Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:06 pm BST

PDB ID	:	2IUS
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 following versions of software and data (see references ①) were used in the production of this report:

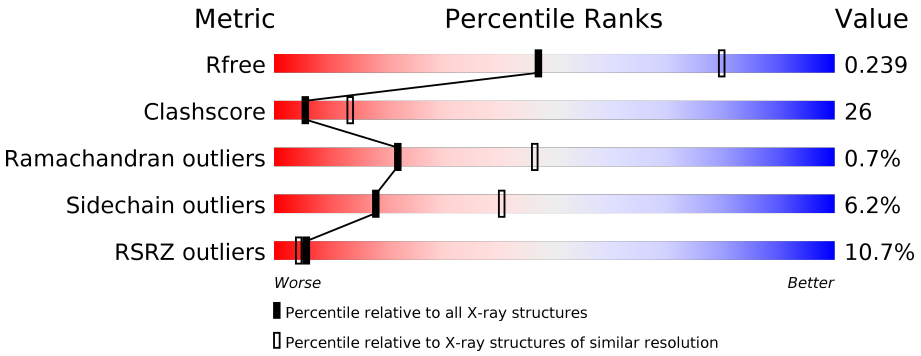
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	512	5% 43% 31% • 23%
1	B	512	5% 46% 27% • 23%
1	C	512	10% 44% 30% • 23%
1	D	512	6% 45% 30% • 23%
1	E	512	10% 43% 28% • 26%
1	F	512	13% 43% 29% • 25%

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

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	O	0	0
			91	91		
2	B	94	Total	O	0	0
			94	94		
2	C	80	Total	O	0	0
			80	80		

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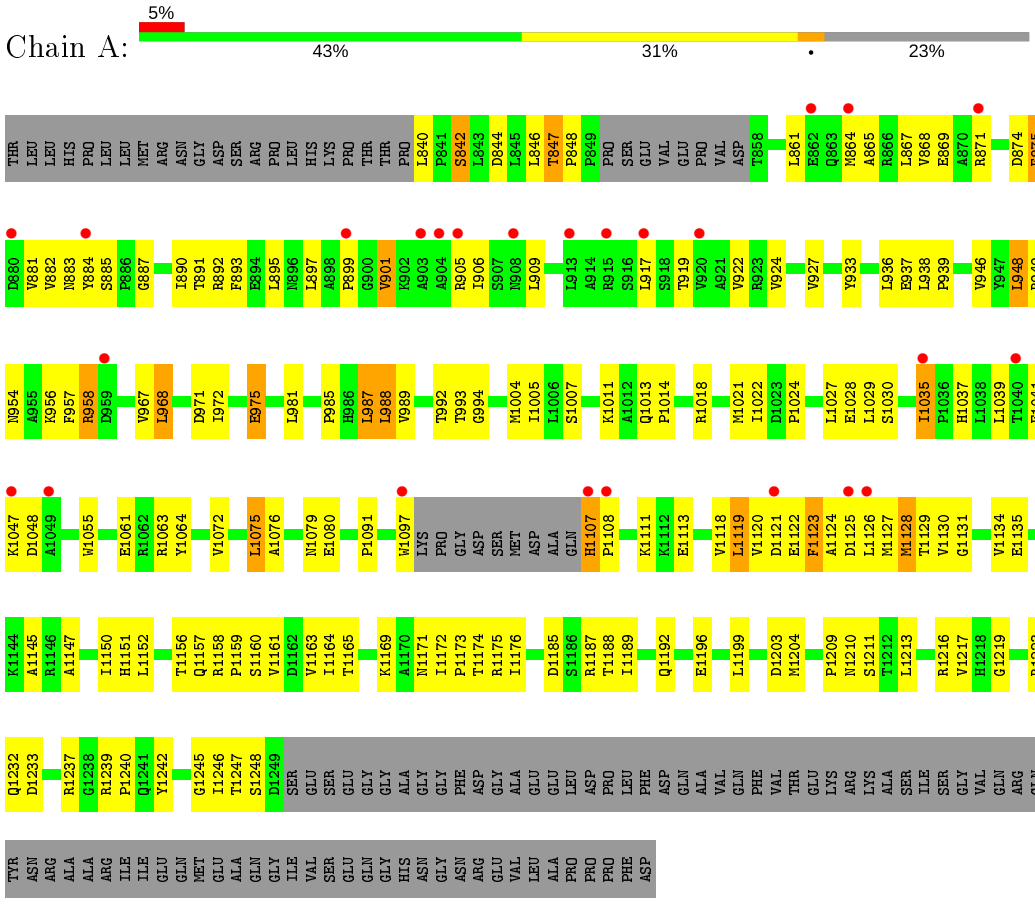
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	116	Total O 116 116	0	0
2	E	99	Total O 99 99	0	0
2	F	73	Total O 73 73	0	0

3 Residue-property plots (i)

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.

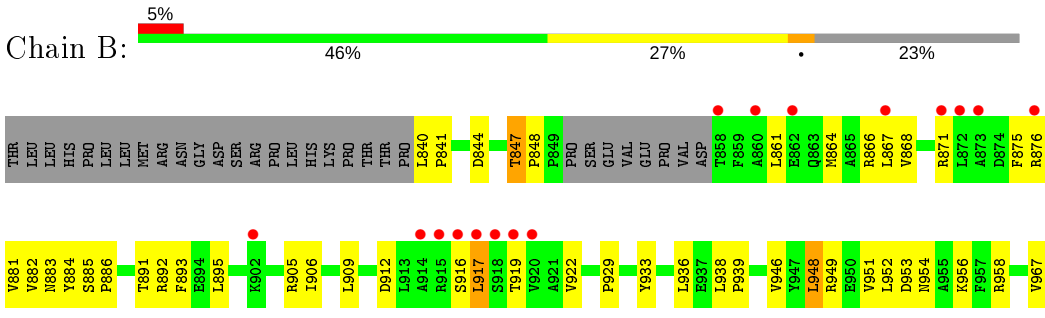
• Molecule 1: DNA TRANSLOCASE FTSK

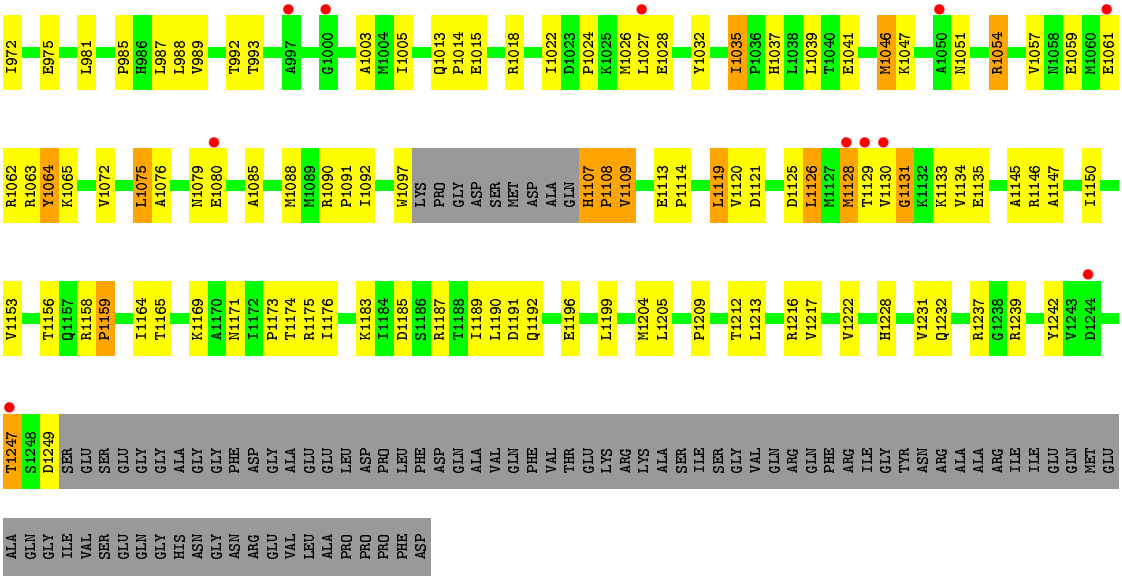
Chain A:



• Molecule 1: DNA TRANSLOCASE FTSK

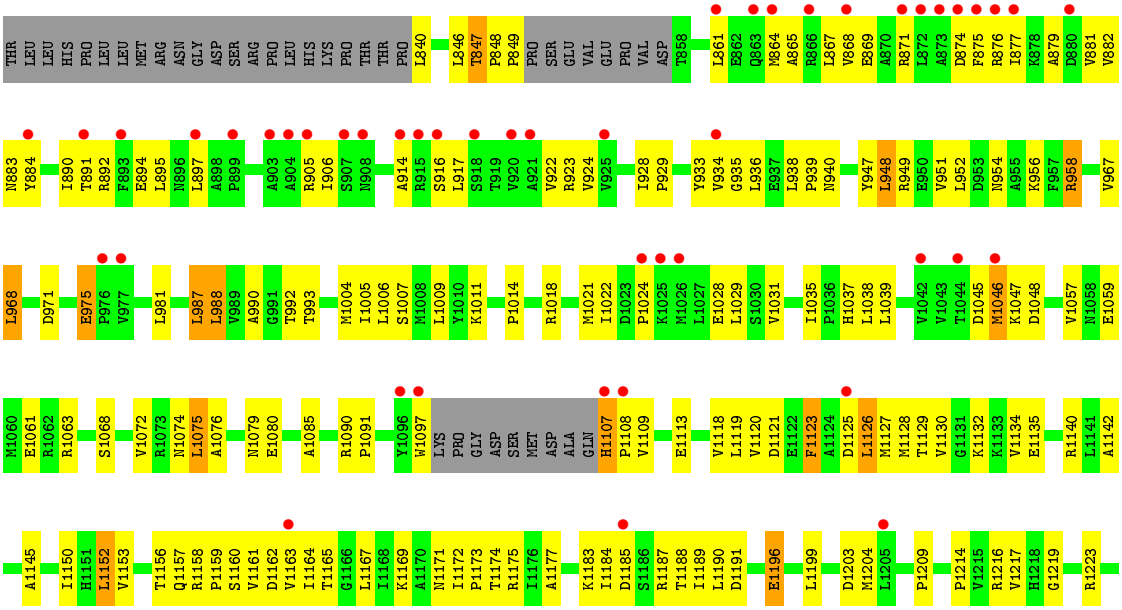
Chain B:





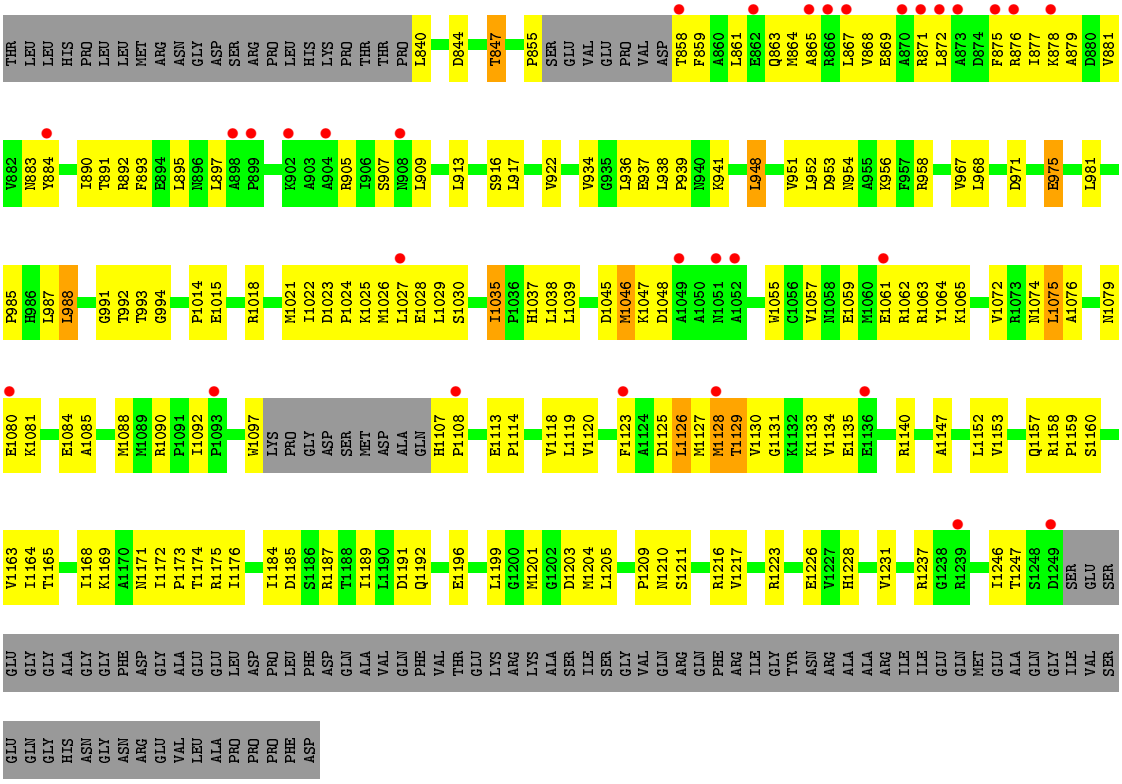
- Molecule 1: DNA TRANSLOCASE FTSK

Chain C:



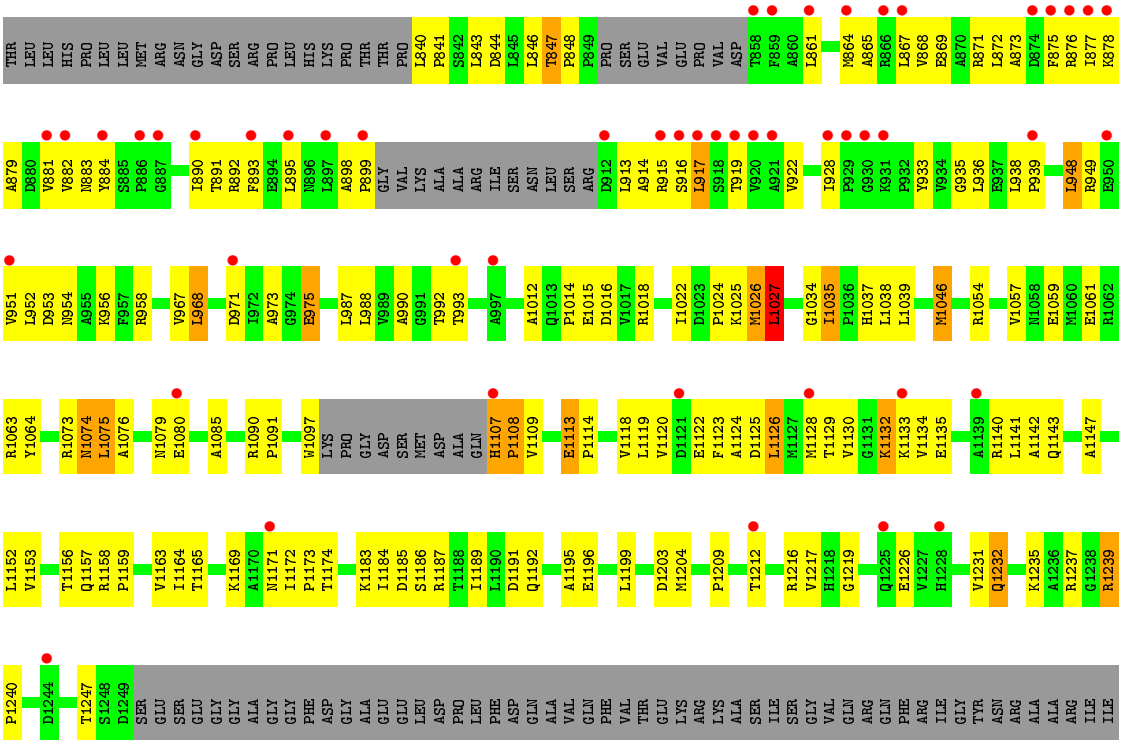
- Molecule 1: DNA TRANSLOCASE FTSK

Chain D:



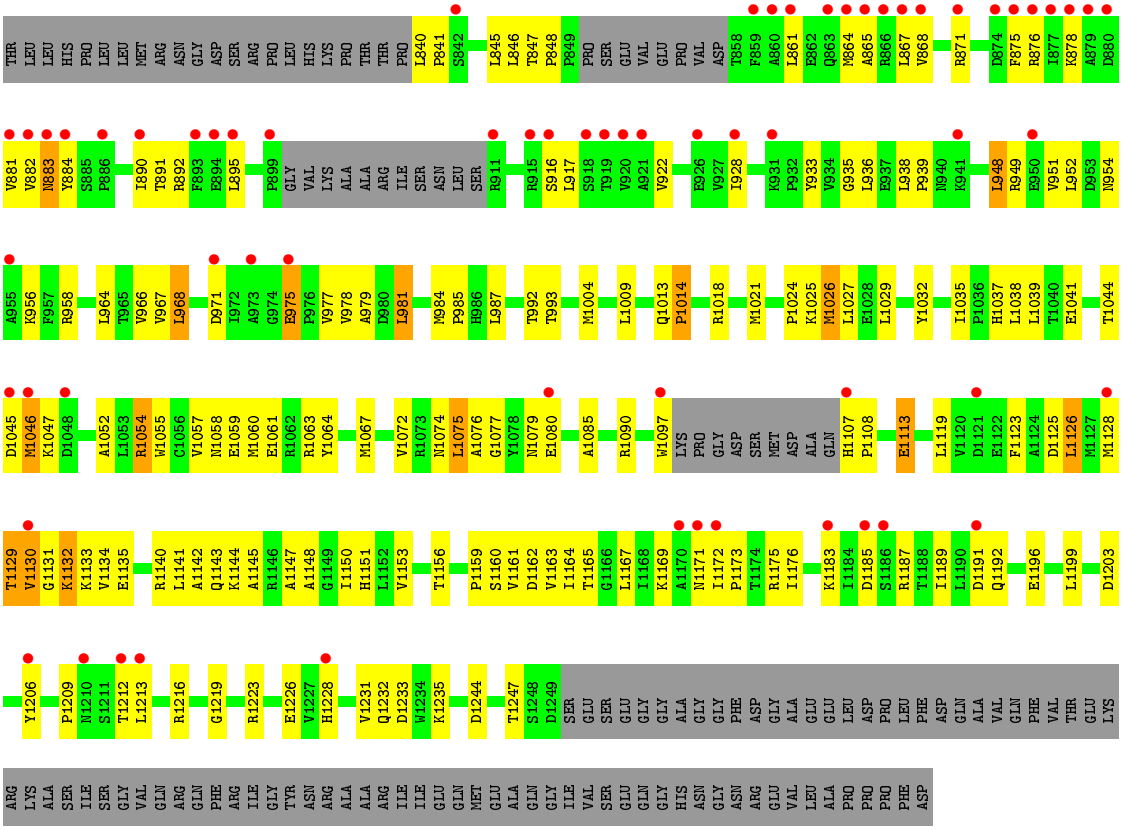
• Molecule 1: DNA TRANSLOCASE FTSK

Chain E:



• Molecule 1: DNA TRANSLOCASE FTSK

Chain F:



4 Data and refinement statistics (i)

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 – 2.70 130.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-2.70) 99.7 (130.58-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.298 0.243 , 0.239	Depositor DCC
R_{free} test set	4056 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18569	wwPDB-VP
Average B, all atoms (Å^2)	48.0	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 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.*

[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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.36	0/3083	0.66	0/4186
1	B	0.39	0/3083	0.66	0/4186
1	C	0.35	0/3083	0.63	0/4186
1	D	0.38	0/3090	0.65	0/4194
1	E	0.38	0/2994	0.67	0/4066
1	F	0.35	0/3005	0.63	0/4080
All	All	0.37	0/18338	0.65	0/24898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3029	0	3146	167	0
1	B	3029	0	3146	157	3
1	C	3029	0	3146	163	0
1	D	3036	0	3153	166	0
1	E	2941	0	3046	159	3
1	F	2952	0	3059	146	0
2	A	91	0	0	18	0
2	B	94	0	0	27	0
2	C	80	0	0	20	0
2	D	116	0	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	99	0	0	22	0
2	F	73	0	0	25	0
All	All	18569	0	18696	948	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 26.

All (948) 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: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: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: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:A:1107:HIS:HD1	1:A:1107:HIS:C	1.73	0.90
1:B:1129:THR:HG23	1:B:1130:VAL:HG23	1.56	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:F:848:PRO:HG3	1:F:949:ARG:NH2	1.90	0.86
1:A:1173:PRO:HB2	1:A:1209:PRO:HB3	1.58	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:E:987:LEU:HB2	2:E:2077:HOH:O	1.77	0.84
1:A:1107:HIS:ND1	1:A:1107:HIS:C	2.30	0.84
1:A:840:LEU:HD22	2:A:2002:HOH:O	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:1046:MET:HE2	1:E:1126:LEU:HG	1.62	0.81
1:E:992:THR:HG22	1:E:993:THR:H	1.45	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: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:D:1107:HIS:ND1	1:D:1107:HIS:C	2.35	0.79
1:C:1097:TRP:CE3	1:C:1107:HIS:HB3	2.18	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: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
1:E:1079:ASN:HD21	1:E:1113:GLU:H	1.33	0.75
1:E:871:ARG:HD2	1:E:916:SER:HB3	1.68	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:ND1	1:F:1107:HIS:C	2.40	0.75
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:1046:MET:HE1	1:D:1126:LEU:HG	1.70	0.74
1:D:1079:ASN:HD21	1:D:1113:GLU:H	1.32	0.74
1:D:954:ASN:HD22	1:D:956:LYS:H	1.33	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:A:1046:MET:HE1	1:A:1126:LEU:HG	1.70	0.73
1:C:848:PRO:HG3	1:C:949:ARG:NH2	2.03	0.73
1:E:1046:MET:CE	1:E:1126:LEU:HG	2.19	0.73
1:E:1129:THR:HG23	1:E:1130:VAL:HG23	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1107:HIS:HD1	1:D:1107:HIS:C	1.91	0.72
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:D:1046:MET:CE	1:D:1126:LEU:HG	2.20	0.72
1:F:1130:VAL:HG12	1:F:1133:LYS:HB3	1.71	0.72
1:F:871:ARG:HD2	1:F:916:SER:HB3	1.72	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:E:1046:MET:HE3	2:E:2048:HOH:O	1.90	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: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:C:1018:ARG:HB3	1:C:1039:LEU:HG	1.73	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:F:1107:HIS:HD1	1:F:1107:HIS:C	1.95	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: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
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: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:1090:ARG:HB2	2:D:2080:HOH:O	1.93	0.68
1:D:864:MET:O	1:D:868:VAL:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1157:GLN:C	1:A:1159:PRO:HD3	2.15	0.67
1:F:1231:VAL:O	1:F:1235:LYS:HG3	1.94	0.67
1:A:1091:PRO:HG2	2:A:2054:HOH:O	1.93	0.67
1:B:1035:ILE:CD1	1:B:1231:VAL:HG13	2.25	0.66
1:B:840:LEU:HD23	2:B:2003:HOH:O	1.94	0.66
1:F:1079:ASN:HD21	1:F:1113:GLU:H	1.43	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:HD12	1:E:917:LEU:N	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:A:1028:GLU:CD	1:A:1028:GLU:H	1.99	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: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
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: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:B:878:LYS:HE2	1:B:878:LYS:C	2.18	0.64
1:E:914:ALA:HB1	2:E:2023:HOH:O	1.97	0.64
1:C:1046:MET:HE1	1:C:1126:LEU:HG	1.80	0.64
1:E:1024:PRO:HB3	1:E:1046:MET:SD	2.38	0.64
1:E:948:LEU:HD22	1:E:952:LEU:HG	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1035:ILE:HG23	1:A:1037:HIS:H	1.64	0.62
1:C:1157:GLN:C	1:C:1159:PRO:HD3	2.20	0.62
1:F:841:PRO:HB3	1:F:1233:ASP:OD1	2.00	0.62
1:D:1046:MET:HA	1:D:1046:MET:CE	2.30	0.62
1:C:954:ASN:HD22	1:C:956:LYS:H	1.48	0.62
1:C:951:VAL:HG11	1:C:967:VAL:HG13	1.82	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:1097:TRP:CE2	1:A:1107:HIS:HE1	2.18	0.61
1:A:1130:VAL:O	1:A:1130:VAL:HG12	2.01	0.61
1:A:987:LEU:HD11	1:A:989:VAL:CG2	2.30	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
1:A:1046:MET:CE	1:A:1046:MET:HA	2.30	0.61
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:A:1046:MET:CE	1:A:1126:LEU:HG	2.31	0.61
1:D:1107:HIS:CE1	1:D:1108:PRO:HD3	2.35	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:1142:ALA:HB3	1:E:1171:ASN:HB3	1.83	0.60
1:E:846:LEU:N	2:E:2002:HOH:O	2.27	0.60
1:F:1026:MET:HE2	1:F:1044:THR:HG21	1.81	0.60
1:B:1156:THR:HG21	1:B:1164:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:951:VAL:HG11	1:D:967:VAL:HG13	1.83	0.60
1:C:1046:MET:CE	1:C:1126:LEU:HG	2.31	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:C:1046:MET:HG2	1:C:1129:THR:HG21	1.83	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: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:B:992:THR:CG2	1:B:993:THR:H	2.15	0.59
1:B:1046:MET:CE	1:B:1046:MET:HA	2.32	0.59
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:C:1130:VAL:HG12	1:C:1130:VAL:O	2.03	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:1111:LYS:HG2	2:A:2058:HOH:O	2.01	0.59
1:A:847:THR:HG22	1:A:1226:GLU:OE2	2.02	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:N	1:F:917:LEU:HD12	2.18	0.58
1:E:1097:TRP:CE3	1:E:1107:HIS:CE1	2.91	0.58
1:E:1035:ILE:CD1	1:E:1231:VAL:HG13	2.33	0.58
1:E:1107:HIS:ND1	1:E:1107:HIS:C	2.57	0.58
1:C:1046:MET:HA	1:C:1046:MET:CE	2.33	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:D:1130:VAL:O	1:D:1134:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:LYS:O	1:A:1175:ARG:NH1	2.37	0.58
1:A:906:ILE:HD12	1:A:906:ILE:N	2.18	0.58
1:C:1018:ARG:NH2	1:C:1039:LEU:HD23	2.18	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: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:A:1127:MET:HE1	2:A:2062:HOH:O	2.03	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:1075:LEU:HD21	1:A:1113:GLU:HB3	1.84	0.57
1:A:946:VAL:HG22	2:A:2024:HOH:O	2.03	0.57
1:B:988:LEU:HD11	1:B:1164:ILE:HG23	1.85	0.57
1:C:1018:ARG:HD2	1:C:1037:HIS:O	2.03	0.57
1:C:929:PRO:HD2	2:C:2013:HOH:O	2.04	0.57
1:A:892:ARG:HD2	2:A:2014:HOH:O	2.04	0.57
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: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:993:THR:HA	1:A:1157:GLN:NE2	2.20	0.57
1:A:887:GLY:HA3	1:A:972:ILE:O	2.05	0.57
1:C:1035:ILE:HG22	1:C:1038:LEU:HG	1.86	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:D:1130:VAL:HG12	1:D:1134:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1145:ALA:HB1	1:C:1150:ILE:HB	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:A:954:ASN:ND2	1:A:956:LYS:H	2.02	0.56
1:C:917:LEU:N	1:C:917:LEU:HD12	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:1057:VAL:O	1:C:1061:GLU:HG3	2.06	0.56
1:C:906:ILE:HD12	1:C:906:ILE:H	1.70	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:B:895:LEU:HD11	1:B:936:LEU:HD12	1.87	0.56
1:E:1027:LEU:HD11	2:E:2043:HOH:O	2.05	0.56
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: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: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:876:ARG:HG3	1:C:905:ARG:HH12	1.70	0.55
1:C:864:MET:SD	1:C:917:LEU:HD23	2.46	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:928:ILE:HD11	1:F:935:GLY:CA	2.36	0.55
1:F:895:LEU:HD11	1:F:936:LEU:CD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1026:MET:O	1:D:1027:LEU:HD23	2.07	0.55
1:D:893:PHE:CE1	1:D:938:LEU:HD12	2.42	0.55
1:E:1126:LEU:HD22	1:E:1134:VAL:HG21	1.89	0.55
1:E:939:PRO:HB3	1:E:1199:LEU:HD13	1.88	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:C:890:ILE:C	1:C:890:ILE:HD12	2.27	0.55
1:A:1169:LYS:HG2	2:A:2067:HOH:O	2.06	0.55
1:C:1048:ASP:CG	1:C:1247:THR:HG23	2.27	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:B:1035:ILE:HD11	1:B:1231:VAL:HA	1.89	0.55
1:D:1107:HIS:ND1	1:D:1108:PRO:HD3	2.22	0.55
1:A:1107:HIS:ND1	1:A:1108:PRO:HD3	2.21	0.55
1:B:1107:HIS:C	1:B:1107:HIS:ND1	2.60	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: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:1169:LYS:O	1:C:1175:ARG:NH1	2.39	0.54
1:C:906:ILE:HD12	1:C:906:ILE:N	2.23	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:1047:LYS:NZ	1:D:847:THR:HB	2.22	0.54
1:B:939:PRO:HB3	1:B:1199:LEU:CD1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:864:MET:O	1:A:868:VAL:HG23	2.08	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:C:1171:ASN:C	1:C:1172:ILE:HD12	2.28	0.54
1:A:844:ASP:N	2:A:2004:HOH:O	2.18	0.54
1:D:988:LEU:HD11	1:D:1164:ILE:HG23	1.90	0.54
1:D:872:LEU:HD21	1:D:913:LEU:HD11	1.90	0.54
1:E:953:ASP:CG	1:E:958:ARG:HH22	2.10	0.54
1:A:1125:ASP:O	1:A:1129:THR:HG22	2.08	0.53
1:C:1046:MET:HA	1:C:1046:MET:HE3	1.88	0.53
1:C:947:TYR:HB3	2:C:2007:HOH:O	2.08	0.53
1:D:1035:ILE:HG23	1:D:1037:HIS:H	1.73	0.53
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:B:895:LEU:HD11	1:B:936:LEU:CD1	2.38	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:C:1167:LEU:HD23	1:F:1167:LEU:HD23	1.89	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:1029:LEU:HD22	2:C:2037:HOH:O	2.08	0.53
1:C:914:ALA:CB	1:C:922:VAL:HG23	2.39	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: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: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:F:890:ILE:HG22	1:F:939:PRO:HA	1.90	0.53
1:C:1107:HIS:ND1	1:C:1107:HIS:N	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1024:PRO:HB3	1:B:1046:MET:SD	2.48	0.52
1:B:919:THR:HG21	1:B:939:PRO:HD2	1.90	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
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:B:953:ASP:CG	1:B:958:ARG:HH22	2.12	0.52
1:D:1187:ARG:HA	1:D:1192:GLN:H	1.75	0.52
1:D:871:ARG:HH21	1:D:871:ARG:HG2	1.74	0.52
1:F:1175:ARG:HD2	1:F:1189:ILE:O	2.08	0.52
1:F:890:ILE:HD12	1:F:890:ILE:C	2.29	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:A:1046:MET:HG2	1:A:1129:THR:HG21	1.90	0.52
1:A:861:LEU:HD22	1:A:891:THR:HG21	1.92	0.52
1:E:1027:LEU:O	1:E:1027:LEU:HD12	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:C:849:PRO:C	2:C:2008:HOH:O	2.48	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:1187:ARG:HA	1:B:1192:GLN:H	1.75	0.52
1:B:1185:ASP:O	1:B:1189:ILE:HG12	2.10	0.52
1:B:1145:ALA:HB1	1:B:1150:ILE:HB	1.92	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:867:LEU:O	1:C:871:ARG:HG2	2.09	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:A:1046:MET:HA	1:A:1046:MET:HE3	1.91	0.51
1:B:1165:THR:O	1:B:1169:LYS:HG3	2.10	0.51
1:B:946:VAL:HG13	1:B:970:LYS:HD2	1.91	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
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:1126:LEU:HD22	1:B:1134:VAL:HG21	1.92	0.51
1:B:1174:THR:OG1	1:B:1209:PRO:HD3	2.11	0.51
1:B:987:LEU:HD12	2:B:2031:HOH:O	2.09	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:1046:MET:SD	1:D:1126:LEU:HA	2.51	0.51
1:D:993:THR:HA	1:D:1157:GLN:NE2	2.25	0.51
1:D:890:ILE:HD13	1:D:937:GLU:HG2	1.92	0.51
1:C:1175:ARG:HD2	1:C:1189:ILE:O	2.11	0.51
1:F:1032:TYR:O	1:F:1035:ILE:HB	2.10	0.51
1:C:1127:MET:HE3	1:C:1135:GLU:HG3	1.93	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: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:1156:THR:HG21	1:C:1164:ILE:HD11	1.93	0.50
1:C:992:THR:HG22	1:C:993:THR:N	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1046:MET:HG2	1:F:1129:THR:HG23	1.94	0.50
1:F:840:LEU:N	1:F:841:PRO:HD2	2.26	0.50
1:D:916:SER:C	1:D:917:LEU:HD12	2.32	0.50
1:A:1028:GLU:CD	1:A:1028:GLU:N	2.65	0.50
1:A:876:ARG:O	1:A:876:ARG:HG3	2.11	0.50
1:C:1063:ARG:NH1	1:C:1113:GLU:HG3	2.25	0.50
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:F:1026:MET:CE	1:F:1044:THR:HG21	2.41	0.49
1:D:1057:VAL:O	1:D:1061:GLU:HG3	2.12	0.49
1:D:985:PRO:HD2	1:D:1173:PRO:CG	2.42	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:C:1018:ARG:NH2	1:C:1039:LEU:HA	2.27	0.49
1:C:1127:MET:CE	1:C:1135:GLU:HG3	2.42	0.49
1:F:1072:VAL:HG21	1:F:1077:GLY:C	2.32	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:1046:MET:HA	1:F:1046:MET:CE	2.43	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: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: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:D:994:GLY:N	2:D:2059:HOH:O	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1158:ARG:N	1:B:1159:PRO:HD3	2.28	0.49
1:B:876:ARG:HG3	1:B:876:ARG:O	2.12	0.49
1:D:1018:ARG:NH2	1:D:1039:LEU:HD23	2.28	0.49
1:D:1157:GLN:C	1:D:1159:PRO:HD3	2.32	0.49
1:F:840:LEU:HD22	2:F:2010:HOH:O	2.13	0.49
1:B:939:PRO:HB3	1:B:1199:LEU:HD13	1.95	0.49
1:B:840:LEU:HD12	1:B:1013:GLN:NE2	2.17	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
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:1024:PRO:HB3	1:A:1046:MET:HE3	1.95	0.48
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: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:1025:LYS:O	1:E:1026:MET:C	2.51	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:1061:GLU:OE2	1:F:1140:ARG:NH1	2.47	0.48
1:F:916:SER:C	1:F:917:LEU:HD12	2.34	0.48
1:F:977:VAL:HA	2:F:2020:HOH:O	2.13	0.48
1:C:865:ALA:HB1	1:C:881:VAL:HG11	1.95	0.48
1:D:1171:ASN:C	1:D:1172:ILE:HD12	2.34	0.48
1:E:1172:ILE:HD12	1:E:1172:ILE:N	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:HG2	1:C:1011:LYS:O	2.14	0.48
1:B:1047:LYS:HZ2	1:D:847:THR:HB	1.78	0.48
1:E:1143:GLN:HG3	1:E:1171:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:844:ASP:CA	2:E:2002:HOH:O	2.56	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:E:1061:GLU:OE2	1:E:1140:ARG:NH1	2.47	0.47
1:F:1125:ASP:O	1:F:1129:THR:CG2	2.55	0.47
1:D:1035:ILE:HD11	1:D:1231:VAL:HA	1.96	0.47
1:D:871:ARG:HD3	2:D:2026:HOH:O	2.14	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:E:1123:PHE:CZ	1:E:1163:VAL:HG12	2.49	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:B:1035:ILE:HD12	1:B:1231:VAL:HG13	1.97	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:844:ASP:C	2:E:2002:HOH:O	2.52	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:D:875:PHE:C	1:D:877:ILE:H	2.16	0.47
1:E:875:PHE:C	1:E:877:ILE:H	2.18	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:D:876:ARG:O	1:D:876:ARG:HG3	2.13	0.47
1:A:875:PHE:CD1	1:A:875:PHE:N	2.83	0.47
1:C:1239:ARG:HB2	1:C:1240:PRO:HD2	1.95	0.47
1:D:1075:LEU:HD21	1:D:1113:GLU:HB3	1.96	0.47
1:D:884:TYR:HA	1:D:892:ARG:O	2.15	0.47
1:B:1027:LEU:CD1	1:D:941:LYS:O	2.63	0.47
1:B:987:LEU:HD21	1:B:1153:VAL:HG22	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:1046:MET:HA	1:D:1046:MET:HE3	1.95	0.47
1:D:1160:SER:OG	1:D:1163:VAL:HG23	2.14	0.47
1:D:869:GLU:HG3	1:D:879:ALA:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1061:GLU:OE2	1:C:1140:ARG:NH1	2.48	0.47
1:C:990:ALA:HB3	1:C:1189:ILE:HD12	1.97	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: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: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: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:O	1:B:1130:VAL:HG12	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: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:E:871:ARG:HH21	1:E:871:ARG:HG2	1.80	0.46
1:E:876:ARG:HG3	1:E:876:ARG:O	2.16	0.46
1:E:878:LYS:HE2	1:E:878:LYS:O	2.16	0.46
1:F:1107:HIS:C	2:F:2046:HOH:O	2.54	0.46
1:F:971:ASP:HB3	1:F:975:GLU:H	1.80	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:A:847:THR:HA	1:A:848:PRO:HD3	1.73	0.46
1:B:840:LEU:N	1:B:841:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:TYR:HA	1:C:892:ARG:O	2.16	0.46
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:E:1035:ILE:HD11	1:E:1231:VAL:HA	1.97	0.46
1:E:1022:ILE:HB	1:E:1120:VAL:HA	1.97	0.46
1:E:1157:GLN:C	1:E:1159:PRO:HD3	2.36	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:D:907:SER:C	1:D:909:LEU:H	2.19	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:1164:ILE:HB	1:C:1188:THR:HG22	1.97	0.45
1:C:846:LEU:HD23	1:C:1226:GLU:HB3	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:1118:VAL:HB	1:A:1152:LEU:HD12	1.97	0.45
1:A:987:LEU:HD12	1:A:988:LEU:N	2.32	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:1045:ASP:OD2	1:C:1047:LYS:HB2	2.16	0.45
1:C:971:ASP:OD2	1:C:975:GLU:HB2	2.16	0.45
1:D:1021:MET:HB3	1:D:1029:LEU:HD13	1.98	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:1079:ASN:ND2	1:D:1113:GLU:H	2.08	0.45
1:D:855:PRO:HD3	2:D:2011:HOH:O	2.17	0.45
1:C:916:SER:HB2	1:C:917:LEU:HD12	1.98	0.45
1:F:1132:LYS:HB3	1:F:1132:LYS:HE3	1.85	0.45
1:F:876:ARG:O	1:F:876:ARG:HG3	2.17	0.45
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:890:ILE:HD13	1:A:937:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:ASP:O	1:A:953:ASP:OD1	2.35	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:CG	1:E:1239:ARG:HH21	2.27	0.45
1:F:1059:GLU:O	1:F:1063:ARG:HG3	2.17	0.45
1:F:1169:LYS:NZ	1:F:1191:ASP:OD2	2.38	0.45
1:A:840:LEU:HA	1:A:840:LEU:HD23	1.72	0.44
1:B:1176:ILE:HD13	1:B:1204:MET:HE1	1.99	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:C:875:PHE:C	1:C:877:ILE:H	2.21	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:D:1023:ASP:OD2	2:D:2063:HOH:O	2.20	0.44
1:F:882:VAL:HG21	1:F:933:TYR:CE1	2.52	0.44
1:A:1143:GLN:HE21	1:A:1171:ASN:HD21	1.65	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:1034:GLY:O	1:E:1240:PRO:HD3	2.18	0.44
1:E:840:LEU:N	1:E:841:PRO:HD2	2.32	0.44
1:F:1067:MET:CE	1:F:1148:ALA:HA	2.47	0.44
1:F:1223:ARG:HB2	1:F:1226:GLU:HG3	1.99	0.44
1:F:939:PRO:HB3	1:F:1199:LEU:CD1	2.48	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
1:F:1143:GLN:HG3	1:F:1171:ASN:ND2	2.33	0.44
1:A:1172:ILE:O	1:A:1172:ILE:HG22	2.17	0.44
1:A:1041:GLU:HG2	1:A:1242:TYR:CE1	2.53	0.44
1:D:987:LEU:HA	1:D:1174:THR:O	2.18	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:F:985:PRO:O	1:F:1151:HIS:HD2	2.00	0.44
1:B:878:LYS:HE2	1:B:878:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:1051:ASN:HD22	1.62	0.44
1:E:1122:GLU:OE2	1:E:1124:ALA:HB3	2.18	0.44
1:E:890:ILE:C	1:E:890:ILE:HD12	2.39	0.44
1:E:922:VAL:HG22	1:E:938:LEU:HD23	2.00	0.44
1:F:1009:LEU:HD11	1:F:1035:ILE:HD11	1.99	0.44
1:A:1122:GLU:C	1:A:1124:ALA:H	2.21	0.43
1:B:936:LEU:HA	1:B:936:LEU:HD23	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:E:1079:ASN:ND2	1:E:1113:GLU:H	2.09	0.43
1:E:913:LEU:HD23	1:E:913:LEU:O	2.18	0.43
1:E:916:SER:C	1:E:917:LEU:HD12	2.38	0.43
1:A:1134:VAL:O	1:A:1135:GLU:C	2.57	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:F:1046:MET:HA	1:F:1046:MET:HE2	1.99	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:1176:ILE:HD13	1:A:1204:MET:HE1	1.99	0.43
1:B:917:LEU:CD1	1:B:917:LEU:N	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:HH21	1:B:876:ARG:HG2	1.83	0.43
1:C:1046:MET:SD	1:C:1126:LEU:HA	2.58	0.43
1:C:1160:SER:C	1:C:1162:ASP:H	2.21	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: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:1187:ARG:HA	1:A:1192:GLN:H	1.84	0.43
1:A:847:THR:CG2	1:A:1226:GLU:OE2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:ASN:CG	1:A:884:TYR:H	2.22	0.43
1:B:1237:ARG:HD3	2:B:2034:HOH:O	2.18	0.43
1:B:919:THR:HG22	1:B:939:PRO:HG2	2.01	0.43
1:C:916:SER:C	1:C:917:LEU:HD12	2.39	0.43
1:D:844:ASP:HB3	2:D:2051:HOH:O	2.19	0.43
1:E:1164:ILE:HG22	1:E:1169:LYS:CG	2.49	0.43
1:E:992:THR:CG2	1:E:993:THR:H	2.25	0.43
1:A:939:PRO:HB3	1:A:1199:LEU:HD11	2.00	0.43
1:C:871:ARG:HH21	1:C:871:ARG:HG2	1.84	0.43
1:C:881:VAL:HG22	1:C:895:LEU:CD2	2.48	0.43
1:E:1074:ASN:N	1:E:1074:ASN:OD1	2.52	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: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:D:953:ASP:CG	1:D:958:ARG:HH22	2.23	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: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:C:1160:SER:C	1:C:1162:ASP:N	2.72	0.42
1:E:875:PHE:N	1:E:875:PHE:CD1	2.87	0.42
1:E:865:ALA:HB1	1:E:881:VAL:HG11	1.99	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: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
1:E:1046:MET:CE	2:E:2048:HOH:O	2.58	0.42
1:E:1107:HIS:ND1	1:E:1108:PRO:HG2	2.34	0.42
1:E:971:ASP:OD2	1:E:975:GLU:HB2	2.19	0.42
1:F:861:LEU:HD22	1:F:891:THR:HG21	2.01	0.42
1:F:936:LEU:HA	1:F:936:LEU:HD23	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:1064:TYR:OH	1:D:1147:ALA:HB3	2.19	0.42
1:D:875:PHE:N	1:D:875:PHE:CD1	2.88	0.42
1:A:884:TYR:HA	1:A:892:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:957:PHE:CZ	1:A:1011:LYS:HE2	2.54	0.42
1:A:954:ASN:O	1:A:958:ARG:HB2	2.19	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:1122:GLU:OE2	1:A:1124:ALA:CB	2.67	0.42
1:A:869:GLU:HG3	1:A:879:ALA:O	2.20	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:F:1212:THR:O	1:F:1212:THR:HG22	2.19	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:1190:LEU:O	1:C:1191:ASP:HB2	2.20	0.42
1:C:940:ASN:CB	2:C:2019:HOH:O	2.68	0.42
1:E:1090:ARG:HG2	2:E:2062:HOH:O	2.20	0.42
1:E:1132:LYS:HE3	1:E:1132:LYS:HB3	1.83	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: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:953:ASP:CG	1:A:958:ARG:HH22	2.24	0.42
1:B:1249:ASP:N	2:B:2094:HOH:O	2.53	0.42
1:B:884:TYR:HA	1:B:892:ARG:O	2.18	0.42
1:B:916:SER:C	1:B:917:LEU:HD12	2.40	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:1041:GLU:H	1:F:1041:GLU:HG3	1.64	0.42
1:F:883:ASN:ND2	1:F:884:TYR:N	2.59	0.42
1:B:1130:VAL:O	1:B:1131:GLY:C	2.59	0.41
1:C:1161:VAL:HG12	1:C:1161:VAL:O	2.19	0.41
1:C:869:GLU:HG3	1:C:879:ALA:O	2.19	0.41
1:C:940:ASN:ND2	1:C:940:ASN:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1172:ILE:HD12	1:C:1172:ILE:N	2.35	0.41
1:F:1085:ALA:HB1	1:F:1090:ARG:O	2.19	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:A:871:ARG:O	1:A:874:ASP:HB3	2.20	0.41
1:B:844:ASP:N	1:B:844:ASP:OD2	2.51	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:1164:ILE:HG22	1:C:1169:LYS:CG	2.51	0.41
1:C:876:ARG:HG3	1:C:905:ARG:NH1	2.36	0.41
1:E:1129:THR:CG2	1:E:1130:VAL:N	2.83	0.41
1:E:867:LEU:HD22	1:E:871:ARG:HH22	1.84	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:D:878:LYS:HE2	1:D:878:LYS:C	2.40	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
1:F:978:VAL:HG12	1:F:979:ALA:N	2.36	0.41
1:A:1039:LEU:HA	1:A:1039:LEU:HD23	1.83	0.41
1:A:985:PRO:O	1:A:1151:HIS:HD2	2.04	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:HB3	1:F:1183:LYS:HE2	1.84	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:A:867:LEU:O	1:A:871:ARG:HG2	2.21	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:B:875:PHE:C	1:B:877:ILE:H	2.24	0.41
1:C:882:VAL:HG21	1:C:933:TYR:CE1	2.55	0.41
1:D:1048:ASP:CG	1:D:1247:THR:HG23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:SER:OG	1:A:1163:VAL:HG23	2.21	0.41
1:A:1161:VAL:O	1:A:1161:VAL:HG12	2.20	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: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:D:1039:LEU:HD23	1:D:1039:LEU:HA	1.90	0.41
1:D:1035:ILE:HD12	1:D:1231:VAL:HG13	2.02	0.41
1:E:1185:ASP:O	1:E:1189:ILE:HG12	2.21	0.41
1:E:846:LEU:CD2	1:E:1226:GLU:HB3	2.51	0.41
1:A:1135:GLU:OE1	1:A:1165:THR:HG21	2.21	0.41
1:B:1026:MET:O	1:B:1027:LEU:HD23	2.20	0.41
1:C:1004:MET:O	1:C:1007:SER:HB2	2.20	0.41
1:F:1097:TRP:C	2:F:2042:HOH:O	2.60	0.41
1:A:1013:GLN:O	1:A:1014:PRO:C	2.58	0.41
1:A:1048:ASP:CG	1:A:1247:THR:HG23	2.41	0.41
1:B:1135:GLU:OE1	1:B:1165:THR:HG21	2.21	0.41
1:B:875:PHE:CE2	1:B:909:LEU:HD11	2.56	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:C:1125:ASP:OD1	1:C:1158:ARG:NH1	2.46	0.40
1:C:875:PHE:N	1:C:875:PHE:CD1	2.88	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:1063:ARG:NE	1:A:1113:GLU:HG2	2.36	0.40
1:A:1035:ILE:HD11	1:A:1231:VAL:HA	2.04	0.40
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:NH2	1:D:871:ARG:HG2	2.34	0.40
1:F:1052:ALA:O	1:F:1055:TRP:HB3	2.21	0.40
1:F:1067:MET:HE1	1:F:1148:ALA:HA	2.03	0.40
1:F:846:LEU:HD23	1:F:1226:GLU:HB3	2.02	0.40
1:A:875:PHE:C	1:A:877:ILE:H	2.24	0.40
1:C:1107:HIS:HA	1:C:1108:PRO:HD2	1.66	0.40
1:D:1018:ARG:NH2	1:D:1039:LEU:HA	2.36	0.40
1:D:987:LEU:H	1:D:987:LEU:HD23	1.85	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:1176:ILE:HG12	1:F:1206:TYR:HD1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:954:ASN:ND2	1:F:956:LYS:H	2.19	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:1028:GLU:HB3	1:B:1121:ASP:OD1	2.21	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:C:1031:VAL:O	1:C:1031:VAL:HG22	2.21	0.40
1:D:1123:PHE:O	1:D:1127:MET:HG2	2.22	0.40
1:D:844:ASP:CB	2:D:2051:HOH:O	2.69	0.40
1:E:869:GLU:HG3	1:E:879:ALA:O	2.22	0.40
1:E:936:LEU:HA	1:E:936:LEU:HD23	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%)	19 43
1	B	387/512 (76%)	360 (93%)	23 (6%)	4 (1%)	15 37
1	C	387/512 (76%)	354 (92%)	33 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	387/512 (76%)	355 (92%)	30 (8%)	2 (0%)	29	54
1	E	373/512 (73%)	347 (93%)	22 (6%)	4 (1%)	14	34
1	F	374/512 (73%)	347 (93%)	24 (6%)	3 (1%)	19	43
All	All	2295/3072 (75%)	2118 (92%)	161 (7%)	16 (1%)	22	46

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%)	310 (94%)	20 (6%)	18	41
1	B	330/429 (77%)	310 (94%)	20 (6%)	18	41
1	C	330/429 (77%)	309 (94%)	21 (6%)	17	39
1	D	331/429 (77%)	314 (95%)	17 (5%)	24	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	321/429 (75%)	300 (94%)	21 (6%)	17 38
1	F	322/429 (75%)	299 (93%)	23 (7%)	14 34
All	All	1964/2574 (76%)	1842 (94%)	122 (6%)	18 40

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	842	SER
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	1196	GLU
1	B	847	THR
1	B	917	LEU
1	B	948	LEU
1	B	968	LEU
1	B	981	LEU
1	B	1014	PRO
1	B	1035	ILE
1	B	1046	MET
1	B	1054	ARG
1	B	1064	TYR
1	B	1072	VAL
1	B	1075	LEU
1	B	1107	HIS
1	B	1109	VAL

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Mol	Chain	Res	Type
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	1046	MET
1	C	1072	VAL
1	C	1074	ASN
1	C	1075	LEU
1	C	1107	HIS
1	C	1119	LEU
1	C	1123	PHE
1	C	1126	LEU
1	C	1128	MET
1	C	1132	LYS
1	C	1152	LEU
1	C	1196	GLU
1	D	847	THR
1	D	863	GLN
1	D	948	LEU
1	D	968	LEU
1	D	975	GLU
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	1119	LEU
1	D	1126	LEU

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Mol	Chain	Res	Type
1	D	1128	MET
1	D	1196	GLU
1	E	847	THR
1	E	917	LEU
1	E	948	LEU
1	E	968	LEU
1	E	975	GLU
1	E	1014	PRO
1	E	1027	LEU
1	E	1035	ILE
1	E	1046	MET
1	E	1054	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	1196	GLU
1	E	1232	GLN
1	E	1239	ARG
1	E	1247	THR
1	F	847	THR
1	F	883	ASN
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	1046	MET
1	F	1054	ARG
1	F	1074	ASN
1	F	1075	LEU
1	F	1113	GLU
1	F	1119	LEU
1	F	1126	LEU
1	F	1128	MET
1	F	1129	THR

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Mol	Chain	Res	Type
1	F	1196	GLU
1	F	1232	GLN
1	F	1244	ASP
1	F	1247	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	863	GLN
1	A	883	ASN
1	A	940	ASN
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	1157	GLN
1	A	1171	ASN
1	A	1192	GLN
1	A	1210	ASN
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	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	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

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Mol	Chain	Res	Type
1	C	1079	ASN
1	C	1143	GLN
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	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
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	1143	GLN
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	1051	ASN
1	F	1058	ASN
1	F	1079	ASN
1	F	1107	HIS

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Mol	Chain	Res	Type
1	F	1143	GLN
1	F	1151	HIS
1	F	1157	GLN
1	F	1171	ASN
1	F	1192	GLN
1	F	1210	ASN
1	F	1232	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	28 (7%) 16 14	18, 43, 85, 100	0
1	B	393/512 (76%)	0.63	28 (7%) 16 14	14, 37, 77, 94	0
1	C	393/512 (76%)	1.00	49 (12%) 3 3	21, 49, 106, 120	0
1	D	394/512 (76%)	0.68	31 (7%) 12 10	16, 37, 76, 103	0
1	E	381/512 (74%)	1.01	50 (13%) 3 2	20, 45, 106, 128	0
1	F	382/512 (74%)	1.11	65 (17%) 1 1	19, 51, 118, 138	0
All	All	2336/3072 (76%)	0.85	251 (10%) 6 4	14, 43, 96, 138	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	918	SER	13.5
1	C	904	ALA	10.7
1	E	920	VAL	10.2
1	E	877	ILE	9.3
1	F	874	ASP	8.7
1	F	884	TYR	8.5
1	C	1108	PRO	8.4
1	E	915	ARG	8.3
1	E	921	ALA	8.2
1	C	868	VAL	8.0
1	E	884	TYR	7.8
1	F	867	LEU	7.3
1	C	872	LEU	7.2
1	F	860	ALA	7.2
1	F	918	SER	7.0
1	F	861	LEU	7.0
1	E	899	PRO	6.9
1	E	876	ARG	6.7
1	E	874	ASP	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	914	ALA	6.6
1	E	875	PHE	6.5
1	F	915	ARG	6.3
1	C	908	ASN	6.3
1	C	875	PHE	6.2
1	F	921	ALA	6.2
1	F	899	PRO	5.9
1	F	895	LEU	5.9
1	F	893	PHE	5.8
1	F	920	VAL	5.6
1	C	877	ILE	5.6
1	F	1183	LYS	5.6
1	C	880	ASP	5.6
1	C	915	ARG	5.6
1	F	865	ALA	5.5
1	F	875	PHE	5.4
1	F	881	VAL	5.4
1	D	878	LYS	5.3
1	F	1171	ASN	5.0
1	C	903	ALA	5.0
1	A	1108	PRO	5.0
1	F	877	ILE	4.9
1	E	861	LEU	4.9
1	F	876	ARG	4.9
1	E	859	PHE	4.8
1	F	859	PHE	4.8
1	A	904	ALA	4.7
1	C	918	SER	4.6
1	E	1228	HIS	4.3
1	F	941	LYS	4.3
1	C	1249	ASP	4.3
1	C	907	SER	4.2
1	B	858	THR	4.2
1	E	858	THR	4.1
1	E	916	SER	4.1
1	C	921	ALA	4.1
1	F	1130	VAL	4.1
1	F	1107	HIS	4.0
1	F	1185	ASP	4.0
1	F	866	ARG	4.0
1	B	917	LEU	4.0
1	E	881	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	919	THR	3.9
1	F	916	SER	3.9
1	A	903	ALA	3.9
1	F	975	GLU	3.9
1	C	1046	MET	3.8
1	D	876	ARG	3.8
1	F	863	GLN	3.8
1	D	1080	GLU	3.8
1	E	895	LEU	3.8
1	F	1213	LEU	3.8
1	C	884	TYR	3.8
1	A	862	GLU	3.8
1	C	874	ASP	3.7
1	B	918	SER	3.7
1	E	890	ILE	3.7
1	F	971	ASP	3.7
1	C	861	LEU	3.7
1	F	911	ARG	3.6
1	F	950	GLU	3.6
1	E	928	ILE	3.6
1	C	916	SER	3.6
1	C	934	VAL	3.6
1	E	893	PHE	3.5
1	A	1125	ASP	3.4
1	E	919	THR	3.4
1	C	864	MET	3.4
1	C	1107	HIS	3.4
1	F	926	GLU	3.4
1	D	902	LYS	3.4
1	B	1080	GLU	3.3
1	D	862	GLU	3.3
1	B	876	ARG	3.3
1	F	868	VAL	3.3
1	F	1212	THR	3.3
1	A	1035	ILE	3.3
1	F	864	MET	3.3
1	E	1080	GLU	3.2
1	B	1000	GLY	3.2
1	C	1097	TRP	3.2
1	F	880	ASP	3.2
1	D	870	ALA	3.1
1	E	886	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	905	ARG	3.1
1	E	951	VAL	3.1
1	E	1128	MET	3.1
1	C	863	GLN	3.1
1	F	1045	ASP	3.1
1	C	1232	GLN	3.1
1	F	1080	GLU	3.1
1	A	915	ARG	3.1
1	B	867	LEU	3.0
1	E	866	ARG	3.0
1	C	891	THR	3.0
1	E	997	ALA	3.0
1	E	917	LEU	3.0
1	D	1128	MET	3.0
1	C	1125	ASP	3.0
1	B	916	SER	3.0
1	C	1044	THR	3.0
1	D	866	ARG	2.9
1	B	1128	MET	2.9
1	F	871	ARG	2.9
1	F	882	VAL	2.9
1	C	893	PHE	2.9
1	E	939	PRO	2.9
1	C	1096	TYR	2.9
1	A	917	LEU	2.8
1	C	873	ALA	2.8
1	E	882	VAL	2.8
1	B	915	ARG	2.8
1	B	1027	LEU	2.8
1	E	887	GLY	2.8
1	E	1133	LYS	2.8
1	A	876	ARG	2.8
1	C	1024	PRO	2.8
1	E	864	MET	2.8
1	F	878	LYS	2.8
1	E	867	LEU	2.8
1	F	1172	ILE	2.8
1	C	876	ARG	2.8
1	F	1206	TYR	2.8
1	A	1049	ALA	2.7
1	B	1129	THR	2.7
1	C	866	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	864	MET	2.7
1	A	1097	TRP	2.7
1	A	959	ASP	2.7
1	E	878	LYS	2.7
1	F	883	ASN	2.7
1	A	878	LYS	2.7
1	D	1049	ALA	2.7
1	A	1046	MET	2.7
1	A	920	VAL	2.6
1	D	1051	ASN	2.6
1	C	897	LEU	2.6
1	B	914	ALA	2.6
1	F	842	SER	2.6
1	F	894	GLU	2.6
1	A	1047	LYS	2.6
1	D	1108	PRO	2.5
1	B	920	VAL	2.5
1	C	871	ARG	2.5
1	D	1123	PHE	2.5
1	E	1107	HIS	2.5
1	C	977	VAL	2.5
1	C	1025	LYS	2.5
1	E	1244	ASP	2.5
1	F	879	ALA	2.5
1	C	1042	VAL	2.5
1	D	858	THR	2.5
1	A	913	LEU	2.5
1	D	1027	LEU	2.5
1	A	1126	LEU	2.4
1	C	925	VAL	2.4
1	E	950	GLU	2.4
1	E	1171	ASN	2.4
1	F	1121	ASP	2.4
1	B	873	ALA	2.4
1	D	865	ALA	2.4
1	C	920	VAL	2.4
1	F	1191	ASP	2.4
1	F	1228	HIS	2.4
1	C	1185	ASP	2.4
1	A	884	TYR	2.4
1	F	1046	MET	2.4
1	D	867	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	1170	ALA	2.4
1	F	919	THR	2.3
1	D	1052	ALA	2.3
1	F	928	ILE	2.3
1	D	1239	ARG	2.3
1	E	897	LEU	2.3
1	A	905	ARG	2.3
1	D	872	LEU	2.3
1	B	1050	ALA	2.3
1	D	904	ALA	2.3
1	E	912	ASP	2.3
1	E	971	ASP	2.3
1	A	1107	HIS	2.3
1	B	862	GLU	2.3
1	C	899	PRO	2.3
1	C	1026	MET	2.3
1	D	873	ALA	2.3
1	C	1163	VAL	2.3
1	B	1244	ASP	2.2
1	D	871	ARG	2.2
1	F	955	ALA	2.2
1	B	860	ALA	2.2
1	B	879	ALA	2.2
1	D	899	PRO	2.2
1	D	1136	GLU	2.2
1	A	871	ARG	2.2
1	A	899	PRO	2.2
1	B	1061	GLU	2.2
1	D	884	TYR	2.2
1	B	872	LEU	2.2
1	C	1205	LEU	2.2
1	B	997	ALA	2.2
1	F	1210	ASN	2.1
1	E	1121	ASP	2.1
1	F	890	ILE	2.1
1	F	931	LYS	2.1
1	D	898	ALA	2.1
1	A	880	ASP	2.1
1	E	1212	THR	2.1
1	E	1225	GLN	2.1
1	A	908	ASN	2.1
1	A	1121	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	929	PRO	2.1
1	F	973	ALA	2.1
1	A	1040	THR	2.1
1	E	931	LYS	2.1
1	E	993	THR	2.1
1	F	1097	TRP	2.1
1	D	1249	ASP	2.1
1	D	1061	GLU	2.1
1	B	1130	VAL	2.1
1	D	1093	PRO	2.1
1	E	1139	ALA	2.1
1	C	976	PRO	2.0
1	B	902	LYS	2.0
1	B	871	ARG	2.0
1	D	908	ASN	2.0
1	B	1247	THR	2.0
1	F	1048	ASP	2.0
1	D	875	PHE	2.0
1	F	1128	MET	2.0
1	E	930	GLY	2.0
1	F	1186	SER	2.0
1	F	886	PRO	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.