



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:19 AM GMT

PDB ID : 3E5Q
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

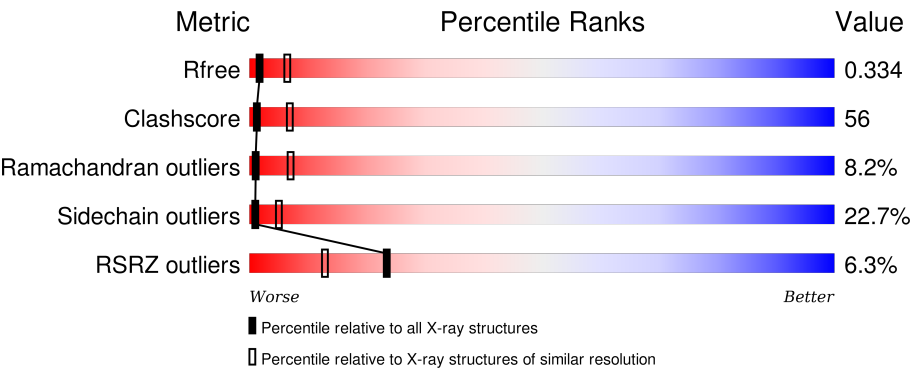
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	250	
1	C	250	
1	D	250	
1	E	250	

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Mol	Chain	Length	Quality of chain
1	F	250	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%26%38%14%•19%</div></div>

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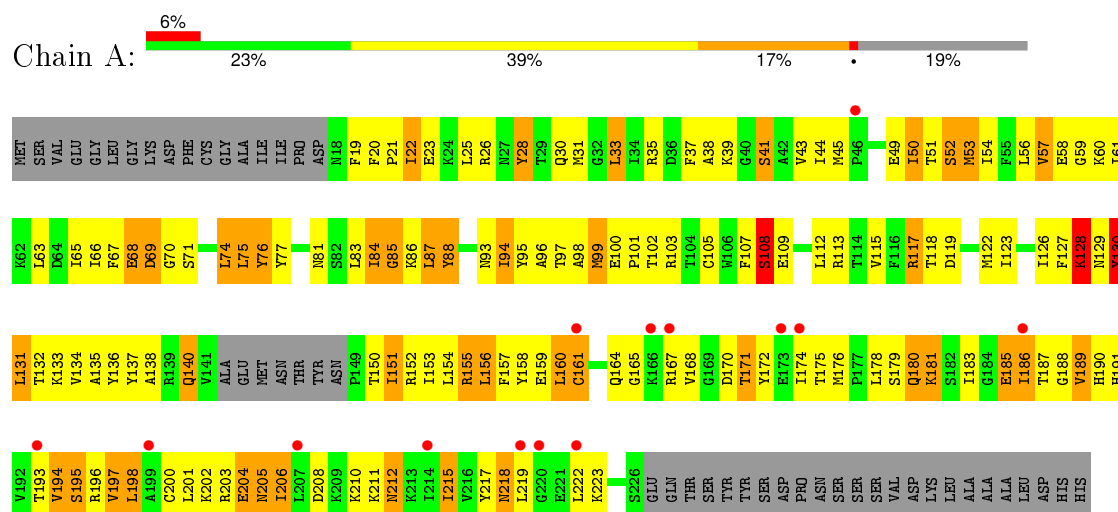
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Chain	Residue	Modelled	Actual	Comment	Reference
F	244	ALA	-	EXPRESSION TAG	UNP Q18R04
F	245	ALA	-	EXPRESSION TAG	UNP Q18R04
F	246	ALA	-	EXPRESSION TAG	UNP Q18R04
F	247	LEU	-	EXPRESSION TAG	UNP Q18R04
F	248	ASP	-	EXPRESSION TAG	UNP Q18R04
F	249	HIS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

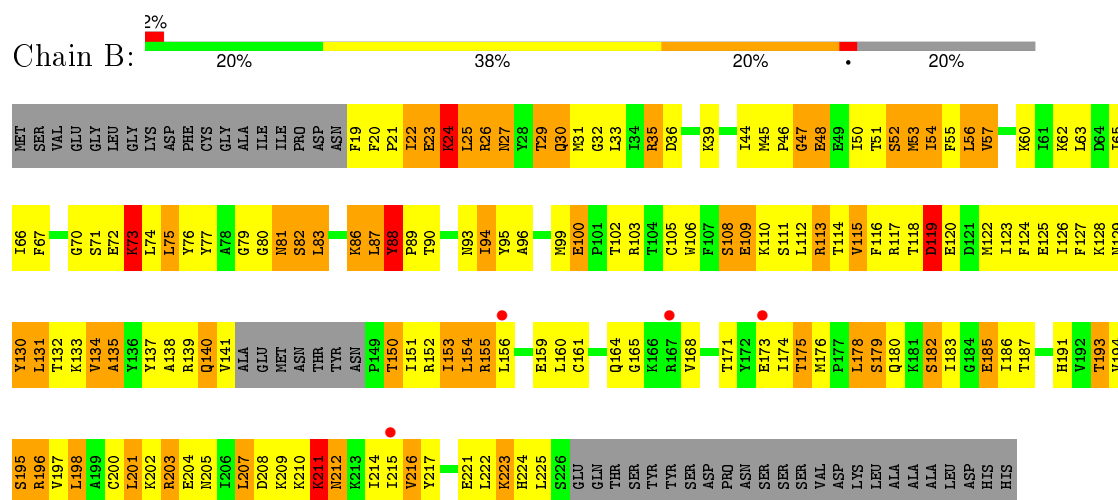
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

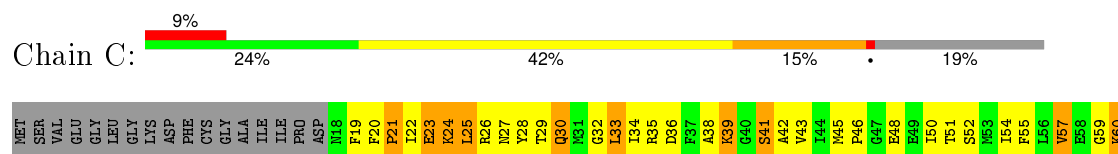
• Molecule 1: Cyclic nucleotide-binding protein

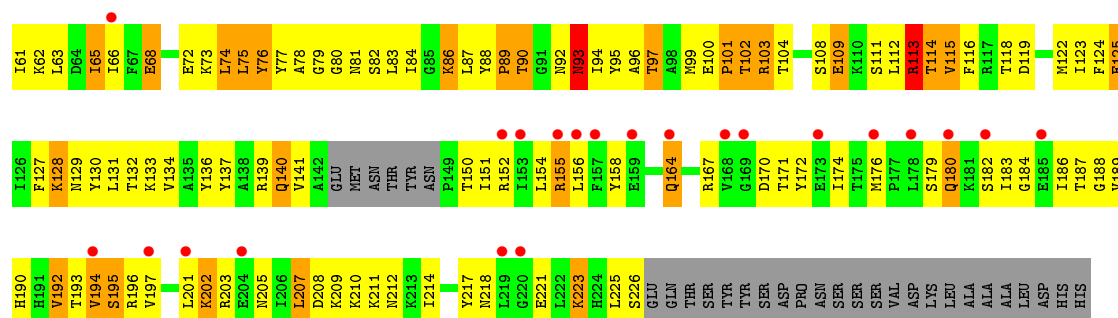


• Molecule 1: Cyclic nucleotide-binding protein

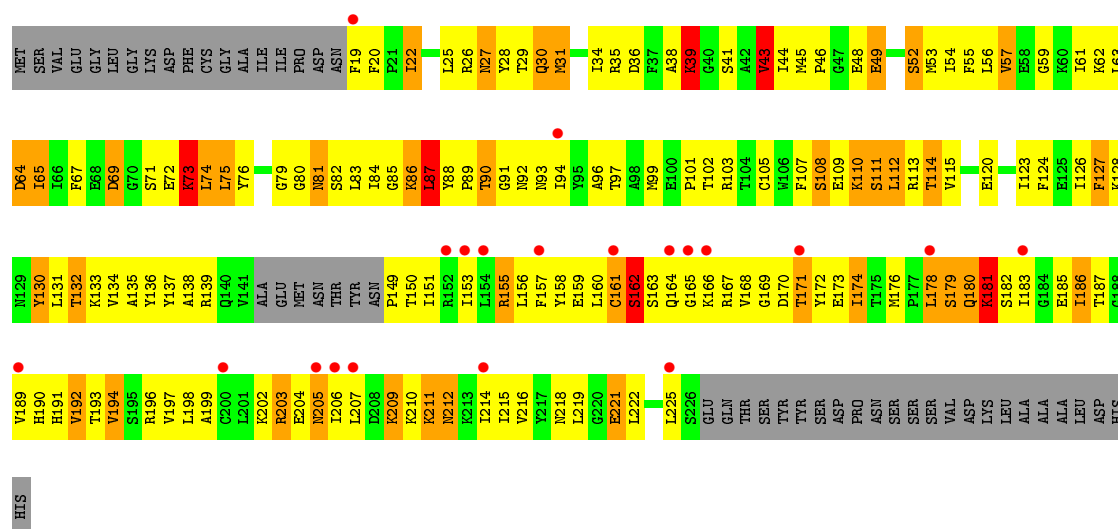
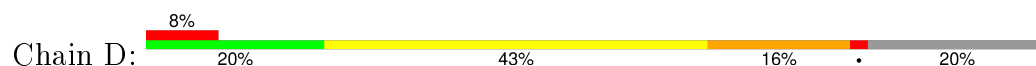


• Molecule 1: Cyclic nucleotide-binding protein

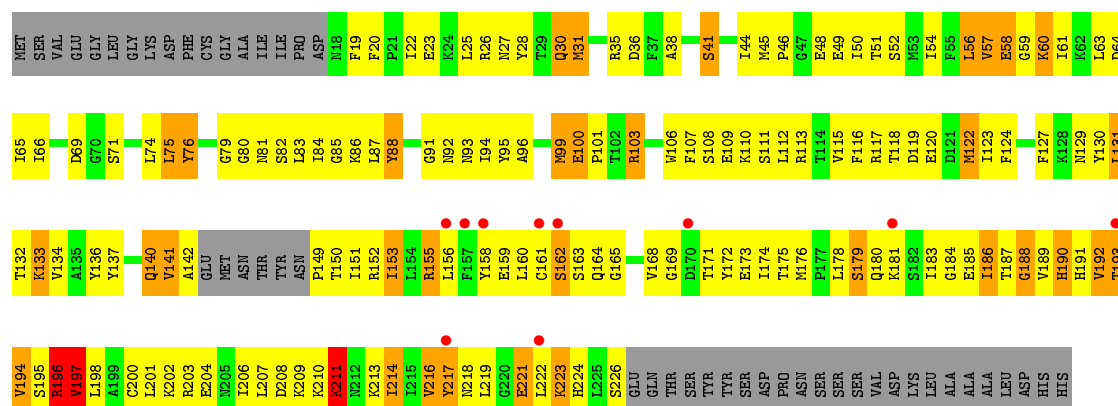
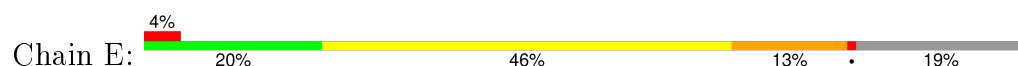




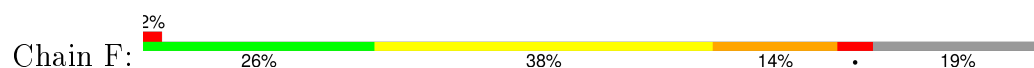
• Molecule 1: Cyclic nucleotide-binding protein

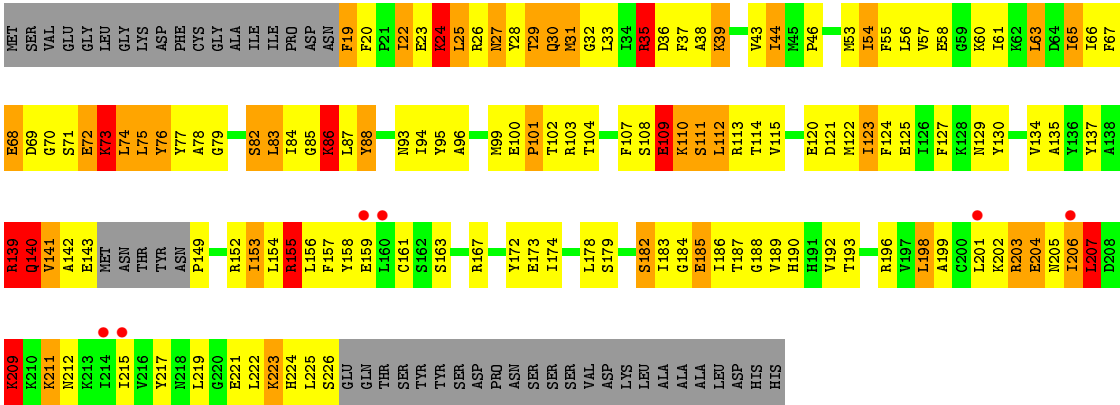


• Molecule 1: Cyclic nucleotide-binding protein



• 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 46.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	79.8 (142.86-3.20) 70.4 (46.52-3.20)	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 0.329 , 0.334	Depositor DCC
R_{free} test set	1711 reflections (10.01%)	DCC
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 , 59.0	EDS
Estimated twinning fraction	0.048 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 17150 reflections (0.017%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.15	4/1630 (0.2%)	1.19	5/2200 (0.2%)
1	B	1.17	5/1641 (0.3%)	1.26	12/2209 (0.5%)
1	C	1.02	1/1635 (0.1%)	1.09	0/2207
1	D	0.92	1/1635 (0.1%)	1.01	2/2202 (0.1%)
1	E	0.98	0/1635	1.11	6/2207 (0.3%)
1	F	0.97	2/1645 (0.1%)	1.08	8/2215 (0.4%)
All	All	1.04	13/9821 (0.1%)	1.13	33/13240 (0.2%)

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	161	CYS	CB-SG	7.62	1.95	1.82
1	A	130	TYR	CE2-CZ	6.38	1.46	1.38
1	A	130	TYR	CG-CD1	6.17	1.47	1.39
1	C	23	GLU	CG-CD	6.17	1.61	1.51
1	B	109	GLU	CG-CD	5.92	1.60	1.51
1	B	23	GLU	CG-CD	5.83	1.60	1.51
1	F	88	TYR	CE1-CZ	5.65	1.45	1.38
1	B	88	TYR	CD2-CE2	5.59	1.47	1.39
1	B	88	TYR	CE2-CZ	5.40	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	TYR	CG-CD2	5.31	1.46	1.39
1	A	161	CYS	CB-SG	5.18	1.91	1.82
1	F	39	LYS	CE-NZ	5.15	1.61	1.49
1	A	88	TYR	CG-CD2	5.07	1.45	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	E	83	LEU	CA-CB-CG	-8.52	95.70	115.30
1	B	119	ASP	CB-CG-OD1	-8.05	111.06	118.30
1	F	207	LEU	CA-CB-CG	7.33	132.15	115.30
1	B	130	TYR	CA-CB-CG	-7.25	99.62	113.40
1	B	56	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	87	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	E	103	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	F	155	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	56	LEU	CB-CG-CD1	-5.92	100.94	111.00
1	F	112	LEU	CA-CB-CG	-5.84	101.87	115.30
1	E	83	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	F	113	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	D	112	LEU	CA-CB-CG	-5.59	102.45	115.30
1	F	35	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	88	TYR	N-CA-C	-5.54	96.04	111.00
1	A	131	LEU	CA-CB-CG	5.53	128.01	115.30
1	E	130	TYR	CA-CB-CG	-5.52	102.91	113.40
1	B	26	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	201	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	131	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	54	ILE	CB-CA-C	-5.30	101.00	111.60
1	B	178	LEU	N-CA-C	-5.24	96.86	111.00
1	F	25	LEU	CA-CB-CG	5.21	127.28	115.30
1	D	130	TYR	CA-CB-CG	-5.19	103.53	113.40
1	B	119	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	83	LEU	CB-CG-CD2	-5.14	102.27	111.00
1	F	140	GLN	C-N-CA	5.13	134.53	121.70
1	A	85	GLY	N-CA-C	5.12	125.90	113.10
1	F	207	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	E	196	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	194	VAL	CB-CA-C	-5.03	101.85	111.40
1	A	83	LEU	CA-CB-CG	5.02	126.84	115.30

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	200	0
1	B	1611	0	1643	226	0
1	C	1605	0	1606	195	0
1	D	1605	0	1632	206	1
1	E	1605	0	1606	200	0
1	F	1615	0	1637	190	1
All	All	9641	0	9725	1081	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 56.

All (1081) 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	1.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:F:27:ASN:N	1.52	1.03
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:A:131:LEU:HD21	1:B:53:MET:HE1	1.42	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:D:189:VAL:CG1	1:D:193:THR:HB	1.94	0.97
1:B:54:ILE:O	1:B:54:ILE:HG22	1.60	0.97
1:D:110:LYS:O	1:D:112:LEU:N	1.98	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:D:86:LYS:HZ1	1:D:90:THR:H	1.00	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:151:ILE:O	1:D:155:ARG:HG3	1.67	0.93
1:D:65:ILE:O	1:D:72:GLU:O	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:123:ILE:HG23	1:F:123:ILE:HG23	1.51	0.91
1:F:73:LYS:HZ2	1:F:74:LEU:H	1.13	0.90
1:B:74:LEU:HD11	1:B:77:TYR:HE1	1.34	0.90
1:D:86:LYS:HZ1	1:D:90:THR:N	1.69	0.89
1:E:209:LYS:HG3	1:E:214:ILE:HG23	1.52	0.89
1:D:156:LEU:O	1:D:160:LEU:HB2	1.71	0.88
1:C:155:ARG:HD3	1:D:185:GLU:OE1	1.72	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: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:F:63:LEU:HD12	1:F:63:LEU:N	1.87	0.87
1:C:186:ILE:HG12	1:D:156:LEU:HA	1.54	0.87
1:C:123:ILE:HD11	1:D:123:ILE:HD13	1.53	0.87
1:E:159:GLU:HG3	1:F:186:ILE:HD11	1.57	0.87
1:E:155:ARG:HB3	1:F:186:ILE:HG13	1.53	0.87
1:E:60:LYS:CD	1:E:99:MET:HE3	2.00	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:E:60:LYS:HD3	1:E:99:MET:CE	2.02	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: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:O	1:B:175:THR:HG22	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:D:92:ASN:O	1:D:94:ILE:HG12	1.77	0.85
1:D:172:TYR:CE1	1:D:219:LEU:HB2	2.11	0.85
1:A:217:TYR:O	1:A:218:ASN:HB2	1.77	0.85
1:E:142:ALA:HB1	1:F:73:LYS:HD3	1.60	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:B:30:GLN:HE21	1:B:30:GLN:H	1.22	0.84
1:B:35:ARG:HB3	1:B:35:ARG:HH11	1.42	0.84
1:C:50:ILE:HB	1:C:86:LYS:CE	2.06	0.84
1:D:111:SER:O	1:D:115:VAL:HG23	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:GLN:OE1	1:F:30:GLN:N	2.12	0.83
1:B:45:MET:HB2	1:B:48:GLU:CB	2.08	0.83
1:C:22:ILE:O	1:C:22:ILE:HG23	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:O	1:E:57:VAL:CG2	2.27	0.82
1:B:22:ILE:CG1	1:B:22:ILE:O	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:B:46:PRO:C	1:B:93:ASN:OD1	2.18	0.81
1:F:30:GLN:CD	1:F:30:GLN:H	1.83	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:F:149:PRO:HB3	1:F:152:ARG:CD	2.11	0.81
1:B:122:MET:HA	1:B:125:GLU:HB2	1.59	0.81
1:F:55:PHE:CB	1:F:107:PHE:HE1	1.93	0.81
1:E:188:GLY:HA3	1:F:152:ARG:NE	1.95	0.81
1:E:44:ILE:HG12	1:E:50:ILE:HD12	1.62	0.81
1:A:23:GLU:HG3	1:A:81:ASN:ND2	1.96	0.81
1:A:164:GLN:HG2	1:B:164:GLN:CD	2.01	0.80
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: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:75:LEU:C	1:A:76:TYR:HD1	1.85	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:F:27:ASN:N	1:F:27:ASN:ND2	2.26	0.78
1:E:152:ARG:HD3	1:F:188:GLY:N	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:LEU:HD23	1:F:109:GLU:HG2	1.65	0.78
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:H	1:F:63:LEU:HD12	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:C:28:TYR:CD2	1:C:115:VAL:HG13	2.20	0.77
1:F:60:LYS:N	1:F:100:GLU:OE2	2.17	0.77
1:D:198:LEU:O	1:D:202:LYS:HB2	1.85	0.77
1:A:130:TYR:CE2	1:B:131:LEU:HD23	2.18	0.76
1:B:66:ILE:HD11	1:B:95:TYR:HB2	1.66	0.76
1:A:202:LYS:HE2	1:A:208:ASP:OD2	1.85	0.76
1:B:179:SER:HA	1:B:209:LYS:NZ	2.00	0.76
1:D:193:THR:O	1:D:197:VAL:HB	1.85	0.76
1:D:55:PHE:HB2	1:D:83:LEU:HD13	1.66	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:D:63:LEU:HD21	1:D:84:ILE:CD1	2.16	0.76
1:C:50:ILE:CB	1:C:86:LYS:HE2	2.13	0.75
1:A:75:LEU:HD22	1:A:76:TYR:CE1	2.21	0.75
1:C:46:PRO:CB	1:C:93:ASN:HD21	1.98	0.75
1:D:172:TYR:CZ	1:D:219:LEU:HD22	2.21	0.75
1:F:140:GLN:C	1:F:142:ALA:HB3	2.07	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:E:140:GLN:O	1:E:142:ALA:N	2.17	0.75
1:A:74:LEU:O	1:A:74:LEU:HD23	1.87	0.75
1:A:189:VAL:HG12	1:A:194:VAL:HG22	1.69	0.74
1:A:67:PHE:C	1:A:69:ASP:H	1.91	0.74
1:A:35:ARG:HH21	1:E:35:ARG:CZ	2.00	0.74
1:E:161:CYS:O	1:E:165:GLY:HA3	1.87	0.74
1:D:86:LYS:NZ	1:D:90:THR:H	1.84	0.74
1:D:45:MET:HB2	1:D:48:GLU:HB2	1.70	0.74
1:E:56:LEU:HD13	1:E:79:GLY:O	1.88	0.74
1:D:191:HIS:HA	1:D:194:VAL:CG2	2.17	0.74
1:C:42:ALA:HA	1:C:97:THR:HG22	1.70	0.74
1:E:192:VAL:O	1:E:195:SER:HB2	1.88	0.74
1:F:141:VAL:N	1:F:142:ALA:HB3	2.01	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:D:204:GLU:O	1:D:205:ASN:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:164:GLN:HB3	1:B:174:ILE:HG23	1.69	0.73
1:A:61:ILE:HG21	1:A:96:ALA:HB1	1.71	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:F:56:LEU:HD13	1:F:79:GLY:O	1.89	0.72
1:C:136:TYR:O	1:C:139:ARG:HB3	1.90	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: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: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:86:LYS:HZ3	1:D:90:THR:HG23	1.55	0.72
1:A:66:ILE:HA	1:A:71:SER:O	1.90	0.71
1:F:54:ILE:HD12	1:F:84:ILE:HD12	1.71	0.71
1:C:155:ARG:HH11	1:C:155:ARG:HG3	1.55	0.71
1:E:48:GLU:HG2	1:E:49:GLU:O	1.90	0.71
1:C:164:GLN:HB3	1:C:174:ILE:HG23	1.73	0.71
1:C:23:GLU:HG3	1:C:81:ASN:ND2	2.06	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: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: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:55:PHE:C	1:C:55:PHE:CD2	2.64	0.70
1:C:63:LEU:HG	1:C:96:ALA:HB2	1.72	0.70
1:C:103:ARG:O	1:C:103:ARG:HG2	1.92	0.70
1:A:156:LEU:HB2	1:B:186:ILE:HG23	1.72	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
1:C:55:PHE:HE2	1:C:57:VAL:HA	1.56	0.70
1:B:46:PRO:CA	1:B:93:ASN:HD21	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:TYR:HB3	1:D:137:TYR:HB3	1.72	0.70
1:C:100:GLU:O	1:C:102:THR:OG1	2.08	0.70
1:B:66:ILE:HD11	1:B:95:TYR:CB	2.22	0.70
1:D:124:PHE:CA	1:D:127:PHE:HB2	2.18	0.69
1:B:179:SER:HA	1:B:209:LYS:HZ3	1.55	0.69
1:D:63:LEU:HD21	1:D:84:ILE:HD13	1.72	0.69
1:A:65:ILE:CG1	1:A:66:ILE:N	2.55	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: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:C:100:GLU:O	1:C:101:PRO:C	2.28	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:D:86:LYS:NZ	1:D:90:THR:HG23	2.06	0.69
1:C:38:ALA:O	1:C:41:SER:HB2	1.93	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:F:27:ASN:ND2	1:F:27:ASN:H	1.91	0.67
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:C:28:TYR:HA	1:C:30:GLN:HE22	1.59	0.67
1:C:66:ILE:HG13	1:C:72:GLU:HG3	1.77	0.67
1:A:59:GLY:HA3	1:A:102:THR:HG23	1.76	0.67
1:F:139:ARG:C	1:F:141:VAL:CB	2.62	0.67
1:B:171:THR:HG22	1:B:217:TYR:HA	1.76	0.67
1:F:26:ARG:HB2	1:F:27:ASN:ND2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:PRO:HD3	1:F:95:TYR:CD2	2.30	0.67
1:B:151:ILE:HA	1:B:154:LEU:HD12	1.75	0.67
1:D:56:LEU:HD23	1:D:59:GLY:O	1.94	0.67
1:D:49:GLU:O	1:D:49:GLU:HG2	1.93	0.67
1:F:110:LYS:HE3	1:F:110:LYS:O	1.95	0.67
1:F:155:ARG:HH11	1:F:155:ARG:HB3	1.59	0.67
1:A:123:ILE:HG22	1:A:123:ILE:O	1.93	0.67
1:E:173:GLU:C	1:E:174:ILE:HD12	2.14	0.66
1:E:152:ARG:CD	1:F:188:GLY:CA	2.73	0.66
1:C:130:TYR:CE2	1:D:131:LEU:HG	2.29	0.66
1:E:123:ILE:HG23	1:F:123:ILE:CG2	2.23	0.66
1:C:174:ILE:HG22	1:C:176:MET:HG2	1.76	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: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:A:61:ILE:CG2	1:A:96:ALA:HB1	2.26	0.66
1:A:65:ILE:HG13	1:A:66:ILE:H	1.60	0.66
1:D:22:ILE:CD1	1:D:22:ILE:O	2.44	0.66
1:A:33:LEU:CD2	1:E:36:ASP:O	2.43	0.66
1:F:44:ILE:HB	1:F:96:ALA:HB3	1.77	0.66
1:E:57:VAL:HG13	1:E:103:ARG:O	1.96	0.66
1:B:161:CYS:O	1:B:165:GLY:HA3	1.96	0.65
1:D:110:LYS:O	1:D:111:SER:C	2.32	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:C:127:PHE:CZ	1:D:130:TYR:CE1	2.84	0.65
1:D:130:TYR:O	1:D:134:VAL:HG23	1.96	0.65
1:D:88:TYR:O	1:D:89:PRO:C	2.35	0.65
1:C:174:ILE:HB	1:C:214:ILE:HB	1.78	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:E:198:LEU:CD1	1:E:201:LEU:HD12	2.23	0.65
1:E:140:GLN:C	1:E:142:ALA:H	1.98	0.65
1:F:19:PHE:CE2	1:F:79:GLY:HA3	2.31	0.65
1:A:53:MET:HB2	1:A:107:PHE:HB2	1.79	0.65
1:C:92:ASN:O	1:C:93:ASN:C	2.35	0.65
1:F:199:ALA:O	1:F:202:LYS:CB	2.44	0.65
1:F:87:LEU:HB2	1:F:88:TYR:CE1	2.31	0.65
1:A:98:ALA:HB1	1:A:100:GLU:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:PHE:CD1	1:D:133:LYS:HG2	2.31	0.65
1:A:74:LEU:HD11	1:A:77:TYR:CE1	2.31	0.65
1:E:129:ASN:O	1:E:133:LYS:HG2	1.97	0.65
1:C:179:SER:HB2	1:C:182:SER:OG	1.97	0.65
1:A:164:GLN:HG2	1:B:164:GLN:NE2	2.11	0.65
1:C:122:MET:O	1:C:123:ILE:C	2.32	0.65
1:E:188:GLY:HA3	1:F:152:ARG:HE	1.62	0.65
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: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: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:E:87:LEU:HD22	1:E:109:GLU:HB2	1.80	0.64
1:C:190:HIS:HD2	1:C:192:VAL:HG23	1.62	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:D:206:ILE:HG23	1:D:218:ASN:HB3	1.80	0.63
1:C:127:PHE:CZ	1:C:131:LEU:HD21	2.34	0.63
1:B:46:PRO:HA	1:B:94:ILE:O	1.98	0.63
1:B:168:VAL:O	1:B:168:VAL:HG12	1.97	0.63
1:F:108:SER:O	1:F:111:SER:N	2.32	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:D:180:GLN:HE22	1:D:194:VAL:HB	1.63	0.63
1:D:64:ASP:HB2	1:D:72:GLU:OE1	1.98	0.63
1:B:194:VAL:O	1:B:198:LEU:HB2	1.99	0.63
1:A:60:LYS:HG2	1:A:99:MET:CE	2.28	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:A:58:GLU:O	1:A:102:THR:HA	2.00	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:B:62:LYS:O	1:B:96:ALA:HA	1.99	0.62
1:C:26:ARG:HD2	1:C:81:ASN:OD1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:HD23	1:B:76:TYR:CD1	2.35	0.62
1:A:21:PRO:HA	1:A:81:ASN:O	1.98	0.62
1:D:61:ILE:HD11	1:D:102:THR:HG21	1.82	0.62
1:E:219:LEU:HA	1:E:222:LEU:HB3	1.82	0.62
1:D:172:TYR:OH	1:D:219:LEU:HD23	1.99	0.62
1:B:120:GLU:O	1:B:123:ILE:N	2.21	0.62
1:A:189:VAL:CG1	1:A:194:VAL:HG22	2.28	0.62
1:E:201:LEU:HD22	1:E:207:LEU:CB	2.30	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:F:22:ILE:HG13	1:F:22:ILE:O	1.99	0.62
1:E:198:LEU:HA	1:E:201:LEU:HD12	1.82	0.62
1:B:35:ARG:HB3	1:B:35:ARG:NH1	2.14	0.62
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:186:ILE:HG23	1:D:156:LEU:HB2	1.82	0.61
1:C:61:ILE:HG22	1:C:96:ALA:HB1	1.82	0.61
1:D:190:HIS:CD2	1:D:192:VAL:HG23	2.36	0.61
1:A:185:GLU:O	1:B:152:ARG:CG	2.46	0.61
1:E:190:HIS:CD2	1:E:190:HIS:C	2.73	0.61
1:F:53:MET:HG2	1:F:87:LEU:HD11	1.81	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:H	1:E:211:LYS:HE3	1.66	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
1:D:22:ILE:HD13	1:D:22:ILE:C	2.21	0.61
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:E:186:ILE:CG1	1:F:155:ARG:HB3	2.30	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:F:26:ARG:HB2	1:F:27:ASN:HD22	1.65	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:223:LYS:HG3	1:F:224:HIS:N	2.16	0.60
1:A:74:LEU:O	1:A:74:LEU:CD2	2.48	0.60
1:D:124:PHE:HA	1:D:127:PHE:CB	2.21	0.60
1:D:88:TYR:O	1:D:90:THR:CG2	2.50	0.60
1:D:166:LYS:O	1:D:173:GLU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:VAL:H	1:F:143:GLU:N	1.97	0.60
1:E:63:LEU:HD11	1:E:84:ILE:CG2	2.31	0.60
1:C:190:HIS:O	1:C:194:VAL:HG23	2.02	0.60
1:A:161:CYS:HA	1:A:174:ILE:HD11	1.83	0.60
1:D:151:ILE:O	1:D:155:ARG:CG	2.48	0.60
1:B:27:ASN:N	1:B:27:ASN:HD22	1.99	0.60
1:C:30:GLN:C	1:C:32:GLY:H	2.04	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:C:46:PRO:HG3	1:C:95:TYR:HB2	1.84	0.60
1:F:37:PHE:CE2	1:F:43:VAL:HA	2.37	0.60
1:B:76:TYR:CD1	1:B:137:TYR:OH	2.54	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:F:141:VAL:H	1:F:142:ALA:C	2.05	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:D:54:ILE:C	1:D:83:LEU:HD12	2.23	0.59
1:F:157:PHE:CG	1:F:207:LEU:HD11	2.36	0.59
1:D:112:LEU:O	1:D:113:ARG:C	2.39	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:E:30:GLN:CD	1:E:30:GLN:H	2.05	0.59
1:D:190:HIS:O	1:D:194:VAL:HG23	2.03	0.59
1:D:149:PRO:CD	1:D:151:ILE:CG1	2.81	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
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:127:PHE:CE1	1:B:130:TYR:CE1	2.91	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: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:A:76:TYR:CD1	1:A:76:TYR:N	2.71	0.58
1:E:79:GLY:N	1:E:82:SER:OG	2.29	0.58
1:A:134:VAL:O	1:A:135:ALA:C	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:O	1:A:118:THR:C	2.38	0.58
1:A:185:GLU:O	1:A:186:ILE:C	2.40	0.58
1:E:186:ILE:HG23	1:F:156:LEU:HB2	1.86	0.58
1:D:207:LEU:CD1	1:D:216:VAL:HG22	2.30	0.57
1:D:155:ARG:NH1	1:D:159:GLU:OE1	2.32	0.57
1:C:152:ARG:NH2	1:C:189:VAL:HG22	2.09	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:A:22:ILE:HG12	1:A:22:ILE:O	2.04	0.57
1:E:201:LEU:HD22	1:E:207:LEU:HB2	1.86	0.57
1:D:34:ILE:HG21	1:D:103:ARG:HD3	1.87	0.57
1:D:179:SER:O	1:D:180:GLN:C	2.43	0.57
1:F:74:LEU:CD2	1:F:75:LEU:H	2.17	0.57
1:A:152:ARG:O	1:A:156:LEU:N	2.35	0.57
1:F:58:GLU:O	1:F:102:THR:HG23	2.05	0.57
1:B:112:LEU:HD22	1:B:116:PHE:CZ	2.39	0.57
1:F:65:ILE:HG23	1:F:67:PHE:CE1	2.39	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: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:D:86:LYS:NZ	1:D:90:THR:N	2.48	0.57
1:C:55:PHE:CD2	1:C:55:PHE:O	2.58	0.57
1:D:46:PRO:HA	1:D:94:ILE:O	2.05	0.57
1:B:46:PRO:O	1:B:93:ASN:OD1	2.23	0.57
1:D:64:ASP:HA	1:D:74:LEU:HA	1.87	0.57
1:C:152:ARG:HH21	1:C:189:VAL:CG2	2.10	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:B:46:PRO:HA	1:B:93:ASN:HD21	1.68	0.57
1:A:128:LYS:HE3	1:B:88:TYR:CE2	2.39	0.57
1:F:55:PHE:HB2	1:F:107:PHE:HE1	1.67	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: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:E:216:VAL:HG11	1:E:222:LEU:HD22	1.86	0.56
1:B:66:ILE:CD1	1:B:95:TYR:CB	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:O	1:A:155:ARG:CG	2.53	0.56
1:C:108:SER:C	1:C:111:SER:OG	2.44	0.56
1:F:28:TYR:HB3	1:F:31:MET:HG3	1.86	0.56
1:A:127:PHE:HE1	1:B:130:TYR:CE1	2.23	0.56
1:D:216:VAL:HG11	1:D:222:LEU:CD2	2.34	0.56
1:D:172:TYR:HB2	1:D:216:VAL:HB	1.86	0.56
1:C:65:ILE:HD11	1:C:92:ASN:ND2	2.20	0.56
1:C:207:LEU:HD23	1:C:208:ASP:C	2.25	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: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:CB	1:F:155:ARG:HH11	2.17	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: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:F:19:PHE:CD2	1:F:79:GLY:HA3	2.41	0.56
1:B:20:PHE:N	1:B:21:PRO:CD	2.69	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: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: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:D:150:THR:HA	1:D:153:ILE:HD12	1.87	0.55
1:B:209:LYS:HG2	1:B:209:LYS:O	2.06	0.55
1:B:32:GLY:HA3	1:B:105:CYS:SG	2.45	0.55
1:E:188:GLY:HA3	1:F:152:ARG:NH2	2.21	0.55
1:A:179:SER:O	1:A:181:LYS:N	2.39	0.55
1:B:19:PHE:CD1	1:B:79:GLY:HA3	2.41	0.55
1:E:161:CYS:SG	1:E:172:TYR:CB	2.88	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:D:53:MET:HE1	1:D:130:TYR:OH	2.07	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:A:26:ARG:NH2	1:A:57:VAL:HG23	2.22	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:D:86:LYS:NZ	1:D:88:TYR:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ILE:HG12	1:F:156:LEU:N	2.22	0.55
1:C:36:ASP:OD1	1:C:103:ARG:HB2	2.06	0.55
1:F:198:LEU:HD11	1:F:209:LYS:HB2	1.89	0.55
1:F:141:VAL:N	1:F:143:GLU:N	2.55	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:F:183:ILE:O	1:F:187:THR:CG2	2.51	0.55
1:C:89:PRO:O	1:C:90:THR:HG22	2.07	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:D:27:ASN:ND2	1:D:27:ASN:N	2.55	0.55
1:E:142:ALA:HB1	1:F:73:LYS:CD	2.35	0.54
1:C:130:TYR:HA	1:C:133:LYS:HB2	1.89	0.54
1:B:130:TYR:O	1:B:131:LEU:C	2.46	0.54
1:B:46:PRO:CB	1:B:93:ASN:HD21	2.19	0.54
1:F:108:SER:O	1:F:109:GLU:C	2.44	0.54
1:E:134:VAL:HG21	1:F:130:TYR:CD2	2.42	0.54
1:E:19:PHE:CG	1:E:79:GLY:HA3	2.43	0.54
1:F:25:LEU:O	1:F:26:ARG:C	2.45	0.54
1:F:65:ILE:CG2	1:F:67:PHE:CE1	2.90	0.54
1:A:86:LYS:HG3	1:A:88:TYR:O	2.07	0.54
1:C:108:SER:O	1:C:111:SER:CB	2.56	0.54
1:B:27:ASN:ND2	1:B:27:ASN:N	2.55	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:A:164:GLN:CG	1:B:164:GLN:CD	2.75	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:CZ	1:E:203:ARG:HB3	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:D:219:LEU:CD1	1:D:222:LEU:HD23	2.37	0.54
1:C:92:ASN:HD21	1:D:139:ARG:HB2	1.73	0.54
1:D:185:GLU:O	1:D:186:ILE:C	2.45	0.54
1:E:206:ILE:HG12	1:E:221:GLU:HB3	1.89	0.54
1:D:191:HIS:CA	1:D:194:VAL:HG23	2.38	0.54
1:F:55:PHE:HB2	1:F:107:PHE:CE1	2.43	0.54
1:A:155:ARG:HB3	1:A:155:ARG:NH1	2.23	0.54
1:A:87:LEU:C	1:A:88:TYR:CD1	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLU:HA	1:B:72:GLU:OE2	2.08	0.54
1:B:22:ILE:O	1:B:23:GLU:C	2.46	0.54
1:D:110:LYS:C	1:D:112:LEU:N	2.55	0.54
1:F:74:LEU:HD11	1:F:77:TYR:HE1	1.72	0.54
1:D:62:LYS:HB3	1:D:97:THR:HB	1.90	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:E:190:HIS:HD2	1:E:191:HIS:N	2.05	0.53
1:B:54:ILE:O	1:B:54:ILE:CG2	2.29	0.53
1:F:60:LYS:HB3	1:F:99:MET:HB2	1.91	0.53
1:D:204:GLU:O	1:D:205:ASN:CB	2.56	0.53
1:C:122:MET:HA	1:C:125:GLU:HB2	1.90	0.53
1:F:153:ILE:HG13	1:F:187:THR:CG2	2.31	0.53
1:D:156:LEU:HD22	1:D:186:ILE:HG21	1.88	0.53
1:D:189:VAL:HG13	1:D:193:THR:CB	2.26	0.53
1:C:155:ARG:NH1	1:C:155:ARG:HG3	2.21	0.53
1:F:108:SER:H	1:F:111:SER:HB3	1.73	0.53
1:C:55:PHE:HE2	1:C:57:VAL:CA	2.21	0.53
1:A:35:ARG:HE	1:E:35:ARG:HE	1.57	0.53
1:A:130:TYR:C	1:A:132:THR:H	2.12	0.53
1:B:75:LEU:CD2	1:B:76:TYR:CD1	2.92	0.53
1:B:77:TYR:N	1:B:77:TYR:CD1	2.74	0.53
1:E:190:HIS:CD2	1:E:192:VAL:H	2.27	0.53
1:D:27:ASN:HD22	1:D:27:ASN:N	2.06	0.53
1:A:33:LEU:O	1:A:105:CYS:HA	2.08	0.53
1:A:95:TYR:CE1	1:A:97:THR:HG23	2.44	0.53
1:F:74:LEU:HD11	1:F:77:TYR:CE1	2.44	0.53
1:A:100:GLU:O	1:A:102:THR:OG1	2.25	0.53
1:E:56:LEU:HD22	1:E:56:LEU:O	2.09	0.53
1:B:36:ASP:O	1:C:33:LEU:HD23	2.09	0.53
1:D:156:LEU:O	1:D:160:LEU:CB	2.53	0.53
1:E:57:VAL:O	1:E:57:VAL:HG23	2.08	0.53
1:A:23:GLU:HG3	1:A:81:ASN:HD22	1.74	0.53
1:C:45:MET:HB2	1:C:48:GLU:HB2	1.91	0.53
1:A:30:GLN:H	1:A:30:GLN:CD	2.12	0.53
1:A:127:PHE:O	1:A:131:LEU:HB2	2.09	0.53
1:F:67:PHE:O	1:F:70:GLY:N	2.38	0.53
1:D:63:LEU:HD21	1:D:84:ILE:HD12	1.90	0.52
1:C:130:TYR:N	1:C:130:TYR:CD1	2.77	0.52
1:B:57:VAL:HG13	1:B:103:ARG:HG2	1.91	0.52
1:B:20:PHE:N	1:B:21:PRO:HD2	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:GLY:HA2	1:E:189:VAL:O	2.08	0.52
1:C:42:ALA:HA	1:C:97:THR:CG2	2.39	0.52
1:B:77:TYR:N	1:B:77:TYR:HD1	2.07	0.52
1:E:30:GLN:H	1:E:30:GLN:NE2	2.07	0.52
1:D:176:MET:N	1:D:212:ASN:O	2.43	0.52
1:B:30:GLN:N	1:B:30:GLN:HE21	2.01	0.52
1:C:207:LEU:HD21	1:C:214:ILE:HG23	1.92	0.52
1:A:93:ASN:C	1:A:94:ILE:HD13	2.30	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:B:208:ASP:HB2	1:B:217:TYR:HE1	1.74	0.52
1:D:26:ARG:NH2	1:D:57:VAL:O	2.36	0.52
1:E:59:GLY:O	1:E:60:LYS:HB2	2.10	0.52
1:C:50:ILE:HG12	1:C:86:LYS:NZ	2.24	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:C:43:VAL:HG23	1:C:97:THR:HA	1.92	0.52
1:D:22:ILE:CD1	1:D:22:ILE:C	2.78	0.52
1:F:55:PHE:HB3	1:F:107:PHE:CE1	2.39	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: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:A:119:ASP:OD1	1:A:119:ASP:C	2.47	0.52
1:E:183:ILE:HG22	1:E:194:VAL:HG22	1.91	0.52
1:C:88:TYR:CD1	1:D:128:LYS:HB2	2.45	0.51
1:E:56:LEU:CD2	1:E:56:LEU:C	2.78	0.51
1:E:56:LEU:HG	1:E:61:ILE:HD11	1.91	0.51
1:C:65:ILE:CD1	1:C:92:ASN:HD22	2.23	0.51
1:F:120:GLU:C	1:F:122:MET:H	2.11	0.51
1:F:120:GLU:O	1:F:122:MET:N	2.43	0.51
1:A:123:ILE:O	1:A:123:ILE:CG2	2.57	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: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:A:167:ARG:HA	1:A:172:TYR:HA	1.92	0.51
1:E:219:LEU:HD12	1:E:222:LEU:HD23	1.92	0.51
1:F:58:GLU:O	1:F:102:THR:HA	2.10	0.51
1:F:20:PHE:O	1:F:129:ASN:ND2	2.38	0.51
1:A:130:TYR:O	1:A:132:THR:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:LEU:HD22	1:E:207:LEU:HB3	1.92	0.51
1:D:219:LEU:HD13	1:D:222:LEU:HD23	1.93	0.51
1:B:67:PHE:HE1	1:B:73:LYS:HB2	1.74	0.51
1:E:44:ILE:HG12	1:E:50:ILE:CD1	2.35	0.51
1:B:32:GLY:O	1:B:33:LEU:HD23	2.10	0.51
1:E:56:LEU:HG	1:E:61:ILE:CD1	2.41	0.51
1:D:150:THR:HG23	1:D:197:VAL:CG2	2.40	0.51
1:F:54:ILE:HD12	1:F:84:ILE:CD1	2.39	0.51
1:C:55:PHE:CE2	1:C:57:VAL:HA	2.42	0.51
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:HB2	1:A:77:TYR:O	2.10	0.51
1:C:22:ILE:CG2	1:C:22:ILE:O	2.52	0.51
1:A:76:TYR:HD1	1:A:76:TYR:N	2.05	0.51
1:C:60:LYS:HG2	1:C:99:MET:HE1	1.92	0.51
1:D:43:VAL:HG23	1:D:96:ALA:O	2.12	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:E:52:SER:O	1:E:54:ILE:HG13	2.12	0.50
1:A:101:PRO:HG2	1:A:101:PRO:O	2.11	0.50
1:F:25:LEU:HD23	1:F:55:PHE:CD1	2.46	0.50
1:A:128:LYS:HG3	1:B:88:TYR:CZ	2.47	0.50
1:E:155:ARG:CB	1:F:186:ILE:HG13	2.33	0.50
1:C:80:GLY:O	1:C:81:ASN:HB2	2.10	0.50
1:D:209:LYS:O	1:D:209:LYS:HG2	2.11	0.50
1:C:218:ASN:OD1	1:C:221:GLU:HB2	2.10	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:F:55:PHE:CB	1:F:107:PHE:CE1	2.84	0.50
1:E:136:TYR:CE2	1:E:140:GLN:NE2	2.79	0.50
1:F:189:VAL:HG12	1:F:193:THR:HB	1.93	0.50
1:E:112:LEU:HA	1:E:115:VAL:HB	1.93	0.50
1:B:106:TRP:CD1	1:B:106:TRP:N	2.77	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:B:66:ILE:HD13	1:B:93:ASN:ND2	2.26	0.50
1:F:74:LEU:HD22	1:F:75:LEU:N	2.26	0.50
1:F:44:ILE:HG21	1:F:94:ILE:CG2	2.42	0.50
1:A:187:THR:OG1	1:A:189:VAL:HB	2.11	0.50
1:E:23:GLU:CD	1:E:23:GLU:H	2.15	0.50
1:D:74:LEU:HD23	1:D:75:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LYS:HG3	1:B:88:TYR:O	2.10	0.50
1:B:179:SER:HA	1:B:209:LYS:HZ1	1.77	0.50
1:A:33:LEU:HD23	1:E:36:ASP:O	2.12	0.50
1:B:126:ILE:HG22	1:B:130:TYR:HD1	1.77	0.50
1:A:44:ILE:HB	1:A:96:ALA:H	1.76	0.50
1:B:182:SER:O	1:B:186:ILE:HG13	2.12	0.49
1:D:52:SER:N	1:D:86:LYS:O	2.44	0.49
1:F:53:MET:HG2	1:F:87:LEU:CD1	2.42	0.49
1:C:87:LEU:HD11	1:C:112:LEU:HD12	1.93	0.49
1:D:180:GLN:O	1:D:182:SER:N	2.44	0.49
1:C:151:ILE:HG23	1:C:154:LEU:HD12	1.94	0.49
1:B:72:GLU:O	1:B:73:LYS:O	2.30	0.49
1:E:92:ASN:OD1	1:F:139:ARG:HG3	2.12	0.49
1:C:123:ILE:HD13	1:D:123:ILE:HG21	1.94	0.49
1:B:19:PHE:CE1	1:B:79:GLY:HA3	2.47	0.49
1:F:203:ARG:O	1:F:205:ASN:ND2	2.44	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:E:51:THR:O	1:E:87:LEU:HD23	2.13	0.49
1:A:167:ARG:HA	1:A:171:THR:O	2.12	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:D:69:ASP:N	1:D:69:ASP:OD1	2.45	0.49
1:E:19:PHE:O	1:E:20:PHE:C	2.50	0.49
1:F:141:VAL:N	1:F:142:ALA:C	2.66	0.49
1:D:150:THR:HA	1:D:153:ILE:CD1	2.42	0.49
1:B:131:LEU:O	1:B:132:THR:C	2.50	0.49
1:F:74:LEU:HD22	1:F:75:LEU:H	1.77	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:E:159:GLU:O	1:E:160:LEU:HD12	2.13	0.49
1:B:140:GLN:O	1:B:141:VAL:O	2.30	0.49
1:B:134:VAL:O	1:B:135:ALA:C	2.51	0.49
1:B:19:PHE:HB2	1:B:21:PRO:HD3	1.95	0.49
1:F:120:GLU:C	1:F:122:MET:N	2.66	0.49
1:D:108:SER:OG	1:D:109:GLU:N	2.46	0.49
1:D:53:MET:CE	1:D:85:GLY:O	2.61	0.49
1:F:219:LEU:O	1:F:223:LYS:HB3	2.13	0.49
1:E:28:TYR:OH	1:E:119:ASP:HB2	2.12	0.49
1:B:55:PHE:HB2	1:B:83:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:TYR:O	1:B:133:LYS:N	2.46	0.49
1:A:138:ALA:HA	1:B:137:TYR:CD2	2.48	0.49
1:A:137:TYR:CE1	1:B:138:ALA:HB2	2.48	0.49
1:C:223:LYS:HE3	1:C:223:LYS:O	2.12	0.49
1:C:155:ARG:NH1	1:C:158:TYR:CD2	2.71	0.48
1:B:200:CYS:O	1:B:204:GLU:HG2	2.13	0.48
1:B:204:GLU:HA	1:B:204:GLU:OE1	2.12	0.48
1:A:43:VAL:HG11	1:A:61:ILE:HD13	1.95	0.48
1:B:115:VAL:O	1:B:116:PHE:C	2.51	0.48
1:E:224:HIS:CG	1:E:224:HIS:O	2.66	0.48
1:F:38:ALA:O	1:F:39:LYS:C	2.51	0.48
1:E:198:LEU:CD1	1:E:201:LEU:CD1	2.87	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:86:LYS:HG3	1:E:88:TYR:O	2.13	0.48
1:F:39:LYS:HB2	1:F:101:PRO:HD3	1.95	0.48
1:E:80:GLY:O	1:E:81:ASN:HB2	2.13	0.48
1:F:173:GLU:HG2	1:F:215:ILE:HG12	1.95	0.48
1:B:36:ASP:OD1	1:B:103:ARG:HG3	2.13	0.48
1:A:186:ILE:HD11	1:B:159:GLU:HG3	1.95	0.48
1:B:155:ARG:HG3	1:B:155:ARG:NH1	2.25	0.48
1:E:63:LEU:CD1	1:E:76:TYR:CD2	2.96	0.48
1:A:168:VAL:N	1:A:171:THR:O	2.46	0.48
1:A:68:GLU:CD	1:B:139:ARG:HH22	2.16	0.48
1:D:199:ALA:O	1:D:203:ARG:HB2	2.13	0.48
1:B:80:GLY:O	1:B:81:ASN:CB	2.43	0.48
1:B:45:MET:HB3	1:B:46:PRO:CD	2.44	0.48
1:A:186:ILE:O	1:B:152:ARG:HB3	2.14	0.48
1:F:221:GLU:O	1:F:225:LEU:HD12	2.13	0.48
1:C:150:THR:HG23	1:C:197:VAL:HG11	1.96	0.48
1:F:43:VAL:O	1:F:43:VAL:HG12	2.13	0.48
1:A:159:GLU:CD	1:B:182:SER:OG	2.52	0.48
1:E:44:ILE:O	1:E:95:TYR:HA	2.13	0.48
1:A:57:VAL:HG13	1:A:103:ARG:HG2	1.96	0.48
1:E:197:VAL:HG12	1:E:198:LEU:N	2.29	0.48
1:D:178:LEU:HG	1:D:183:ILE:CD1	2.32	0.48
1:E:218:ASN:HB3	1:E:221:GLU:HB2	1.95	0.48
1:C:60:LYS:HG2	1:C:99:MET:CE	2.43	0.48
1:F:35:ARG:N	1:F:104:THR:O	2.42	0.48
1:C:151:ILE:HA	1:C:154:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:LYS:HG3	1:E:214:ILE:CG2	2.35	0.48
1:C:186:ILE:CG2	1:D:156:LEU:HD13	2.43	0.48
1:A:115:VAL:O	1:A:119:ASP:N	2.41	0.48
1:B:127:PHE:O	1:B:128:LYS:C	2.51	0.48
1:A:35:ARG:NH2	1:E:35:ARG:CZ	2.74	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:184:GLY:O	1:F:186:ILE:N	2.47	0.48
1:F:76:TYR:CD1	1:F:137:TYR:OH	2.62	0.48
1:A:130:TYR:HE1	1:A:133:LYS:NZ	2.11	0.48
1:E:164:GLN:O	1:E:174:ILE:HG13	2.13	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
1:C:63:LEU:HG	1:C:96:ALA:CB	2.43	0.48
1:C:54:ILE:CG2	1:C:104:THR:HB	2.44	0.48
1:B:23:GLU:O	1:B:24:LYS:C	2.52	0.48
1:D:20:PHE:CE1	1:D:133:LYS:HG2	2.49	0.48
1:F:122:MET:O	1:F:123:ILE:C	2.52	0.48
1:A:44:ILE:HG22	1:A:45:MET:O	2.14	0.47
1:A:49:GLU:C	1:A:50:ILE:HD13	2.33	0.47
1:A:54:ILE:HB	1:A:84:ILE:HG13	1.95	0.47
1:B:222:LEU:O	1:B:223:LYS:C	2.52	0.47
1:F:158:TYR:CE1	1:F:223:LYS:HB2	2.49	0.47
1:E:131:LEU:O	1:E:132:THR:C	2.52	0.47
1:E:127:PHE:CE1	1:F:130:TYR:CD1	2.99	0.47
1:E:207:LEU:HD21	1:E:214:ILE:HG22	1.97	0.47
1:D:110:LYS:C	1:D:112:LEU:H	2.18	0.47
1:F:73:LYS:HZ3	1:F:73:LYS:HA	1.79	0.47
1:F:203:ARG:HD2	1:F:204:GLU:OE1	2.14	0.47
1:A:67:PHE:HB2	1:A:69:ASP:OD1	2.14	0.47
1:D:45:MET:HB2	1:D:48:GLU:CB	2.41	0.47
1:F:112:LEU:HD23	1:F:112:LEU:HA	1.67	0.47
1:D:193:THR:O	1:D:197:VAL:CB	2.60	0.47
1:B:47:GLY:N	1:B:93:ASN:OD1	2.47	0.47
1:D:168:VAL:N	1:D:171:THR:O	2.43	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:D:80:GLY:O	1:D:81:ASN:HB2	2.15	0.47
1:B:161:CYS:HA	1:B:174:ILE:HD11	1.96	0.47
1:E:60:LYS:C	1:E:61:ILE:HG13	2.34	0.47
1:A:154:LEU:O	1:A:158:TYR:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLN:N	1:B:30:GLN:NE2	2.48	0.47
1:E:113:ARG:NH1	1:F:121:ASP:OD1	2.44	0.47
1:B:65:ILE:HB	1:B:75:LEU:HD12	1.97	0.47
1:E:63:LEU:CD1	1:E:76:TYR:CE2	2.98	0.47
1:A:63:LEU:N	1:A:63:LEU:HD12	2.29	0.47
1:B:211:LYS:HB2	1:B:212:ASN:OD1	2.15	0.47
1:B:48:GLU:HG2	1:B:50:ILE:CD1	2.42	0.47
1:B:122:MET:O	1:B:123:ILE:C	2.50	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:E:66:ILE:HB	1:E:93:ASN:HB3	1.97	0.47
1:B:19:PHE:CE1	1:B:79:GLY:CA	2.98	0.47
1:E:149:PRO:O	1:E:152:ARG:HB2	2.15	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:140:GLN:H	1:E:140:GLN:HG2	1.49	0.46
1:F:74:LEU:CD2	1:F:75:LEU:N	2.78	0.46
1:F:36:ASP:OD1	1:F:103:ARG:HG3	2.16	0.46
1:D:53:MET:HG2	1:D:87:LEU:HD11	1.96	0.46
1:A:75:LEU:O	1:A:76:TYR:HD1	1.97	0.46
1:A:22:ILE:O	1:A:22:ILE:CG1	2.62	0.46
1:C:87:LEU:HA	1:C:87:LEU:HD23	1.68	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:A:94:ILE:HD13	1:A:94:ILE:N	2.30	0.46
1:F:78:ALA:HB1	1:F:82:SER:HB3	1.98	0.46
1:B:173:GLU:HG2	1:B:215:ILE:HG12	1.97	0.46
1:E:152:ARG:CD	1:F:188:GLY:HA2	2.40	0.46
1:B:44:ILE:CD1	1:B:50:ILE:HG21	2.46	0.46
1:D:161:CYS:C	1:D:163:SER:H	2.18	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:F:141:VAL:N	1:F:142:ALA:CB	2.75	0.46
1:B:126:ILE:HG22	1:B:130:TYR:CD1	2.50	0.46
1:B:52:SER:HB3	1:B:108:SER:HA	1.98	0.46
1:A:113:ARG:O	1:A:117:ARG:HG3	2.14	0.46
1:D:29:THR:C	1:D:31:MET:H	2.19	0.46
1:F:179:SER:HG	1:F:182:SER:H	1.63	0.46
1:E:172:TYR:CE1	1:E:219:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:GLU:H	1:F:68:GLU:CD	2.19	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:D:75:LEU:HB3	1:D:76:TYR:CD1	2.51	0.45
1:B:63:LEU:HD12	1:B:63:LEU:N	2.30	0.45
1:B:202:LYS:C	1:B:204:GLU:H	2.18	0.45
1:D:22:ILE:HD13	1:D:22:ILE:O	2.12	0.45
1:A:57:VAL:O	1:A:57:VAL:CG2	2.63	0.45
1:F:85:GLY:C	1:F:86:LYS:HG2	2.35	0.45
1:F:65:ILE:CG2	1:F:67:PHE:HE1	2.29	0.45
1:D:53:MET:SD	1:D:87:LEU:HD13	2.57	0.45
1:F:221:GLU:O	1:F:225:LEU:CG	2.64	0.45
1:F:66:ILE:HD12	1:F:93:ASN:O	2.16	0.45
1:A:52:SER:OG	1:A:108:SER:N	2.50	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: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:113:ARG:O	1:B:114:THR:C	2.52	0.45
1:C:180:GLN:NE2	1:C:194:VAL:O	2.50	0.45
1:C:136:TYR:O	1:C:139:ARG:CB	2.63	0.45
1:E:116:PHE:CD1	1:E:122:MET:HB3	2.51	0.45
1:E:56:LEU:C	1:E:56:LEU:HD23	2.36	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:A:87:LEU:CB	1:A:88:TYR:CD1	2.96	0.45
1:F:140:GLN:O	1:F:143:GLU:CB	2.65	0.45
1:C:60:LYS:CG	1:C:99:MET:HE1	2.47	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:153:ILE:H	1:A:153:ILE:HD12	1.82	0.45
1:A:188:GLY:N	1:B:152:ARG:HD3	2.32	0.44
1:A:203:ARG:O	1:A:204:GLU:C	2.54	0.44
1:D:180:GLN:O	1:D:181:LYS:C	2.56	0.44
1:A:128:LYS:CG	1:B:88:TYR:CE1	2.93	0.44
1:F:155:ARG:HA	1:F:155:ARG:HD2	1.51	0.44
1:B:122:MET:HB3	1:B:122:MET:HE2	1.42	0.44
1:D:49:GLU:O	1:D:49:GLU:CG	2.59	0.44
1:A:26:ARG:HH22	1:A:57:VAL:HG23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:ARG:NH1	1:E:188:GLY:O	2.50	0.44
1:A:123:ILE:CD1	1:B:123:ILE:HD13	2.48	0.44
1:A:67:PHE:C	1:A:69:ASP:N	2.65	0.44
1:E:87:LEU:CD2	1:E:109:GLU:HB2	2.48	0.44
1:C:66:ILE:HD11	1:C:95:TYR:HB2	1.98	0.44
1:E:151:ILE:O	1:E:155:ARG:HB2	2.18	0.44
1:C:183:ILE:O	1:C:187:THR:OG1	2.32	0.44
1:F:206:ILE:O	1:F:217:TYR:N	2.50	0.44
1:C:139:ARG:O	1:C:140:GLN:C	2.55	0.44
1:B:23:GLU:O	1:B:26:ARG:N	2.47	0.44
1:F:23:GLU:O	1:F:25:LEU:N	2.50	0.44
1:A:201:LEU:HA	1:A:206:ILE:HD12	2.00	0.44
1:E:74:LEU:HD23	1:E:75:LEU:N	2.33	0.44
1:A:67:PHE:O	1:A:69:ASP:N	2.45	0.44
1:C:167:ARG:HG3	1:C:172:TYR:CZ	2.52	0.44
1:F:24:LYS:HD2	1:F:125:GLU:OE1	2.17	0.44
1:C:88:TYR:CD1	1:D:128:LYS:HE3	2.53	0.44
1:B:36:ASP:O	1:C:33:LEU:CD2	2.65	0.44
1:E:187:THR:O	1:E:188:GLY:C	2.55	0.44
1:E:140:GLN:C	1:E:142:ALA:N	2.62	0.44
1:F:158:TYR:HE1	1:F:223:LYS:HB2	1.82	0.44
1:F:46:PRO:HA	1:F:94:ILE:O	2.18	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:D:44:ILE:H	1:D:96:ALA:HB3	1.83	0.43
1:C:123:ILE:CD1	1:D:123:ILE:CD1	2.78	0.43
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:D:34:ILE:HD13	1:D:105:CYS:SG	2.58	0.43
1:B:108:SER:HG	1:B:111:SER:H	1.58	0.43
1:E:189:VAL:HG12	1:E:190:HIS:H	1.82	0.43
1:C:74:LEU:HD11	1:C:77:TYR:CE1	2.52	0.43
1:D:52:SER:HA	1:D:107:PHE:O	2.18	0.43
1:A:60:LYS:HG2	1:A:99:MET:HE2	1.98	0.43
1:C:45:MET:O	1:C:48:GLU:HB3	2.18	0.43
1:A:28:TYR:N	1:A:28:TYR:CD1	2.87	0.43
1:B:216:VAL:HG12	1:B:216:VAL:O	2.18	0.43
1:A:159:GLU:CD	1:B:182:SER:HG	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:O	1:A:131:LEU:CB	2.67	0.43
1:F:198:LEU:HA	1:F:198:LEU:HD22	1.77	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:C:115:VAL:O	1:C:118:THR:N	2.52	0.43
1:E:152:ARG:HG2	1:F:185:GLU:O	2.19	0.43
1:A:186:ILE:HG13	1:B:155:ARG:HB3	2.00	0.43
1:C:127:PHE:HE2	1:D:53:MET:SD	2.42	0.43
1:D:65:ILE:HG23	1:D:73:LYS:O	2.19	0.43
1:C:155:ARG:CG	1:D:185:GLU:OE1	2.66	0.43
1:E:131:LEU:O	1:E:134:VAL:N	2.51	0.43
1:F:43:VAL:O	1:F:44:ILE:HG12	2.18	0.43
1:C:65:ILE:CD1	1:C:92:ASN:ND2	2.81	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:28:TYR:CE2	1:C:115:VAL:HG13	2.53	0.43
1:E:216:VAL:HG11	1:E:222:LEU:CD2	2.48	0.43
1:B:46:PRO:HA	1:B:93:ASN:ND2	2.34	0.43
1:D:53:MET:HG2	1:D:87:LEU:CD1	2.49	0.43
1:C:65:ILE:HD11	1:C:92:ASN:HD22	1.83	0.43
1:A:138:ALA:HA	1:B:137:TYR:HD2	1.84	0.43
1:E:156:LEU:N	1:F:186:ILE:HG12	2.34	0.43
1:B:35:ARG:NH1	1:C:35:ARG:HE	2.16	0.43
1:A:190:HIS:C	1:A:190:HIS:CD2	2.92	0.43
1:E:158:TYR:CZ	1:E:223:LYS:HD2	2.54	0.43
1:E:100:GLU:O	1:E:101:PRO:C	2.56	0.43
1:E:188:GLY:CA	1:F:152:ARG:HE	2.30	0.43
1:D:112:LEU:O	1:D:115:VAL:N	2.52	0.43
1:B:195:SER:O	1:B:197:VAL:N	2.51	0.43
1:E:46:PRO:HB3	1:E:66:ILE:HD13	1.99	0.43
1:E:25:LEU:HA	1:E:25:LEU:HD23	1.63	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:B:112:LEU:HA	1:B:112:LEU:HD23	1.66	0.43
1:B:156:LEU:HD13	1:B:186:ILE:HG21	2.01	0.42
1:D:64:ASP:N	1:D:64:ASP:OD2	2.51	0.42
1:E:28:TYR:O	1:E:31:MET:HG3	2.18	0.42
1:A:30:GLN:CD	1:A:30:GLN:N	2.72	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:GLN:N	1:F:142:ALA:HB3	2.34	0.42
1:D:189:VAL:CG1	1:D:190:HIS:O	2.62	0.42
1:A:195:SER:C	1:A:197:VAL:H	2.22	0.42
1:F:74:LEU:HD23	1:F:75:LEU:H	1.84	0.42
1:A:107:PHE:HB3	1:A:112:LEU:HG	2.00	0.42
1:A:99:MET:HB2	1:A:99:MET:HE2	1.76	0.42
1:C:193:THR:C	1:C:195:SER:H	2.22	0.42
1:F:57:VAL:O	1:F:57:VAL:HG23	2.18	0.42
1:C:50:ILE:HG12	1:C:86:LYS:HZ1	1.83	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:160:LEU:HD21	1:A:176:MET:SD	2.60	0.42
1:A:152:ARG:O	1:A:155:ARG:HB2	2.19	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:A:28:TYR:OH	1:A:119:ASP:OD2	2.21	0.42
1:C:46:PRO:CA	1:C:94:ILE:O	2.68	0.42
1:A:74:LEU:O	1:A:74:LEU:HG	2.06	0.42
1:F:87:LEU:CB	1:F:88:TYR:CE1	3.02	0.42
1:C:132:THR:O	1:C:133:LYS:C	2.57	0.42
1:E:28:TYR:HB3	1:E:115:VAL:HG22	2.01	0.42
1:C:180:GLN:HB3	1:C:180:GLN:HE21	1.70	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: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: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:A:101:PRO:CG	1:A:101:PRO:O	2.68	0.42
1:E:109:GLU:C	1:E:111:SER:N	2.73	0.42
1:C:60:LYS:HA	1:C:78:ALA:O	2.19	0.42
1:F:33:LEU:HD23	1:F:33:LEU:N	2.34	0.42
1:B:87:LEU:C	1:B:88:TYR:CD1	2.93	0.42
1:E:190:HIS:CD2	1:E:191:HIS:N	2.86	0.42
1:B:46:PRO:HD3	1:B:95:TYR:CE2	2.55	0.42
1:C:94:ILE:HG22	1:C:95:TYR:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:LEU:HA	1:C:83:LEU:HD12	1.51	0.42
1:C:86:LYS:HB2	1:C:88:TYR:O	2.20	0.42
1:D:92:ASN:O	1:D:94:ILE:CG1	2.59	0.42
1:C:115:VAL:O	1:C:119:ASP:N	2.38	0.42
1:B:87:LEU:HB3	1:B:88:TYR:CE1	2.55	0.42
1:E:159:GLU:CG	1:F:186:ILE:HD11	2.39	0.42
1:A:219:LEU:O	1:A:222:LEU:HB3	2.20	0.42
1:E:161:CYS:SG	1:E:174:ILE:HD11	2.60	0.41
1:D:62:LYS:HG3	1:D:74:LEU:HD12	2.02	0.41
1:C:57:VAL:HG23	1:C:57:VAL:O	2.20	0.41
1:D:189:VAL:HG11	1:D:193:THR:HB	1.91	0.41
1:E:161:CYS:O	1:E:165:GLY:CA	2.64	0.41
1:E:75:LEU:HD23	1:E:75:LEU:HA	1.53	0.41
1:E:45:MET:O	1:E:48:GLU:HB3	2.19	0.41
1:D:209:LYS:HZ2	1:D:209:LYS:C	2.23	0.41
1:B:140:GLN:H	1:B:140:GLN:HG2	1.56	0.41
1:A:151:ILE:O	1:A:155:ARG:HG2	2.20	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:C:26:ARG:HA	1:C:29:THR:HG23	2.03	0.41
1:B:114:THR:O	1:B:115:VAL:C	2.57	0.41
1:E:86:LYS:CG	1:E:88:TYR:O	2.68	0.41
1:D:67:PHE:HB2	1:D:71:SER:OG	2.20	0.41
1:A:160:LEU:O	1:A:164:GLN:HB2	2.20	0.41
1:C:186:ILE:HG23	1:D:156:LEU:CB	2.48	0.41
1:A:126:ILE:O	1:A:129:ASN:HB3	2.20	0.41
1:B:86:LYS:O	1:B:86:LYS:HG2	2.21	0.41
1:A:160:LEU:HD21	1:A:176:MET:CE	2.50	0.41
1:C:128:LYS:O	1:C:129:ASN:C	2.59	0.41
1:F:158:TYR:HD2	1:F:159:GLU:OE1	2.03	0.41
1:F:158:TYR:HA	1:F:222:LEU:HD21	2.02	0.41
1:A:123:ILE:HD11	1:B:123:ILE:HD13	2.02	0.41
1:C:184:GLY:O	1:C:188:GLY:N	2.54	0.41
1:C:151:ILE:HA	1:C:154:LEU:CG	2.49	0.41
1:A:160:LEU:HD12	1:A:174:ILE:HD13	2.02	0.41
1:D:53:MET:HB3	1:D:83:LEU:HD11	2.03	0.41
1:E:151:ILE:HG23	1:E:226:SER:HA	2.03	0.41
1:E:116:PHE:HE1	1:E:122:MET:HB3	1.79	0.41
1:A:108:SER:OG	1:A:109:GLU:N	2.51	0.41
1:C:19:PHE:CD1	1:C:19:PHE:N	2.83	0.41
1:B:191:HIS:C	1:B:193:THR:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ALA:O	1:D:39:LYS:C	2.59	0.41
1:B:20:PHE:HA	1:B:21:PRO:HD2	1.90	0.41
1:A:164:GLN:HB3	1:A:174:ILE:HG12	2.02	0.41
1:E:131:LEU:HD23	1:F:130:TYR:CZ	2.56	0.41
1:D:93:ASN:O	1:D:94:ILE:HD13	2.21	0.41
1:C:116:PHE:CE1	1:C:123:ILE:HA	2.56	0.41
1:A:128:LYS:O	1:A:129:ASN:C	2.59	0.41
1:A:130:TYR:C	1:A:132:THR:N	2.71	0.41
1:B:35:ARG:HH11	1:C:35:ARG:HE	1.69	0.41
1:A:75:LEU:HD13	1:A:76:TYR:CE1	2.56	0.41
1:A:66:ILE:HB	1:A:93:ASN:ND2	2.36	0.41
1:C:74:LEU:HD21	1:C:76:TYR:HA	2.03	0.41
1:B:52:SER:HA	1:B:87:LEU:HD13	2.03	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:133:LYS:O	1:D:137:TYR:HD1	2.04	0.41
1:E:120:GLU:O	1:E:123:ILE:HG13	2.21	0.41
1:C:111:SER:O	1:C:114:THR:OG1	2.37	0.41
1:B:109:GLU:O	1:B:113:ARG:N	2.46	0.41
1:E:108:SER:OG	1:E:111:SER:HB3	2.21	0.41
1:B:29:THR:HG22	1:B:105:CYS:CB	2.50	0.41
1:C:20:PHE:N	1:C:21:PRO:CD	2.83	0.41
1:A:186:ILE:HG12	1:B:156:LEU:N	2.37	0.40
1:D:130:TYR:O	1:D:133:LYS:HB2	2.20	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:F:115:VAL:HG23	1:F:115:VAL:H	1.69	0.40
1:E:175:THR:O	1:E:176:MET:HB3	2.21	0.40
1:D:29:THR:C	1:D:31:MET:N	2.73	0.40
1:B:195:SER:O	1:B:198:LEU:N	2.54	0.40
1:A:140:GLN:H	1:A:140:GLN:HG2	1.71	0.40
1:C:19:PHE:HB2	1:C:21:PRO:HD3	2.03	0.40
1:F:161:CYS:HB2	1:F:174:ILE:HD11	2.02	0.40
1:B:224:HIS:CD2	1:B:224:HIS:O	2.74	0.40
1:C:124:PHE:HZ	1:D:112:LEU:HB3	1.87	0.40
1:D:161:CYS:HG	1:D:172:TYR:CB	2.35	0.40
1:F:67:PHE:HB2	1:F:71:SER:OG	2.20	0.40
1:F:189:VAL:CG1	1:F:193:THR:HB	2.51	0.40
1:C:186:ILE:HG23	1:D:156:LEU:HD13	2.03	0.40
1:E:54:ILE:HD13	1:E:106:TRP:CZ2	2.56	0.40
1:E:109:GLU:C	1:E:111:SER:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:LEU:HA	1:F:178:LEU:HD12	1.91	0.40
1:E:171:THR:HG22	1:E:217:TYR:HA	2.03	0.40
1:F:86:LYS:HG3	1:F:86:LYS:HZ3	1.62	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
1:C:128:LYS:HG3	1:D:88:TYR:CD1	2.56	0.40
1:D:167:ARG:CA	1:D:171:THR:O	2.60	0.40
1:C:130:TYR:HE2	1:D:131:LEU:HG	1.83	0.40
1:A:198:LEU:HA	1:A:198:LEU:HD13	1.86	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%)	1	6
1	B	197/250 (79%)	146 (74%)	31 (16%)	20 (10%)	1	4
1	C	199/250 (80%)	151 (76%)	36 (18%)	12 (6%)	2	16
1	D	197/250 (79%)	144 (73%)	31 (16%)	22 (11%)	0	3
1	E	199/250 (80%)	152 (76%)	34 (17%)	13 (6%)	1	13
1	F	199/250 (80%)	156 (78%)	29 (15%)	14 (7%)	1	10
All	All	1189/1500 (79%)	889 (75%)	202 (17%)	98 (8%)	1	7

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	131 (77%)	39 (23%)	1	4
1	B	174/220 (79%)	133 (76%)	41 (24%)	1	4
1	C	170/220 (77%)	130 (76%)	40 (24%)	1	4
1	D	173/220 (79%)	134 (78%)	39 (22%)	1	5
1	E	170/220 (77%)	137 (81%)	33 (19%)	2	9
1	F	172/220 (78%)	130 (76%)	42 (24%)	1	3
All	All	1029/1320 (78%)	795 (77%)	234 (23%)	1	5

All (234) 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	41	SER
1	A	50	ILE

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Mol	Chain	Res	Type
1	A	51	THR
1	A	52	SER
1	A	53	MET
1	A	56	LEU
1	A	57	VAL
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	117	ARG
1	A	128	LYS
1	A	130	TYR
1	A	140	GLN
1	A	155	ARG
1	A	156	LEU
1	A	160	LEU
1	A	170	ASP
1	A	171	THR
1	A	175	THR
1	A	180	GLN
1	A	181	LYS
1	A	185	GLU
1	A	189	VAL
1	A	195	SER
1	A	196	ARG
1	A	197	VAL
1	A	198	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	35	ARG
1	B	39	LYS
1	B	48	GLU

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Mol	Chain	Res	Type
1	B	51	THR
1	B	52	SER
1	B	53	MET
1	B	56	LEU
1	B	57	VAL
1	B	73	LYS
1	B	75	LEU
1	B	82	SER
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	113	ARG
1	B	119	ASP
1	B	134	VAL
1	B	140	GLN
1	B	154	LEU
1	B	155	ARG
1	B	160	LEU
1	B	175	THR
1	B	179	SER
1	B	180	GLN
1	B	182	SER
1	B	193	THR
1	B	196	ARG
1	B	198	LEU
1	B	207	LEU
1	B	211	LYS
1	B	212	ASN
1	B	216	VAL
1	B	223	LYS
1	C	21	PRO
1	C	25	LEU
1	C	30	GLN
1	C	33	LEU
1	C	34	ILE
1	C	39	LYS
1	C	41	SER
1	C	51	THR
1	C	52	SER

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Mol	Chain	Res	Type
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	76	TYR
1	C	86	LYS
1	C	90	THR
1	C	93	ASN
1	C	97	THR
1	C	102	THR
1	C	103	ARG
1	C	113	ARG
1	C	114	THR
1	C	125	GLU
1	C	128	LYS
1	C	140	GLN
1	C	155	ARG
1	C	164	GLN
1	C	170	ASP
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	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	39	LYS
1	D	41	SER
1	D	43	VAL
1	D	49	GLU
1	D	57	VAL
1	D	64	ASP

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Mol	Chain	Res	Type
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	99	MET
1	D	108	SER
1	D	126	ILE
1	D	127	PHE
1	D	132	THR
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	196	ARG
1	D	209	LYS
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	30	GLN
1	E	31	MET
1	E	41	SER
1	E	56	LEU
1	E	57	VAL
1	E	60	LYS
1	E	69	ASP
1	E	75	LEU
1	E	76	TYR
1	E	99	MET
1	E	100	GLU
1	E	122	MET
1	E	131	LEU
1	E	133	LYS

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Mol	Chain	Res	Type
1	E	140	GLN
1	E	153	ILE
1	E	155	ARG
1	E	162	SER
1	E	163	SER
1	E	178	LEU
1	E	179	SER
1	E	180	GLN
1	E	185	GLU
1	E	190	HIS
1	E	192	VAL
1	E	196	ARG
1	E	197	VAL
1	E	211	LYS
1	E	214	ILE
1	E	216	VAL
1	E	217	TYR
1	E	221	GLU
1	E	223	LYS
1	F	19	PHE
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	54	ILE
1	F	63	LEU
1	F	65	ILE
1	F	73	LYS
1	F	74	LEU
1	F	75	LEU
1	F	76	TYR
1	F	83	LEU
1	F	86	LYS
1	F	101	PRO
1	F	109	GLU
1	F	110	LYS
1	F	111	SER
1	F	114	THR

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Mol	Chain	Res	Type
1	F	139	ARG
1	F	153	ILE
1	F	154	LEU
1	F	155	ARG
1	F	163	SER
1	F	167	ARG
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	207	LEU
1	F	209	LYS
1	F	211	LYS
1	F	212	ASN
1	F	223	LYS
1	F	226	SER

Some 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	164	GLN
1	A	190	HIS
1	B	27	ASN
1	B	30	GLN
1	B	224	HIS
1	C	92	ASN
1	C	93	ASN
1	C	164	GLN
1	C	180	GLN
1	C	190	HIS
1	C	212	ASN
1	D	27	ASN
1	D	180	GLN
1	D	190	HIS
1	D	191	HIS
1	D	205	ASN
1	E	30	GLN
1	E	140	GLN

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Mol	Chain	Res	Type
1	E	190	HIS
1	E	191	HIS
1	F	27	ASN
1	F	190	HIS
1	F	191	HIS
1	F	212	ASN

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 carbohydrates 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%)	0.39	14 (6%)	20 11	74, 81, 85, 90	0
1	B	201/250 (80%)	0.30	4 (1%)	68 54	74, 79, 84, 87	0
1	C	203/250 (81%)	0.62	22 (10%)	8 4	73, 80, 85, 91	0
1	D	201/250 (80%)	0.47	20 (9%)	9 5	73, 80, 85, 89	0
1	E	203/250 (81%)	0.26	10 (4%)	33 20	75, 80, 84, 90	0
1	F	203/250 (81%)	0.23	6 (2%)	54 39	75, 80, 84, 87	0
All	All	1213/1500 (80%)	0.38	76 (6%)	23 13	73, 80, 85, 91	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	8.0
1	C	153	ILE	7.4
1	D	161	CYS	6.2
1	E	161	CYS	6.1
1	C	201	LEU	5.2
1	D	165	GLY	5.0
1	A	174	ILE	5.0
1	C	178	LEU	4.9
1	C	159	GLU	4.7
1	C	219	LEU	4.7
1	E	162	SER	4.7
1	A	173	GLU	4.5
1	A	161	CYS	4.5
1	C	180	GLN	4.3
1	D	178	LEU	4.1
1	C	157	PHE	4.0
1	A	207	LEU	3.6
1	D	214	ILE	3.6
1	C	168	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	156	LEU	3.5
1	D	154	LEU	3.5
1	C	197	VAL	3.5
1	D	183	ILE	3.4
1	C	220	GLY	3.3
1	D	157	PHE	3.1
1	D	166	LYS	3.1
1	F	215	ILE	3.1
1	B	215	ILE	3.1
1	E	158	TYR	3.0
1	C	155	ARG	2.9
1	E	170	ASP	2.9
1	C	182	SER	2.9
1	D	189	VAL	2.8
1	D	206	ILE	2.8
1	A	193	THR	2.8
1	A	166	LYS	2.8
1	B	173	GLU	2.7
1	A	220	GLY	2.6
1	A	222	LEU	2.6
1	D	164	GLN	2.6
1	C	169	GLY	2.6
1	D	205	ASN	2.6
1	D	200	CYS	2.6
1	D	171	THR	2.6
1	D	207	LEU	2.5
1	D	152	ARG	2.5
1	F	159	GLU	2.5
1	F	214	ILE	2.5
1	D	94	ILE	2.5
1	F	160	LEU	2.5
1	F	206	ILE	2.4
1	C	194	VAL	2.4
1	A	219	LEU	2.4
1	C	164	GLN	2.4
1	A	214	ILE	2.3
1	D	225	LEU	2.3
1	A	186	ILE	2.3
1	E	181	LYS	2.3
1	C	152	ARG	2.3
1	E	217	TYR	2.2
1	E	157	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	185	GLU	2.2
1	E	156	LEU	2.2
1	E	222	LEU	2.2
1	C	204	GLU	2.1
1	C	66	ILE	2.1
1	C	176	MET	2.1
1	D	19	PHE	2.1
1	A	46	PRO	2.1
1	E	193	THR	2.1
1	A	167	ARG	2.0
1	C	173	GLU	2.0
1	D	153	ILE	2.0
1	B	167	ARG	2.0
1	A	199	ALA	2.0
1	F	201	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 carbohydrates 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.