HA	1:A:171:THR:O	2.12	0.49
1:A:178:LEU:HG	1:A:183:ILE:HD11	1.94	0.49
1:A:183:ILE:O	1:A:187:THR:OG1	2.18	0.49
1:B:19:PHE:CE1	1:B:79:GLY:HA3	2.47	0.49
1:C:123:ILE:HD13	1:D:123:ILE:HG21	1.94	0.49
1:E:51:THR:O	1:E:87:LEU:HD23	2.13	0.49
1:E:56:LEU:C	1:E:56:LEU:HD23	2.36	0.49
1:E:92:ASN:OD1	1:F:139:ARG:HG3	2.12	0.49
1:F:203:ARG:O	1:F:205:ASN:ND2	2.44	0.49
1:A:151:ILE:O	1:A:155:ARG:HG3	2.13	0.49
1:C:128:LYS:O	1:C:131:LEU:N	2.41	0.49
1:C:130:TYR:HE2	1:D:131:LEU:CD2	2.25	0.49
1:A:203:ARG:O	1:A:204:GLU:C	2.54	0.49
1:D:69:ASP:N	1:D:69:ASP:OD1	2.45	0.49
1:B:140:GLN:O	1:B:141:VAL:O	2.30	0.49
1:C:155:ARG:HG2	1:D:185:GLU:OE1	2.12	0.49
1:C:205:ASN:O	1:C:217:TYR:CB	2.60	0.49
1:D:150:THR:HA	1:D:153:ILE:CD1	2.42	0.49
1:D:180:GLN:O	1:D:181:LYS:C	2.56	0.49
1:E:159:GLU:O	1:E:160:LEU:HD12	2.13	0.49
1:F:74:LEU:HD22	1:F:75:LEU:H	1.77	0.49
1:B:19:PHE:HB2	1:B:21:PRO:HD3	1.95	0.49
1:D:53:MET:CE	1:D:85:GLY:O	2.61	0.49
1:E:28:TYR:OH	1:E:119:ASP:HB2	2.12	0.49
1:F:219:LEU:O	1:F:223:LYS:HB3	2.13	0.49
1:A:137:TYR:CE1	1:B:138:ALA:HB2	2.48	0.49
1:A:138:ALA:HA	1:B:137:TYR:CD2	2.48	0.49
1:B:55:PHE:HB2	1:B:83:LEU:HD12	1.94	0.49
1:B:130:TYR:O	1:B:133:LYS:N	2.46	0.49
1:C:139:ARG:O	1:C:140:GLN:C	2.55	0.49
1:C:223:LYS:HE3	1:C:223:LYS:O	2.12	0.49
1:E:187:THR:O	1:E:188:GLY:C	2.55	0.49
1:A:43:VAL:HG11	1:A:61:ILE:HD13	1.95	0.48
1:B:200:CYS:O	1:B:204:GLU:HG2	2.13	0.48
1:B:204:GLU:OE1	1:B:204:GLU:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ARG:NH1	1:C:158:TYR:CD2	2.71	0.48
1:E:53:MET:HE3	1:E:84:ILE:O	2.13	0.48
1:E:224:HIS:CG	1:E:224:HIS:O	2.66	0.48
1:B:45:MET:HB2	1:B:48:GLU:HB2	1.94	0.48
1:C:66:ILE:CD1	1:C:95:TYR:HB2	2.42	0.48
1:C:92:ASN:HD21	1:D:139:ARG:HD2	1.78	0.48
1:E:80:GLY:O	1:E:81:ASN:HB2	2.13	0.48
1:E:86:LYS:HG3	1:E:88:TYR:O	2.13	0.48
1:E:198:LEU:CD1	1:E:201:LEU:CD1	2.87	0.48
1:F:39:LYS:HB2	1:F:101:PRO:HD3	1.95	0.48
1:F:173:GLU:HG2	1:F:215:ILE:HG12	1.95	0.48
1:A:168:VAL:N	1:A:171:THR:O	2.46	0.48
1:A:186:ILE:HD11	1:B:159:GLU:HG3	1.95	0.48
1:B:36:ASP:OD1	1:B:103:ARG:HG3	2.13	0.48
1:B:155:ARG:HG3	1:B:155:ARG:NH1	2.25	0.48
1:D:199:ALA:O	1:D:203:ARG:HB2	2.13	0.48
1:E:63:LEU:CD1	1:E:76:TYR:CD2	2.96	0.48
1:A:186:ILE:O	1:B:152:ARG:HB3	2.14	0.48
1:B:45:MET:HB3	1:B:46:PRO:CD	2.44	0.48
1:F:221:GLU:O	1:F:225:LEU:HD12	2.13	0.48
1:A:57:VAL:HG13	1:A:103:ARG:HG2	1.96	0.48
1:C:150:THR:HG23	1:C:197:VAL:HG11	1.96	0.48
1:E:44:ILE:O	1:E:95:TYR:HA	2.13	0.48
1:F:43:VAL:HG12	1:F:43:VAL:O	2.13	0.48
1:D:178:LEU:HG	1:D:183:ILE:CD1	2.32	0.48
1:E:197:VAL:HG12	1:E:198:LEU:N	2.29	0.48
1:E:218:ASN:HB3	1:E:221:GLU:HB2	1.95	0.48
1:F:35:ARG:N	1:F:104:THR:O	2.42	0.48
1:A:115:VAL:O	1:A:119:ASP:N	2.41	0.48
1:C:151:ILE:HA	1:C:154:LEU:HG	1.96	0.48
1:C:186:ILE:CG2	1:D:156:LEU:HD13	2.43	0.48
1:E:209:LYS:HG3	1:E:214:ILE:CG2	2.35	0.48
1:A:35:ARG:NH2	1:E:35:ARG:CZ	2.74	0.48
1:E:140:GLN:C	1:E:142:ALA:N	2.62	0.48
1:E:153:ILE:CG1	1:E:189:VAL:HG21	2.43	0.48
1:E:155:ARG:HB3	1:F:186:ILE:HG12	1.94	0.48
1:F:76:TYR:CD1	1:F:137:TYR:OH	2.62	0.48
1:F:184:GLY:O	1:F:186:ILE:N	2.47	0.48
1:A:130:TYR:HE1	1:A:133:LYS:NZ	2.11	0.48
1:B:155:ARG:HH11	1:B:155:ARG:CG	2.24	0.48
1:C:46:PRO:HA	1:C:94:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ILE:CG2	1:C:104:THR:HB	2.44	0.48
1:C:63:LEU:HG	1:C:96:ALA:CB	2.43	0.48
1:E:164:GLN:O	1:E:174:ILE:HG13	2.13	0.48
1:D:20:PHE:CE1	1:D:133:LYS:HG2	2.49	0.48
1:A:44:ILE:HG22	1:A:45:MET:O	2.14	0.47
1:A:54:ILE:HB	1:A:84:ILE:HG13	1.95	0.47
1:E:100:GLU:O	1:E:101:PRO:C	2.56	0.47
1:F:158:TYR:CE1	1:F:223:LYS:HB2	2.49	0.47
1:E:127:PHE:CE1	1:F:130:TYR:CD1	2.99	0.47
1:A:67:PHE:HB2	1:A:69:ASP:OD1	2.14	0.47
1:A:99:MET:HE2	1:A:99:MET:HB2	1.78	0.47
1:D:45:MET:HB2	1:D:48:GLU:CB	2.41	0.47
1:E:207:LEU:HD21	1:E:214:ILE:HG22	1.97	0.47
1:F:73:LYS:HA	1:F:73:LYS:HZ3	1.79	0.47
1:F:112:LEU:HA	1:F:112:LEU:HD23	1.67	0.47
1:F:203:ARG:HD2	1:F:204:GLU:OE1	2.14	0.47
1:A:131:LEU:CD2	1:B:53:MET:HE1	2.41	0.47
1:B:47:GLY:N	1:B:93:ASN:OD1	2.47	0.47
1:D:80:GLY:O	1:D:81:ASN:HB2	2.15	0.47
1:D:168:VAL:N	1:D:171:THR:O	2.43	0.47
1:D:193:THR:O	1:D:197:VAL:CB	2.60	0.47
1:E:28:TYR:OH	1:E:119:ASP:CB	2.63	0.47
1:E:108:SER:O	1:E:111:SER:OG	2.15	0.47
1:A:190:HIS:CD2	1:A:190:HIS:C	2.92	0.47
1:A:195:SER:C	1:A:197:VAL:H	2.22	0.47
1:B:161:CYS:HA	1:B:174:ILE:HD11	1.96	0.47
1:A:63:LEU:N	1:A:63:LEU:HD12	2.29	0.47
1:A:154:LEU:O	1:A:158:TYR:N	2.45	0.47
1:B:30:GLN:NE2	1:B:30:GLN:N	2.48	0.47
1:B:65:ILE:HB	1:B:75:LEU:HD12	1.97	0.47
1:B:211:LYS:HB2	1:B:212:ASN:OD1	2.15	0.47
1:C:132:THR:O	1:C:133:LYS:C	2.57	0.47
1:C:193:THR:C	1:C:195:SER:H	2.22	0.47
1:E:63:LEU:CD1	1:E:76:TYR:CE2	2.98	0.47
1:E:113:ARG:NH1	1:F:121:ASP:OD1	2.44	0.47
1:B:48:GLU:HG2	1:B:50:ILE:CD1	2.42	0.47
1:D:45:MET:HE3	1:D:46:PRO:HD2	1.96	0.47
1:E:66:ILE:HB	1:E:93:ASN:HB3	1.97	0.47
1:E:79:GLY:H	1:E:82:SER:CB	2.27	0.47
1:E:94:ILE:HG22	1:E:95:TYR:N	2.29	0.47
1:B:19:PHE:CE1	1:B:79:GLY:CA	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LEU:C	1:B:88:TYR:CD1	2.93	0.47
1:B:156:LEU:CD2	1:B:183:ILE:HG23	2.45	0.47
1:D:53:MET:O	1:D:107:PHE:HB2	2.15	0.47
1:E:149:PRO:O	1:E:152:ARG:HB2	2.15	0.47
1:E:140:GLN:H	1:E:140:GLN:HG2	1.49	0.46
1:F:36:ASP:OD1	1:F:103:ARG:HG3	2.16	0.46
1:F:74:LEU:CD2	1:F:75:LEU:N	2.78	0.46
1:A:22:ILE:O	1:A:22:ILE:CG1	2.62	0.46
1:A:30:GLN:CD	1:A:30:GLN:N	2.72	0.46
1:A:75:LEU:O	1:A:76:TYR:HD1	1.97	0.46
1:C:87:LEU:HD23	1:C:87:LEU:HA	1.68	0.46
1:D:53:MET:HG2	1:D:87:LEU:HD11	1.96	0.46
1:E:109:GLU:C	1:E:111:SER:N	2.73	0.46
1:A:94:ILE:HD13	1:A:94:ILE:N	2.30	0.46
1:B:173:GLU:HG2	1:B:215:ILE:HG12	1.97	0.46
1:B:207:LEU:HD21	1:B:214:ILE:HG23	1.97	0.46
1:D:161:CYS:SG	1:D:172:TYR:CB	3.03	0.46
1:F:78:ALA:HB1	1:F:82:SER:HB3	1.98	0.46
1:B:44:ILE:CD1	1:B:50:ILE:HG21	2.46	0.46
1:E:152:ARG:CD	1:F:188:GLY:HA2	2.40	0.46
1:B:114:THR:O	1:B:115:VAL:C	2.57	0.46
1:B:118:THR:O	1:B:119:ASP:HB3	2.14	0.46
1:C:150:THR:O	1:C:154:LEU:CG	2.47	0.46
1:E:107:PHE:HB3	1:E:111:SER:OG	2.16	0.46
1:C:89:PRO:O	1:C:90:THR:CG2	2.63	0.46
1:C:128:LYS:O	1:C:129:ASN:C	2.59	0.46
1:F:30:GLN:CD	1:F:30:GLN:N	2.53	0.46
1:A:113:ARG:O	1:A:117:ARG:HG3	2.14	0.46
1:B:52:SER:HB3	1:B:108:SER:HA	1.98	0.46
1:B:126:ILE:HG22	1:B:130:TYR:CD1	2.50	0.46
1:D:38:ALA:O	1:D:39:LYS:C	2.59	0.46
1:F:141:VAL:N	1:F:142:ALA:CB	2.75	0.46
1:B:191:HIS:C	1:B:193:THR:N	2.73	0.46
1:D:29:THR:C	1:D:31:MET:N	2.73	0.46
1:E:172:TYR:CE1	1:E:219:LEU:HD22	2.51	0.46
1:A:128:LYS:O	1:A:129:ASN:C	2.59	0.46
1:A:130:TYR:C	1:A:132:THR:N	2.71	0.46
1:B:154:LEU:H	1:B:154:LEU:HG	1.31	0.46
1:C:187:THR:O	1:D:187:THR:HA	2.16	0.45
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.66	0.45
1:A:57:VAL:CG2	1:A:57:VAL:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:N	1:B:63:LEU:HD12	2.30	0.45
1:D:22:ILE:O	1:D:22:ILE:HD13	2.12	0.45
1:D:75:LEU:HB3	1:D:76:TYR:CD1	2.51	0.45
1:A:52:SER:OG	1:A:108:SER:N	2.50	0.45
1:D:53:MET:SD	1:D:87:LEU:HD13	2.57	0.45
1:F:65:ILE:CG2	1:F:67:PHE:HE1	2.29	0.45
1:F:66:ILE:HD12	1:F:93:ASN:O	2.16	0.45
1:F:221:GLU:O	1:F:225:LEU:CG	2.64	0.45
1:B:44:ILE:CD1	1:B:50:ILE:HG13	2.34	0.45
1:B:124:PHE:O	1:B:127:PHE:HB2	2.16	0.45
1:D:209:LYS:C	1:D:209:LYS:HZ2	2.24	0.45
1:C:180:GLN:NE2	1:C:194:VAL:O	2.50	0.45
1:D:157:PHE:O	1:D:161:CYS:HB2	2.17	0.45
1:E:57:VAL:HG13	1:E:103:ARG:HG2	1.99	0.45
1:B:26:ARG:C	1:B:28:TYR:H	2.25	0.45
1:C:136:TYR:O	1:C:139:ARG:CB	2.63	0.45
1:E:109:GLU:C	1:E:111:SER:H	2.24	0.45
1:E:116:PHE:CD1	1:E:122:MET:HB3	2.51	0.45
1:A:75:LEU:C	1:A:76:TYR:CD1	2.77	0.45
1:A:87:LEU:CB	1:A:88:TYR:CD1	2.96	0.45
1:B:26:ARG:HG2	1:B:55:PHE:CZ	2.52	0.45
1:B:129:ASN:O	1:B:133:LYS:HG3	2.16	0.45
1:F:140:GLN:O	1:F:143:GLU:CB	2.65	0.45
1:A:153:ILE:HD12	1:A:153:ILE:H	1.82	0.45
1:C:109:GLU:CG	1:C:113:ARG:HH21	2.26	0.45
1:C:115:VAL:HG11	1:C:122:MET:HG3	1.98	0.45
1:F:58:GLU:O	1:F:102:THR:CG2	2.65	0.45
1:A:188:GLY:N	1:B:152:ARG:HD3	2.32	0.44
1:F:208:ASP:OD2	1:F:208:ASP:C	2.59	0.44
1:A:26:ARG:HH22	1:A:57:VAL:HG23	1.83	0.44
1:A:128:LYS:CG	1:B:88:TYR:CE1	2.93	0.44
1:D:49:GLU:O	1:D:49:GLU:CG	2.59	0.44
1:E:210:LYS:C	1:E:211:LYS:HE3	2.42	0.44
1:F:155:ARG:HD2	1:F:155:ARG:HA	1.51	0.44
1:A:123:ILE:CD1	1:B:123:ILE:HD13	2.48	0.44
1:E:87:LEU:CD2	1:E:109:GLU:HB2	2.48	0.44
1:E:152:ARG:NH1	1:E:188:GLY:O	2.50	0.44
1:B:45:MET:C	1:B:47:GLY:N	2.76	0.44
1:C:66:ILE:HD11	1:C:95:TYR:HB2	1.98	0.44
1:C:114:THR:O	1:C:115:VAL:C	2.60	0.44
1:C:183:ILE:O	1:C:187:THR:OG1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ILE:O	1:E:155:ARG:HB2	2.18	0.44
1:A:18:ASN:C	1:A:20:PHE:H	2.24	0.44
1:F:206:ILE:O	1:F:217:TYR:N	2.50	0.44
1:A:67:PHE:O	1:A:69:ASP:N	2.45	0.44
1:A:201:LEU:HA	1:A:206:ILE:HD12	2.00	0.44
1:B:23:GLU:O	1:B:26:ARG:N	2.47	0.44
1:C:167:ARG:HG3	1:C:172:TYR:CZ	2.52	0.44
1:D:111:SER:C	1:D:114:THR:HB	2.42	0.44
1:E:74:LEU:HD23	1:E:75:LEU:N	2.33	0.44
1:F:23:GLU:O	1:F:25:LEU:N	2.50	0.44
1:F:24:LYS:HD2	1:F:125:GLU:OE1	2.17	0.44
1:B:36:ASP:O	1:C:33:LEU:CD2	2.65	0.44
1:C:88:TYR:CD1	1:D:128:LYS:HE3	2.53	0.44
1:D:108:SER:OG	1:D:109:GLU:N	2.46	0.44
1:F:158:TYR:HE1	1:F:223:LYS:HB2	1.82	0.44
1:C:50:ILE:HG12	1:C:86:LYS:HZ1	1.81	0.44
1:D:53:MET:CE	1:D:130:TYR:OH	2.66	0.44
1:E:76:TYR:CD1	1:E:76:TYR:N	2.85	0.44
1:F:29:THR:O	1:F:32:GLY:N	2.48	0.44
1:F:46:PRO:HA	1:F:94:ILE:O	2.18	0.44
1:A:130:TYR:HE2	1:B:131:LEU:CD2	2.16	0.43
1:B:63:LEU:HD22	1:B:76:TYR:CE2	2.52	0.43
1:C:123:ILE:CD1	1:D:123:ILE:CD1	2.78	0.43
1:D:34:ILE:HD13	1:D:105:CYS:SG	2.58	0.43
1:D:44:ILE:H	1:D:96:ALA:HB3	1.83	0.43
1:A:109:GLU:CD	1:A:113:ARG:HH21	2.26	0.43
1:A:127:PHE:O	1:A:128:LYS:C	2.60	0.43
1:B:108:SER:HG	1:B:111:SER:H	1.58	0.43
1:C:74:LEU:HD11	1:C:77:TYR:CE1	2.52	0.43
1:E:189:VAL:HG12	1:E:190:HIS:H	1.82	0.43
1:A:28:TYR:N	1:A:28:TYR:CD1	2.87	0.43
1:B:216:VAL:O	1:B:216:VAL:HG12	2.18	0.43
1:C:45:MET:O	1:C:48:GLU:HB3	2.18	0.43
1:D:52:SER:HA	1:D:107:PHE:O	2.18	0.43
1:D:88:TYR:HA	1:D:89:PRO:HD2	1.88	0.43
1:D:165:GLY:HA2	1:D:174:ILE:HG12	2.00	0.43
1:E:164:GLN:NE2	1:F:164:GLN:CD	2.76	0.43
1:A:127:PHE:O	1:A:131:LEU:CB	2.67	0.43
1:C:19:PHE:HB3	1:C:82:SER:OG	2.18	0.43
1:F:161:CYS:SG	1:F:172:TYR:HB3	2.58	0.43
1:F:198:LEU:HA	1:F:198:LEU:HD22	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HG13	1:B:155:ARG:HB3	2.00	0.43
1:C:115:VAL:O	1:C:118:THR:N	2.52	0.43
1:C:127:PHE:HE2	1:D:53:MET:SD	2.42	0.43
1:C:155:ARG:CG	1:D:185:GLU:OE1	2.66	0.43
1:D:22:ILE:HD11	1:D:122:MET:HE1	2.00	0.43
1:D:65:ILE:HG23	1:D:73:LYS:O	2.19	0.43
1:E:131:LEU:O	1:E:134:VAL:N	2.51	0.43
1:E:152:ARG:HG2	1:F:185:GLU:O	2.19	0.43
1:A:60:LYS:HG2	1:A:99:MET:HE2	1.98	0.43
1:A:151:ILE:C	1:A:155:ARG:HG3	2.43	0.43
1:B:73:LYS:HZ1	1:B:74:LEU:H	1.67	0.43
1:C:45:MET:HE3	1:C:48:GLU:HG3	2.00	0.43
1:C:65:ILE:CD1	1:C:92:ASN:ND2	2.81	0.43
1:F:43:VAL:O	1:F:44:ILE:HG12	2.18	0.43
1:A:127:PHE:HZ	1:B:53:MET:HE2	1.76	0.43
1:A:138:ALA:HA	1:B:137:TYR:HD2	1.84	0.43
1:B:35:ARG:NH1	1:C:35:ARG:HE	2.16	0.43
1:B:46:PRO:HA	1:B:93:ASN:ND2	2.34	0.43
1:C:28:TYR:CE2	1:C:115:VAL:HG13	2.53	0.43
1:C:65:ILE:HD11	1:C:92:ASN:HD22	1.83	0.43
1:D:53:MET:HG2	1:D:87:LEU:CD1	2.49	0.43
1:E:156:LEU:N	1:F:186:ILE:HG12	2.34	0.43
1:E:158:TYR:CZ	1:E:223:LYS:HD2	2.54	0.43
1:E:216:VAL:HG11	1:E:222:LEU:CD2	2.48	0.43
1:B:195:SER:O	1:B:197:VAL:N	2.51	0.43
1:C:30:GLN:C	1:C:32:GLY:N	2.73	0.43
1:D:112:LEU:O	1:D:115:VAL:N	2.52	0.43
1:E:24:LYS:O	1:E:25:LEU:C	2.61	0.43
1:E:25:LEU:HA	1:E:25:LEU:HD23	1.63	0.43
1:E:46:PRO:HB3	1:E:66:ILE:HD13	1.99	0.43
1:E:188:GLY:CA	1:F:152:ARG:HE	2.30	0.43
1:B:112:LEU:HD23	1:B:112:LEU:HA	1.66	0.43
1:B:183:ILE:O	1:B:187:THR:N	2.34	0.43
1:D:136:TYR:O	1:D:139:ARG:HB3	2.18	0.43
1:E:124:PHE:HB3	1:F:88:TYR:OH	2.19	0.43
1:A:28:TYR:HB3	1:A:31:MET:HG3	2.00	0.42
1:A:68:GLU:OE2	1:B:139:ARG:NH2	2.52	0.42
1:B:131:LEU:C	1:B:134:VAL:HG23	2.44	0.42
1:B:156:LEU:HD13	1:B:186:ILE:HG21	2.01	0.42
1:D:64:ASP:OD2	1:D:64:ASP:N	2.51	0.42
1:E:28:TYR:O	1:E:31:MET:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PHE:HB3	1:A:112:LEU:HG	2.00	0.42
1:D:189:VAL:CG1	1:D:190:HIS:O	2.62	0.42
1:F:57:VAL:O	1:F:57:VAL:HG23	2.18	0.42
1:F:74:LEU:HD23	1:F:75:LEU:H	1.84	0.42
1:F:87:LEU:C	1:F:88:TYR:CG	2.97	0.42
1:F:140:GLN:N	1:F:142:ALA:HB3	2.34	0.42
1:A:152:ARG:O	1:A:155:ARG:HB2	2.19	0.42
1:A:160:LEU:HD21	1:A:176:MET:SD	2.60	0.42
1:A:211:LYS:C	1:A:213:LYS:H	2.27	0.42
1:C:94:ILE:CG2	1:C:95:TYR:N	2.82	0.42
1:E:63:LEU:HD13	1:E:76:TYR:CE2	2.55	0.42
1:E:153:ILE:HD12	1:E:197:VAL:HG11	2.01	0.42
1:E:164:GLN:O	1:E:174:ILE:HG23	2.18	0.42
1:A:74:LEU:O	1:A:74:LEU:HG	2.06	0.42
1:C:46:PRO:CA	1:C:94:ILE:O	2.68	0.42
1:C:180:GLN:HE21	1:C:180:GLN:HB3	1.70	0.42
1:E:28:TYR:HB3	1:E:115:VAL:HG22	2.01	0.42
1:F:19:PHE:CE1	1:F:78:ALA:C	2.97	0.42
1:F:87:LEU:CB	1:F:88:TYR:CE1	3.02	0.42
1:B:47:GLY:CA	1:B:93:ASN:OD1	2.68	0.42
1:D:88:TYR:O	1:D:90:THR:N	2.52	0.42
1:E:84:ILE:HB	1:E:85:GLY:H	1.56	0.42
1:A:87:LEU:C	1:A:88:TYR:CG	2.98	0.42
1:A:90:THR:O	1:A:91:GLY:C	2.63	0.42
1:A:161:CYS:O	1:A:165:GLY:N	2.53	0.42
1:B:75:LEU:CD2	1:B:76:TYR:CE1	3.03	0.42
1:C:207:LEU:HD23	1:C:208:ASP:N	2.35	0.42
1:F:124:PHE:HA	1:F:127:PHE:HB2	2.01	0.42
1:A:101:PRO:O	1:A:101:PRO:CG	2.68	0.42
1:C:60:LYS:HA	1:C:78:ALA:O	2.19	0.42
1:C:164:GLN:HB3	1:C:174:ILE:CG2	2.47	0.42
1:C:202:LYS:HD3	1:C:203:ARG:N	2.34	0.42
1:F:33:LEU:N	1:F:33:LEU:HD23	2.34	0.42
1:F:38:ALA:C	1:F:39:LYS:O	2.63	0.42
1:B:46:PRO:HD3	1:B:95:TYR:CE2	2.55	0.42
1:B:65:ILE:O	1:B:72:GLU:O	2.38	0.42
1:B:75:LEU:HD22	1:B:76:TYR:CE1	2.54	0.42
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.51	0.42
1:C:94:ILE:HG22	1:C:95:TYR:N	2.33	0.42
1:E:190:HIS:CD2	1:E:191:HIS:N	2.86	0.42
1:A:121:ASP:O	1:A:122:MET:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LYS:HB2	1:C:88:TYR:O	2.20	0.42
1:A:219:LEU:O	1:A:222:LEU:HB3	2.20	0.42
1:B:87:LEU:HB3	1:B:88:TYR:CE1	2.55	0.42
1:B:120:GLU:O	1:B:121:ASP:C	2.62	0.42
1:C:115:VAL:O	1:C:119:ASP:N	2.38	0.42
1:D:92:ASN:O	1:D:94:ILE:CG1	2.59	0.42
1:E:159:GLU:CG	1:F:186:ILE:HD11	2.39	0.42
1:A:137:TYR:O	1:A:138:ALA:C	2.62	0.41
1:C:57:VAL:O	1:C:57:VAL:HG23	2.20	0.41
1:D:62:LYS:HG3	1:D:74:LEU:HD12	2.02	0.41
1:E:161:CYS:SG	1:E:174:ILE:HD11	2.60	0.41
1:B:140:GLN:H	1:B:140:GLN:HG2	1.56	0.41
1:D:189:VAL:HG11	1:D:193:THR:HB	1.91	0.41
1:E:45:MET:O	1:E:48:GLU:HB3	2.19	0.41
1:E:75:LEU:HA	1:E:75:LEU:HD23	1.53	0.41
1:E:161:CYS:O	1:E:165:GLY:CA	2.64	0.41
1:A:151:ILE:O	1:A:155:ARG:HG2	2.20	0.41
1:B:202:LYS:C	1:B:204:GLU:N	2.77	0.41
1:C:26:ARG:HA	1:C:29:THR:HG23	2.03	0.41
1:C:134:VAL:HG21	1:D:130:TYR:CD2	2.50	0.41
1:D:55:PHE:N	1:D:83:LEU:HD12	2.35	0.41
1:D:67:PHE:HB2	1:D:71:SER:OG	2.20	0.41
1:E:86:LYS:CG	1:E:88:TYR:O	2.68	0.41
1:A:160:LEU:O	1:A:164:GLN:HB2	2.20	0.41
1:C:109:GLU:C	1:C:111:SER:N	2.77	0.41
1:C:186:ILE:HG23	1:D:156:LEU:CB	2.48	0.41
1:F:86:LYS:HZ3	1:F:86:LYS:HG3	1.61	0.41
1:A:123:ILE:HD11	1:B:123:ILE:HD13	2.02	0.41
1:A:126:ILE:O	1:A:129:ASN:HB3	2.20	0.41
1:A:160:LEU:HD21	1:A:176:MET:CE	2.50	0.41
1:B:122:MET:HB3	1:B:122:MET:HE3	1.40	0.41
1:C:184:GLY:O	1:C:188:GLY:N	2.54	0.41
1:F:158:TYR:HA	1:F:222:LEU:HD21	2.02	0.41
1:F:158:TYR:HD2	1:F:159:GLU:OE1	2.03	0.41
1:A:108:SER:OG	1:A:109:GLU:N	2.51	0.41
1:A:160:LEU:HD12	1:A:174:ILE:HD13	2.02	0.41
1:C:19:PHE:CD1	1:C:19:PHE:N	2.83	0.41
1:C:151:ILE:HA	1:C:154:LEU:CG	2.49	0.41
1:D:53:MET:HB3	1:D:83:LEU:HD11	2.03	0.41
1:E:116:PHE:HE1	1:E:122:MET:HB3	1.79	0.41
1:E:151:ILE:HG23	1:E:226:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:LEU:C	1:E:207:LEU:O	2.64	0.41
1:E:218:ASN:CG	1:E:221:GLU:HB2	2.46	0.41
1:A:164:GLN:HB3	1:A:174:ILE:HG12	2.02	0.41
1:B:20:PHE:HA	1:B:21:PRO:HD2	1.90	0.41
1:E:131:LEU:HD23	1:F:130:TYR:CZ	2.56	0.41
1:A:66:ILE:HB	1:A:93:ASN:ND2	2.36	0.41
1:A:75:LEU:HD13	1:A:76:TYR:CE1	2.56	0.41
1:B:35:ARG:HH11	1:C:35:ARG:HE	1.69	0.41
1:B:51:THR:C	1:B:52:SER:OG	2.63	0.41
1:B:91:GLY:C	1:B:92:ASN:OD1	2.63	0.41
1:C:74:LEU:HD21	1:C:76:TYR:HA	2.03	0.41
1:C:116:PHE:CE1	1:C:123:ILE:HA	2.56	0.41
1:D:93:ASN:O	1:D:94:ILE:HD13	2.21	0.41
1:B:29:THR:HG22	1:B:105:CYS:CB	2.50	0.41
1:B:52:SER:HA	1:B:87:LEU:HD13	2.03	0.41
1:B:109:GLU:O	1:B:113:ARG:N	2.46	0.41
1:B:210:LYS:C	1:B:211:LYS:HG3	2.45	0.41
1:C:20:PHE:N	1:C:21:PRO:CD	2.83	0.41
1:C:111:SER:O	1:C:114:THR:OG1	2.37	0.41
1:D:86:LYS:HZ1	1:D:90:THR:HG23	1.84	0.41
1:D:121:ASP:O	1:D:122:MET:C	2.62	0.41
1:D:133:LYS:O	1:D:137:TYR:HD1	2.04	0.41
1:E:108:SER:OG	1:E:111:SER:HB3	2.21	0.41
1:E:120:GLU:O	1:E:123:ILE:HG13	2.21	0.41
1:E:149:PRO:HG2	1:E:150:THR:H	1.86	0.41
1:E:153:ILE:HD11	1:E:189:VAL:HG11	2.03	0.41
1:D:100:GLU:O	1:D:102:THR:OG1	2.25	0.41
1:D:155:ARG:HH12	1:D:159:GLU:CD	2.26	0.41
1:A:186:ILE:HG12	1:B:156:LEU:N	2.37	0.40
1:B:122:MET:HE3	1:B:122:MET:CA	2.43	0.40
1:C:74:LEU:HG	1:C:75:LEU:N	2.31	0.40
1:C:190:HIS:CD2	1:C:192:VAL:HG23	2.50	0.40
1:D:130:TYR:O	1:D:133:LYS:HB2	2.20	0.40
1:E:175:THR:O	1:E:176:MET:HB3	2.21	0.40
1:F:115:VAL:H	1:F:115:VAL:HG23	1.69	0.40
1:A:140:GLN:HG2	1:A:140:GLN:H	1.71	0.40
1:B:195:SER:O	1:B:198:LEU:N	2.54	0.40
1:B:224:HIS:O	1:B:224:HIS:CD2	2.74	0.40
1:C:19:PHE:HB2	1:C:21:PRO:HD3	2.03	0.40
1:E:60:LYS:CD	1:E:99:MET:CE	2.81	0.40
1:E:137:TYR:O	1:E:138:ALA:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:CYS:HB2	1:F:174:ILE:HD11	2.02	0.40
1:C:124:PHE:HZ	1:D:112:LEU:HB3	1.87	0.40
1:F:67:PHE:HB2	1:F:71:SER:OG	2.20	0.40
1:C:186:ILE:HG23	1:D:156:LEU:HD13	2.03	0.40
1:D:149:PRO:C	1:D:151:ILE:N	2.80	0.40
1:E:54:ILE:HD13	1:E:106:TRP:CZ2	2.56	0.40
1:E:171:THR:HG22	1:E:217:TYR:HA	2.03	0.40
1:F:178:LEU:HD12	1:F:178:LEU:HA	1.91	0.40
1:F:189:VAL:CG1	1:F:193:THR:HB	2.51	0.40
1:A:122:MET:O	1:A:123:ILE:C	2.63	0.40
1:A:198:LEU:HD13	1:A:198:LEU:HA	1.86	0.40
1:B:32:GLY:C	1:B:33:LEU:HD23	2.47	0.40
1:C:128:LYS:HG3	1:D:88:TYR:CD1	2.56	0.40
1:C:130:TYR:HE2	1:D:131:LEU:HG	1.83	0.40
1:D:167:ARG:CA	1:D:171:THR:O	2.60	0.40
1:E:190:HIS:NE2	1:E:192:VAL:HB	2.37	0.40
1:F:43:VAL:HG21	1:F:61:ILE:HD11	2.03	0.40

All (1) 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)
1:D:35:ARG:NH1	1:F:35:ARG:NH1[1_656]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	198/250 (79%)	140 (71%)	41 (21%)	17 (9%)	0 3
1	B	197/250 (79%)	146 (74%)	31 (16%)	20 (10%)	0 2
1	C	199/250 (80%)	151 (76%)	36 (18%)	12 (6%)	1 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	197/250 (79%)	144 (73%)	31 (16%)	22 (11%)	0	2
1	E	199/250 (80%)	152 (76%)	34 (17%)	13 (6%)	1	8
1	F	199/250 (80%)	156 (78%)	29 (15%)	14 (7%)	1	6
All	All	1189/1500 (79%)	889 (75%)	202 (17%)	98 (8%)	0	4

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ILE
1	A	205	ASN
1	A	206	ILE
1	A	212	ASN
1	A	218	ASN
1	B	24	LYS
1	B	108	SER
1	B	119	ASP
1	B	150	THR
1	B	153	ILE
1	C	68	GLU
1	C	73	LYS
1	C	93	ASN
1	C	109	GLU
1	C	113	ARG
1	C	210	LYS
1	D	73	LYS
1	D	75	LEU
1	D	111	SER
1	D	180	GLN
1	D	181	LYS
1	D	205	ASN
1	E	58	GLU
1	E	141	VAL
1	F	24	LYS
1	F	68	GLU
1	F	72	GLU
1	F	82	SER
1	F	109	GLU
1	F	141	VAL
1	A	70	GLY
1	A	122	MET
1	A	180	GLN

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Mol	Chain	Res	Type
1	B	81	ASN
1	B	196	ARG
1	B	203	ARG
1	B	211	LYS
1	C	24	LYS
1	D	39	LYS
1	D	43	VAL
1	D	81	ASN
1	D	110	LYS
1	D	169	GLY
1	D	179	SER
1	D	192	VAL
1	D	203	ARG
1	D	211	LYS
1	E	26	ARG
1	E	110	LYS
1	F	140	GLN
1	F	206	ILE
1	A	210	LYS
1	B	27	ASN
1	B	73	LYS
1	B	135	ALA
1	B	195	SER
1	B	210	LYS
1	C	101	PRO
1	C	194	VAL
1	D	52	SER
1	D	186	ILE
1	E	71	SER
1	E	211	LYS
1	F	185	GLU
1	F	209	LYS
1	F	211	LYS
1	A	25	LEU
1	A	68	GLU
1	A	84	ILE
1	A	128	LYS
1	B	25	LEU
1	B	70	GLY
1	D	30	GLN
1	D	162	SER
1	D	210	LYS

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Mol	Chain	Res	Type
1	E	169	GLY
1	F	123	ILE
1	A	108	SER
1	B	115	VAL
1	B	117	ARG
1	B	185	GLU
1	E	188	GLY
1	F	73	LYS
1	F	86	LYS
1	C	89	PRO
1	D	101	PRO
1	D	114	THR
1	E	118	THR
1	A	186	ILE
1	E	194	VAL
1	C	141	VAL
1	B	89	PRO
1	E	197	VAL
1	A	85	GLY
1	E	186	ILE
1	A	215	ILE
1	C	115	VAL
1	E	22	ILE

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	170/220 (77%)	118 (69%)	52 (31%)	0	1
1	B	174/220 (79%)	126 (72%)	48 (28%)	0	2
1	C	170/220 (77%)	130 (76%)	40 (24%)	1	4
1	D	173/220 (79%)	132 (76%)	41 (24%)	1	4
1	E	170/220 (77%)	124 (73%)	46 (27%)	0	2
1	F	172/220 (78%)	124 (72%)	48 (28%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1029/1320 (78%)	754 (73%)	275 (27%)	0 3

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	28	TYR
1	A	33	LEU
1	A	34	ILE
1	A	41	SER
1	A	43	VAL
1	A	48	GLU
1	A	50	ILE
1	A	51	THR
1	A	52	SER
1	A	53	MET
1	A	54	ILE
1	A	56	LEU
1	A	57	VAL
1	A	66	ILE
1	A	69	ASP
1	A	74	LEU
1	A	75	LEU
1	A	76	TYR
1	A	94	ILE
1	A	99	MET
1	A	108	SER
1	A	109	GLU
1	A	117	ARG
1	A	118	THR
1	A	120	GLU
1	A	128	LYS
1	A	130	TYR
1	A	134	VAL
1	A	140	GLN
1	A	154	LEU
1	A	155	ARG
1	A	156	LEU
1	A	160	LEU
1	A	168	VAL
1	A	170	ASP
1	A	171	THR

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Mol	Chain	Res	Type
1	A	175	THR
1	A	180	GLN
1	A	181	LYS
1	A	185	GLU
1	A	189	VAL
1	A	194	VAL
1	A	195	SER
1	A	196	ARG
1	A	197	VAL
1	A	198	LEU
1	A	201	LEU
1	A	204	GLU
1	A	211	LYS
1	A	212	ASN
1	A	215	ILE
1	B	22	ILE
1	B	24	LYS
1	B	29	THR
1	B	30	GLN
1	B	31	MET
1	B	33	LEU
1	B	35	ARG
1	B	44	ILE
1	B	48	GLU
1	B	49	GLU
1	B	51	THR
1	B	52	SER
1	B	53	MET
1	B	56	LEU
1	B	57	VAL
1	B	72	GLU
1	B	73	LYS
1	B	75	LEU
1	B	82	SER
1	B	83	LEU
1	B	86	LYS
1	B	87	LEU
1	B	90	THR
1	B	94	ILE
1	B	100	GLU
1	B	110	LYS
1	B	119	ASP

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Mol	Chain	Res	Type
1	B	134	VAL
1	B	140	GLN
1	B	141	VAL
1	B	153	ILE
1	B	154	LEU
1	B	155	ARG
1	B	156	LEU
1	B	160	LEU
1	B	175	THR
1	B	179	SER
1	B	180	GLN
1	B	182	SER
1	B	183	ILE
1	B	193	THR
1	B	196	ARG
1	B	198	LEU
1	B	204	GLU
1	B	207	LEU
1	B	211	LYS
1	B	212	ASN
1	B	216	VAL
1	C	21	PRO
1	C	25	LEU
1	C	33	LEU
1	C	34	ILE
1	C	39	LYS
1	C	41	SER
1	C	43	VAL
1	C	49	GLU
1	C	51	THR
1	C	52	SER
1	C	57	VAL
1	C	60	LYS
1	C	65	ILE
1	C	68	GLU
1	C	74	LEU
1	C	75	LEU
1	C	86	LYS
1	C	90	THR
1	C	93	ASN
1	C	97	THR
1	C	102	THR

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Mol	Chain	Res	Type
1	C	103	ARG
1	C	114	THR
1	C	125	GLU
1	C	128	LYS
1	C	140	GLN
1	C	155	ARG
1	C	160	LEU
1	C	164	GLN
1	C	180	GLN
1	C	192	VAL
1	C	195	SER
1	C	196	ARG
1	C	201	LEU
1	C	202	LYS
1	C	207	LEU
1	C	212	ASN
1	C	221	GLU
1	C	223	LYS
1	C	225	LEU
1	D	22	ILE
1	D	27	ASN
1	D	30	GLN
1	D	31	MET
1	D	36	ASP
1	D	41	SER
1	D	43	VAL
1	D	49	GLU
1	D	57	VAL
1	D	60	LYS
1	D	64	ASP
1	D	65	ILE
1	D	69	ASP
1	D	73	LYS
1	D	74	LEU
1	D	86	LYS
1	D	87	LEU
1	D	90	THR
1	D	94	ILE
1	D	99	MET
1	D	101	PRO
1	D	108	SER
1	D	126	ILE

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Mol	Chain	Res	Type
1	D	127	PHE
1	D	132	THR
1	D	153	ILE
1	D	155	ARG
1	D	162	SER
1	D	170	ASP
1	D	171	THR
1	D	174	ILE
1	D	178	LEU
1	D	181	LYS
1	D	194	VAL
1	D	197	VAL
1	D	211	LYS
1	D	212	ASN
1	D	214	ILE
1	D	215	ILE
1	D	221	GLU
1	D	225	LEU
1	E	27	ASN
1	E	30	GLN
1	E	31	MET
1	E	41	SER
1	E	50	ILE
1	E	56	LEU
1	E	57	VAL
1	E	61	ILE
1	E	75	LEU
1	E	76	TYR
1	E	84	ILE
1	E	94	ILE
1	E	99	MET
1	E	100	GLU
1	E	102	THR
1	E	122	MET
1	E	128	LYS
1	E	131	LEU
1	E	133	LYS
1	E	140	GLN
1	E	141	VAL
1	E	153	ILE
1	E	155	ARG
1	E	160	LEU

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Mol	Chain	Res	Type
1	E	162	SER
1	E	163	SER
1	E	174	ILE
1	E	176	MET
1	E	178	LEU
1	E	179	SER
1	E	183	ILE
1	E	185	GLU
1	E	190	HIS
1	E	192	VAL
1	E	196	ARG
1	E	197	VAL
1	E	198	LEU
1	E	203	ARG
1	E	206	ILE
1	E	211	LYS
1	E	214	ILE
1	E	216	VAL
1	E	217	TYR
1	E	221	GLU
1	E	222	LEU
1	E	223	LYS
1	F	22	ILE
1	F	24	LYS
1	F	27	ASN
1	F	29	THR
1	F	30	GLN
1	F	31	MET
1	F	35	ARG
1	F	44	ILE
1	F	45	MET
1	F	50	ILE
1	F	54	ILE
1	F	57	VAL
1	F	63	LEU
1	F	65	ILE
1	F	68	GLU
1	F	73	LYS
1	F	74	LEU
1	F	75	LEU
1	F	83	LEU
1	F	84	ILE

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Mol	Chain	Res	Type
1	F	86	LYS
1	F	101	PRO
1	F	108	SER
1	F	109	GLU
1	F	110	LYS
1	F	111	SER
1	F	114	THR
1	F	125	GLU
1	F	134	VAL
1	F	139	ARG
1	F	153	ILE
1	F	154	LEU
1	F	155	ARG
1	F	163	SER
1	F	182	SER
1	F	190	HIS
1	F	192	VAL
1	F	196	ARG
1	F	198	LEU
1	F	203	ARG
1	F	204	GLU
1	F	206	ILE
1	F	207	LEU
1	F	209	LYS
1	F	211	LYS
1	F	212	ASN
1	F	223	LYS
1	F	226	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	190	HIS
1	B	27	ASN
1	B	30	GLN
1	B	191	HIS
1	B	224	HIS
1	C	30	GLN
1	C	92	ASN
1	C	93	ASN
1	C	164	GLN

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Mol	Chain	Res	Type
1	C	180	GLN
1	C	190	HIS
1	C	191	HIS
1	C	212	ASN
1	D	27	ASN
1	D	180	GLN
1	D	205	ASN
1	E	30	GLN
1	E	81	ASN
1	E	140	GLN
1	E	190	HIS
1	E	191	HIS
1	F	27	ASN
1	F	190	HIS
1	F	191	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	202/250 (80%)	1.17	38 (18%) 3 2	74, 81, 85, 90	0
1	B	201/250 (80%)	1.06	27 (13%) 7 6	74, 79, 84, 87	0
1	C	203/250 (81%)	1.23	42 (20%) 2 2	73, 80, 85, 91	0
1	D	201/250 (80%)	1.13	33 (16%) 4 3	73, 80, 85, 89	0
1	E	203/250 (81%)	1.03	26 (12%) 7 6	75, 80, 84, 90	0
1	F	203/250 (81%)	0.82	19 (9%) 14 9	75, 80, 84, 87	0
All	All	1213/1500 (80%)	1.07	185 (15%) 5 4	73, 80, 85, 91	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	161	CYS	8.1
1	C	156	LEU	7.1
1	C	201	LEU	6.5
1	A	161	CYS	6.4
1	D	206	ILE	5.9
1	A	173	GLU	5.8
1	C	153	ILE	5.2
1	D	165	GLY	5.2
1	C	159	GLU	5.1
1	C	178	LEU	4.9
1	E	222	LEU	4.8
1	D	214	ILE	4.8
1	A	207	LEU	4.8
1	E	193	THR	4.6
1	D	200	CYS	4.4
1	C	157	PHE	4.4
1	D	151	ILE	4.4
1	C	197	VAL	4.4
1	D	216	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	174	ILE	4.3
1	C	220	GLY	4.2
1	E	171	THR	4.1
1	D	154	LEU	4.0
1	F	201	LEU	3.9
1	B	164	GLN	3.7
1	A	193	THR	3.7
1	C	90	THR	3.7
1	D	153	ILE	3.6
1	D	178	LEU	3.6
1	F	188	GLY	3.6
1	F	178	LEU	3.6
1	C	59	GLY	3.5
1	A	46	PRO	3.4
1	B	173	GLU	3.4
1	E	168	VAL	3.3
1	D	184	GLY	3.3
1	A	166	LYS	3.3
1	D	199	ALA	3.3
1	E	162	SER	3.3
1	D	160	LEU	3.3
1	E	140	GLN	3.3
1	B	215	ILE	3.3
1	F	95	TYR	3.2
1	D	162	SER	3.2
1	D	126	ILE	3.2
1	C	193	THR	3.2
1	B	199	ALA	3.2
1	D	28	TYR	3.1
1	D	186	ILE	3.1
1	F	136	TYR	3.1
1	A	180	GLN	3.1
1	F	149	PRO	3.1
1	A	222	LEU	3.0
1	B	156	LEU	3.0
1	D	222	LEU	3.0
1	F	207	LEU	3.0
1	A	219	LEU	3.0
1	D	161	CYS	3.0
1	B	56	LEU	2.9
1	B	137	TYR	2.9
1	A	162	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	226	SER	2.9
1	D	157	PHE	2.9
1	D	179	SER	2.9
1	E	170	ASP	2.9
1	F	169	GLY	2.9
1	B	78	ALA	2.8
1	F	159	GLU	2.8
1	C	210	LYS	2.8
1	E	87	LEU	2.8
1	A	224	HIS	2.8
1	A	49	GLU	2.7
1	E	158	TYR	2.7
1	B	51	THR	2.7
1	E	190	HIS	2.7
1	D	204	GLU	2.7
1	C	175	THR	2.7
1	D	94	ILE	2.6
1	E	149	PRO	2.6
1	C	168	VAL	2.6
1	C	219	LEU	2.6
1	C	182	SER	2.6
1	B	136	TYR	2.6
1	A	211	LYS	2.6
1	E	58	GLU	2.6
1	A	115	VAL	2.6
1	C	215	ILE	2.6
1	D	189	VAL	2.6
1	A	150	THR	2.6
1	A	22	ILE	2.5
1	A	170	ASP	2.5
1	F	33	LEU	2.5
1	F	216	VAL	2.5
1	C	98	ALA	2.5
1	F	93	ASN	2.5
1	B	20	PHE	2.5
1	A	83	LEU	2.5
1	E	200	CYS	2.5
1	A	216	VAL	2.5
1	A	220	GLY	2.5
1	A	130	TYR	2.5
1	B	214	ILE	2.4
1	A	221	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	204	GLU	2.4
1	C	212	ASN	2.4
1	C	180	GLN	2.4
1	B	177	PRO	2.4
1	C	224	HIS	2.4
1	C	135	ALA	2.4
1	B	58	GLU	2.4
1	A	141	VAL	2.4
1	F	28	TYR	2.4
1	D	164	GLN	2.4
1	E	156	LEU	2.4
1	C	188	GLY	2.4
1	B	96	ALA	2.4
1	D	172	TYR	2.4
1	A	199	ALA	2.3
1	B	176	MET	2.3
1	E	160	LEU	2.3
1	E	109	GLU	2.3
1	C	202	LYS	2.3
1	F	158	TYR	2.3
1	A	167	ARG	2.3
1	B	167	ARG	2.3
1	C	152	ARG	2.3
1	D	167	ARG	2.3
1	D	158	TYR	2.3
1	F	89	PRO	2.3
1	B	206	ILE	2.2
1	B	85	GLY	2.2
1	C	70	GLY	2.2
1	E	224	HIS	2.2
1	C	162	SER	2.2
1	D	174	ILE	2.2
1	C	142	ALA	2.2
1	C	169	GLY	2.2
1	A	99	MET	2.2
1	B	25	LEU	2.2
1	C	173	GLU	2.2
1	E	178	LEU	2.2
1	E	219	LEU	2.2
1	C	200	CYS	2.2
1	B	191	HIS	2.2
1	A	182	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	157	PHE	2.2
1	D	171	THR	2.1
1	C	176	MET	2.1
1	C	20	PHE	2.1
1	A	35	ARG	2.1
1	B	188	GLY	2.1
1	E	194	VAL	2.1
1	A	214	ILE	2.1
1	C	171	THR	2.1
1	D	201	LEU	2.1
1	D	223	LYS	2.1
1	C	155	ARG	2.1
1	B	149	PRO	2.1
1	F	143	GLU	2.1
1	B	127	PHE	2.1
1	D	205	ASN	2.1
1	C	170	ASP	2.1
1	A	187	THR	2.1
1	C	102	THR	2.1
1	B	53	MET	2.1
1	E	78	ALA	2.1
1	B	82	SER	2.1
1	F	190	HIS	2.1
1	A	31	MET	2.1
1	F	208	ASP	2.1
1	E	90	THR	2.1
1	A	129	ASN	2.0
1	A	186	ILE	2.0
1	E	81	ASN	2.0
1	E	212	ASN	2.0
1	C	105	CYS	2.0
1	A	165	GLY	2.0
1	D	19	PHE	2.0
1	A	58	GLU	2.0
1	C	185	GLU	2.0
1	B	194	VAL	2.0
1	A	206	ILE	2.0
1	C	78	ALA	2.0
1	F	20	PHE	2.0
1	C	160	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.