



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:25 AM UTC

PDB ID : 2IUS / pdb_00002ius
Title : E. coli FtsK motor domain
Authors : Massey, T.H.; Mercogliano, C.P.; Yates, J.; Sherratt, D.J.; Lowe, J.
Deposited on : 2006-06-07
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

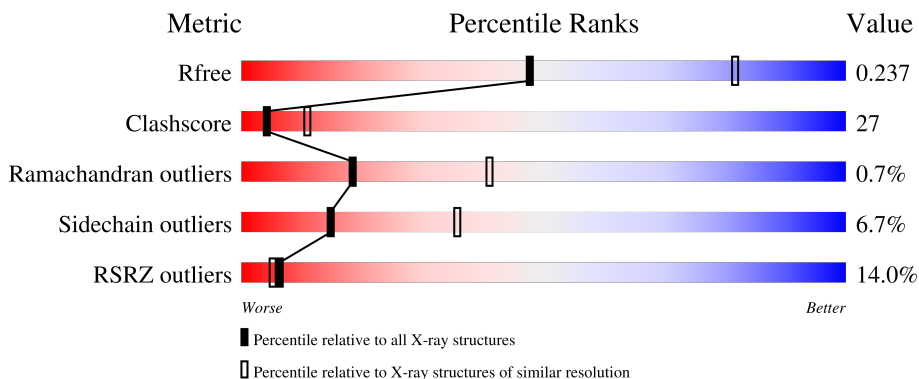
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



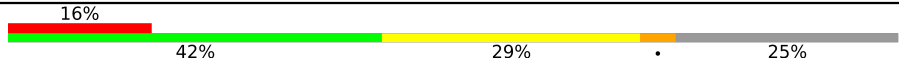
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	512	 7% 40% 32% 23%
1	B	512	 5% 44% 29% 23%
1	C	512	 15% 41% 33% 23%
1	D	512	 6% 42% 32% 23%
1	E	512	 15% 40% 28% 5% 26%

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Mol	Chain	Length	Quality of chain
1	F	512	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (16%), a green segment (42%), a yellow segment (29%), and a grey segment (25%). A small black dot is located on the yellow segment.</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18569 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 DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	393	Total 3029	C 1930	N 532	O 551	S 16	0	0	1
1	B	393	Total 3029	C 1930	N 532	O 551	S 16	0	0	1
1	C	393	Total 3029	C 1930	N 532	O 551	S 16	0	0	1
1	D	394	Total 3036	C 1935	N 533	O 552	S 16	0	0	1
1	E	381	Total 2941	C 1877	N 512	O 536	S 16	0	0	1
1	F	382	Total 2952	C 1883	N 516	O 537	S 16	0	0	1

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	997	ALA	LYS	engineered mutation	UNP P46889
B	997	ALA	LYS	engineered mutation	UNP P46889
C	997	ALA	LYS	engineered mutation	UNP P46889
D	997	ALA	LYS	engineered mutation	UNP P46889
E	997	ALA	LYS	engineered mutation	UNP P46889
F	997	ALA	LYS	engineered mutation	UNP P46889

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total 91	O 91	0	0
2	B	94	Total 94	O 94	0	0
2	C	80	Total 80	O 80	0	0

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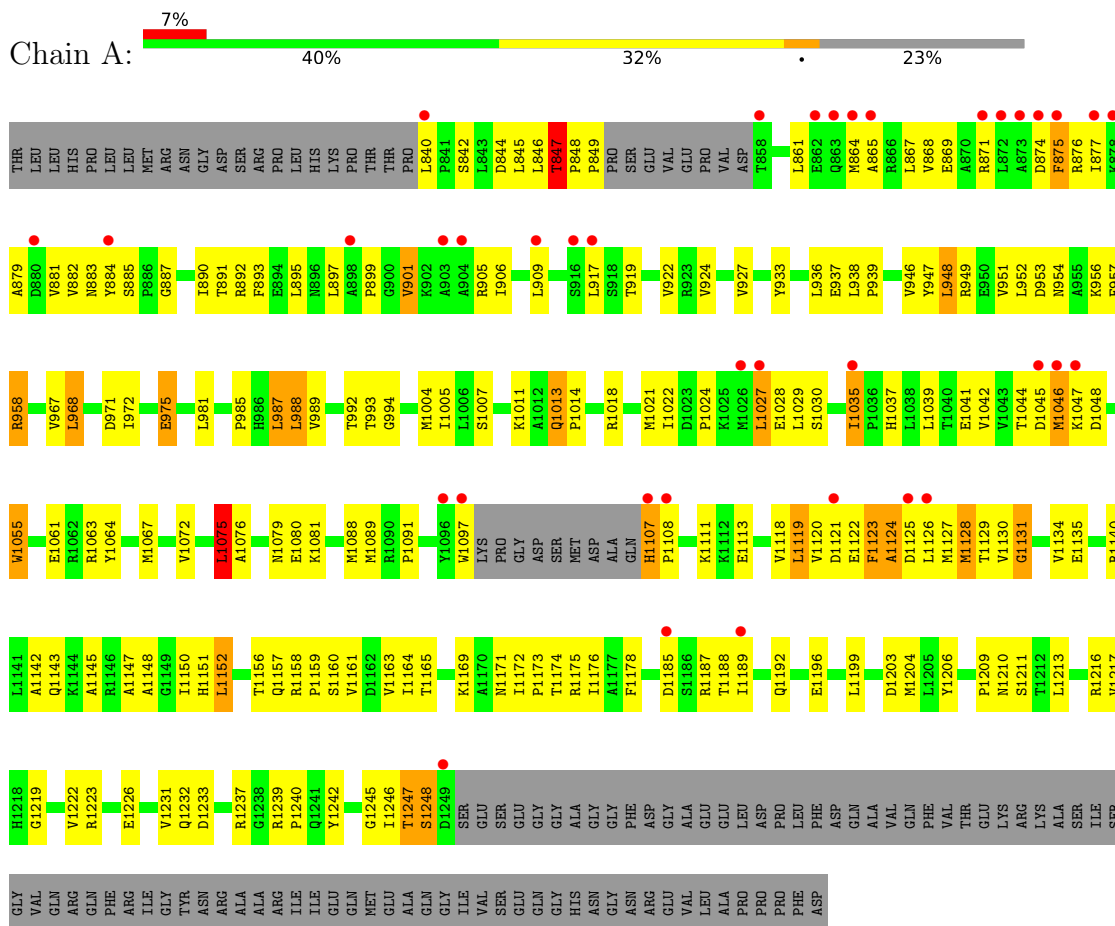
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	116	Total 116	O 116	0	0
2	E	99	Total 99	O 99	0	0
2	F	73	Total 73	O 73	0	0

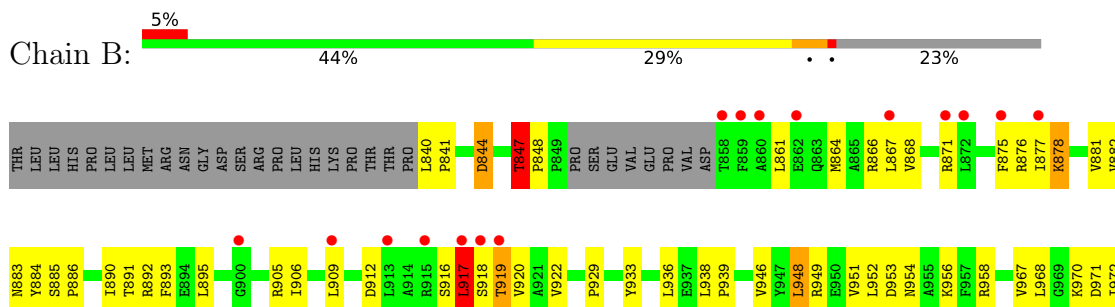
3 Residue-property plots i

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

• Molecule 1: DNA TRANSLOCASE FTSK

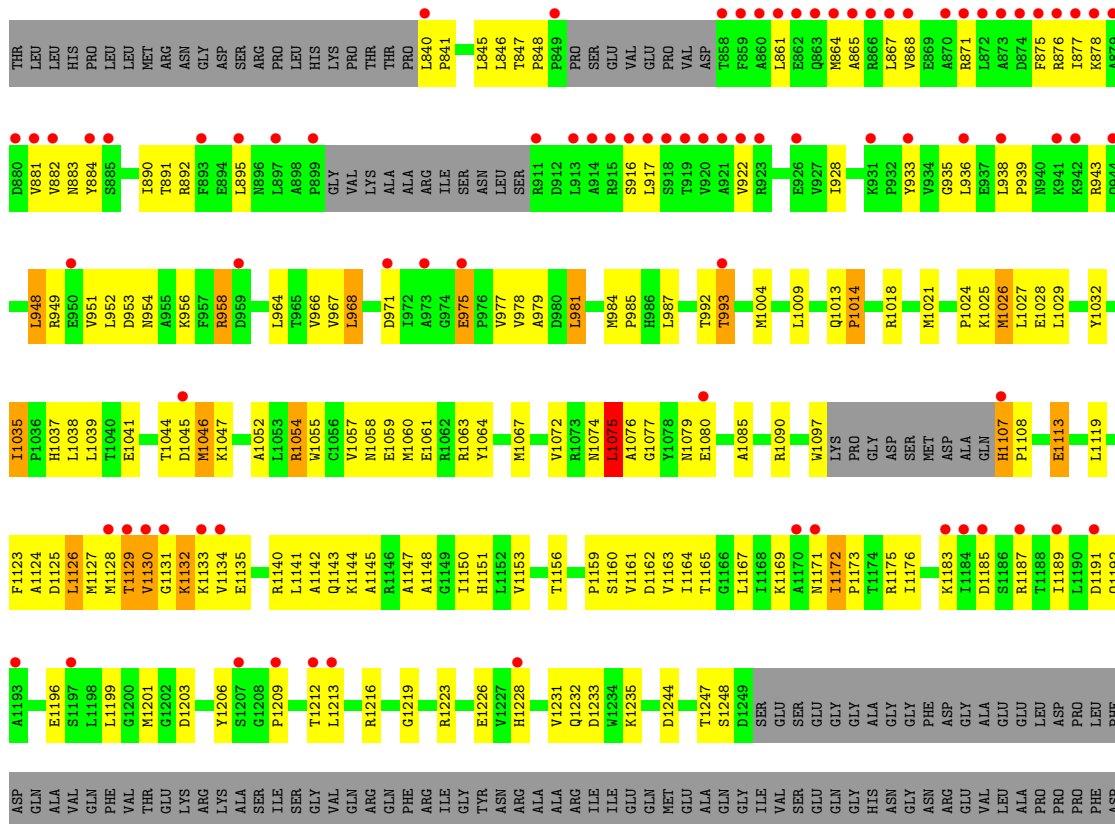


• Molecule 1: DNA TRANSLOCASE FTSK



ARG	LYS	ALA	SER	ILE	PRO	SER	GLY	VAL	GLN	ARG	GLN	ARG	GLN	PHE	ARG	PHE	ARG	ILE	ILE	GLY	TVR	ARG	ASN	ASN	GLN	ALA	ALA	GLN	GLY	ILE	VAL	SER	SER	GLU	GLN	GLN	GLY	GLY	HIS	ASN	ASN	GLY	ASN	ASN	ARG	ARG	GLU	GLU	VAL	VAL	LEU	ALA	ALA	PRO	PRO	PRO	PHE	PHE	ASP
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● Molecule 1: DNA TRANSLOCASE FTSK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.60Å 117.20Å 132.80Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	100.00 – 2.70 100.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-2.70) 99.8 (100.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.298 0.243 , 0.237	Depositor DCC
R_{free} test set	4056 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtrriage
Anisotropy	0.266	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	18569	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.21 % 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 4.8823e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality 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	0.47	1/3083 (0.0%)	1.01	10/4186 (0.2%)
1	B	0.53	2/3083 (0.1%)	1.02	17/4186 (0.4%)
1	C	0.45	1/3083 (0.0%)	1.01	12/4186 (0.3%)
1	D	0.49	1/3090 (0.0%)	1.00	12/4194 (0.3%)
1	E	0.51	1/2994 (0.0%)	1.05	17/4066 (0.4%)
1	F	0.45	1/3005 (0.0%)	0.97	6/4080 (0.1%)
All	All	0.48	7/18338 (0.0%)	1.01	74/24898 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	918	SER	CA-C	7.14	1.59	1.53
1	D	1248	SER	C-N	-6.04	1.24	1.33
1	B	1248	SER	C-N	-5.76	1.25	1.33
1	E	1248	SER	C-N	-5.49	1.25	1.33
1	F	1248	SER	C-N	-5.37	1.25	1.33
1	A	1248	SER	C-N	-5.27	1.25	1.33
1	C	1248	SER	C-N	-5.25	1.26	1.33

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	1107	HIS	CA-C-N	9.42	131.62	119.84
1	E	1107	HIS	C-N-CA	9.42	131.62	119.84
1	B	918	SER	N-CA-C	9.29	122.30	109.11
1	A	1075	LEU	N-CA-C	-9.05	100.83	112.23
1	D	993	THR	N-CA-C	8.26	121.03	111.11
1	C	1013	GLN	N-CA-C	-8.26	99.59	110.40
1	C	1107	HIS	CA-C-N	8.23	130.13	119.84
1	C	1107	HIS	C-N-CA	8.23	130.13	119.84
1	E	993	THR	N-CA-C	7.68	120.33	111.11
1	E	917	LEU	N-CA-C	-6.97	99.21	108.34
1	F	1028	GLU	N-CA-C	6.92	118.62	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1013	GLN	N-CA-C	-6.80	101.49	110.40
1	A	1013	GLN	N-CA-C	-6.75	101.31	110.36
1	F	1075	LEU	N-CA-C	-6.66	103.84	112.23
1	C	847	THR	CA-C-N	6.47	127.05	120.38
1	C	847	THR	C-N-CA	6.47	127.05	120.38
1	D	887	GLY	CA-C-N	6.43	126.36	119.28
1	D	887	GLY	C-N-CA	6.43	126.36	119.28
1	B	1172	ILE	CA-C-N	6.43	126.01	119.19
1	B	1172	ILE	C-N-CA	6.43	126.01	119.19
1	B	993	THR	N-CA-C	6.42	118.28	111.28
1	F	1124	ALA	N-CA-C	-6.36	104.27	111.07
1	D	847	THR	CA-C-N	6.16	126.73	120.38
1	D	847	THR	C-N-CA	6.16	126.73	120.38
1	E	1172	ILE	CA-C-N	6.09	125.49	118.85
1	E	1172	ILE	C-N-CA	6.09	125.49	118.85
1	E	845	LEU	N-CA-C	-6.08	105.86	113.28
1	D	1178	PHE	N-CA-C	-6.04	101.00	110.36
1	B	1178	PHE	N-CA-C	-5.97	101.11	110.36
1	C	1172	ILE	CA-C-N	5.88	125.58	119.05
1	C	1172	ILE	C-N-CA	5.88	125.58	119.05
1	D	1013	GLN	N-CA-C	-5.85	102.52	110.36
1	A	1027	LEU	N-CA-C	5.84	120.10	111.87
1	C	1081	LYS	N-CA-C	-5.77	104.91	111.14
1	B	1107	HIS	CA-C-N	5.76	127.04	119.84
1	B	1107	HIS	C-N-CA	5.76	127.04	119.84
1	B	1143	GLN	N-CA-C	5.75	117.22	111.07
1	B	1108	PRO	N-CA-C	5.73	124.27	112.47
1	D	1075	LEU	N-CA-C	-5.72	105.19	111.82
1	E	1131	GLY	N-CA-C	5.71	118.14	110.43
1	C	1109	VAL	N-CA-C	-5.69	100.28	108.53
1	A	845	LEU	N-CA-C	-5.69	106.11	113.16
1	E	918	SER	N-CA-C	5.62	122.78	110.80
1	D	1143	GLN	N-CA-C	5.62	117.08	111.07
1	C	845	LEU	N-CA-C	-5.61	106.20	113.16
1	C	1143	GLN	N-CA-C	5.58	117.44	111.36
1	B	847	THR	CA-C-N	5.49	126.03	120.38
1	B	847	THR	C-N-CA	5.49	126.03	120.38
1	B	919	THR	CB-CA-C	-5.46	99.72	109.71
1	A	1081	LYS	N-CA-C	-5.42	105.46	111.36
1	E	1178	PHE	N-CA-C	-5.41	102.88	110.35
1	B	1189	ILE	CB-CA-C	-5.39	105.15	111.94
1	A	1055	TRP	N-CA-C	-5.38	105.11	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1181	SER	N-CA-C	5.38	118.31	111.69
1	E	1075	LEU	N-CA-C	-5.35	105.48	112.23
1	E	1124	ALA	N-CA-C	-5.31	105.50	111.28
1	E	1204	MET	N-CA-C	5.30	116.86	108.96
1	C	1178	PHE	N-CA-C	-5.29	103.71	110.53
1	E	919	THR	CB-CA-C	-5.26	100.08	109.71
1	F	1172	ILE	CA-C-N	5.25	124.58	118.85
1	F	1172	ILE	C-N-CA	5.25	124.58	118.85
1	E	1108	PRO	N-CA-C	5.25	123.29	112.47
1	B	917	LEU	N-CA-C	-5.22	98.98	108.65
1	A	1178	PHE	N-CA-C	-5.18	103.08	110.59
1	B	1204	MET	N-CA-C	5.16	116.65	108.96
1	A	847	THR	CA-C-N	5.16	125.69	120.38
1	A	847	THR	C-N-CA	5.16	125.69	120.38
1	E	1189	ILE	CB-CA-C	-5.15	105.17	111.92
1	A	1124	ALA	N-CA-C	-5.14	105.76	111.36
1	D	1189	ILE	CB-CA-C	-5.11	105.22	111.92
1	D	1012	ALA	N-CA-C	5.10	117.80	109.59
1	D	1092	ILE	CB-CA-C	-5.08	105.06	110.95
1	F	993	THR	N-CA-C	5.07	119.69	111.37
1	B	1191	ASP	N-CA-C	-5.04	104.94	111.74

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	3029	0	3146	180	0
1	B	3029	0	3146	165	3
1	C	3029	0	3146	171	0
1	D	3036	0	3153	173	0
1	E	2941	0	3046	173	3
1	F	2952	0	3059	152	0
2	A	91	0	0	19	0
2	B	94	0	0	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	80	0	0	20	0
2	D	116	0	0	26	0
2	E	99	0	0	23	0
2	F	73	0	0	26	0
All	All	18569	0	18696	1003	3

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 27.

All (1003) 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:E:1046:MET:HG2	1:E:1129:THR:HG21	1.20	1.10
1:E:1046:MET:HE2	1:E:1126:LEU:HG	1.34	1.08
1:D:1159:PRO:HB3	1:D:1189:ILE:HD11	1.38	1.06
1:E:1159:PRO:HB3	1:E:1189:ILE:HD11	1.34	1.05
1:B:1159:PRO:HB3	1:B:1189:ILE:HD11	1.33	1.05
1:F:1035:ILE:HG22	1:F:1038:LEU:HG	1.45	0.99
1:F:1159:PRO:HB3	1:F:1189:ILE:HD11	1.45	0.98
1:E:1046:MET:CG	1:E:1129:THR:HG21	1.94	0.96
1:C:958:ARG:HA	2:C:2023:HOH:O	1.65	0.95
1:E:1173:PRO:HB2	1:E:1209:PRO:HB3	1.48	0.95
1:A:1129:THR:HG23	1:A:1130:VAL:HG23	1.48	0.95
1:A:1107:HIS:C	1:A:1107:HIS:HD1	1.73	0.95
1:C:1173:PRO:HB2	1:C:1209:PRO:HB3	1.47	0.94
1:C:1129:THR:HG23	1:C:1130:VAL:HG23	1.49	0.92
1:C:1127:MET:HE1	1:C:1135:GLU:HG3	1.52	0.92
1:B:840:LEU:HD12	1:B:1013:GLN:HE22	1.36	0.91
1:D:992:THR:HG22	1:D:993:THR:H	1.33	0.91
1:F:1125:ASP:O	1:F:1129:THR:HG22	1.71	0.91
1:F:1173:PRO:HB2	1:F:1209:PRO:HB3	1.49	0.91
1:A:992:THR:HG22	1:A:993:THR:H	1.36	0.90
1:F:1067:MET:HE1	1:F:1148:ALA:HA	1.51	0.90
1:A:1107:HIS:C	1:A:1107:HIS:ND1	2.30	0.89
1:B:1129:THR:HG23	1:B:1130:VAL:HG23	1.56	0.88
1:A:1046:MET:HE3	1:A:1046:MET:HA	1.53	0.88
1:F:841:PRO:HB2	2:F:2025:HOH:O	1.73	0.88
1:D:987:LEU:HB2	2:D:2101:HOH:O	1.74	0.87
1:A:1159:PRO:HB3	1:A:1189:ILE:HD11	1.57	0.87
1:D:1046:MET:HE3	1:D:1046:MET:HA	1.54	0.86
1:F:848:PRO:HG3	1:F:949:ARG:NH2	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:PRO:HB2	1:A:1209:PRO:HB3	1.58	0.85
1:F:1026:MET:HE2	1:F:1044:THR:HG21	1.57	0.85
1:E:1184:ILE:HB	2:E:2084:HOH:O	1.76	0.85
1:C:883:ASN:ND2	1:C:884:TYR:H	1.75	0.85
1:B:1046:MET:HE3	1:B:1046:MET:HA	1.56	0.84
1:C:1046:MET:HE3	1:C:1046:MET:HA	1.56	0.84
1:E:987:LEU:HB2	2:E:2077:HOH:O	1.77	0.84
1:A:840:LEU:HD22	2:A:2002:HOH:O	1.77	0.84
1:D:1107:HIS:ND1	1:D:1107:HIS:C	2.35	0.84
1:B:987:LEU:HD21	1:B:1153:VAL:HG13	1.60	0.83
1:D:1173:PRO:HB2	1:D:1209:PRO:HB3	1.61	0.82
1:B:1173:PRO:HB2	1:B:1209:PRO:HB3	1.59	0.82
1:A:1169:LYS:HE3	2:A:2067:HOH:O	1.78	0.82
1:E:840:LEU:HD22	2:E:2001:HOH:O	1.80	0.81
1:C:992:THR:HG22	1:C:993:THR:H	1.44	0.81
1:D:1067:MET:HE1	1:D:1148:ALA:HA	1.62	0.81
1:E:992:THR:HG22	1:E:993:THR:H	1.45	0.81
1:D:1046:MET:HE2	1:D:1126:LEU:HG	1.62	0.81
1:A:1022:ILE:HG22	1:A:1024:PRO:HD3	1.63	0.80
1:A:919:THR:HA	2:A:2020:HOH:O	1.81	0.80
1:D:941:LYS:HG2	2:D:2042:HOH:O	1.82	0.80
1:F:1107:HIS:ND1	1:F:1107:HIS:C	2.40	0.79
1:A:1126:LEU:HD22	1:A:1134:VAL:HG21	1.64	0.79
1:C:1223:ARG:HB2	1:C:1226:GLU:HG3	1.63	0.79
1:C:1097:TRP:CE3	1:C:1107:HIS:HB3	2.18	0.79
1:C:1127:MET:HE1	1:C:1135:GLU:CG	2.12	0.79
1:B:987:LEU:HB2	2:B:2031:HOH:O	1.81	0.79
1:B:992:THR:HG22	1:B:993:THR:H	1.47	0.79
1:E:971:ASP:HB2	2:E:2093:HOH:O	1.82	0.78
1:F:1025:LYS:HB2	2:F:2029:HOH:O	1.84	0.78
1:E:1025:LYS:HE3	1:E:1122:GLU:HG2	1.66	0.78
1:C:987:LEU:HD23	1:C:1153:VAL:HG22	1.66	0.77
1:B:1067:MET:HE1	1:B:1148:ALA:HA	1.66	0.77
1:D:1107:HIS:C	1:D:1107:HIS:HD1	1.91	0.77
1:F:1046:MET:HE3	1:F:1046:MET:HA	1.67	0.76
1:F:987:LEU:HD21	1:F:1153:VAL:HG13	1.67	0.76
1:A:954:ASN:HD22	1:A:956:LYS:H	1.34	0.76
1:E:987:LEU:HD21	1:E:1153:VAL:HG22	1.68	0.76
1:B:883:ASN:ND2	1:B:884:TYR:H	1.84	0.76
1:B:1079:ASN:HD21	1:B:1113:GLU:H	1.32	0.75
1:C:1006:LEU:HD12	2:C:2030:HOH:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:871:ARG:HD2	1:E:916:SER:HB3	1.68	0.75
1:E:1079:ASN:HD21	1:E:1113:GLU:H	1.33	0.75
1:F:992:THR:HG22	1:F:993:THR:H	1.52	0.75
1:B:1228:HIS:HB3	2:B:2087:HOH:O	1.86	0.75
1:F:1107:HIS:C	1:F:1107:HIS:HD1	1.95	0.74
1:C:1079:ASN:HD21	1:C:1113:GLU:H	1.35	0.74
1:E:883:ASN:ND2	1:E:884:TYR:H	1.83	0.74
1:D:954:ASN:HD22	1:D:956:LYS:H	1.33	0.74
1:D:1079:ASN:HD21	1:D:1113:GLU:H	1.32	0.74
1:D:1126:LEU:HD22	1:D:1134:VAL:HG21	1.68	0.74
1:C:1209:PRO:HD2	2:C:2067:HOH:O	1.85	0.74
1:C:848:PRO:HG3	1:C:949:ARG:NH2	2.03	0.73
1:E:1129:THR:HG23	1:E:1130:VAL:HG23	1.71	0.73
1:F:1060:MET:SD	2:F:2050:HOH:O	2.46	0.73
1:A:1079:ASN:HD21	1:A:1113:GLU:H	1.34	0.73
1:B:992:THR:HG22	1:B:993:THR:N	2.03	0.73
1:D:992:THR:HG22	1:D:993:THR:N	2.03	0.72
1:F:951:VAL:HG11	1:F:967:VAL:HG13	1.70	0.72
1:F:871:ARG:HD2	1:F:916:SER:HB3	1.72	0.72
1:F:1130:VAL:HG12	1:F:1133:LYS:HB3	1.71	0.72
1:E:843:LEU:O	2:E:2002:HOH:O	2.08	0.71
1:F:883:ASN:ND2	1:F:884:TYR:H	1.86	0.71
1:C:847:THR:HG22	1:C:1226:GLU:OE2	1.91	0.71
1:E:987:LEU:CD2	1:E:1153:VAL:HG22	2.20	0.71
1:D:1046:MET:CE	1:D:1126:LEU:HG	2.20	0.71
1:D:864:MET:SD	1:D:917:LEU:HD23	2.30	0.71
1:F:1161:VAL:HB	2:F:2052:HOH:O	1.90	0.71
1:A:1067:MET:HE1	1:A:1148:ALA:HA	1.72	0.71
1:A:1157:GLN:C	1:A:1159:PRO:HD3	2.15	0.70
1:C:1018:ARG:HB3	1:C:1039:LEU:HG	1.73	0.70
1:A:1028:GLU:CD	1:A:1028:GLU:H	1.99	0.70
1:C:1126:LEU:HD22	1:C:1134:VAL:HG21	1.74	0.70
1:B:917:LEU:N	1:B:917:LEU:HD12	2.07	0.70
1:F:987:LEU:CD2	1:F:1153:VAL:HG22	2.22	0.70
1:A:1165:THR:O	1:A:1169:LYS:HG3	1.91	0.69
1:A:1223:ARG:HB2	1:A:1226:GLU:HG3	1.73	0.69
1:D:1024:PRO:HB3	1:D:1046:MET:HE1	1.73	0.69
1:A:848:PRO:HG3	1:A:949:ARG:NH2	2.07	0.69
1:E:1035:ILE:HG22	1:E:1038:LEU:HG	1.74	0.69
1:A:1018:ARG:HB3	1:A:1039:LEU:HG	1.74	0.69
1:A:1203:ASP:OD1	1:A:1216:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:LEU:CD2	1:C:1153:VAL:HG22	2.23	0.69
1:D:1097:TRP:CZ2	1:D:1107:HIS:CE1	2.81	0.69
1:C:1159:PRO:HB3	1:C:1189:ILE:HD11	1.74	0.69
1:F:846:LEU:HG	2:F:2024:HOH:O	1.92	0.69
1:B:878:LYS:HE2	1:B:878:LYS:C	2.18	0.68
1:A:883:ASN:ND2	1:A:884:TYR:H	1.91	0.68
1:D:1024:PRO:HB3	1:D:1046:MET:CE	2.23	0.68
1:D:864:MET:O	1:D:868:VAL:HG23	1.93	0.68
1:D:1090:ARG:HB2	2:D:2080:HOH:O	1.93	0.68
1:B:951:VAL:HG11	1:B:967:VAL:HG13	1.76	0.68
1:E:895:LEU:HD11	1:E:936:LEU:HD12	1.76	0.68
1:E:922:VAL:HG23	2:E:2023:HOH:O	1.92	0.67
1:E:1239:ARG:HH21	1:E:1239:ARG:HG3	1.59	0.67
1:E:1018:ARG:HB3	1:E:1039:LEU:HG	1.76	0.67
1:C:917:LEU:HB3	2:C:2016:HOH:O	1.93	0.67
1:F:1231:VAL:O	1:F:1235:LYS:HG3	1.94	0.67
1:C:1157:GLN:C	1:C:1159:PRO:HD3	2.20	0.67
1:A:1091:PRO:HG2	2:A:2054:HOH:O	1.93	0.67
1:C:1067:MET:HE1	1:C:1148:ALA:HA	1.77	0.66
1:B:840:LEU:HD23	2:B:2003:HOH:O	1.94	0.66
1:B:1035:ILE:CD1	1:B:1231:VAL:HG13	2.25	0.66
1:F:1079:ASN:HD21	1:F:1113:GLU:H	1.43	0.66
1:E:1046:MET:CE	1:E:1126:LEU:HG	2.19	0.66
1:F:1018:ARG:HB3	1:F:1039:LEU:HG	1.77	0.66
1:F:1133:LYS:HE2	2:F:2049:HOH:O	1.94	0.66
1:E:846:LEU:O	2:E:2002:HOH:O	2.13	0.66
1:E:917:LEU:N	1:E:917:LEU:HD12	2.10	0.66
1:A:948:LEU:HD22	1:A:952:LEU:HG	1.77	0.66
1:C:928:ILE:HA	2:C:2013:HOH:O	1.95	0.66
1:F:1142:ALA:HB3	1:F:1171:ASN:HB3	1.76	0.66
1:C:1009:LEU:HD12	2:C:2030:HOH:O	1.94	0.66
1:D:1133:LYS:HD3	2:D:2090:HOH:O	1.96	0.66
1:E:844:ASP:HA	2:E:2002:HOH:O	1.95	0.66
1:E:848:PRO:HG3	1:E:949:ARG:NH2	2.11	0.66
1:F:1046:MET:HG2	1:F:1129:THR:CG2	2.26	0.66
1:B:866:ARG:HD3	2:B:2011:HOH:O	1.95	0.65
1:D:881:VAL:HG22	1:D:895:LEU:CD2	2.26	0.65
1:E:1127:MET:HE1	1:E:1135:GLU:OE1	1.95	0.65
1:E:1232:GLN:HG2	2:E:2096:HOH:O	1.96	0.65
1:A:1027:LEU:HB3	1:A:1030:SER:OG	1.97	0.65
1:A:1204:MET:HG2	1:A:1217:VAL:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:881:VAL:HG21	2:D:2019:HOH:O	1.96	0.65
1:D:1097:TRP:CE2	1:D:1107:HIS:HE1	2.15	0.64
1:A:1024:PRO:HB3	1:A:1046:MET:SD	2.37	0.64
1:C:1046:MET:HE2	1:C:1126:LEU:HG	1.78	0.64
1:E:1203:ASP:OD1	1:E:1216:ARG:NH1	2.30	0.64
1:C:1024:PRO:HB3	1:C:1046:MET:CE	2.28	0.64
1:E:914:ALA:HB1	2:E:2023:HOH:O	1.97	0.64
1:E:948:LEU:HD22	1:E:952:LEU:HG	1.80	0.64
1:E:1024:PRO:HB3	1:E:1046:MET:SD	2.38	0.64
1:A:1024:PRO:HB3	1:A:1046:MET:CE	2.28	0.63
1:A:1107:HIS:ND1	1:A:1107:HIS:O	2.30	0.63
1:A:992:THR:HG22	1:A:993:THR:N	2.13	0.63
1:B:1027:LEU:HD12	1:D:941:LYS:O	1.99	0.63
1:B:1107:HIS:ND1	1:B:1108:PRO:HD2	2.14	0.63
1:E:1107:HIS:ND1	1:E:1107:HIS:C	2.57	0.63
1:F:1097:TRP:CE2	1:F:1107:HIS:HE1	2.16	0.63
1:D:1228:HIS:HB3	2:D:2114:HOH:O	1.99	0.62
1:D:985:PRO:HD2	1:D:1173:PRO:HG3	1.80	0.62
1:F:1107:HIS:ND1	1:F:1108:PRO:HD3	2.14	0.62
1:E:864:MET:O	1:E:868:VAL:HG23	1.98	0.62
1:E:1026:MET:HE2	1:E:1044:THR:HG23	1.81	0.62
1:A:1035:ILE:HG23	1:A:1037:HIS:H	1.64	0.62
1:F:841:PRO:HB3	1:F:1233:ASP:OD1	2.00	0.62
1:C:951:VAL:HG11	1:C:967:VAL:HG13	1.82	0.62
1:C:954:ASN:HD22	1:C:956:LYS:H	1.48	0.62
1:F:1097:TRP:CE2	1:F:1107:HIS:CE1	2.88	0.62
1:F:1161:VAL:HG13	2:F:2054:HOH:O	1.99	0.62
1:B:1003:ALA:HA	2:B:2033:HOH:O	2.00	0.62
1:E:1183:LYS:HD2	2:E:2082:HOH:O	1.98	0.62
1:C:1046:MET:HG2	1:C:1129:THR:CG2	2.28	0.61
1:F:864:MET:O	1:F:868:VAL:HG23	2.00	0.61
1:E:992:THR:HG22	1:E:993:THR:N	2.15	0.61
1:C:1022:ILE:HG22	1:C:1024:PRO:HD3	1.81	0.61
1:D:971:ASP:OD2	1:D:975:GLU:HB2	2.00	0.61
1:E:951:VAL:HG11	1:E:967:VAL:HG13	1.82	0.61
1:A:987:LEU:HD11	1:A:989:VAL:CG2	2.30	0.61
1:A:1097:TRP:CE2	1:A:1107:HIS:HE1	2.18	0.61
1:A:1130:VAL:HG12	1:A:1130:VAL:O	2.01	0.61
1:A:1046:MET:CE	1:A:1126:LEU:HG	2.31	0.61
1:E:1026:MET:O	1:E:1027:LEU:HB3	1.99	0.61
1:F:992:THR:HG22	1:F:993:THR:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1107:HIS:N	2:C:2052:HOH:O	2.33	0.61
1:E:1204:MET:HG2	1:E:1217:VAL:O	2.00	0.61
1:C:1035:ILE:HG23	1:C:1037:HIS:H	1.65	0.61
1:C:1107:HIS:N	2:C:2051:HOH:O	2.33	0.61
1:E:968:LEU:O	1:E:1219:GLY:HA2	2.00	0.61
1:F:1018:ARG:HD2	1:F:1037:HIS:O	2.01	0.61
1:D:1107:HIS:CE1	1:D:1108:PRO:HD3	2.35	0.61
1:F:1026:MET:HE2	1:F:1044:THR:CG2	2.30	0.61
1:D:922:VAL:HG22	1:D:938:LEU:CD2	2.31	0.60
1:A:922:VAL:HG22	1:A:938:LEU:CD2	2.32	0.60
1:B:936:LEU:HB3	2:B:2023:HOH:O	2.01	0.60
1:D:1237:ARG:HD3	2:D:2062:HOH:O	2.01	0.60
1:E:846:LEU:N	2:E:2002:HOH:O	2.27	0.60
1:E:1142:ALA:HB3	1:E:1171:ASN:HB3	1.83	0.60
1:A:1046:MET:HA	1:A:1046:MET:CE	2.30	0.60
1:B:1156:THR:HG21	1:B:1164:ILE:HD11	1.84	0.60
1:D:951:VAL:HG11	1:D:967:VAL:HG13	1.83	0.60
1:D:840:LEU:N	2:D:2004:HOH:O	2.32	0.60
1:E:1035:ILE:HD13	1:E:1231:VAL:HG13	1.83	0.60
1:F:1107:HIS:CE1	1:F:1108:PRO:HD3	2.37	0.60
1:A:951:VAL:HG11	1:A:967:VAL:HG13	1.84	0.60
1:A:988:LEU:HB2	1:A:1172:ILE:HG21	1.83	0.60
1:E:1118:VAL:HB	1:E:1152:LEU:HD12	1.84	0.60
1:E:1135:GLU:OE1	1:E:1165:THR:HG21	2.02	0.60
1:E:1133:LYS:HE2	2:E:2071:HOH:O	2.01	0.60
1:C:864:MET:O	1:C:868:VAL:HG23	2.02	0.60
1:B:987:LEU:CD2	1:B:1153:VAL:HG22	2.31	0.60
1:E:953:ASP:CG	1:E:958:ARG:HH22	2.10	0.60
1:C:890:ILE:C	1:C:890:ILE:HD12	2.27	0.59
1:C:1046:MET:CE	1:C:1126:LEU:HG	2.31	0.59
1:C:1046:MET:HG2	1:C:1129:THR:HG21	1.83	0.59
1:C:1048:ASP:CG	1:C:1247:THR:HG23	2.27	0.59
1:E:1046:MET:HG2	1:E:1129:THR:CG2	2.13	0.59
1:F:1054:ARG:HG3	2:F:2003:HOH:O	2.01	0.59
1:B:1046:MET:HG2	1:B:1129:THR:HG21	1.83	0.59
1:B:1107:HIS:ND1	1:B:1107:HIS:C	2.60	0.59
1:C:1203:ASP:OD1	1:C:1216:ARG:NH1	2.35	0.59
1:F:1203:ASP:OD1	1:F:1216:ARG:NH1	2.35	0.59
1:A:906:ILE:HG22	1:A:924:VAL:HG21	1.85	0.59
1:A:1127:MET:HE1	1:A:1135:GLU:HG3	1.83	0.59
1:B:992:THR:CG2	1:B:993:THR:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:883:ASN:HD22	1:E:884:TYR:H	1.50	0.59
1:E:895:LEU:HD11	1:E:936:LEU:CD1	2.33	0.59
1:B:1085:ALA:HB1	1:B:1090:ARG:O	2.02	0.59
1:B:840:LEU:HA	2:B:2003:HOH:O	2.02	0.59
1:B:864:MET:O	1:B:868:VAL:HG23	2.02	0.59
1:D:1035:ILE:CD1	1:D:1231:VAL:HG13	2.33	0.59
1:A:847:THR:HG22	1:A:1226:GLU:OE2	2.02	0.59
1:A:1111:LYS:HG2	2:A:2058:HOH:O	2.01	0.59
1:B:1175:ARG:HD2	1:B:1189:ILE:O	2.03	0.59
1:F:968:LEU:O	1:F:1219:GLY:HA2	2.02	0.59
1:F:1076:ALA:O	1:F:1080:GLU:HG3	2.02	0.58
1:F:917:LEU:HD12	1:F:917:LEU:N	2.18	0.58
1:C:1171:ASN:C	1:C:1172:ILE:HD12	2.28	0.58
1:E:1035:ILE:CD1	1:E:1231:VAL:HG13	2.33	0.58
1:E:1097:TRP:CE3	1:E:1107:HIS:CE1	2.91	0.58
1:D:1024:PRO:HB3	1:D:1046:MET:SD	2.43	0.58
1:F:840:LEU:HD13	2:F:2010:HOH:O	2.03	0.58
1:C:1130:VAL:HG12	1:C:1130:VAL:O	2.03	0.58
1:D:1130:VAL:O	1:D:1134:VAL:HG23	2.03	0.58
1:A:906:ILE:HD12	1:A:906:ILE:N	2.18	0.58
1:A:1169:LYS:O	1:A:1175:ARG:NH1	2.37	0.58
1:C:840:LEU:N	2:C:2001:HOH:O	2.37	0.58
1:C:871:ARG:HD2	1:C:916:SER:HB3	1.86	0.58
1:C:1018:ARG:NH2	1:C:1039:LEU:HD23	2.18	0.58
1:D:876:ARG:HG3	1:D:905:ARG:HH12	1.68	0.58
1:F:840:LEU:HB3	2:F:2069:HOH:O	2.02	0.58
1:D:987:LEU:CD2	1:D:1153:VAL:HG22	2.33	0.58
1:E:1174:THR:OG1	1:E:1209:PRO:HD3	2.03	0.58
1:F:890:ILE:C	1:F:890:ILE:HD12	2.29	0.58
1:B:1097:TRP:CE3	1:B:1107:HIS:CE1	2.91	0.58
1:C:1024:PRO:HB3	1:C:1046:MET:SD	2.43	0.58
1:C:1118:VAL:HB	1:C:1152:LEU:HD12	1.86	0.58
1:D:1187:ARG:O	1:D:1191:ASP:N	2.35	0.58
1:E:872:LEU:HD21	1:E:913:LEU:HD11	1.86	0.58
1:F:1107:HIS:N	2:F:2046:HOH:O	2.37	0.58
1:A:946:VAL:HG22	2:A:2024:HOH:O	2.03	0.57
1:A:1075:LEU:HD21	1:A:1113:GLU:HB3	1.84	0.57
1:B:988:LEU:HD11	1:B:1164:ILE:HG23	1.85	0.57
1:C:929:PRO:HD2	2:C:2013:HOH:O	2.04	0.57
1:C:1018:ARG:HD2	1:C:1037:HIS:O	2.03	0.57
1:A:892:ARG:HD2	2:A:2014:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:ARG:HB2	1:A:1240:PRO:HD2	1.86	0.57
1:B:971:ASP:OD2	1:B:975:GLU:HB2	2.04	0.57
1:C:1031:VAL:N	2:C:2040:HOH:O	2.36	0.57
1:C:1177:ALA:HB2	1:C:1189:ILE:HG21	1.86	0.57
1:B:893:PHE:CE1	1:B:938:LEU:HD12	2.39	0.57
1:E:867:LEU:O	1:E:871:ARG:HG2	2.04	0.57
1:E:881:VAL:HG22	1:E:895:LEU:CD2	2.33	0.57
1:A:840:LEU:HD21	2:A:2011:HOH:O	2.05	0.57
1:C:1035:ILE:CD1	1:C:1231:VAL:HG13	2.34	0.57
1:E:987:LEU:HD12	2:E:2077:HOH:O	2.04	0.57
1:B:953:ASP:CG	1:B:958:ARG:HH22	2.12	0.57
1:A:1245:GLY:HA2	1:A:1248:SER:HG	1.70	0.57
1:E:883:ASN:ND2	1:E:884:TYR:N	2.53	0.57
1:F:895:LEU:HD11	1:F:936:LEU:HD12	1.85	0.57
1:A:887:GLY:HA3	1:A:972:ILE:O	2.05	0.57
1:A:993:THR:HA	1:A:1157:GLN:NE2	2.20	0.57
1:C:1035:ILE:HG22	1:C:1038:LEU:HG	1.86	0.57
1:D:1046:MET:HA	1:D:1046:MET:CE	2.30	0.57
1:C:883:ASN:ND2	1:C:884:TYR:N	2.51	0.57
1:D:1035:ILE:HG22	1:D:1038:LEU:HG	1.87	0.57
1:C:864:MET:HE1	2:C:2016:HOH:O	2.05	0.56
1:C:1046:MET:HA	1:C:1046:MET:CE	2.33	0.56
1:D:876:ARG:CG	1:D:905:ARG:HH12	2.17	0.56
1:D:992:THR:CG2	1:D:993:THR:H	2.10	0.56
1:D:1130:VAL:HG12	1:D:1134:VAL:HG23	1.86	0.56
1:C:1145:ALA:HB1	1:C:1150:ILE:HB	1.86	0.56
1:A:954:ASN:ND2	1:A:956:LYS:H	2.02	0.56
1:C:917:LEU:HD12	1:C:917:LEU:N	2.20	0.56
1:C:1024:PRO:HB3	1:C:1046:MET:HE1	1.86	0.56
1:C:1097:TRP:CZ3	1:C:1107:HIS:HB3	2.39	0.56
1:E:1107:HIS:ND1	1:E:1108:PRO:HD2	2.20	0.56
1:F:1057:VAL:O	1:F:1061:GLU:HG3	2.05	0.56
1:A:1046:MET:HG2	1:A:1129:THR:CG2	2.35	0.56
1:B:922:VAL:HG22	1:B:938:LEU:HD23	1.87	0.56
1:A:1245:GLY:HA2	1:A:1248:SER:OG	2.05	0.56
1:C:906:ILE:H	1:C:906:ILE:HD12	1.70	0.56
1:C:1057:VAL:O	1:C:1061:GLU:HG3	2.06	0.56
1:B:895:LEU:HD11	1:B:936:LEU:HD12	1.87	0.56
1:B:1107:HIS:ND1	1:B:1108:PRO:CD	2.68	0.56
1:B:1247:THR:HG21	2:B:2041:HOH:O	2.06	0.56
1:E:1027:LEU:HD11	2:E:2043:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1024:PRO:HB3	1:F:1046:MET:SD	2.46	0.56
1:E:1129:THR:HG23	1:E:1130:VAL:N	2.20	0.56
1:F:1097:TRP:CZ2	1:F:1107:HIS:CE1	2.94	0.56
1:F:1145:ALA:HB2	2:F:2050:HOH:O	2.04	0.56
1:C:849:PRO:C	2:C:2008:HOH:O	2.48	0.56
1:A:1061:GLU:OE2	1:A:1140:ARG:NH1	2.38	0.56
1:B:936:LEU:HD13	2:B:2023:HOH:O	2.06	0.56
1:B:1046:MET:HA	1:B:1046:MET:CE	2.32	0.56
1:C:1076:ALA:O	1:C:1080:GLU:HG3	2.06	0.56
1:C:1130:VAL:HG12	1:C:1134:VAL:HG23	1.87	0.56
1:C:1204:MET:HG2	1:C:1217:VAL:O	2.06	0.56
1:D:1107:HIS:ND1	1:D:1107:HIS:O	2.33	0.56
1:E:919:THR:HG21	1:E:939:PRO:HD2	1.88	0.56
1:B:1222:VAL:HB	2:B:2033:HOH:O	2.05	0.55
1:B:922:VAL:HG22	1:B:938:LEU:CD2	2.37	0.55
1:C:864:MET:SD	1:C:917:LEU:HD23	2.46	0.55
1:C:876:ARG:HG3	1:C:905:ARG:HH12	1.70	0.55
1:D:858:THR:N	2:D:2014:HOH:O	2.40	0.55
1:F:1141:LEU:HA	2:F:2050:HOH:O	2.07	0.55
1:F:895:LEU:HD11	1:F:936:LEU:CD1	2.36	0.55
1:F:928:ILE:HD11	1:F:935:GLY:CA	2.36	0.55
1:B:867:LEU:O	1:B:871:ARG:HG2	2.07	0.55
1:C:922:VAL:HG22	1:C:938:LEU:CD2	2.37	0.55
1:E:890:ILE:HG22	1:E:939:PRO:HA	1.88	0.55
1:F:1228:HIS:HB3	2:F:2068:HOH:O	2.05	0.55
1:A:1021:MET:HB3	1:A:1029:LEU:HD13	1.87	0.55
1:B:1205:LEU:HD23	1:B:1216:ARG:HA	1.88	0.55
1:B:1242:TYR:CE1	1:D:993:THR:HG22	2.41	0.55
1:D:893:PHE:CE1	1:D:938:LEU:HD12	2.42	0.55
1:D:1026:MET:O	1:D:1027:LEU:HD23	2.07	0.55
1:E:939:PRO:HB3	1:E:1199:LEU:HD13	1.88	0.55
1:E:1126:LEU:HD22	1:E:1134:VAL:HG21	1.89	0.55
1:F:948:LEU:HD22	1:F:952:LEU:HG	1.89	0.55
1:B:881:VAL:HG22	1:B:895:LEU:CD2	2.37	0.55
1:A:1169:LYS:HG2	2:A:2067:HOH:O	2.06	0.55
1:D:1184:ILE:HG13	1:D:1185:ASP:N	2.21	0.55
1:F:864:MET:SD	1:F:917:LEU:HD23	2.47	0.55
1:F:1072:VAL:HG21	1:F:1077:GLY:C	2.32	0.55
1:B:1035:ILE:HD11	1:B:1231:VAL:HA	1.89	0.55
1:D:916:SER:C	1:D:917:LEU:HD12	2.32	0.55
1:D:1107:HIS:ND1	1:D:1108:PRO:HD3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:GLU:CD	1:A:1028:GLU:N	2.65	0.55
1:A:1107:HIS:ND1	1:A:1108:PRO:HD3	2.21	0.55
1:D:922:VAL:HG22	1:D:938:LEU:HD23	1.89	0.55
1:F:1046:MET:HG2	1:F:1129:THR:HG21	1.89	0.55
1:F:1046:MET:HE2	1:F:1126:LEU:HG	1.89	0.55
1:C:1158:ARG:N	1:C:1159:PRO:HD3	2.22	0.54
1:B:871:ARG:HD2	1:B:916:SER:HB3	1.88	0.54
1:C:906:ILE:HD12	1:C:906:ILE:N	2.23	0.54
1:C:1169:LYS:O	1:C:1175:ARG:NH1	2.39	0.54
1:D:987:LEU:HD21	1:D:1153:VAL:HG22	1.90	0.54
1:E:1231:VAL:O	1:E:1235:LYS:HG3	2.07	0.54
1:A:1158:ARG:N	1:A:1159:PRO:HD3	2.22	0.54
1:D:987:LEU:HD21	1:D:1153:VAL:HG13	1.88	0.54
1:E:892:ARG:NH2	1:E:928:ILE:HG23	2.23	0.54
1:A:1028:GLU:HB2	1:A:1121:ASP:OD1	2.07	0.54
1:B:939:PRO:HB3	1:B:1199:LEU:CD1	2.38	0.54
1:B:1047:LYS:NZ	1:D:847:THR:HB	2.22	0.54
1:D:876:ARG:HB3	1:D:905:ARG:NH1	2.21	0.54
1:E:1076:ALA:O	1:E:1080:GLU:HG3	2.07	0.54
1:A:871:ARG:HG2	1:A:871:ARG:HH21	1.72	0.54
1:D:1125:ASP:O	1:D:1129:THR:HG22	2.07	0.54
1:D:1129:THR:HG23	1:D:1130:VAL:HG23	1.90	0.54
1:B:1092:ILE:HD11	2:B:2056:HOH:O	2.06	0.54
1:B:1125:ASP:O	1:B:1129:THR:HG22	2.08	0.54
1:F:881:VAL:HG22	1:F:895:LEU:CD2	2.38	0.54
1:B:929:PRO:HD2	2:B:2016:HOH:O	2.08	0.54
1:C:954:ASN:ND2	1:C:956:LYS:H	2.05	0.54
1:A:864:MET:O	1:A:868:VAL:HG23	2.08	0.54
1:A:1064:TYR:OH	1:A:1147:ALA:HB3	2.07	0.54
1:A:1107:HIS:HD1	1:A:1108:PRO:HD3	1.73	0.54
1:A:1145:ALA:HB1	1:A:1150:ILE:HB	1.90	0.54
1:B:987:LEU:HD23	1:B:1153:VAL:HA	1.90	0.54
1:E:1057:VAL:O	1:E:1061:GLU:HG3	2.08	0.54
1:A:844:ASP:N	2:A:2004:HOH:O	2.18	0.54
1:D:872:LEU:HD21	1:D:913:LEU:HD11	1.90	0.54
1:D:988:LEU:HD11	1:D:1164:ILE:HG23	1.90	0.54
1:A:1125:ASP:O	1:A:1129:THR:HG22	2.08	0.53
1:C:947:TYR:HB3	2:C:2007:HOH:O	2.08	0.53
1:D:875:PHE:C	1:D:877:ILE:H	2.16	0.53
1:D:1035:ILE:HG23	1:D:1037:HIS:H	1.73	0.53
1:D:1157:GLN:C	1:D:1159:PRO:HD3	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1075:LEU:HD21	1:E:1113:GLU:HB3	1.89	0.53
1:A:1156:THR:HG21	1:A:1164:ILE:HD11	1.89	0.53
1:E:1046:MET:HE2	1:E:1126:LEU:CG	2.22	0.53
1:F:1169:LYS:NZ	1:F:1191:ASP:OD2	2.38	0.53
1:B:895:LEU:HD11	1:B:936:LEU:CD1	2.38	0.53
1:C:1167:LEU:HD23	1:F:1167:LEU:HD23	1.89	0.53
1:D:1097:TRP:CE2	1:D:1107:HIS:CE1	2.96	0.53
1:E:1239:ARG:HG3	1:E:1239:ARG:NH2	2.22	0.53
1:B:1035:ILE:HG23	1:B:1037:HIS:H	1.73	0.53
1:B:1059:GLU:O	1:B:1063:ARG:HG3	2.08	0.53
1:B:1079:ASN:ND2	1:B:1113:GLU:H	2.04	0.53
1:B:1183:LYS:HD2	2:B:2075:HOH:O	2.09	0.53
1:C:1022:ILE:HG13	1:C:1120:VAL:HG22	1.90	0.53
1:F:1145:ALA:HB1	1:F:1150:ILE:HB	1.90	0.53
1:B:992:THR:CG2	1:B:993:THR:N	2.71	0.53
1:C:914:ALA:CB	1:C:922:VAL:HG23	2.39	0.53
1:C:1029:LEU:HD22	2:C:2037:HOH:O	2.08	0.53
1:D:1085:ALA:HB1	1:D:1090:ARG:O	2.08	0.53
1:C:1233:ASP:OD1	1:C:1237:ARG:NH2	2.42	0.53
1:D:859:PHE:N	2:D:2014:HOH:O	2.41	0.53
1:E:1025:LYS:O	1:E:1026:MET:C	2.51	0.53
1:E:1091:PRO:HB2	1:E:1109:VAL:HG11	1.91	0.53
1:F:954:ASN:HD22	1:F:956:LYS:HB2	1.73	0.53
1:A:954:ASN:HD22	1:A:956:LYS:N	2.06	0.53
1:D:991:GLY:O	1:D:1157:GLN:HA	2.08	0.53
1:F:890:ILE:HG22	1:F:939:PRO:HA	1.90	0.53
1:F:916:SER:C	1:F:917:LEU:HD12	2.34	0.53
1:F:1064:TYR:OH	1:F:1147:ALA:HB3	2.09	0.53
1:F:1142:ALA:CB	1:F:1171:ASN:HB3	2.38	0.53
1:C:1107:HIS:N	1:C:1107:HIS:ND1	2.57	0.53
1:D:1171:ASN:C	1:D:1172:ILE:HD12	2.34	0.53
1:C:1005:ILE:HG22	2:C:2030:HOH:O	2.09	0.53
1:C:1068:SER:OG	1:F:1213:LEU:HD12	2.09	0.53
1:D:867:LEU:O	1:D:871:ARG:HG2	2.09	0.53
1:E:1142:ALA:CB	1:E:1171:ASN:HB3	2.39	0.53
1:D:1061:GLU:OE2	1:D:1140:ARG:NH1	2.42	0.53
1:A:1035:ILE:CD1	1:A:1231:VAL:HG13	2.39	0.52
1:B:919:THR:HG21	1:B:939:PRO:HD2	1.90	0.52
1:B:1024:PRO:HB3	1:B:1046:MET:SD	2.48	0.52
1:D:895:LEU:HD11	1:D:936:LEU:HD12	1.90	0.52
1:D:987:LEU:HD12	2:D:2101:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:840:LEU:CD1	1:B:1013:GLN:HE22	2.15	0.52
1:B:1091:PRO:HB2	1:B:1109:VAL:HG21	1.89	0.52
1:A:1046:MET:HE2	1:A:1126:LEU:HG	1.91	0.52
1:D:871:ARG:HG2	1:D:871:ARG:HH21	1.74	0.52
1:D:1187:ARG:HA	1:D:1192:GLN:H	1.75	0.52
1:F:1175:ARG:HD2	1:F:1189:ILE:O	2.08	0.52
1:B:948:LEU:HD22	1:B:952:LEU:HG	1.89	0.52
1:C:939:PRO:HB3	1:C:1199:LEU:CD1	2.39	0.52
1:D:1175:ARG:HD2	1:D:1189:ILE:O	2.09	0.52
1:A:1097:TRP:CZ2	1:A:1107:HIS:CE1	2.97	0.52
1:C:1183:LYS:HA	1:C:1196:GLU:HG2	1.91	0.52
1:D:993:THR:HB	2:D:2059:HOH:O	2.09	0.52
1:E:844:ASP:C	2:E:2002:HOH:O	2.52	0.52
1:A:861:LEU:HD22	1:A:891:THR:HG21	1.92	0.52
1:A:1046:MET:HG2	1:A:1129:THR:HG21	1.90	0.52
1:E:1027:LEU:HD12	1:E:1027:LEU:O	2.10	0.52
1:A:1076:ALA:O	1:A:1080:GLU:HG3	2.10	0.52
1:D:1018:ARG:HB3	1:D:1039:LEU:HG	1.91	0.52
1:D:1076:ALA:O	1:D:1080:GLU:HG3	2.09	0.52
1:F:1021:MET:HB3	1:F:1029:LEU:HD13	1.92	0.52
1:A:1185:ASP:O	1:A:1189:ILE:HG12	2.09	0.52
1:C:1165:THR:O	1:C:1169:LYS:HG3	2.10	0.52
1:D:922:VAL:CG1	1:D:936:LEU:HD22	2.40	0.52
1:D:948:LEU:HD22	1:D:952:LEU:HG	1.91	0.52
1:A:1018:ARG:HD2	1:A:1037:HIS:O	2.09	0.52
1:B:1185:ASP:O	1:B:1189:ILE:HG12	2.10	0.52
1:B:1187:ARG:HA	1:B:1192:GLN:H	1.75	0.52
1:B:909:LEU:HD12	1:B:912:ASP:HB2	1.92	0.51
1:B:954:ASN:HD22	1:B:956:LYS:H	1.57	0.51
1:B:1145:ALA:HB1	1:B:1150:ILE:HB	1.92	0.51
1:C:867:LEU:O	1:C:871:ARG:HG2	2.09	0.51
1:E:875:PHE:C	1:E:877:ILE:H	2.18	0.51
1:E:1085:ALA:HB1	1:E:1090:ARG:O	2.10	0.51
1:E:1107:HIS:ND1	1:E:1108:PRO:CD	2.73	0.51
1:F:892:ARG:NH2	1:F:928:ILE:HG23	2.25	0.51
1:B:946:VAL:HG13	1:B:970:LYS:HD2	1.91	0.51
1:B:1165:THR:O	1:B:1169:LYS:HG3	2.10	0.51
1:E:1046:MET:CE	2:E:2048:HOH:O	2.58	0.51
1:E:1073:ARG:HA	2:E:2057:HOH:O	2.11	0.51
1:B:1076:ALA:O	1:B:1080:GLU:HG3	2.11	0.51
1:C:876:ARG:HG3	1:C:876:ARG:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:917:LEU:HD12	1:D:917:LEU:N	2.25	0.51
1:E:939:PRO:HB3	1:E:1199:LEU:CD1	2.40	0.51
1:F:1187:ARG:HA	1:F:1192:GLN:H	1.76	0.51
1:A:906:ILE:HD12	1:A:906:ILE:H	1.74	0.51
1:A:987:LEU:HD11	1:A:989:VAL:HG22	1.92	0.51
1:B:1047:LYS:HZ1	1:D:847:THR:HB	1.74	0.51
1:B:1126:LEU:HD22	1:B:1134:VAL:HG21	1.92	0.51
1:B:987:LEU:HD12	2:B:2031:HOH:O	2.09	0.51
1:B:1046:MET:HE2	1:B:1126:LEU:HG	1.91	0.51
1:B:1174:THR:OG1	1:B:1209:PRO:HD3	2.11	0.51
1:A:917:LEU:HD12	1:A:917:LEU:N	2.25	0.51
1:B:848:PRO:HG3	1:B:949:ARG:NH2	2.26	0.51
1:D:890:ILE:HD13	1:D:937:GLU:HG2	1.92	0.51
1:D:993:THR:HA	1:D:1157:GLN:NE2	2.25	0.51
1:D:1046:MET:SD	1:D:1126:LEU:HA	2.51	0.51
1:C:1175:ARG:HD2	1:C:1189:ILE:O	2.11	0.51
1:F:943:ARG:NH2	1:F:1201:MET:HE3	2.25	0.51
1:F:1032:TYR:O	1:F:1035:ILE:HB	2.10	0.51
1:D:865:ALA:HA	2:D:2019:HOH:O	2.11	0.50
1:E:919:THR:HG22	1:E:939:PRO:HG2	1.93	0.50
1:F:1107:HIS:C	2:F:2046:HOH:O	2.54	0.50
1:C:895:LEU:HD11	1:C:936:LEU:CD1	2.42	0.50
1:D:1185:ASP:O	1:D:1189:ILE:HG12	2.10	0.50
1:A:1232:GLN:NE2	2:A:2086:HOH:O	2.33	0.50
1:B:1091:PRO:HB2	1:B:1109:VAL:CG2	2.41	0.50
1:C:992:THR:HG22	1:C:993:THR:N	2.21	0.50
1:C:1156:THR:HG21	1:C:1164:ILE:HD11	1.93	0.50
1:E:1157:GLN:C	1:E:1159:PRO:HD3	2.36	0.50
1:F:865:ALA:HB1	1:F:881:VAL:HG11	1.94	0.50
1:A:1120:VAL:HG11	1:A:1126:LEU:HD12	1.92	0.50
1:D:907:SER:C	1:D:909:LEU:H	2.19	0.50
1:D:1140:ARG:NE	2:D:2091:HOH:O	2.45	0.50
1:E:915:ARG:HB2	2:E:2021:HOH:O	2.10	0.50
1:C:940:ASN:N	1:C:940:ASN:HD22	2.07	0.50
1:D:1045:ASP:OD2	1:D:1047:LYS:HB2	2.12	0.50
1:E:1165:THR:O	1:E:1169:LYS:HG3	2.12	0.50
1:F:840:LEU:N	1:F:841:PRO:HD2	2.26	0.50
1:F:1046:MET:HG2	1:F:1129:THR:HG23	1.94	0.50
1:A:876:ARG:HG3	1:A:876:ARG:O	2.11	0.50
1:A:1046:MET:HE2	1:A:1126:LEU:CD2	2.42	0.50
1:C:1063:ARG:NH1	1:C:1113:GLU:HG3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1015:GLU:O	1:D:1114:PRO:HB3	2.11	0.50
1:E:893:PHE:CE1	1:E:938:LEU:HD12	2.47	0.50
1:D:1165:THR:O	1:D:1169:LYS:HG3	2.12	0.50
1:B:1130:VAL:HG12	1:B:1133:LYS:HB3	1.93	0.49
1:D:1172:ILE:HD12	1:D:1172:ILE:N	2.27	0.49
1:F:966:VAL:HB	1:F:1004:MET:HG2	1.93	0.49
1:A:875:PHE:CE2	1:A:909:LEU:HD21	2.46	0.49
1:A:971:ASP:OD2	1:A:975:GLU:HB2	2.11	0.49
1:A:994:GLY:N	2:A:2034:HOH:O	2.19	0.49
1:C:914:ALA:HB2	1:C:922:VAL:HG23	1.94	0.49
1:C:968:LEU:O	1:C:1219:GLY:HA2	2.13	0.49
1:D:985:PRO:HD2	1:D:1173:PRO:CG	2.42	0.49
1:D:1057:VAL:O	1:D:1061:GLU:HG3	2.12	0.49
1:E:898:ALA:HB1	1:E:899:PRO:HD2	1.95	0.49
1:F:1172:ILE:N	1:F:1172:ILE:HD12	2.27	0.49
1:A:1123:PHE:CE2	1:A:1163:VAL:HG12	2.47	0.49
1:A:1127:MET:HE1	1:A:1135:GLU:CG	2.41	0.49
1:C:1018:ARG:NH2	1:C:1039:LEU:HA	2.27	0.49
1:A:895:LEU:HD11	1:A:936:LEU:HD12	1.95	0.49
1:C:882:VAL:HG22	1:C:894:GLU:O	2.13	0.49
1:A:1018:ARG:NH2	1:A:1039:LEU:HD23	2.27	0.49
1:B:1057:VAL:O	1:B:1061:GLU:HG3	2.13	0.49
1:B:1088:MET:HB3	2:B:2055:HOH:O	2.12	0.49
1:F:922:VAL:HG22	1:F:938:LEU:CD2	2.43	0.49
1:A:1045:ASP:OD2	1:A:1047:LYS:HB2	2.12	0.49
1:B:871:ARG:HG2	1:B:871:ARG:HH21	1.77	0.49
1:A:939:PRO:HB3	1:A:1199:LEU:CD1	2.42	0.49
1:C:875:PHE:C	1:C:877:ILE:H	2.21	0.49
1:C:1035:ILE:HD13	1:C:1231:VAL:HG13	1.94	0.49
1:C:1174:THR:OG1	1:C:1209:PRO:HD3	2.13	0.49
1:D:994:GLY:N	2:D:2059:HOH:O	2.25	0.49
1:D:1018:ARG:HD2	1:D:1037:HIS:O	2.13	0.49
1:D:1059:GLU:O	1:D:1063:ARG:HG3	2.13	0.49
1:B:876:ARG:O	1:B:876:ARG:HG3	2.12	0.49
1:B:1158:ARG:N	1:B:1159:PRO:HD3	2.28	0.49
1:D:1018:ARG:NH2	1:D:1039:LEU:HD23	2.28	0.49
1:F:840:LEU:HD22	2:F:2010:HOH:O	2.13	0.49
1:B:840:LEU:HD12	1:B:1013:GLN:NE2	2.17	0.49
1:B:939:PRO:HB3	1:B:1199:LEU:HD13	1.95	0.49
1:B:988:LEU:HD11	1:B:1164:ILE:HD12	1.95	0.49
1:C:1209:PRO:O	1:F:1144:LYS:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:987:LEU:HD21	1:E:1153:VAL:HG13	1.95	0.49
1:E:1143:GLN:HG3	1:E:1171:ASN:HD22	1.78	0.49
1:A:1097:TRP:CE2	1:A:1107:HIS:CE1	2.99	0.48
1:B:840:LEU:HG	2:B:2067:HOH:O	2.11	0.48
1:C:895:LEU:HD11	1:C:936:LEU:HD12	1.95	0.48
1:F:981:LEU:HA	1:F:984:MET:HG3	1.95	0.48
1:A:865:ALA:HB1	1:A:881:VAL:HG11	1.95	0.48
1:B:1097:TRP:CD1	1:B:1108:PRO:HG3	2.48	0.48
1:C:1214:PRO:HG3	2:C:2062:HOH:O	2.13	0.48
1:E:1022:ILE:HG13	1:E:1120:VAL:HG22	1.96	0.48
1:A:864:MET:SD	1:A:917:LEU:HD23	2.54	0.48
1:A:1122:GLU:C	1:A:1124:ALA:H	2.21	0.48
1:C:1075:LEU:HD21	1:C:1113:GLU:HB3	1.95	0.48
1:D:1092:ILE:HD11	2:D:2083:HOH:O	2.13	0.48
1:E:1035:ILE:HG23	1:E:1037:HIS:H	1.77	0.48
1:C:1091:PRO:HB2	1:C:1109:VAL:HG11	1.95	0.48
1:F:977:VAL:HA	2:F:2020:HOH:O	2.13	0.48
1:F:1061:GLU:OE2	1:F:1140:ARG:NH1	2.47	0.48
1:A:1134:VAL:O	1:A:1135:GLU:C	2.57	0.48
1:C:865:ALA:HB1	1:C:881:VAL:HG11	1.95	0.48
1:E:916:SER:C	1:E:917:LEU:HD12	2.38	0.48
1:E:1172:ILE:N	1:E:1172:ILE:HD12	2.27	0.48
1:A:895:LEU:HD11	1:A:936:LEU:CD1	2.43	0.48
1:C:883:ASN:HD22	1:C:884:TYR:H	1.60	0.48
1:C:939:PRO:HB3	1:C:1199:LEU:HD13	1.96	0.48
1:D:883:ASN:ND2	1:D:884:TYR:H	2.12	0.48
1:E:1156:THR:HG21	1:E:1164:ILE:HD11	1.96	0.48
1:F:987:LEU:HD21	1:F:1153:VAL:HG22	1.96	0.48
1:C:1011:LYS:O	1:C:1011:LYS:HG2	2.14	0.48
1:E:844:ASP:CA	2:E:2002:HOH:O	2.56	0.48
1:E:1143:GLN:HG3	1:E:1171:ASN:ND2	2.29	0.48
1:A:882:VAL:HG21	1:A:933:TYR:CE1	2.49	0.48
1:D:1081:LYS:O	1:D:1084:GLU:HB3	2.14	0.48
1:F:846:LEU:N	2:F:2024:HOH:O	2.47	0.48
1:A:883:ASN:CG	1:A:884:TYR:H	2.22	0.47
1:B:1026:MET:HE2	1:D:943:ARG:HD3	1.94	0.47
1:B:1176:ILE:HG23	1:B:1204:MET:HE3	1.96	0.47
1:C:916:SER:C	1:C:917:LEU:HD12	2.39	0.47
1:C:1160:SER:C	1:C:1162:ASP:H	2.21	0.47
1:E:890:ILE:HD12	1:E:890:ILE:C	2.39	0.47
1:E:1061:GLU:OE2	1:E:1140:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1125:ASP:O	1:F:1129:THR:CG2	2.55	0.47
1:D:871:ARG:HD3	2:D:2026:HOH:O	2.14	0.47
1:D:1035:ILE:HD11	1:D:1231:VAL:HA	1.96	0.47
1:E:954:ASN:HD22	1:E:956:LYS:HB2	1.79	0.47
1:F:845:LEU:HD12	2:F:2025:HOH:O	2.14	0.47
1:A:1005:ILE:HD11	1:A:1119:LEU:CD1	2.45	0.47
1:D:953:ASP:CG	1:D:958:ARG:HH22	2.23	0.47
1:E:1123:PHE:CZ	1:E:1163:VAL:HG12	2.49	0.47
1:B:1035:ILE:HD12	1:B:1231:VAL:HG13	1.97	0.47
1:B:1054:ARG:HD3	2:B:2042:HOH:O	2.14	0.47
1:B:1059:GLU:OE2	1:B:1062:ARG:NH2	2.47	0.47
1:C:948:LEU:HD22	1:C:952:LEU:HG	1.96	0.47
1:D:1026:MET:HB2	1:D:1028:GLU:OE2	2.13	0.47
1:E:873:ALA:HA	1:E:877:ILE:O	2.15	0.47
1:F:1123:PHE:CZ	1:F:1163:VAL:HG12	2.49	0.47
1:A:846:LEU:HD23	1:A:1226:GLU:HB3	1.95	0.47
1:E:878:LYS:NZ	2:E:2009:HOH:O	2.37	0.47
1:A:1175:ARG:NE	2:A:2067:HOH:O	2.46	0.47
1:B:1061:GLU:O	1:B:1065:LYS:HG3	2.14	0.47
1:B:1107:HIS:HB2	2:B:2060:HOH:O	2.15	0.47
1:C:1160:SER:C	1:C:1162:ASP:N	2.72	0.47
1:D:876:ARG:HG3	1:D:876:ARG:O	2.13	0.47
1:A:875:PHE:N	1:A:875:PHE:CD1	2.83	0.47
1:A:1176:ILE:HG23	1:A:1204:MET:HE3	1.97	0.47
1:B:987:LEU:HD21	1:B:1153:VAL:HG22	1.96	0.47
1:B:1027:LEU:CD1	1:D:941:LYS:O	2.63	0.47
1:C:1239:ARG:HB2	1:C:1240:PRO:HD2	1.95	0.47
1:D:884:TYR:HA	1:D:892:ARG:O	2.15	0.47
1:D:1075:LEU:HD21	1:D:1113:GLU:HB3	1.96	0.47
1:E:988:LEU:HD11	1:E:1164:ILE:HG23	1.96	0.47
1:A:1209:PRO:HD2	2:A:2079:HOH:O	2.15	0.47
1:D:869:GLU:HG3	1:D:879:ALA:O	2.14	0.47
1:D:1160:SER:OG	1:D:1163:VAL:HG23	2.14	0.47
1:F:1130:VAL:HB	1:F:1134:VAL:CG2	2.45	0.47
1:A:881:VAL:HG22	1:A:895:LEU:CD2	2.45	0.47
1:A:899:PRO:HB2	2:A:2017:HOH:O	2.13	0.47
1:A:968:LEU:O	1:A:1219:GLY:HA2	2.15	0.47
1:B:1046:MET:HG2	1:B:1129:THR:CG2	2.44	0.47
1:C:928:ILE:HD11	1:C:935:GLY:CA	2.45	0.47
1:D:1158:ARG:N	1:D:1159:PRO:HD3	2.30	0.47
1:F:1126:LEU:HD22	1:F:1134:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1204:MET:HG2	1:B:1217:VAL:O	2.14	0.47
1:B:1239:ARG:NH1	1:D:992:THR:HG23	2.30	0.47
1:C:990:ALA:HB3	1:C:1189:ILE:HD12	1.97	0.47
1:C:1061:GLU:OE2	1:C:1140:ARG:NH1	2.48	0.47
1:D:1169:LYS:NZ	1:D:1191:ASP:OD2	2.42	0.47
1:F:1107:HIS:HD1	1:F:1108:PRO:HD3	1.79	0.47
1:E:1064:TYR:OH	1:E:1147:ALA:HB3	2.15	0.46
1:A:953:ASP:CG	1:A:958:ARG:HH22	2.24	0.46
1:B:916:SER:C	1:B:917:LEU:HD12	2.40	0.46
1:C:897:LEU:HD11	1:C:934:VAL:HG21	1.97	0.46
1:C:954:ASN:HD22	1:C:956:LYS:N	2.14	0.46
1:D:858:THR:N	2:D:2015:HOH:O	2.48	0.46
1:B:1015:GLU:O	1:B:1114:PRO:HB3	2.15	0.46
1:B:1130:VAL:O	1:B:1131:GLY:C	2.59	0.46
1:C:861:LEU:HD22	1:C:891:THR:HG21	1.96	0.46
1:D:1059:GLU:OE2	1:D:1062:ARG:NH2	2.49	0.46
1:C:1125:ASP:O	1:C:1129:THR:HG22	2.15	0.46
1:D:878:LYS:C	1:D:878:LYS:HE2	2.40	0.46
1:D:1088:MET:HB3	2:D:2080:HOH:O	2.15	0.46
1:F:878:LYS:O	1:F:878:LYS:HE2	2.15	0.46
1:A:1004:MET:O	1:A:1007:SER:HB2	2.15	0.46
1:B:882:VAL:HG21	1:B:933:TYR:CE1	2.50	0.46
2:B:2039:HOH:O	1:D:1201:MET:HG2	2.15	0.46
1:C:1097:TRP:CD2	1:C:1107:HIS:HB3	2.50	0.46
1:A:1233:ASP:OD1	1:A:1237:ARG:NH2	2.49	0.46
1:B:1018:ARG:HD2	1:B:1037:HIS:O	2.16	0.46
1:B:1130:VAL:HG12	1:B:1130:VAL:O	2.16	0.46
1:C:871:ARG:O	1:C:874:ASP:HB3	2.15	0.46
1:C:923:ARG:HD3	1:C:1216:ARG:HH21	1.79	0.46
1:E:871:ARG:HG2	1:E:871:ARG:HH21	1.80	0.46
1:E:876:ARG:O	1:E:876:ARG:HG3	2.16	0.46
1:E:878:LYS:HE2	1:E:878:LYS:O	2.16	0.46
1:E:1067:MET:HE1	1:E:1148:ALA:HA	1.97	0.46
1:E:1125:ASP:O	1:E:1129:THR:HG22	2.15	0.46
1:E:1169:LYS:NZ	1:E:1191:ASP:OD2	2.48	0.46
1:F:971:ASP:HB3	1:F:975:GLU:H	1.80	0.46
1:A:847:THR:HA	1:A:848:PRO:HD3	1.73	0.46
1:A:1107:HIS:HD1	1:A:1108:PRO:CD	2.28	0.46
1:A:1107:HIS:CE1	1:A:1108:PRO:HD3	2.50	0.46
1:B:840:LEU:N	1:B:841:PRO:HD2	2.31	0.46
1:C:884:TYR:HA	1:C:892:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1128:MET:O	1:D:1129:THR:HB	2.16	0.46
1:E:1212:THR:HG22	1:E:1212:THR:O	2.15	0.46
1:A:922:VAL:HG22	1:A:938:LEU:HD23	1.98	0.46
1:D:988:LEU:HD11	1:D:1164:ILE:HD12	1.98	0.46
1:B:875:PHE:C	1:B:877:ILE:H	2.24	0.46
1:D:1046:MET:HE2	1:D:1126:LEU:CG	2.39	0.46
1:D:1048:ASP:CG	1:D:1247:THR:HG23	2.41	0.46
1:E:1022:ILE:HB	1:E:1120:VAL:HA	1.97	0.46
1:E:1035:ILE:HD11	1:E:1231:VAL:HA	1.97	0.46
1:E:1164:ILE:HG22	1:E:1169:LYS:HG2	1.97	0.46
1:F:883:ASN:HD22	1:F:884:TYR:H	1.62	0.46
1:D:1204:MET:HG2	1:D:1217:VAL:O	2.16	0.45
1:E:861:LEU:HD22	1:E:891:THR:HG21	1.98	0.45
1:F:1075:LEU:HD21	1:F:1113:GLU:HB3	1.98	0.45
1:A:876:ARG:HG3	1:A:905:ARG:HH12	1.81	0.45
1:B:1064:TYR:OH	1:B:1147:ALA:HB3	2.16	0.45
1:C:846:LEU:HD23	1:C:1226:GLU:HB3	1.97	0.45
1:C:1164:ILE:HB	1:C:1188:THR:HG22	1.97	0.45
1:D:1203:ASP:OD1	1:D:1216:ARG:NH1	2.45	0.45
1:D:1205:LEU:HD23	1:D:1216:ARG:HA	1.98	0.45
1:E:1059:GLU:OE2	1:E:1063:ARG:NE	2.49	0.45
1:A:987:LEU:HD12	1:A:988:LEU:N	2.32	0.45
1:A:1013:GLN:O	1:A:1014:PRO:C	2.58	0.45
1:A:1048:ASP:CG	1:A:1247:THR:HG23	2.41	0.45
1:A:1118:VAL:HB	1:A:1152:LEU:HD12	1.97	0.45
1:C:1187:ARG:O	1:C:1191:ASP:N	2.48	0.45
1:E:922:VAL:HG22	1:E:938:LEU:CD2	2.47	0.45
1:B:875:PHE:CD2	1:B:909:LEU:HD21	2.52	0.45
1:C:971:ASP:OD2	1:C:975:GLU:HB2	2.16	0.45
1:C:1045:ASP:OD2	1:C:1047:LYS:HB2	2.16	0.45
1:D:1021:MET:HB3	1:D:1029:LEU:HD13	1.98	0.45
1:F:1097:TRP:C	2:F:2042:HOH:O	2.60	0.45
1:B:1018:ARG:HB3	1:B:1039:LEU:HG	1.97	0.45
1:B:1075:LEU:HD21	1:B:1113:GLU:HB3	1.98	0.45
1:C:922:VAL:HG22	1:C:938:LEU:HD23	1.99	0.45
1:D:1176:ILE:HG13	2:D:2101:HOH:O	2.16	0.45
1:D:855:PRO:HD3	2:D:2011:HOH:O	2.17	0.45
1:D:1079:ASN:ND2	1:D:1113:GLU:H	2.08	0.45
1:C:916:SER:HB2	1:C:917:LEU:HD12	1.98	0.45
1:F:876:ARG:HG3	1:F:876:ARG:O	2.17	0.45
1:F:1132:LYS:HB3	1:F:1132:LYS:HE3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:883:ASN:ND2	1:B:884:TYR:N	2.60	0.45
1:F:1013:GLN:O	1:F:1014:PRO:C	2.55	0.45
1:A:883:ASN:CG	1:A:884:TYR:N	2.75	0.45
1:C:1176:ILE:HG23	1:C:1204:MET:HE3	1.98	0.45
1:A:890:ILE:HD13	1:A:937:GLU:HG2	1.98	0.45
1:A:953:ASP:OD1	1:A:953:ASP:O	2.35	0.45
1:C:878:LYS:C	1:C:878:LYS:HE2	2.41	0.45
1:C:1059:GLU:O	1:C:1063:ARG:HG3	2.17	0.45
1:D:861:LEU:HD22	1:D:891:THR:HG21	1.99	0.45
1:E:1239:ARG:HH21	1:E:1239:ARG:CG	2.27	0.45
1:F:1059:GLU:O	1:F:1063:ARG:HG3	2.17	0.45
1:A:840:LEU:HA	1:A:840:LEU:HD23	1.72	0.44
1:A:875:PHE:C	1:A:877:ILE:H	2.24	0.44
1:B:875:PHE:CE2	1:B:909:LEU:HD21	2.53	0.44
1:C:988:LEU:HB2	1:C:1172:ILE:HG21	1.99	0.44
1:D:939:PRO:HB3	1:D:1199:LEU:CD1	2.47	0.44
1:E:1216:ARG:C	1:E:1217:VAL:HG23	2.42	0.44
1:D:1061:GLU:O	1:D:1065:LYS:HG3	2.17	0.44
1:D:1074:ASN:ND2	2:D:2077:HOH:O	2.50	0.44
1:D:1210:ASN:O	1:D:1211:SER:HB2	2.17	0.44
1:E:1012:ALA:HB1	1:E:1016:ASP:HB2	1.99	0.44
1:A:842:SER:HB3	1:A:844:ASP:OD2	2.17	0.44
1:A:947:TYR:O	1:A:948:LEU:C	2.59	0.44
1:D:1023:ASP:OD2	2:D:2063:HOH:O	2.20	0.44
1:E:1026:MET:HE2	1:E:1044:THR:CG2	2.46	0.44
1:F:882:VAL:HG21	1:F:933:TYR:CE1	2.52	0.44
1:F:1046:MET:HA	1:F:1046:MET:CE	2.43	0.44
1:A:1143:GLN:HE21	1:A:1171:ASN:HD21	1.65	0.44
1:B:890:ILE:HD12	1:B:890:ILE:C	2.42	0.44
1:B:1005:ILE:HD11	1:B:1119:LEU:HD13	1.99	0.44
1:B:1164:ILE:HG22	1:B:1169:LYS:CG	2.47	0.44
1:D:1135:GLU:OE1	1:D:1165:THR:HG21	2.17	0.44
1:E:1158:ARG:N	1:E:1159:PRO:HD3	2.32	0.44
1:A:1044:THR:HG22	2:A:2041:HOH:O	2.17	0.44
1:D:922:VAL:HG11	1:D:936:LEU:HD22	1.99	0.44
1:E:840:LEU:N	1:E:841:PRO:HD2	2.32	0.44
1:E:1034:GLY:O	1:E:1240:PRO:HD3	2.18	0.44
1:F:939:PRO:HB3	1:F:1199:LEU:CD1	2.48	0.44
1:F:1223:ARG:HB2	1:F:1226:GLU:HG3	1.99	0.44
1:B:1232:GLN:HB3	2:B:2017:HOH:O	2.17	0.44
1:E:1171:ASN:O	1:E:1173:PRO:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1025:LYS:C	1:F:1026:MET:HG3	2.42	0.44
1:F:1143:GLN:HG3	1:F:1171:ASN:ND2	2.33	0.44
1:A:1041:GLU:HG2	1:A:1242:TYR:CE1	2.53	0.44
1:A:1172:ILE:O	1:A:1172:ILE:HG22	2.17	0.44
1:B:1245:GLY:O	1:B:1246:ILE:C	2.59	0.44
1:D:987:LEU:HA	1:D:1174:THR:O	2.18	0.44
1:F:985:PRO:O	1:F:1151:HIS:HD2	2.00	0.44
1:F:1045:ASP:OD2	1:F:1047:LYS:HB2	2.18	0.44
1:F:1185:ASP:O	1:F:1189:ILE:HG12	2.17	0.44
1:B:878:LYS:HE2	1:B:878:LYS:O	2.17	0.44
1:B:922:VAL:CG1	1:B:936:LEU:HD22	2.48	0.44
1:C:1142:ALA:HB3	1:C:1171:ASN:HB3	2.00	0.44
1:F:987:LEU:CD2	1:F:1153:VAL:HG13	2.40	0.44
1:F:1160:SER:OG	1:F:1163:VAL:HG23	2.17	0.44
1:A:893:PHE:CE1	1:A:938:LEU:HD12	2.52	0.44
1:B:1022:ILE:HB	1:B:1120:VAL:HA	2.00	0.44
1:B:1051:ASN:HD22	1:B:1051:ASN:HA	1.62	0.44
1:E:922:VAL:HG22	1:E:938:LEU:HD23	2.00	0.44
1:E:1122:GLU:OE2	1:E:1124:ALA:HB3	2.18	0.44
1:F:1009:LEU:HD11	1:F:1035:ILE:HD11	1.99	0.44
1:B:936:LEU:HD23	1:B:936:LEU:HA	1.88	0.43
1:E:1091:PRO:HB2	1:E:1109:VAL:CG1	2.48	0.43
1:F:871:ARG:HH21	1:F:871:ARG:HG2	1.83	0.43
1:F:875:PHE:CD1	1:F:875:PHE:N	2.86	0.43
1:B:972:ILE:HG12	2:B:2085:HOH:O	2.18	0.43
1:A:1204:MET:HE2	1:A:1206:TYR:HB2	2.01	0.43
1:E:842:SER:HG	1:E:844:ASP:CG	2.26	0.43
1:E:913:LEU:O	1:E:913:LEU:HD23	2.18	0.43
1:E:1079:ASN:ND2	1:E:1113:GLU:H	2.09	0.43
1:A:988:LEU:HD11	1:A:1164:ILE:HG23	2.00	0.43
1:C:1021:MET:HB3	1:C:1029:LEU:HD13	2.00	0.43
1:C:1085:ALA:HB1	1:C:1090:ARG:O	2.17	0.43
1:B:1041:GLU:HG3	2:B:2038:HOH:O	2.18	0.43
1:C:1028:GLU:HB2	1:C:1121:ASP:OD1	2.18	0.43
1:D:847:THR:HG22	1:D:1226:GLU:OE2	2.19	0.43
1:A:849:PRO:C	2:A:2008:HOH:O	2.60	0.43
1:B:917:LEU:N	1:B:917:LEU:CD1	2.78	0.43
1:E:1034:GLY:HA3	1:E:1235:LYS:HE3	1.99	0.43
1:A:840:LEU:HD12	1:A:1013:GLN:HE22	1.83	0.43
1:B:876:ARG:HG2	1:B:876:ARG:HH21	1.83	0.43
1:B:919:THR:O	1:B:920:VAL:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1046:MET:SD	1:C:1126:LEU:HA	2.58	0.43
1:C:1237:ARG:HD3	2:C:2032:HOH:O	2.18	0.43
1:D:939:PRO:HB3	1:D:1199:LEU:HD13	2.01	0.43
1:E:919:THR:O	1:E:920:VAL:C	2.60	0.43
1:E:1015:GLU:O	1:E:1114:PRO:HB3	2.18	0.43
1:F:1156:THR:HG21	1:F:1164:ILE:HD11	2.00	0.43
1:A:847:THR:CG2	1:A:1226:GLU:OE2	2.65	0.43
1:A:1131:GLY:C	2:A:2062:HOH:O	2.60	0.43
1:A:1187:ARG:HA	1:A:1192:GLN:H	1.84	0.43
1:B:919:THR:HG22	1:B:939:PRO:HG2	2.01	0.43
1:B:1237:ARG:HD3	2:B:2034:HOH:O	2.18	0.43
1:C:907:SER:C	1:C:909:LEU:H	2.26	0.43
1:D:844:ASP:HB3	2:D:2051:HOH:O	2.19	0.43
1:E:992:THR:CG2	1:E:993:THR:H	2.25	0.43
1:E:1164:ILE:HG22	1:E:1169:LYS:CG	2.49	0.43
1:A:939:PRO:HB3	1:A:1199:LEU:HD11	2.00	0.43
1:A:1024:PRO:HB3	1:A:1046:MET:HE1	2.00	0.43
1:B:1157:GLN:C	1:B:1159:PRO:HD3	2.43	0.43
1:C:871:ARG:HG2	1:C:871:ARG:HH21	1.84	0.43
1:C:881:VAL:HG22	1:C:895:LEU:CD2	2.48	0.43
1:E:847:THR:HA	1:E:848:PRO:HD3	1.82	0.43
1:E:881:VAL:HG22	1:E:895:LEU:HD23	1.99	0.43
1:E:1074:ASN:OD1	1:E:1074:ASN:N	2.52	0.43
1:F:867:LEU:O	1:F:871:ARG:HG2	2.19	0.43
1:F:939:PRO:HB3	1:F:1199:LEU:HD13	2.01	0.43
1:B:1107:HIS:CE1	1:B:1108:PRO:HG2	2.53	0.43
1:C:922:VAL:CG1	1:C:936:LEU:HD22	2.49	0.43
1:D:871:ARG:HG3	1:D:917:LEU:HD11	2.01	0.43
1:F:916:SER:HB2	1:F:917:LEU:HD12	2.01	0.43
1:F:964:LEU:HB3	1:F:981:LEU:HB3	2.00	0.43
1:A:1041:GLU:O	1:A:1042:VAL:C	2.62	0.42
1:A:1142:ALA:HB3	1:A:1171:ASN:HB3	2.00	0.42
1:B:906:ILE:N	1:B:906:ILE:HD12	2.33	0.42
1:C:1079:ASN:ND2	1:C:1113:GLU:H	2.11	0.42
1:E:865:ALA:HB1	1:E:881:VAL:HG11	1.99	0.42
1:E:875:PHE:CD1	1:E:875:PHE:N	2.87	0.42
1:E:990:ALA:CB	1:E:1189:ILE:HD12	2.49	0.42
1:F:1018:ARG:NH2	1:F:1039:LEU:HA	2.33	0.42
1:F:1127:MET:HE1	1:F:1135:GLU:OE1	2.19	0.42
1:B:840:LEU:HD21	2:B:2067:HOH:O	2.19	0.42
1:D:1118:VAL:HB	1:D:1152:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:971:ASP:OD2	1:E:975:GLU:HB2	2.19	0.42
1:E:1107:HIS:ND1	1:E:1108:PRO:HG2	2.34	0.42
1:F:861:LEU:HD22	1:F:891:THR:HG21	2.01	0.42
1:F:936:LEU:HD23	1:F:936:LEU:HA	1.89	0.42
1:B:861:LEU:HD22	1:B:891:THR:HG21	2.01	0.42
1:C:990:ALA:CB	1:C:1189:ILE:HD12	2.49	0.42
1:D:875:PHE:CD1	1:D:875:PHE:N	2.88	0.42
1:D:1064:TYR:OH	1:D:1147:ALA:HB3	2.19	0.42
1:D:1245:GLY:O	1:D:1246:ILE:C	2.62	0.42
1:F:875:PHE:C	1:F:877:ILE:H	2.27	0.42
1:A:884:TYR:HA	1:A:892:ARG:O	2.19	0.42
1:B:1047:LYS:HB2	1:D:1223:ARG:CZ	2.50	0.42
1:D:879:ALA:HB2	1:D:897:LEU:HD23	2.02	0.42
1:A:954:ASN:O	1:A:958:ARG:HB2	2.19	0.42
1:A:957:PHE:CZ	1:A:1011:LYS:HE2	2.54	0.42
1:D:1223:ARG:HB2	1:D:1226:GLU:HG3	2.02	0.42
1:E:841:PRO:HA	1:E:1237:ARG:HH12	1.85	0.42
1:A:869:GLU:HG3	1:A:879:ALA:O	2.20	0.42
1:A:1122:GLU:OE2	1:A:1124:ALA:CB	2.67	0.42
1:D:864:MET:SD	1:D:917:LEU:CD2	3.05	0.42
1:D:988:LEU:HB2	1:D:1172:ILE:HG21	2.02	0.42
1:E:1187:ARG:HA	1:E:1192:GLN:H	1.85	0.42
1:A:985:PRO:HD2	1:A:1173:PRO:HG3	2.02	0.42
1:B:909:LEU:CD1	1:B:912:ASP:HB2	2.49	0.42
1:C:940:ASN:CB	2:C:2019:HOH:O	2.68	0.42
1:C:1190:LEU:O	1:C:1191:ASP:HB2	2.20	0.42
1:E:1090:ARG:HG2	2:E:2062:HOH:O	2.20	0.42
1:E:1127:MET:HE2	1:E:1163:VAL:O	2.20	0.42
1:E:1132:LYS:HE3	1:E:1132:LYS:HB3	1.83	0.42
1:F:1212:THR:O	1:F:1212:THR:HG22	2.19	0.42
1:A:1209:PRO:HD2	2:A:2031:HOH:O	2.19	0.42
1:D:875:PHE:CD2	1:D:909:LEU:HD21	2.55	0.42
1:F:953:ASP:CG	1:F:958:ARG:HH22	2.28	0.42
1:F:1162:ASP:N	2:F:2052:HOH:O	2.52	0.42
1:A:897:LEU:HB3	1:A:901:VAL:HB	2.00	0.42
1:B:1171:ASN:O	1:B:1173:PRO:HD3	2.20	0.42
1:D:868:VAL:HB	2:D:2019:HOH:O	2.20	0.42
1:E:882:VAL:HG21	1:E:933:TYR:CE1	2.55	0.42
1:F:1135:GLU:OE1	1:F:1165:THR:HG21	2.20	0.42
1:F:1171:ASN:HA	2:F:2056:HOH:O	2.19	0.42
1:A:1127:MET:HE1	1:A:1135:GLU:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:884:TYR:HA	1:B:892:ARG:O	2.18	0.42
1:B:1249:ASP:N	2:B:2094:HOH:O	2.53	0.42
1:D:1165:THR:OG1	1:D:1168:ILE:HG12	2.20	0.42
1:E:928:ILE:HD11	1:E:935:GLY:CA	2.49	0.42
1:F:883:ASN:ND2	1:F:884:TYR:N	2.59	0.42
1:F:1041:GLU:H	1:F:1041:GLU:HG3	1.64	0.42
1:C:869:GLU:HG3	1:C:879:ALA:O	2.19	0.41
1:C:940:ASN:N	1:C:940:ASN:ND2	2.68	0.41
1:C:1161:VAL:HG12	1:C:1161:VAL:O	2.19	0.41
1:D:928:ILE:O	1:D:929:PRO:C	2.61	0.41
1:E:1013:GLN:O	1:E:1014:PRO:C	2.61	0.41
1:E:1186:SER:HB2	1:E:1195:ALA:HB3	2.02	0.41
1:F:987:LEU:HD21	1:F:1153:VAL:CG1	2.45	0.41
1:C:1172:ILE:HD12	1:C:1172:ILE:N	2.35	0.41
1:D:907:SER:C	1:D:909:LEU:N	2.77	0.41
1:F:1085:ALA:HB1	1:F:1090:ARG:O	2.19	0.41
1:A:871:ARG:O	1:A:874:ASP:HB3	2.20	0.41
1:A:1055:TRP:CD2	1:A:1246:ILE:HG12	2.55	0.41
1:A:1063:ARG:NH1	1:A:1113:GLU:HG3	2.35	0.41
1:B:954:ASN:ND2	1:B:956:LYS:H	2.18	0.41
1:C:1035:ILE:HG22	1:C:1038:LEU:H	1.86	0.41
1:F:1035:ILE:CG2	1:F:1038:LEU:HG	2.32	0.41
1:F:1058:ASN:ND2	2:F:2033:HOH:O	2.53	0.41
1:A:1018:ARG:CZ	1:A:1039:LEU:HD23	2.49	0.41
1:B:1213:LEU:HD23	2:B:2083:HOH:O	2.19	0.41
1:C:876:ARG:HG3	1:C:905:ARG:NH1	2.36	0.41
1:C:1164:ILE:HG22	1:C:1169:LYS:CG	2.51	0.41
1:C:1204:MET:HE2	1:C:1206:TYR:HB2	2.03	0.41
1:E:867:LEU:HD22	1:E:871:ARG:HH22	1.84	0.41
1:E:1129:THR:CG2	1:E:1130:VAL:N	2.83	0.41
1:A:1079:ASN:ND2	1:A:1113:GLU:H	2.10	0.41
1:B:864:MET:SD	1:B:917:LEU:CD2	3.09	0.41
1:B:885:SER:HA	1:B:886:PRO:HD2	1.98	0.41
1:D:1022:ILE:HG22	1:D:1024:PRO:HD3	2.03	0.41
1:D:1055:TRP:CD2	1:D:1246:ILE:HG12	2.56	0.41
1:E:1196:GLU:OE2	1:E:1196:GLU:C	2.63	0.41
1:F:1009:LEU:CD1	1:F:1035:ILE:HD11	2.51	0.41
1:A:871:ARG:HG2	1:A:871:ARG:NH2	2.36	0.41
1:B:847:THR:HA	1:B:848:PRO:HD3	1.74	0.41
1:B:988:LEU:HD23	1:B:989:VAL:N	2.36	0.41
1:E:1063:ARG:NH1	1:E:1113:GLU:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:978:VAL:HG12	1:F:979:ALA:N	2.36	0.41
1:A:985:PRO:O	1:A:1151:HIS:HD2	2.04	0.41
1:A:1039:LEU:HD23	1:A:1039:LEU:HA	1.83	0.41
1:A:1122:GLU:C	1:A:1124:ALA:N	2.79	0.41
1:D:1022:ILE:HG13	1:D:1120:VAL:HG22	2.02	0.41
1:F:1161:VAL:HG22	2:F:2054:HOH:O	2.20	0.41
1:F:1183:LYS:HE2	1:F:1183:LYS:HB3	1.84	0.41
1:A:867:LEU:O	1:A:871:ARG:HG2	2.21	0.41
1:A:1046:MET:SD	1:A:1126:LEU:HA	2.61	0.41
1:A:1174:THR:OG1	1:A:1209:PRO:HD3	2.20	0.41
1:B:844:ASP:OD2	1:B:844:ASP:N	2.51	0.41
1:B:1005:ILE:HG21	1:B:1032:TYR:CE2	2.55	0.41
1:B:1097:TRP:CD2	1:B:1107:HIS:CE1	3.09	0.41
1:C:882:VAL:HG21	1:C:933:TYR:CE1	2.55	0.41
1:E:1097:TRP:C	2:E:2066:HOH:O	2.63	0.41
1:A:1135:GLU:OE1	1:A:1165:THR:HG21	2.21	0.41
1:A:1160:SER:OG	1:A:1163:VAL:HG23	2.21	0.41
1:A:1164:ILE:HB	1:A:1188:THR:HG22	2.03	0.41
1:B:840:LEU:CD2	2:B:2067:HOH:O	2.68	0.41
1:B:1026:MET:O	1:B:1027:LEU:HD23	2.20	0.41
1:C:924:VAL:HG12	2:C:2015:HOH:O	2.21	0.41
1:C:968:LEU:HB3	1:C:1217:VAL:HG11	2.02	0.41
1:C:1004:MET:O	1:C:1007:SER:HB2	2.20	0.41
1:D:1035:ILE:HD12	1:D:1231:VAL:HG13	2.02	0.41
1:D:1039:LEU:HD23	1:D:1039:LEU:HA	1.90	0.41
1:E:846:LEU:CD2	1:E:1226:GLU:HB3	2.51	0.41
1:E:1185:ASP:O	1:E:1189:ILE:HG12	2.21	0.41
1:B:875:PHE:CE2	1:B:909:LEU:HD11	2.56	0.41
1:B:1135:GLU:OE1	1:B:1165:THR:HG21	2.21	0.41
1:C:953:ASP:CG	1:C:958:ARG:HH2	2.29	0.41
1:E:1107:HIS:CE1	1:E:1108:PRO:HG2	2.55	0.41
1:A:927:VAL:HG11	1:A:1213:LEU:CD2	2.50	0.40
1:A:1161:VAL:O	1:A:1161:VAL:HG12	2.20	0.40
1:C:875:PHE:N	1:C:875:PHE:CD1	2.88	0.40
1:C:1125:ASP:OD1	1:C:1158:ARG:NH1	2.46	0.40
1:D:897:LEU:HD11	1:D:934:VAL:HG21	2.03	0.40
1:F:884:TYR:HA	1:F:892:ARG:O	2.20	0.40
1:F:917:LEU:HB3	2:F:2012:HOH:O	2.20	0.40
1:A:1035:ILE:HD11	1:A:1231:VAL:HA	2.04	0.40
1:A:1063:ARG:NE	1:A:1113:GLU:HG2	2.36	0.40
1:A:1088:MET:O	1:A:1089:MET:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:876:ARG:HG3	1:B:905:ARG:HH12	1.87	0.40
1:C:1091:PRO:HB2	1:C:1109:VAL:CG1	2.52	0.40
1:C:1184:ILE:HG13	1:C:1185:ASP:N	2.36	0.40
1:D:871:ARG:HG2	1:D:871:ARG:NH2	2.34	0.40
1:E:1048:ASP:CG	1:E:1247:THR:HG23	2.47	0.40
1:F:846:LEU:HD23	1:F:1226:GLU:HB3	2.02	0.40
1:F:1052:ALA:O	1:F:1055:TRP:HB3	2.21	0.40
1:F:1161:VAL:C	2:F:2052:HOH:O	2.64	0.40
1:C:1107:HIS:HA	1:C:1108:PRO:HD2	1.66	0.40
1:D:987:LEU:H	1:D:987:LEU:HD23	1.85	0.40
1:D:1018:ARG:NH2	1:D:1039:LEU:HA	2.36	0.40
1:E:898:ALA:HB1	1:E:899:PRO:CD	2.52	0.40
1:E:971:ASP:OD1	1:E:973:ALA:N	2.50	0.40
1:F:954:ASN:ND2	1:F:956:LYS:H	2.19	0.40
1:F:1176:ILE:HG12	1:F:1206:TYR:HD1	1.87	0.40
1:A:987:LEU:HD11	1:A:989:VAL:HG23	1.99	0.40
1:B:1190:LEU:O	1:B:1191:ASP:HB2	2.21	0.40
1:C:1123:PHE:CE2	1:C:1163:VAL:HG12	2.57	0.40
1:D:1027:LEU:HB3	1:D:1030:SER:OG	2.21	0.40
1:E:1141:LEU:HD23	1:E:1141:LEU:HA	1.96	0.40
1:A:1210:ASN:O	1:A:1211:SER:HB2	2.22	0.40
1:B:895:LEU:O	1:B:933:TYR:HB3	2.22	0.40
1:B:985:PRO:HG3	1:B:1146:ARG:HD2	2.04	0.40
1:B:1028:GLU:HB3	1:B:1121:ASP:OD1	2.21	0.40
1:C:1031:VAL:O	1:C:1031:VAL:HG22	2.21	0.40
1:C:1041:GLU:O	1:C:1042:VAL:C	2.64	0.40
1:D:844:ASP:CB	2:D:2051:HOH:O	2.69	0.40
1:D:1123:PHE:O	1:D:1127:MET:HG2	2.22	0.40
1:E:869:GLU:HG3	1:E:879:ALA:O	2.22	0.40
1:E:913:LEU:C	1:E:915:ARG:H	2.29	0.40
1:E:936:LEU:HD23	1:E:936:LEU:HA	1.88	0.40

All (3) 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:B:919:THR:N	1:E:919:THR:N[1_465]	1.90	0.30
1:B:919:THR:O	1:E:919:THR:O[1_465]	2.09	0.11
1:B:917:LEU:O	1:E:919:THR:CG2[1_465]	2.18	0.02

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	387/512 (76%)	355 (92%)	29 (8%)	3 (1%)	16	37
1	B	387/512 (76%)	360 (93%)	23 (6%)	4 (1%)	12	32
1	C	387/512 (76%)	354 (92%)	33 (8%)	0	100	100
1	D	387/512 (76%)	355 (92%)	30 (8%)	2 (0%)	24	48
1	E	373/512 (73%)	347 (93%)	22 (6%)	4 (1%)	11	29
1	F	374/512 (73%)	347 (93%)	24 (6%)	3 (1%)	16	37
All	All	2295/3072 (75%)	2118 (92%)	161 (7%)	16 (1%)	18	41

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1131	GLY
1	D	1129	THR
1	E	1026	MET
1	E	1027	LEU
1	E	1108	PRO
1	F	1132	LYS
1	B	1108	PRO
1	B	1128	MET
1	D	1131	GLY
1	E	1132	LYS
1	A	1128	MET
1	A	1131	GLY
1	B	1159	PRO
1	A	901	VAL
1	F	1130	VAL
1	F	1131	GLY

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	330/429 (77%)	308 (93%)	22 (7%)	15	36
1	B	330/429 (77%)	309 (94%)	21 (6%)	16	38
1	C	330/429 (77%)	310 (94%)	20 (6%)	17	40
1	D	331/429 (77%)	311 (94%)	20 (6%)	17	41
1	E	321/429 (75%)	296 (92%)	25 (8%)	11	29
1	F	322/429 (75%)	298 (92%)	24 (8%)	12	31
All	All	1964/2574 (76%)	1832 (93%)	132 (7%)	15	36

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	847	THR
1	A	875	PHE
1	A	885	SER
1	A	948	LEU
1	A	958	ARG
1	A	968	LEU
1	A	975	GLU
1	A	981	LEU
1	A	987	LEU
1	A	988	LEU
1	A	1035	ILE
1	A	1046	MET
1	A	1072	VAL
1	A	1075	LEU
1	A	1107	HIS
1	A	1119	LEU
1	A	1123	PHE
1	A	1128	MET
1	A	1152	LEU
1	A	1196	GLU
1	A	1222	VAL
1	A	1247	THR

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Mol	Chain	Res	Type
1	B	844	ASP
1	B	847	THR
1	B	878	LYS
1	B	917	LEU
1	B	948	LEU
1	B	968	LEU
1	B	978	VAL
1	B	981	LEU
1	B	1014	PRO
1	B	1035	ILE
1	B	1046	MET
1	B	1072	VAL
1	B	1075	LEU
1	B	1107	HIS
1	B	1109	VAL
1	B	1119	LEU
1	B	1126	LEU
1	B	1128	MET
1	B	1196	GLU
1	B	1212	THR
1	B	1247	THR
1	C	847	THR
1	C	948	LEU
1	C	958	ARG
1	C	968	LEU
1	C	975	GLU
1	C	981	LEU
1	C	987	LEU
1	C	988	LEU
1	C	1014	PRO
1	C	1035	ILE
1	C	1072	VAL
1	C	1074	ASN
1	C	1075	LEU
1	C	1107	HIS
1	C	1119	LEU
1	C	1126	LEU
1	C	1132	LYS
1	C	1152	LEU
1	C	1196	GLU
1	C	1232	GLN
1	D	847	THR

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Mol	Chain	Res	Type
1	D	863	GLN
1	D	948	LEU
1	D	968	LEU
1	D	975	GLU
1	D	978	VAL
1	D	981	LEU
1	D	988	LEU
1	D	1014	PRO
1	D	1025	LYS
1	D	1035	ILE
1	D	1046	MET
1	D	1072	VAL
1	D	1075	LEU
1	D	1107	HIS
1	D	1119	LEU
1	D	1126	LEU
1	D	1128	MET
1	D	1196	GLU
1	D	1232	GLN
1	E	847	THR
1	E	917	LEU
1	E	948	LEU
1	E	968	LEU
1	E	975	GLU
1	E	988	LEU
1	E	1014	PRO
1	E	1027	LEU
1	E	1035	ILE
1	E	1046	MET
1	E	1054	ARG
1	E	1073	ARG
1	E	1074	ASN
1	E	1075	LEU
1	E	1107	HIS
1	E	1113	GLU
1	E	1119	LEU
1	E	1126	LEU
1	E	1128	MET
1	E	1152	LEU
1	E	1161	VAL
1	E	1196	GLU
1	E	1232	GLN

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Mol	Chain	Res	Type
1	E	1239	ARG
1	E	1247	THR
1	F	847	THR
1	F	948	LEU
1	F	958	ARG
1	F	968	LEU
1	F	975	GLU
1	F	981	LEU
1	F	1014	PRO
1	F	1026	MET
1	F	1027	LEU
1	F	1035	ILE
1	F	1046	MET
1	F	1054	ARG
1	F	1074	ASN
1	F	1075	LEU
1	F	1107	HIS
1	F	1113	GLU
1	F	1119	LEU
1	F	1126	LEU
1	F	1128	MET
1	F	1129	THR
1	F	1196	GLU
1	F	1232	GLN
1	F	1244	ASP
1	F	1247	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	863	GLN
1	A	883	ASN
1	A	940	ASN
1	A	944	GLN
1	A	954	ASN
1	A	1013	GLN
1	A	1037	HIS
1	A	1051	ASN
1	A	1058	ASN
1	A	1079	ASN
1	A	1171	ASN
1	A	1192	GLN

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Mol	Chain	Res	Type
1	A	1210	ASN
1	A	1225	GLN
1	A	1232	GLN
1	B	863	GLN
1	B	883	ASN
1	B	940	ASN
1	B	954	ASN
1	B	1013	GLN
1	B	1037	HIS
1	B	1051	ASN
1	B	1058	ASN
1	B	1079	ASN
1	B	1157	GLN
1	B	1171	ASN
1	B	1192	GLN
1	B	1210	ASN
1	B	1218	HIS
1	B	1232	GLN
1	C	863	GLN
1	C	883	ASN
1	C	940	ASN
1	C	954	ASN
1	C	1051	ASN
1	C	1058	ASN
1	C	1074	ASN
1	C	1079	ASN
1	C	1157	GLN
1	C	1171	ASN
1	C	1192	GLN
1	C	1210	ASN
1	C	1232	GLN
1	D	863	GLN
1	D	883	ASN
1	D	896	ASN
1	D	940	ASN
1	D	954	ASN
1	D	1037	HIS
1	D	1051	ASN
1	D	1058	ASN
1	D	1079	ASN
1	D	1157	GLN
1	D	1171	ASN

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Mol	Chain	Res	Type
1	D	1192	GLN
1	D	1210	ASN
1	D	1232	GLN
1	E	863	GLN
1	E	883	ASN
1	E	940	ASN
1	E	954	ASN
1	E	1013	GLN
1	E	1051	ASN
1	E	1058	ASN
1	E	1079	ASN
1	E	1157	GLN
1	E	1171	ASN
1	E	1192	GLN
1	E	1210	ASN
1	E	1232	GLN
1	F	863	GLN
1	F	883	ASN
1	F	940	ASN
1	F	954	ASN
1	F	1013	GLN
1	F	1051	ASN
1	F	1058	ASN
1	F	1079	ASN
1	F	1107	HIS
1	F	1143	GLN
1	F	1157	GLN
1	F	1171	ASN
1	F	1192	GLN
1	F	1210	ASN
1	F	1232	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	849:PRO	C	855:PRO	N	13.90

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	393/512 (76%)	0.67	37 (9%) 14 12	18, 43, 85, 100	0
1	B	393/512 (76%)	0.40	24 (6%) 27 24	14, 37, 77, 94	0
1	C	393/512 (76%)	1.06	75 (19%) 3 3	21, 49, 106, 120	0
1	D	394/512 (76%)	0.48	31 (7%) 18 16	16, 37, 76, 103	0
1	E	381/512 (74%)	0.98	78 (20%) 2 2	20, 45, 106, 128	0
1	F	382/512 (74%)	1.07	82 (21%) 2 2	19, 51, 118, 138	0
All	All	2336/3072 (76%)	0.77	327 (13%) 6 5	14, 43, 96, 138	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	921	ALA	8.6
1	E	918	SER	8.2
1	C	904	ALA	7.7
1	C	1108	PRO	7.4
1	E	915	ARG	6.0
1	F	1171	ASN	5.9
1	C	1046	MET	5.8
1	F	895	LEU	5.8
1	F	921	ALA	5.8
1	E	920	VAL	5.8
1	E	877	ILE	5.6
1	C	861	LEU	5.5
1	E	913	LEU	5.4
1	F	920	VAL	5.4
1	D	1080	GLU	5.4
1	F	1183	LYS	5.2
1	C	1107	HIS	5.2
1	F	893	PHE	5.1
1	E	1228	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	875	PHE	4.9
1	E	884	TYR	4.9
1	D	855	PRO	4.8
1	A	1249	ASP	4.8
1	F	861	LEU	4.7
1	E	861	LEU	4.7
1	F	918	SER	4.7
1	A	1125	ASP	4.6
1	F	882	VAL	4.6
1	C	903	ALA	4.5
1	A	1108	PRO	4.5
1	F	858	THR	4.4
1	D	862	GLU	4.4
1	B	919	THR	4.4
1	F	859	PHE	4.4
1	E	893	PHE	4.3
1	F	881	VAL	4.3
1	E	875	PHE	4.2
1	E	858	THR	4.2
1	E	866	ARG	4.2
1	E	895	LEU	4.1
1	E	878	LYS	4.1
1	C	868	VAL	4.1
1	C	917	LEU	4.1
1	E	1107	HIS	4.1
1	E	899	PRO	4.1
1	C	921	ALA	4.0
1	C	897	LEU	4.0
1	A	862	GLU	4.0
1	C	872	LEU	4.0
1	E	1171	ASN	4.0
1	F	864	MET	4.0
1	F	867	LEU	3.9
1	C	880	ASP	3.9
1	B	858	THR	3.9
1	F	1130	VAL	3.9
1	C	1125	ASP	3.9
1	B	915	ARG	3.8
1	C	906	ILE	3.8
1	E	882	VAL	3.8
1	A	1046	MET	3.8
1	E	917	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	860	ALA	3.8
1	F	875	PHE	3.8
1	F	880	ASP	3.7
1	F	975	GLU	3.7
1	C	858	THR	3.7
1	C	873	ALA	3.7
1	F	971	ASP	3.7
1	E	881	VAL	3.6
1	E	922	VAL	3.6
1	A	858	THR	3.6
1	E	997	ALA	3.6
1	D	858	THR	3.6
1	F	915	ARG	3.6
1	C	908	ASN	3.6
1	C	1185	ASP	3.6
1	B	917	LEU	3.6
1	F	913	LEU	3.6
1	B	1080	GLU	3.6
1	F	936	LEU	3.6
1	D	873	ALA	3.5
1	A	1107	HIS	3.5
1	A	1126	LEU	3.5
1	A	1047	LYS	3.5
1	A	1097	TRP	3.5
1	E	897	LEU	3.5
1	B	918	SER	3.5
1	F	865	ALA	3.5
1	D	879	ALA	3.4
1	F	1228	HIS	3.4
1	E	1128	MET	3.4
1	F	1128	MET	3.4
1	C	919	THR	3.4
1	B	1249	ASP	3.4
1	C	914	ALA	3.4
1	E	1130	VAL	3.4
1	C	878	LYS	3.4
1	C	907	SER	3.4
1	F	884	TYR	3.3
1	A	840	LEU	3.3
1	E	912	ASP	3.3
1	A	880	ASP	3.3
1	F	840	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	863	GLN	3.3
1	A	904	ALA	3.3
1	E	873	ALA	3.3
1	F	922	VAL	3.3
1	A	1035	ILE	3.3
1	C	1097	TRP	3.3
1	C	1025	LYS	3.3
1	F	874	ASP	3.3
1	F	1045	ASP	3.2
1	F	917	LEU	3.2
1	C	901	VAL	3.2
1	F	1191	ASP	3.2
1	D	1136	GLU	3.2
1	E	1080	GLU	3.2
1	B	1129	THR	3.2
1	C	865	ALA	3.2
1	D	918	SER	3.2
1	B	1061	GLU	3.2
1	D	899	PRO	3.2
1	B	859	PHE	3.2
1	E	1133	LYS	3.1
1	E	929	PRO	3.1
1	C	1026	MET	3.1
1	E	864	MET	3.1
1	C	913	LEU	3.1
1	E	919	THR	3.1
1	F	860	ALA	3.1
1	E	886	PRO	3.1
1	F	877	ILE	3.1
1	E	859	PHE	3.1
1	E	1244	ASP	3.0
1	D	875	PHE	3.0
1	F	1107	HIS	3.0
1	B	1244	ASP	3.0
1	E	1187	ARG	3.0
1	D	859	PHE	2.9
1	D	917	LEU	2.9
1	F	923	ARG	2.9
1	C	877	ILE	2.9
1	B	875	PHE	2.9
1	D	1061	GLU	2.9
1	E	876	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	911	ARG	2.9
1	C	879	ALA	2.9
1	F	919	THR	2.9
1	C	866	ARG	2.8
1	F	866	ARG	2.8
1	F	899	PRO	2.8
1	C	1181	SER	2.8
1	E	928	ILE	2.8
1	A	872	LEU	2.8
1	E	840	LEU	2.8
1	E	993	THR	2.8
1	F	879	ALA	2.8
1	C	893	PHE	2.8
1	E	1209	PRO	2.8
1	D	860	ALA	2.8
1	E	1129	THR	2.8
1	F	1213	LEU	2.8
1	A	1185	ASP	2.8
1	E	869	GLU	2.8
1	D	1108	PRO	2.7
1	D	881	VAL	2.7
1	E	865	ALA	2.7
1	A	884	TYR	2.7
1	F	1133	LYS	2.7
1	F	916	SER	2.7
1	B	862	GLU	2.7
1	C	915	ARG	2.7
1	C	925	VAL	2.7
1	D	867	LEU	2.7
1	C	1248	SER	2.7
1	A	903	ALA	2.7
1	F	870	ALA	2.7
1	C	884	TYR	2.7
1	A	917	LEU	2.7
1	E	951	VAL	2.7
1	C	1027	LEU	2.6
1	F	1170	ALA	2.6
1	E	1212	THR	2.6
1	E	933	TYR	2.6
1	B	867	LEU	2.6
1	B	860	ALA	2.6
1	C	885	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	870	ALA	2.6
1	E	880	ASP	2.6
1	F	959	ASP	2.6
1	C	864	MET	2.6
1	C	1096	TYR	2.6
1	E	916	SER	2.6
1	E	936	LEU	2.6
1	F	950	GLU	2.6
1	F	1080	GLU	2.6
1	F	914	ALA	2.6
1	D	915	ARG	2.5
1	A	898	ALA	2.5
1	A	875	PHE	2.5
1	C	869	GLU	2.5
1	F	933	TYR	2.5
1	C	1192	GLN	2.5
1	C	891	THR	2.4
1	F	1187	ARG	2.4
1	C	918	SER	2.4
1	C	1134	VAL	2.4
1	C	898	ALA	2.4
1	F	993	THR	2.4
1	A	916	SER	2.4
1	C	926	GLU	2.4
1	E	894	GLU	2.4
1	F	1131	GLY	2.4
1	E	941	LYS	2.4
1	F	941	LYS	2.4
1	D	871	ARG	2.4
1	F	876	ARG	2.4
1	A	877	ILE	2.4
1	B	1027	LEU	2.4
1	C	909	LEU	2.4
1	D	1044	THR	2.4
1	E	1184	ILE	2.4
1	F	897	LEU	2.4
1	C	1045	ASP	2.4
1	C	1249	ASP	2.4
1	E	1097	TRP	2.4
1	C	900	GLY	2.4
1	C	881	VAL	2.4
1	E	879	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	909	LEU	2.4
1	F	1184	ILE	2.4
1	B	1107	HIS	2.4
1	F	862	GLU	2.4
1	F	885	SER	2.4
1	F	878	LYS	2.4
1	F	1209	PRO	2.4
1	A	871	ARG	2.4
1	C	1042	VAL	2.4
1	E	927	VAL	2.4
1	F	871	ARG	2.4
1	C	867	LEU	2.3
1	A	1026	MET	2.3
1	C	1047	LYS	2.3
1	C	905	ARG	2.3
1	C	1109	VAL	2.3
1	C	1035	ILE	2.3
1	F	1129	THR	2.3
1	E	887	GLY	2.3
1	C	1139	ALA	2.3
1	E	1201	MET	2.3
1	C	888	PRO	2.3
1	D	959	ASP	2.3
1	C	1126	LEU	2.3
1	F	872	LEU	2.3
1	F	973	ALA	2.3
1	D	1107	HIS	2.3
1	F	942	LYS	2.3
1	C	1024	PRO	2.3
1	C	1048	ASP	2.3
1	D	876	ARG	2.3
1	F	1185	ASP	2.3
1	A	909	LEU	2.3
1	A	865	ALA	2.2
1	B	877	ILE	2.2
1	D	1052	ALA	2.2
1	F	1212	THR	2.2
1	C	896	ASN	2.2
1	F	849	PRO	2.2
1	E	932	PRO	2.2
1	B	900	GLY	2.2
1	C	916	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	938	LEU	2.2
1	E	924	VAL	2.2
1	F	931	LYS	2.2
1	F	1134	VAL	2.2
1	A	878	LYS	2.2
1	E	971	ASP	2.2
1	F	1197	SER	2.2
1	C	920	VAL	2.2
1	D	1046	MET	2.2
1	F	1189	ILE	2.2
1	C	870	ALA	2.2
1	A	863	GLN	2.2
1	C	1119	LEU	2.2
1	E	1213	LEU	2.2
1	E	885	SER	2.2
1	E	1197	SER	2.2
1	F	873	ALA	2.1
1	E	891	THR	2.1
1	B	872	LEU	2.1
1	F	1207	SER	2.1
1	A	873	ALA	2.1
1	F	1193	ALA	2.1
1	F	926	GLU	2.1
1	E	883	ASN	2.1
1	C	922	VAL	2.1
1	C	1163	VAL	2.1
1	D	869	GLU	2.1
1	A	864	MET	2.1
1	C	1232	GLN	2.1
1	E	863	GLN	2.1
1	F	868	VAL	2.1
1	D	866	ARG	2.1
1	E	862	GLU	2.1
1	E	914	ALA	2.1
1	C	886	PRO	2.1
1	A	1027	LEU	2.1
1	B	913	LEU	2.1
1	E	994	GLY	2.1
1	E	1208	GLY	2.1
1	A	1189	ILE	2.1
1	B	1130	VAL	2.1
1	A	874	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1045	ASP	2.0
1	C	1121	ASP	2.0
1	D	1027	LEU	2.0
1	E	867	LEU	2.0
1	B	871	ARG	2.0
1	A	1121	ASP	2.0
1	D	1244	ASP	2.0
1	E	844	ASP	2.0
1	E	870	ALA	2.0
1	E	931	LYS	2.0
1	D	919	THR	2.0
1	F	944	GLN	2.0
1	E	1238	GLY	2.0
1	A	1096	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.