WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 11:46 am BST

PDB ID	:	3P3F
Title	:	Crystal structure of the F36A mutant of the fluoroacetyl-CoA-specific thioesterase FlK
Authors	:	Weeks, A.M.; Coyle, S.M.; Jinek, M.; Doudna, J.A.; Chang, M.C.Y.
Deposited on	:	2010-10-04
Resolution	:	2.30 Å(reported)

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

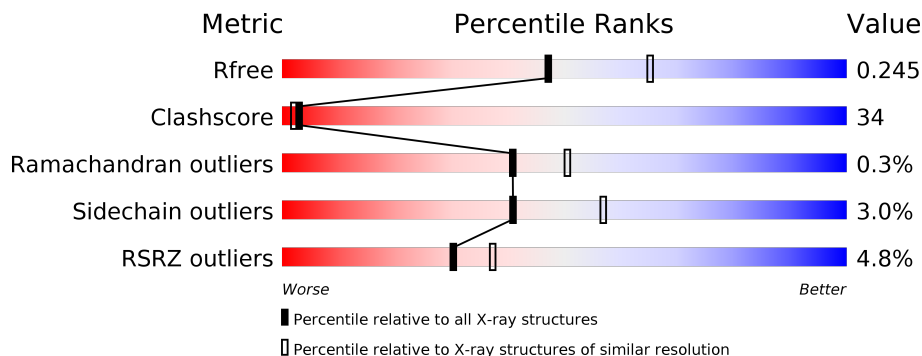|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		34
Ramachandran outliers		0.3%
Sidechain outliers		3.0%
RSRZ outliers		4.8%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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 <=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	143	% 70% 24% 6%
1	B	143	4% 63% 28% • 7%
1	C	143	5% 58% 31% •• 8%
1	D	143	3% 55% 33% • 9%
1	E	143	6% 55% 31% • 11%
1	F	143	6% 55% 38% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6649 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 Fluoroacetyl coenzyme A thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1042	657	188	191	6			
1	B	133	Total	C	N	O	S	0	0	0
			1028	650	185	187	6			
1	C	131	Total	C	N	O	S	0	0	0
			1009	639	180	185	5			
1	D	130	Total	C	N	O	S	0	0	0
			1005	635	181	183	6			
1	E	127	Total	C	N	O	S	0	0	0
			978	620	176	177	5			
1	F	133	Total	C	N	O	S	0	0	0
			1028	650	185	187	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q1EMV2
A	-2	THR	-	EXPRESSION TAG	UNP Q1EMV2
A	-1	GLY	-	EXPRESSION TAG	UNP Q1EMV2
A	0	ALA	-	EXPRESSION TAG	UNP Q1EMV2
A	36	ALA	PHE	ENGINEERED MUTATION	UNP Q1EMV2
B	-3	GLY	-	EXPRESSION TAG	UNP Q1EMV2
B	-2	THR	-	EXPRESSION TAG	UNP Q1EMV2
B	-1	GLY	-	EXPRESSION TAG	UNP Q1EMV2
B	0	ALA	-	EXPRESSION TAG	UNP Q1EMV2
B	36	ALA	PHE	ENGINEERED MUTATION	UNP Q1EMV2
C	-3	GLY	-	EXPRESSION TAG	UNP Q1EMV2
C	-2	THR	-	EXPRESSION TAG	UNP Q1EMV2
C	-1	GLY	-	EXPRESSION TAG	UNP Q1EMV2
C	0	ALA	-	EXPRESSION TAG	UNP Q1EMV2
C	36	ALA	PHE	ENGINEERED MUTATION	UNP Q1EMV2
D	-3	GLY	-	EXPRESSION TAG	UNP Q1EMV2
D	-2	THR	-	EXPRESSION TAG	UNP Q1EMV2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	EXPRESSION TAG	UNP Q1EMV2
D	0	ALA	-	EXPRESSION TAG	UNP Q1EMV2
D	36	ALA	PHE	ENGINEERED MUTATION	UNP Q1EMV2
E	-3	GLY	-	EXPRESSION TAG	UNP Q1EMV2
E	-2	THR	-	EXPRESSION TAG	UNP Q1EMV2
E	-1	GLY	-	EXPRESSION TAG	UNP Q1EMV2
E	0	ALA	-	EXPRESSION TAG	UNP Q1EMV2
E	36	ALA	PHE	ENGINEERED MUTATION	UNP Q1EMV2
F	-3	GLY	-	EXPRESSION TAG	UNP Q1EMV2
F	-2	THR	-	EXPRESSION TAG	UNP Q1EMV2
F	-1	GLY	-	EXPRESSION TAG	UNP Q1EMV2
F	0	ALA	-	EXPRESSION TAG	UNP Q1EMV2
F	36	ALA	PHE	ENGINEERED MUTATION	UNP Q1EMV2

- Molecule 2 is water.

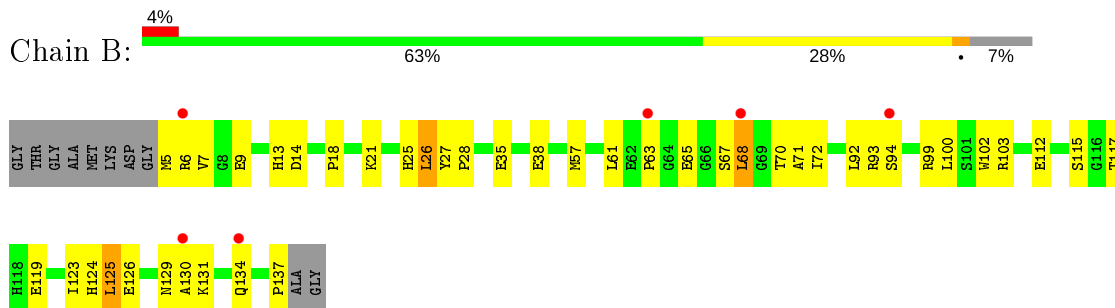| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	96	Total 96	O 96	0	0
2	B	86	Total 86	O 86	0	0
2	C	106	Total 106	O 106	0	0
2	D	97	Total 97	O 97	0	0
2	E	86	Total 86	O 86	0	0
2	F	88	Total 88	O 88	0	0

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 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.
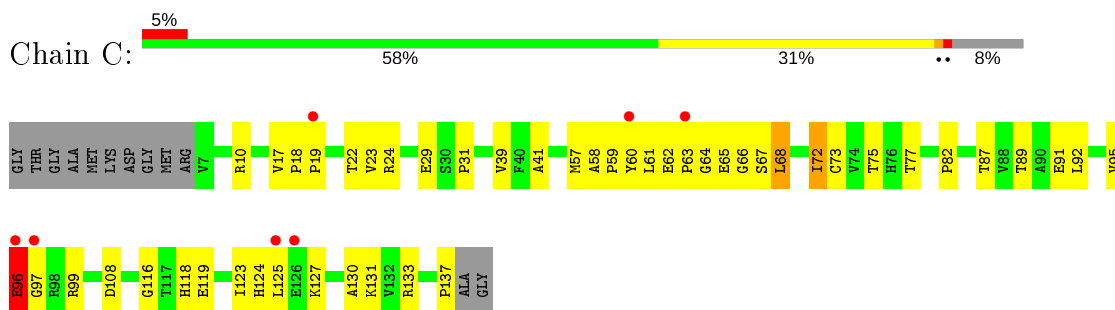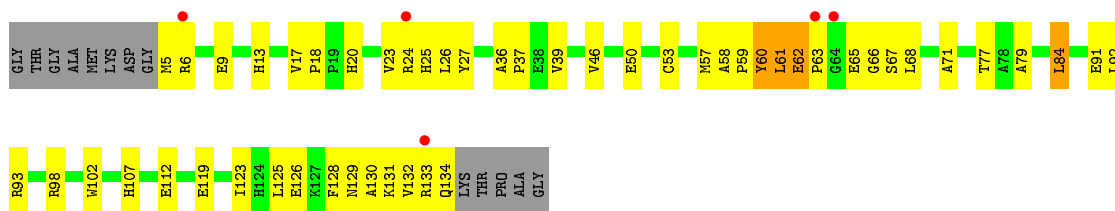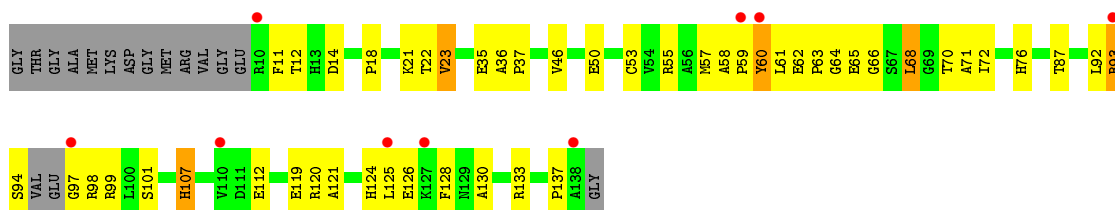
- Molecule 1: Fluoroacetyl coenzyme A thioesterase

- Molecule 1: Fluoroacetyl coenzyme A thioesterase

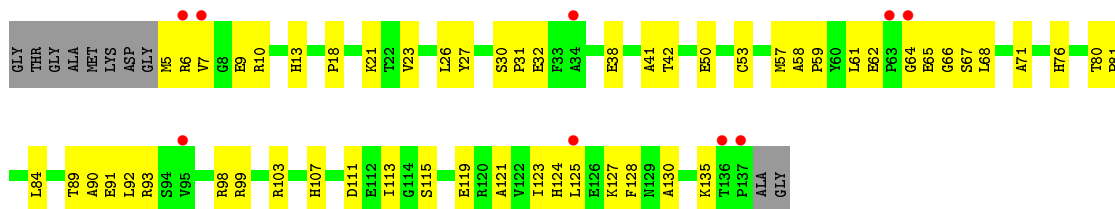- Molecule 1: Fluoroacetyl coenzyme A thioesterase

- Molecule 1: Fluoroacetyl coenzyme A thioesterase

• Molecule 1: Fluoroacetyl coenzyme A thioesterase

Chain E:

• Molecule 1: Fluoroacetyl coenzyme A thioesterase

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.38Å 88.82Å 71.08Å 90.00° 117.97° 90.00°	Depositor
Resolution (Å)	19.75 – 2.30 19.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.75-2.30) 99.1 (19.75-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.29 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.220 , 0.247 0.216 , 0.245	Depositor DCC
R_{free} test set	1722 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 68.9	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6649	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8002e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.82	0/1069	0.79	1/1452 (0.1%)
1	B	0.85	0/1056	0.75	1/1437 (0.1%)
1	C	0.98	0/1037	0.74	0/1413
1	D	0.83	2/1032 (0.2%)	0.73	0/1404
1	E	0.74	2/1005 (0.2%)	0.72	0/1368
1	F	0.75	0/1056	0.70	0/1437
All	All	0.83	4/6255 (0.1%)	0.74	2/8511 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	126	GLU	CB-CG	-5.26	1.42	1.52
1	D	62	GLU	CD-OE1	-5.22	1.20	1.25
1	D	129	ASN	CG-ND2	-5.03	1.20	1.32
1	E	126	GLU	CG-CD	-5.00	1.44	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	26	LEU	CB-CG-CD2	5.45	120.27	111.00
1	A	99	ARG	NE-CZ-NH1	5.42	123.01	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1042	0	1022	52	0
1	B	1028	0	1009	74	0
1	C	1009	0	987	82	3
1	D	1005	0	982	66	3
1	E	978	0	958	67	0
1	F	1028	0	1009	83	0
2	A	96	0	0	11	2
2	B	86	0	0	12	0
2	C	106	0	0	26	0
2	D	97	0	0	19	1
2	E	86	0	0	13	1
2	F	88	0	0	13	1
All	All	6649	0	5967	414	6

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 34.

All (414) 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:F:68:LEU:CD1	1:F:123:ILE:HD13	1.54	1.33
1:A:57:MET:O	1:A:61:LEU:CD1	1.76	1.32
1:C:68:LEU:HD13	2:C:452:HOH:O	1.22	1.30
1:E:99:ARG:NH1	1:E:121:ALA:HB2	1.47	1.28
1:D:71:ALA:HB3	2:D:496:HOH:O	1.31	1.28
1:F:64:GLY:O	1:F:125:LEU:HD13	1.22	1.28
1:B:35:GLU:HG3	2:B:309:HOH:O	1.15	1.27
1:C:24:ARG:HD2	2:C:488:HOH:O	1.17	1.27
1:B:93:ARG:NH1	1:B:117:THR:CG2	1.99	1.25
1:B:93:ARG:NH1	1:B:117:THR:HG21	1.54	1.23
1:F:6:ARG:HD3	2:F:346:HOH:O	1.35	1.23
1:F:26:LEU:CD1	1:F:27:TYR:CD2	2.22	1.22
1:C:60:TYR:CE1	2:C:520:HOH:O	1.91	1.19
1:D:68:LEU:HD11	1:D:123:ILE:CD1	1.75	1.14
1:D:91:GLU:OE1	1:D:93:ARG:NH1	1.80	1.14
1:F:68:LEU:HD11	1:F:123:ILE:CD1	1.79	1.12
1:F:5:MET:N	2:F:544:HOH:O	1.80	1.12
1:F:65:GLU:C	1:F:125:LEU:HD11	1.71	1.11
1:A:57:MET:O	1:A:61:LEU:HD13	1.38	1.11
1:A:68:LEU:HD11	1:A:123:ILE:CD1	1.80	1.09
1:B:112:GLU:HB2	2:B:270:HOH:O	1.54	1.08
1:C:68:LEU:HD21	1:C:123:ILE:HD11	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:HD21	1:C:123:ILE:CD1	1.84	1.06
1:A:103:ARG:NE	2:A:205:HOH:O	1.88	1.05
1:B:26:LEU:CD1	1:B:27:TYR:CD2	2.38	1.05
1:C:66:GLY:N	1:C:125:LEU:HD21	1.71	1.04
1:B:67:SER:C	1:B:68:LEU:HD22	1.77	1.03
1:D:68:LEU:CD1	1:D:123:ILE:HD13	1.88	1.03
1:A:68:LEU:HD11	1:A:123:ILE:HD13	1.41	1.01
1:D:68:LEU:HD11	1:D:123:ILE:HD13	1.01	1.01
1:E:93:ARG:O	1:E:94:SER:HB3	1.56	1.01
1:D:98:ARG:HD3	2:D:254:HOH:O	1.61	1.00
1:C:67:SER:C	1:C:68:LEU:HD22	1.80	1.00
1:E:65:GLU:C	1:E:125:LEU:HD11	1.81	0.99
1:B:26:LEU:CD1	1:B:27:TYR:HD2	1.72	0.99
1:F:26:LEU:HD12	1:F:27:TYR:HD2	1.28	0.99
1:C:60:TYR:CD2	2:C:148:HOH:O	2.15	0.99
1:F:57:MET:O	1:F:61:LEU:HD13	1.64	0.97
1:E:99:ARG:NH1	1:E:121:ALA:CB	2.26	0.97
1:A:91:GLU:OE2	2:A:161:HOH:O	1.80	0.97
1:E:99:ARG:HH11	1:E:121:ALA:HB2	1.30	0.96
1:F:111:ASP:OD2	2:F:364:HOH:O	1.84	0.96
1:B:26:LEU:HD13	1:B:27:TYR:CD2	2.01	0.96
1:E:94:SER:OG	1:E:101:SER:HB3	1.66	0.95
1:C:119:GLU:OE1	2:C:438:HOH:O	1.83	0.94
1:C:68:LEU:CD2	1:C:123:ILE:CD1	2.44	0.94
1:D:9:GLU:HB3	2:D:168:HOH:O	1.66	0.94
1:D:119:GLU:HB3	2:D:496:HOH:O	1.69	0.93
1:E:65:GLU:C	1:E:125:LEU:CD1	2.37	0.92
1:F:81:PRO:HD2	1:F:84:LEU:HD22	1.48	0.92
1:B:103:ARG:NH2	1:B:115:SER:HB2	1.84	0.92
1:F:65:GLU:O	1:F:125:LEU:HD11	1.69	0.91
1:A:68:LEU:CD1	1:A:123:ILE:CD1	2.49	0.91
1:C:66:GLY:N	1:C:125:LEU:CD2	2.35	0.90
1:F:127:LYS:NZ	2:F:504:HOH:O	2.02	0.90
1:F:31:PRO:HD2	1:F:32:GLU:OE2	1.69	0.90
1:B:68:LEU:HD21	1:B:123:ILE:HD11	1.55	0.89
1:B:67:SER:O	1:B:68:LEU:HD22	1.72	0.89
1:F:119:GLU:HB2	2:F:464:HOH:O	1.71	0.89
1:B:68:LEU:CD2	1:B:123:ILE:CD1	2.51	0.89
1:B:68:LEU:CD2	1:B:123:ILE:HD13	2.02	0.88
1:F:26:LEU:HD11	1:F:27:TYR:CE2	2.08	0.88
1:A:103:ARG:CZ	2:A:205:HOH:O	2.17	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:GLY:C	1:F:125:LEU:HD13	1.94	0.88
1:D:112:GLU:HB3	2:D:501:HOH:O	1.72	0.88
1:C:60:TYR:CE2	2:C:148:HOH:O	2.24	0.88
1:F:26:LEU:CD1	1:F:27:TYR:HD2	1.77	0.88
1:F:64:GLY:O	1:F:125:LEU:CD1	2.17	0.88
1:F:68:LEU:HD11	1:F:123:ILE:HD13	0.90	0.88
1:E:76:HIS:O	2:E:291:HOH:O	1.90	0.87
1:B:131:LYS:O	1:B:134:GLN:HB2	1.74	0.87
1:D:68:LEU:CD1	1:D:123:ILE:CD1	2.49	0.87
1:B:38:GLU:OE1	2:B:171:HOH:O	1.93	0.87
1:D:98:ARG:CD	2:D:254:HOH:O	2.19	0.87
1:B:93:ARG:HH12	1:B:117:THR:HG21	1.33	0.86
1:A:68:LEU:HD11	1:A:123:ILE:HD11	1.55	0.86
1:E:66:GLY:N	1:E:125:LEU:HD11	1.90	0.86
1:E:64:GLY:O	1:E:125:LEU:HD13	1.74	0.86
1:B:68:LEU:HD23	1:B:123:ILE:HD13	1.58	0.85
1:F:6:ARG:HG3	2:F:288:HOH:O	1.75	0.85
1:E:124:HIS:CE1	2:E:472:HOH:O	2.29	0.85
1:C:68:LEU:CD2	1:C:123:ILE:HD13	2.07	0.85
1:F:107:HIS:HB3	2:F:145:HOH:O	1.76	0.84
1:F:99:ARG:O	2:F:282:HOH:O	1.94	0.84
1:A:57:MET:O	1:A:61:LEU:HD11	1.76	0.84
1:B:68:LEU:HD21	1:B:123:ILE:CD1	2.08	0.84
1:C:24:ARG:CD	2:C:488:HOH:O	1.88	0.84
1:F:98:ARG:HG3	1:F:98:ARG:HH11	1.43	0.84
1:E:22:THR:HG22	2:E:144:HOH:O	1.77	0.83
1:F:26:LEU:HD11	1:F:27:TYR:CD2	2.11	0.83
1:A:68:LEU:CD1	1:A:123:ILE:HD13	2.07	0.83
1:D:126:GLU:HG3	2:D:383:HOH:O	1.77	0.83
1:B:57:MET:O	1:B:61:LEU:HD23	1.78	0.83
1:F:65:GLU:C	1:F:125:LEU:CD1	2.47	0.83
1:F:68:LEU:HD13	1:F:123:ILE:HG21	1.59	0.82
1:D:6:ARG:NH1	2:D:515:HOH:O	2.12	0.82
1:E:92:LEU:HD13	1:E:93:ARG:N	1.93	0.82
1:C:60:TYR:OH	2:C:415:HOH:O	1.97	0.82
1:F:26:LEU:HD13	1:F:27:TYR:CD2	2.15	0.82
1:C:65:GLU:C	1:C:125:LEU:CD2	2.49	0.81
1:A:103:ARG:NH2	2:A:205:HOH:O	2.12	0.81
1:D:130:ALA:O	1:D:133:ARG:HG3	1.81	0.80
1:E:112:GLU:HG3	2:E:152:HOH:O	1.81	0.80
1:C:67:SER:O	1:C:68:LEU:HD22	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:GLU:CD	2:E:152:HOH:O	2.19	0.79
1:F:68:LEU:CD1	1:F:123:ILE:CD1	2.50	0.79
1:C:60:TYR:CZ	2:C:415:HOH:O	2.34	0.79
1:B:129:ASN:ND2	2:B:400:HOH:O	2.13	0.79
1:E:92:LEU:HD13	1:E:92:LEU:C	2.02	0.79
1:B:93:ARG:NH1	1:B:117:THR:HG22	1.97	0.79
1:E:66:GLY:N	1:E:125:LEU:CD1	2.46	0.79
1:B:93:ARG:HH11	1:B:117:THR:CG2	1.96	0.79
1:E:112:GLU:CG	2:E:152:HOH:O	2.30	0.79
1:F:26:LEU:HD12	1:F:27:TYR:CD2	2.05	0.78
1:F:81:PRO:HD2	1:F:84:LEU:CD2	2.14	0.77
1:B:14:ASP:O	2:B:177:HOH:O	2.03	0.76
1:B:124:HIS:HE1	1:B:126:GLU:HB3	1.50	0.76
1:E:124:HIS:ND1	2:E:472:HOH:O	2.17	0.76
1:B:5:MET:HE1	1:B:102:TRP:HH2	1.50	0.76
1:A:18:PRO:HB2	1:A:20:HIS:CD2	2.21	0.76
1:B:93:ARG:NH2	1:C:91:GLU:OE2	2.19	0.76
1:B:26:LEU:HD12	1:B:27:TYR:HD2	1.50	0.75
1:C:65:GLU:C	1:C:125:LEU:HD21	2.05	0.75
1:F:26:LEU:CD1	1:F:27:TYR:CE2	2.70	0.74
1:A:136:THR:O	2:A:145:HOH:O	2.05	0.74
1:B:124:HIS:CE1	1:B:126:GLU:HB3	2.22	0.74
1:B:93:ARG:NH1	1:B:117:THR:CB	2.50	0.74
1:E:58:ALA:HB3	1:E:59:PRO:HD3	1.70	0.74
1:E:93:ARG:O	1:E:94:SER:CB	2.36	0.74
1:C:60:TYR:OH	2:C:563:HOH:O	2.05	0.73
1:B:103:ARG:NH2	1:B:115:SER:CB	2.51	0.73
1:B:68:LEU:HD23	1:B:123:ILE:CD1	2.15	0.73
1:C:119:GLU:OE2	2:C:140:HOH:O	2.07	0.73
1:F:38:GLU:OE1	2:F:338:HOH:O	2.07	0.73
1:D:126:GLU:CG	2:D:383:HOH:O	2.35	0.72
1:B:131:LYS:HA	1:B:134:GLN:OE1	1.88	0.72
1:F:50:GLU:OE1	2:F:303:HOH:O	2.08	0.71
1:C:108:ASP:O	2:C:168:HOH:O	2.09	0.70
1:F:26:LEU:C	1:F:26:LEU:HD13	2.12	0.70
1:C:58:ALA:N	1:C:59:PRO:CD	2.55	0.70
1:C:57:MET:O	1:C:61:LEU:HD23	1.92	0.70
1:F:68:LEU:HD13	1:F:123:ILE:CG2	2.21	0.70
1:B:63:PRO:O	2:B:304:HOH:O	2.10	0.70
1:C:124:HIS:CB	1:C:127:LYS:HD2	2.22	0.70
1:E:65:GLU:O	1:E:125:LEU:HD11	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:ARG:NH1	2:C:530:HOH:O	2.25	0.69
1:C:66:GLY:CA	1:C:125:LEU:HD21	2.23	0.68
1:D:126:GLU:OE2	1:D:126:GLU:HA	1.93	0.68
1:D:119:GLU:CB	2:D:496:HOH:O	2.34	0.68
1:E:71:ALA:HB3	1:E:119:GLU:HB2	1.76	0.68
1:A:66:GLY:HA3	1:A:125:LEU:HD21	1.75	0.67
1:D:24:ARG:HG3	1:D:24:ARG:NH1	2.09	0.67
1:D:26:LEU:HD13	1:D:27:TYR:CD2	2.30	0.67
1:E:60:TYR:CD2	1:E:60:TYR:N	2.61	0.67
1:D:119:GLU:OE2	2:D:451:HOH:O	2.12	0.67
1:A:91:GLU:OE1	2:A:143:HOH:O	2.11	0.66
1:B:119:GLU:HB2	2:B:354:HOH:O	1.94	0.66
1:C:124:HIS:HB3	1:C:127:LYS:HD2	1.77	0.66
1:C:68:LEU:HD23	1:C:123:ILE:CD1	2.25	0.66
1:E:70:THR:HG21	1:E:99:ARG:NH1	2.10	0.66
1:C:124:HIS:CG	1:C:127:LYS:HD2	2.31	0.66
1:E:23:VAL:HB	2:E:150:HOH:O	1.95	0.66
1:A:66:GLY:N	1:A:125:LEU:CD2	2.58	0.66
1:A:67:SER:O	1:A:68:LEU:HD12	1.95	0.66
1:C:60:TYR:HE1	2:C:520:HOH:O	1.48	0.66
1:E:62:GLU:HB3	1:E:63:PRO:HD2	1.77	0.66
1:F:5:MET:HG2	1:F:92:LEU:HD22	1.76	0.66
1:E:60:TYR:HD2	1:E:60:TYR:N	1.93	0.66
1:B:5:MET:CE	1:B:102:TRP:HH2	2.07	0.65
1:B:103:ARG:NE	2:B:460:HOH:O	1.85	0.65
1:D:24:ARG:HH11	1:D:24:ARG:HG3	1.60	0.65
1:D:20:HIS:HA	1:D:25:HIS:CE1	2.30	0.65
1:C:68:LEU:CD2	1:C:123:ILE:HD11	2.14	0.65
1:A:67:SER:C	1:A:68:LEU:HD12	2.17	0.65
1:F:125:LEU:N	1:F:125:LEU:HD12	2.11	0.65
1:B:67:SER:C	1:B:68:LEU:CD2	2.61	0.64
1:D:71:ALA:CB	2:D:496:HOH:O	2.09	0.64
1:F:10:ARG:HG2	1:F:91:GLU:HG3	1.79	0.64
1:B:25:HIS:O	1:B:28:PRO:HD3	1.97	0.64
1:A:124:HIS:CE1	1:A:126:GLU:HB2	2.33	0.64
1:E:137:PRO:HD3	1:F:84:LEU:HD11	1.80	0.64
1:A:53:CYS:O	1:A:57:MET:HG2	1.99	0.63
1:B:93:ARG:CZ	1:B:117:THR:HG21	2.28	0.63
1:C:63:PRO:HD3	2:C:553:HOH:O	1.97	0.63
1:B:57:MET:O	1:B:61:LEU:CD2	2.47	0.63
1:B:137:PRO:C	2:B:258:HOH:O	2.37	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ARG:CZ	1:E:121:ALA:HB2	2.23	0.63
1:D:5:MET:HE1	1:D:102:TRP:HH2	1.62	0.62
1:B:99:ARG:HG3	2:B:202:HOH:O	1.99	0.62
1:C:60:TYR:CD1	2:C:520:HOH:O	2.34	0.62
1:D:24:ARG:NE	2:D:358:HOH:O	2.33	0.62
1:D:26:LEU:CD1	1:D:27:TYR:CD2	2.83	0.62
1:D:62:GLU:N	1:D:65:GLU:OE2	2.26	0.62
1:C:19:PRO:HG2	2:C:372:HOH:O	1.99	0.62
1:C:65:GLU:CA	1:C:125:LEU:HD23	2.30	0.62
1:F:31:PRO:HD2	1:F:32:GLU:H	1.65	0.62
1:E:46:VAL:HG22	1:E:72:ILE:HG12	1.83	0.61
1:E:92:LEU:C	1:E:92:LEU:CD1	2.68	0.61
1:B:93:ARG:HH11	1:B:117:THR:HB	1.65	0.61
1:A:68:LEU:CD1	1:A:123:ILE:HD11	2.24	0.61
1:C:65:GLU:C	1:C:125:LEU:HD23	2.20	0.61
1:B:93:ARG:NH1	1:B:117:THR:HB	2.16	0.60
1:C:64:GLY:O	1:C:125:LEU:HD23	2.00	0.60
1:E:137:PRO:HD3	1:F:84:LEU:CD1	2.30	0.60
1:D:91:GLU:CD	1:D:93:ARG:HH12	2.05	0.60
1:E:62:GLU:HB3	1:E:63:PRO:CD	2.31	0.60
1:A:68:LEU:HA	2:A:442:HOH:O	2.02	0.60
1:C:60:TYR:CE2	2:C:415:HOH:O	2.53	0.59
1:E:107:HIS:CD2	2:E:425:HOH:O	2.55	0.59
1:C:10:ARG:HH21	1:C:89:THR:HG21	1.67	0.59
1:D:24:ARG:CD	2:D:358:HOH:O	2.50	0.59
1:B:9:GLU:HB2	2:B:547:HOH:O	2.01	0.59
1:C:68:LEU:N	1:C:68:LEU:HD22	2.18	0.59
1:C:68:LEU:HD21	1:C:123:ILE:HD13	1.68	0.59
1:A:65:GLU:C	1:A:125:LEU:CD2	2.71	0.58
1:F:80:THR:HG23	1:F:84:LEU:HD22	1.86	0.58
1:A:61:LEU:N	1:A:61:LEU:HD12	2.18	0.58
1:A:62:GLU:OE1	2:A:518:HOH:O	2.17	0.58
1:B:26:LEU:HD11	1:B:27:TYR:CD2	2.37	0.58
1:D:66:GLY:HA3	1:D:125:LEU:HD21	1.86	0.58
1:D:60:TYR:N	1:D:60:TYR:CD2	2.72	0.58
1:B:5:MET:HG2	1:B:92:LEU:HD22	1.84	0.58
1:A:132:VAL:O	1:A:135:LYS:N	2.33	0.58
1:B:124:HIS:HE1	1:B:126:GLU:CB	2.17	0.57
1:C:99:ARG:HH11	1:C:99:ARG:HG2	1.70	0.57
1:A:136:THR:C	2:A:264:HOH:O	2.43	0.57
1:F:68:LEU:CD1	1:F:123:ILE:HG21	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:SER:C	1:F:68:LEU:HD12	2.26	0.57
1:F:10:ARG:HA	1:F:90:ALA:O	2.05	0.57
1:E:66:GLY:CA	1:E:125:LEU:HD11	2.34	0.57
1:E:94:SER:C	2:E:140:HOH:O	2.43	0.57
1:B:18:PRO:HG2	1:B:21:LYS:HG2	1.87	0.56
1:A:58:ALA:N	1:A:59:PRO:HD2	2.20	0.56
1:D:24:ARG:HH11	1:D:24:ARG:CG	2.19	0.56
1:B:68:LEU:HD22	1:B:68:LEU:N	2.21	0.56
1:C:68:LEU:HD23	1:C:123:ILE:HD13	1.82	0.56
1:A:66:GLY:CA	1:A:125:LEU:HD21	2.34	0.56
1:D:68:LEU:CD1	1:D:123:ILE:CG1	2.83	0.56
1:B:5:MET:CE	1:B:102:TRP:CH2	2.88	0.56
1:E:92:LEU:CD1	1:E:94:SER:H	2.18	0.56
1:A:6:ARG:HG3	1:A:9:GLU:HB2	1.88	0.56
1:F:125:LEU:CD1	1:F:125:LEU:N	2.69	0.55
1:E:99:ARG:HD3	1:E:120:ARG:O	2.06	0.55
1:C:10:ARG:HD3	2:C:351:HOH:O	2.06	0.55
1:A:66:GLY:N	1:A:125:LEU:HD22	2.22	0.55
1:C:67:SER:C	1:C:68:LEU:CD2	2.66	0.55
1:E:35:GLU:HB3	2:E:322:HOH:O	2.05	0.55
1:B:93:ARG:CZ	1:B:117:THR:CG2	2.82	0.55
1:C:61:LEU:HD12	1:C:65:GLU:HB3	1.89	0.55
1:B:93:ARG:HH11	1:B:117:THR:CB	2.15	0.54
1:E:59:PRO:HB2	1:E:60:TYR:CD2	2.43	0.54
1:D:5:MET:CE	1:D:102:TRP:HH2	2.20	0.54
1:B:93:ARG:HG3	1:B:103:ARG:N	2.23	0.54
1:D:67:SER:C	1:D:68:LEU:HD12	2.27	0.54
1:F:53:CYS:O	1:F:57:MET:HG3	2.08	0.54
1:C:87:THR:HG22	2:C:161:HOH:O	2.06	0.54
1:D:68:LEU:HD13	1:D:123:ILE:CG2	2.38	0.54
1:E:64:GLY:C	1:E:125:LEU:HD13	2.29	0.54
1:F:9:GLU:C	1:F:10:ARG:HG3	2.27	0.54
1:C:68:LEU:N	1:C:68:LEU:CD2	2.71	0.53
1:D:77:THR:O	2:D:470:HOH:O	2.18	0.53
1:F:71:ALA:HB3	1:F:119:GLU:HB3	1.91	0.53
1:C:130:ALA:N	1:C:133:ARG:HH21	2.06	0.53
1:D:20:HIS:HA	1:D:25:HIS:NE2	2.24	0.53
1:D:68:LEU:CD1	1:D:123:ILE:HG12	2.39	0.53
1:E:125:LEU:HD12	1:E:125:LEU:H	1.73	0.52
1:F:98:ARG:HG3	1:F:98:ARG:NH1	2.17	0.52
1:D:23:VAL:HG11	1:D:36:ALA:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:CD1	1:A:61:LEU:N	2.73	0.52
1:A:69:GLY:N	2:A:442:HOH:O	2.29	0.52
1:A:84:LEU:HD12	1:A:84:LEU:N	2.24	0.52
1:C:10:ARG:HG2	1:C:91:GLU:HG3	1.90	0.52
1:E:58:ALA:N	1:E:59:PRO:CD	2.73	0.52
1:B:100:LEU:HD12	1:B:100:LEU:N	2.25	0.52
1:B:35:GLU:CG	2:B:309:HOH:O	2.01	0.51
1:D:66:GLY:N	1:D:125:LEU:CD2	2.73	0.51
1:E:125:LEU:H	1:E:125:LEU:CD1	2.24	0.51
1:E:18:PRO:HG2	1:E:21:LYS:HG2	1.93	0.51
1:B:68:LEU:N	1:B:68:LEU:CD2	2.73	0.51
1:C:131:LYS:NZ	2:C:285:HOH:O	1.80	0.51
1:D:68:LEU:N	1:D:68:LEU:HD12	2.25	0.51
1:F:10:ARG:NH2	1:F:89:THR:HG21	2.26	0.51
1:C:22:THR:HG22	2:C:543:HOH:O	2.10	0.51
1:E:68:LEU:HD21	1:E:128:PHE:CE1	2.46	0.51
1:E:92:LEU:HD13	1:E:94:SER:H	1.76	0.51
1:C:62:GLU:O	1:C:65:GLU:HB2	2.11	0.51
1:D:60:TYR:O	1:D:61:LEU:HD23	2.10	0.51
1:D:5:MET:HG2	1:D:92:LEU:HD22	1.92	0.51
1:E:68:LEU:HD21	1:E:128:PHE:CZ	2.45	0.51
1:F:61:LEU:HD22	2:F:151:HOH:O	2.11	0.51
1:F:62:GLU:O	1:F:65:GLU:HB2	2.11	0.51
1:F:119:GLU:CB	2:F:464:HOH:O	2.45	0.50
1:F:9:GLU:O	1:F:91:GLU:HA	2.11	0.50
1:F:26:LEU:CD1	1:F:26:LEU:C	2.80	0.50
1:A:84:LEU:CD1	1:B:137:PRO:HD3	2.41	0.50
1:D:68:LEU:HD13	1:D:123:ILE:HG21	1.93	0.50
1:A:57:MET:O	1:A:61:LEU:HD12	1.98	0.50
1:E:125:LEU:HB2	2:E:146:HOH:O	2.10	0.50
1:B:57:MET:HB3	1:B:61:LEU:HD21	1.94	0.50
1:A:55:ARG:HA	2:A:193:HOH:O	2.12	0.49
1:F:125:LEU:CD1	1:F:125:LEU:H	2.25	0.49
1:F:127:LYS:O	1:F:130:ALA:HB3	2.12	0.49
1:E:93:ARG:O	1:E:93:ARG:CG	2.60	0.49
1:A:96:GLU:CD	1:C:99:ARG:HH21	2.15	0.49
1:F:84:LEU:N	1:F:84:LEU:HD12	2.27	0.49
1:E:125:LEU:HD12	1:E:125:LEU:N	2.27	0.49
1:D:107:HIS:HB2	2:D:187:HOH:O	2.12	0.49
1:A:124:HIS:ND1	1:A:127:LYS:HG3	2.28	0.49
1:D:132:VAL:C	1:D:134:GLN:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:PRO:HD3	1:D:84:LEU:HD13	1.95	0.49
1:F:65:GLU:CA	1:F:125:LEU:CD1	2.91	0.49
1:F:31:PRO:CD	1:F:32:GLU:H	2.24	0.49
1:F:58:ALA:N	1:F:59:PRO:CD	2.76	0.49
1:F:68:LEU:N	1:F:68:LEU:HD12	2.28	0.49
1:E:97:GLY:C	1:E:99:ARG:H	2.16	0.48
1:B:26:LEU:C	1:B:26:LEU:HD13	2.33	0.48
1:C:92:LEU:HD21	1:C:95:VAL:CG2	2.44	0.48
1:C:57:MET:O	1:C:61:LEU:CD2	2.59	0.48
1:D:98:ARG:NE	2:D:254:HOH:O	2.42	0.48
1:E:53:CYS:O	1:E:57:MET:HG2	2.14	0.48
1:F:119:GLU:CG	2:F:464:HOH:O	2.62	0.48
1:E:66:GLY:N	1:E:125:LEU:HD12	2.27	0.47
1:E:60:TYR:HD2	1:E:60:TYR:H	1.60	0.47
1:C:75:THR:HB	1:C:77:THR:HG23	1.96	0.47
1:F:26:LEU:O	1:F:26:LEU:HD13	2.13	0.47
1:D:68:LEU:HD21	1:D:128:PHE:CE1	2.49	0.47
1:C:68:LEU:HD23	1:C:123:ILE:HG12	1.97	0.47
1:D:62:GLU:HB3	1:D:63:PRO:HD2	1.95	0.47
1:F:103:ARG:NH2	1:F:115:SER:HB2	2.29	0.47
1:F:5:MET:HG2	1:F:92:LEU:CD2	2.43	0.47
1:E:70:THR:HG21	1:E:99:ARG:HH11	1.75	0.47
1:F:84:LEU:N	1:F:84:LEU:CD1	2.78	0.47
1:C:29:GLU:O	1:C:31:PRO:HD3	2.15	0.47
1:C:65:GLU:CA	1:C:125:LEU:CD2	2.93	0.47
1:C:57:MET:C	1:C:59:PRO:HD2	2.36	0.46
1:C:22:THR:HA	1:C:39:VAL:O	2.15	0.46
1:D:26:LEU:HD12	1:D:27:TYR:HD2	1.80	0.46
1:D:68:LEU:N	1:D:68:LEU:CD1	2.79	0.46
1:A:84:LEU:HD11	1:B:137:PRO:HD3	1.98	0.45
1:D:24:ARG:HD3	2:D:358:HOH:O	2.14	0.45
1:D:58:ALA:N	1:D:59:PRO:CD	2.79	0.45
1:C:99:ARG:HH11	1:C:99:ARG:CG	2.29	0.45
1:A:68:LEU:HD13	1:A:123:ILE:HG12	1.97	0.45
1:A:7:VAL:HG13	1:A:93:ARG:O	2.16	0.45
1:E:14:ASP:OD2	1:E:87:THR:HG23	2.17	0.45
1:D:26:LEU:CD1	1:D:27:TYR:HD2	2.26	0.45
1:E:59:PRO:HB2	1:E:60:TYR:HD2	1.80	0.45
1:F:66:GLY:N	1:F:125:LEU:HD11	2.24	0.45
1:A:58:ALA:N	1:A:59:PRO:CD	2.80	0.45
1:B:7:VAL:HG22	1:B:94:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:GLY:HA3	1:C:125:LEU:HD21	1.97	0.45
1:F:135:LYS:O	1:F:135:LYS:HG2	2.17	0.45
1:B:124:HIS:CE1	1:B:126:GLU:CB	2.94	0.45
1:B:103:ARG:NH2	1:B:115:SER:OG	2.49	0.44
1:A:66:GLY:HA3	1:A:125:LEU:CD2	2.44	0.44
1:C:124:HIS:HB3	1:C:127:LYS:HB2	1.99	0.44
1:A:66:GLY:CA	1:A:125:LEU:CD2	2.95	0.44
1:C:65:GLU:HG2	2:C:150:HOH:O	2.17	0.44
1:A:103:ARG:HG3	1:A:103:ARG:HH11	1.82	0.44
1:F:76:HIS:HA	1:F:113:ILE:O	2.17	0.44
1:F:124:HIS:CG	1:F:127:LYS:HD2	2.51	0.44
1:F:10:ARG:HG2	1:F:91:GLU:CG	2.46	0.43
1:B:5:MET:HE2	1:B:102:TRP:CH2	2.53	0.43
1:C:68:LEU:HD23	1:C:123:ILE:CG1	2.47	0.43
1:B:130:ALA:O	1:B:134:GLN:HG3	2.18	0.43
1:C:58:ALA:HB3	1:C:59:PRO:HD3	1.99	0.43
1:C:58:ALA:N	1:C:59:PRO:HD2	2.30	0.43
1:F:68:LEU:N	1:F:68:LEU:CD1	2.81	0.43
1:C:96:GLU:HB3	1:C:97:GLY:H	1.59	0.43
1:F:23:VAL:HA	1:F:41:ALA:HB2	2.00	0.43
1:C:64:GLY:C	1:C:125:LEU:HD23	2.39	0.43
1:C:73:CYS:O	1:C:116:GLY:HA3	2.18	0.43
1:D:39:VAL:HG11	1:D:79:ALA:HB1	2.00	0.43
1:C:72:ILE:HD12	1:C:118:HIS:HB2	2.00	0.43
1:B:131:LYS:HA	1:B:134:GLN:CD	2.38	0.43
1:D:26:LEU:CD1	1:D:27:TYR:CE2	3.02	0.42
1:D:50:GLU:OE1	2:D:200:HOH:O	2.21	0.42
1:A:75:THR:HB	1:A:77:THR:HG23	2.00	0.42
1:B:6:ARG:C	1:B:92:LEU:HD23	2.39	0.42
1:C:68:LEU:HD11	1:D:37:PRO:HG2	2.00	0.42
1:B:131:LYS:O	1:B:134:GLN:CB	2.56	0.42
1:B:26:LEU:HD11	1:B:27:TYR:CE2	2.55	0.42
1:F:18:PRO:HG2	1:F:21:LYS:HG2	2.01	0.42
1:D:20:HIS:HA	1:D:25:HIS:CD2	2.55	0.42
1:D:26:LEU:HD13	1:D:27:TYR:CE2	2.55	0.42
1:E:11:PHE:HZ	1:E:55:ARG:CZ	2.33	0.42
1:D:66:GLY:CA	1:D:125:LEU:HD21	2.50	0.41
1:E:124:HIS:O	1:E:125:LEU:C	2.58	0.41
1:E:137:PRO:CD	1:F:84:LEU:HD12	2.50	0.41
1:F:67:SER:HA	1:F:121:ALA:O	2.20	0.41
1:B:72:ILE:HG23	1:B:72:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:THR:CG2	2:C:543:HOH:O	2.67	0.41
1:B:93:ARG:HH11	1:B:117:THR:HG22	1.75	0.41
1:C:82:PRO:HG3	2:C:543:HOH:O	2.20	0.41
1:B:65:GLU:C	1:B:125:LEU:CD2	2.88	0.41
1:C:60:TYR:HB3	2:C:184:HOH:O	2.20	0.41
1:F:93:ARG:HD3	1:F:93:ARG:HA	1.90	0.41
1:A:124:HIS:HE1	1:A:126:GLU:HB2	1.82	0.41
1:C:17:VAL:HA	1:C:18:PRO:HD3	1.98	0.41
1:D:17:VAL:HA	1:D:18:PRO:HD3	1.86	0.41
1:D:53:CYS:O	1:D:57:MET:HG3	2.21	0.41
1:B:70:THR:O	1:B:71:ALA:HB2	2.21	0.41
1:E:12:THR:HG22	2:E:261:HOH:O	2.20	0.41
1:E:36:ALA:HA	1:E:37:PRO:HD3	1.93	0.41
1:A:84:LEU:CD1	1:A:84:LEU:N	2.84	0.40
1:E:130:ALA:HA	1:E:133:ARG:HE	1.86	0.40
1:E:62:GLU:CB	1:E:63:PRO:CD	2.97	0.40
1:F:68:LEU:HD21	1:F:128:PHE:CE1	2.56	0.40
1:F:30:SER:HA	1:F:31:PRO:HD3	1.96	0.40
1:E:50:GLU:OE1	1:F:42:THR:HB	2.22	0.40
1:A:68:LEU:HD13	1:A:123:ILE:CD1	2.44	0.40
1:A:23:VAL:HG23	1:A:23:VAL:H	1.56	0.40
1:C:23:VAL:HA	1:C:41:ALA:HB2	2.02	0.40
1:D:46:VAL:O	1:D:50:GLU:HG3	2.21	0.40

All (6) 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:C:62:GLU:OE1	1:D:131:LYS:CD[4_444]	1.82	0.38
2:A:169:HOH:O	2:E:349:HOH:O[4_444]	2.03	0.17
2:A:203:HOH:O	2:A:290:HOH:O[2_453]	2.13	0.07
1:C:62:GLU:OE1	1:D:131:LYS:NZ[4_444]	2.14	0.06
1:C:97:GLY:O	1:D:134:GLN:OE1[4_444]	2.19	0.01
2:D:147:HOH:O	2:F:155:HOH:O[1_554]	2.19	0.01

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	133/143 (93%)	129 (97%)	4 (3%)	0	100	100
1	B	131/143 (92%)	122 (93%)	9 (7%)	0	100	100
1	C	129/143 (90%)	123 (95%)	5 (4%)	1 (1%)	19	23
1	D	128/143 (90%)	123 (96%)	5 (4%)	0	100	100
1	E	123/143 (86%)	119 (97%)	3 (2%)	1 (1%)	19	23
1	F	131/143 (92%)	128 (98%)	3 (2%)	0	100	100
All	All	775/858 (90%)	744 (96%)	29 (4%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	96	GLU
1	E	98	ARG

5.3.2 Protein sidechains (i)

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	110/113 (97%)	109 (99%)	1 (1%)	78	89
1	B	109/113 (96%)	106 (97%)	3 (3%)	43	60
1	C	107/113 (95%)	104 (97%)	3 (3%)	43	60
1	D	106/113 (94%)	102 (96%)	4 (4%)	33	47
1	E	103/113 (91%)	97 (94%)	6 (6%)	20	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	109/113 (96%)	107 (98%)	2 (2%)	59	75
All	All	644/678 (95%)	625 (97%)	19 (3%)	41	57

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ILE
1	B	13	HIS
1	B	68	LEU
1	B	125	LEU
1	C	68	LEU
1	C	72	ILE
1	C	96	GLU
1	D	13	HIS
1	D	60	TYR
1	D	61	LEU
1	D	84	LEU
1	E	23	VAL
1	E	60	TYR
1	E	61	LEU
1	E	68	LEU
1	E	93	ARG
1	E	107	HIS
1	F	7	VAL
1	F	13	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	25	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 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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	135/143 (94%)	-0.04	2 (1%)	73	79	5, 22, 45, 68	0
1	B	133/143 (93%)	0.08	6 (4%)	33	40	10, 22, 58, 81	0
1	C	131/143 (91%)	0.11	7 (5%)	26	33	10, 24, 57, 79	0
1	D	130/143 (90%)	0.09	5 (3%)	40	47	12, 23, 58, 74	0
1	E	127/143 (88%)	0.33	9 (7%)	16	21	14, 31, 68, 92	0
1	F	133/143 (93%)	0.27	9 (6%)	17	22	13, 29, 60, 82	0
All	All	789/858 (91%)	0.14	38 (4%)	30	37	5, 26, 61, 92	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	60	TYR	5.7
1	E	138	ALA	4.4
1	B	68	LEU	4.2
1	E	60	TYR	3.5
1	E	97	GLY	3.5
1	F	34	ALA	3.4
1	F	125	LEU	3.4
1	B	94	SER	3.3
1	D	133	ARG	3.3
1	E	127	LYS	3.2
1	C	63	PRO	3.2
1	E	125	LEU	3.2
1	D	63	PRO	3.1
1	F	6	ARG	3.1
1	B	134	GLN	3.1
1	F	7	VAL	3.0
1	C	96	GLU	3.0
1	B	6	ARG	2.9
1	C	97	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	6	ARG	2.8
1	C	126	GLU	2.6
1	F	64	GLY	2.5
1	D	24	ARG	2.4
1	A	61	LEU	2.4
1	E	110	VAL	2.4
1	D	64	GLY	2.4
1	F	63	PRO	2.4
1	F	136	THR	2.4
1	E	93	ARG	2.3
1	C	125	LEU	2.2
1	C	19	PRO	2.2
1	E	59	PRO	2.2
1	F	137	PRO	2.1
1	B	63	PRO	2.1
1	F	95	VAL	2.0
1	A	6	ARG	2.0
1	E	10	ARG	2.0
1	B	130	ALA	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.