



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:37 am GMT

PDB ID : 3EK6
Title : Unique GTP-binding Pocket and Allostery of UMP Kinase from a Gram-Negative Phytopathogen Bacterium
Authors : Tu, J.-L.; Chin, K.-H.; Wang, A.H.-J.; Chou, S.-H.
Deposited on : 2008-09-18
Resolution : 2.34 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

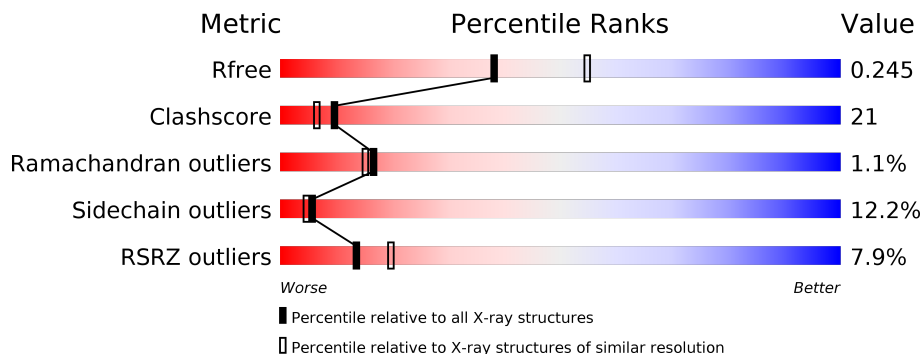
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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

Mol	Chain	Length	Quality of chain
1	A	243	<div> <div>4%</div> <div>68% 29% .</div> </div>
1	B	243	<div> <div>6%</div> <div>64% 28% 7% .</div> </div>
1	C	243	<div> <div>2%</div> <div>69% 25% . .</div> </div>
1	D	243	<div> <div>13%</div> <div>63% 31% 5% .</div> </div>
1	E	243	<div> <div>13%</div> <div>60% 31% 6% .</div> </div>
1	F	243	<div> <div>9%</div> <div>62% 31% 5% .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11284 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 Uridylate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1823	1141	328	343	11			
1	B	240	Total	C	N	O	S	0	0	0
			1804	1131	324	338	11			
1	C	238	Total	C	N	O	S	0	0	0
			1790	1123	322	335	10			
1	D	240	Total	C	N	O	S	0	0	0
			1804	1131	324	338	11			
1	E	238	Total	C	N	O	S	0	0	1
			1784	1120	322	332	10			
1	F	238	Total	C	N	O	S	0	0	0
			1790	1123	322	335	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P59009
A	-1	ASN	-	EXPRESSION TAG	UNP P59009
A	0	ALA	-	EXPRESSION TAG	UNP P59009
B	-2	SER	-	EXPRESSION TAG	UNP P59009
B	-1	ASN	-	EXPRESSION TAG	UNP P59009
B	0	ALA	-	EXPRESSION TAG	UNP P59009
C	-2	SER	-	EXPRESSION TAG	UNP P59009
C	-1	ASN	-	EXPRESSION TAG	UNP P59009
C	0	ALA	-	EXPRESSION TAG	UNP P59009
D	-2	SER	-	EXPRESSION TAG	UNP P59009
D	-1	ASN	-	EXPRESSION TAG	UNP P59009
D	0	ALA	-	EXPRESSION TAG	UNP P59009
E	-2	SER	-	EXPRESSION TAG	UNP P59009
E	-1	ASN	-	EXPRESSION TAG	UNP P59009
E	0	ALA	-	EXPRESSION TAG	UNP P59009
F	-2	SER	-	EXPRESSION TAG	UNP P59009
F	-1	ASN	-	EXPRESSION TAG	UNP P59009

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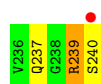
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP P59009

- Molecule 2 is water.

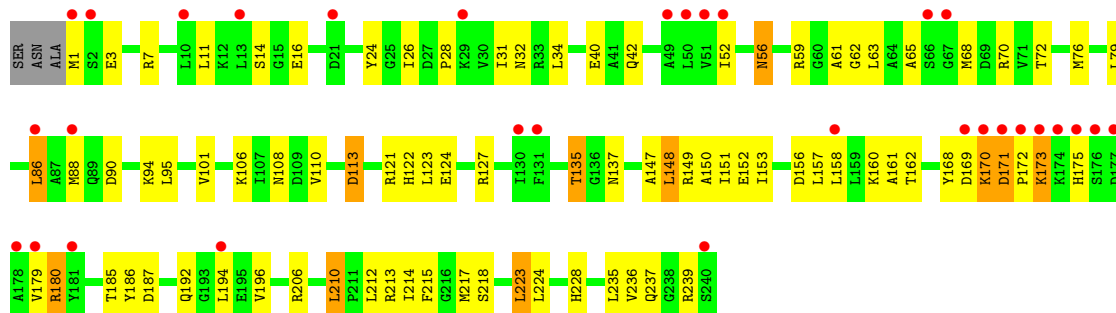
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	102	Total 102	O 102	0	0
2	B	90	Total 90	O 90	0	0
2	C	110	Total 110	O 110	0	0
2	D	69	Total 69	O 69	0	0
2	E	54	Total 54	O 54	0	0
2	F	64	Total 64	O 64	0	0

- Molecule 1: Uridylate kinase

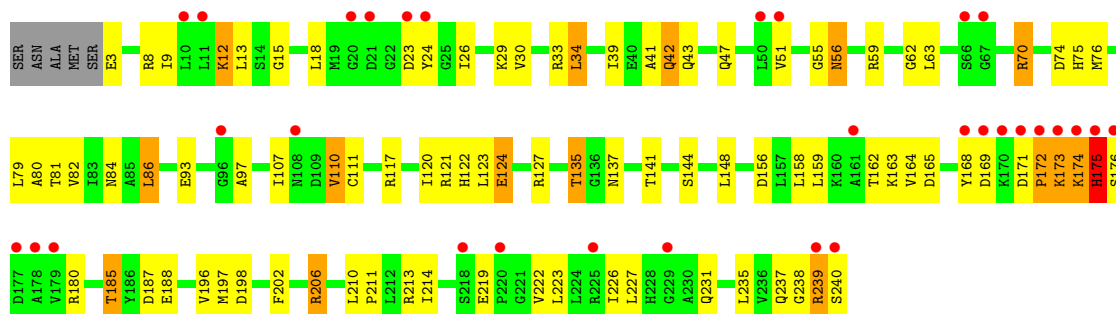




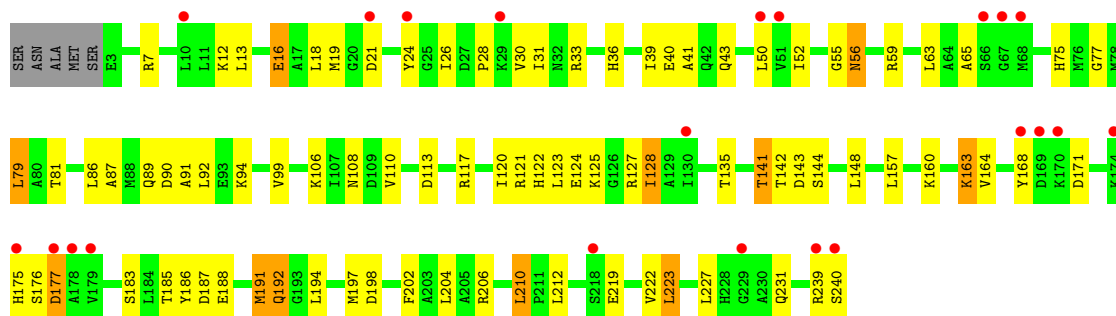
• Molecule 1: Uridylate kinase



• Molecule 1: Uridylate kinase



• Molecule 1: Uridylate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.47Å 120.10Å 125.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 2.34 29.35 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.35-2.34) 98.8 (29.35-2.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.246 0.207 , 0.245	Depositor DCC
R_{free} test set	3603 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11284	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.55	0/1844	0.71	0/2480
1	B	0.56	0/1825	0.72	0/2454
1	C	0.55	0/1811	0.71	0/2436
1	D	0.49	0/1825	0.66	0/2454
1	E	0.45	0/1805	0.60	0/2430
1	F	0.43	0/1811	0.65	0/2436
All	All	0.51	0/10921	0.67	0/14690

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 [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	1823	0	1868	75	0
1	B	1804	0	1852	79	0
1	C	1790	0	1835	87	1
1	D	1804	0	1852	77	1
1	E	1784	0	1830	99	0
1	F	1790	0	1835	73	0
2	A	102	0	0	20	0
2	B	90	0	0	10	0
2	C	110	0	0	24	0
2	D	69	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	54	0	0	10	0
2	F	64	0	0	10	0
All	All	11284	0	11072	470	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (470) 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:C:169:ASP:HB3	2:C:1061:HOH:O	1.22	1.29
1:B:1:MET:HE2	2:B:1438:HOH:O	1.28	1.27
1:C:101:VAL:HB	2:C:1471:HOH:O	1.16	1.26
1:A:3:GLU:HG3	2:A:1440:HOH:O	1.40	1.21
2:A:1451:HOH:O	1:C:68:MET:CE	1.91	1.16
1:C:156:ASP:HB2	2:C:1105:HOH:O	1.49	1.12
1:A:113:ASP:HB2	2:A:1487:HOH:O	1.46	1.11
1:E:196:VAL:HG13	1:E:214:ILE:HD11	1.23	1.10
1:C:108:ASN:ND2	1:C:108:ASN:H	1.41	1.08
1:E:80:ALA:O	2:E:1120:HOH:O	1.70	1.08
1:C:106:LYS:HA	2:C:1315:HOH:O	1.53	1.07
1:C:106:LYS:HD3	2:C:1315:HOH:O	1.52	1.06
1:B:81:THR:HG21	1:B:133:ALA:H	1.19	1.03
1:A:239:ARG:HG2	2:A:1389:HOH:O	1.57	1.02
1:C:108:ASN:HD22	1:C:108:ASN:N	1.56	1.02
1:A:34:LEU:HG	2:A:1453:HOH:O	1.56	1.02
1:A:240:SER:OXT	2:A:1070:HOH:O	1.77	1.01
1:B:183:SER:HB2	2:B:1265:HOH:O	1.58	1.00
1:E:141:THR:HG21	1:E:198:ASP:OD2	1.61	0.99
1:D:90:ASP:OD2	1:D:94:LYS:HE3	1.63	0.98
1:E:196:VAL:HG13	1:E:214:ILE:CD1	1.93	0.98
1:B:81:THR:CG2	1:B:133:ALA:H	1.78	0.97
1:B:185:THR:HG22	1:B:188:GLU:H	1.28	0.97
1:F:90:ASP:HB2	2:F:1135:HOH:O	1.64	0.97
1:B:26:ILE:O	1:D:62:GLY:HA3	1.63	0.97
1:B:141:THR:HG21	1:B:198:ASP:OD2	1.64	0.97
1:F:141:THR:HG22	1:F:144:SER:H	1.28	0.95
1:A:56:ASN:HD22	1:A:56:ASN:H	1.12	0.94
1:E:172:PRO:HA	1:E:175:HIS:NE2	1.86	0.91
1:A:213:ARG:HG3	2:A:1493:HOH:O	1.70	0.90
1:F:231:GLN:HG2	2:F:1415:HOH:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:MET:SD	2:E:1511:HOH:O	2.27	0.90
1:D:185:THR:HG22	1:D:187:ASP:H	1.37	0.89
1:C:3:GLU:HB3	2:C:1396:HOH:O	1.72	0.89
1:C:101:VAL:CB	2:C:1471:HOH:O	1.89	0.89
1:A:188:GLU:HG3	2:A:1070:HOH:O	1.72	0.88
1:F:191:MET:HE2	2:F:1241:HOH:O	1.72	0.88
1:F:55:GLY:O	1:F:59:ARG:HD3	1.71	0.88
1:E:173:LYS:H	1:E:175:HIS:CE1	1.92	0.88
1:F:206:ARG:NH1	2:F:1145:HOH:O	2.05	0.88
1:B:151:ILE:HD13	1:B:208:SER:OG	1.74	0.88
1:F:89:GLN:HG3	1:F:99:VAL:HG21	1.54	0.88
1:E:164:VAL:HG21	1:E:168:TYR:OH	1.74	0.87
1:E:164:VAL:HG11	1:E:168:TYR:CE2	2.10	0.86
2:A:1451:HOH:O	1:C:68:MET:HE2	1.61	0.86
1:D:56:ASN:H	1:D:56:ASN:HD22	1.22	0.86
1:C:108:ASN:ND2	1:C:108:ASN:N	2.18	0.86
1:A:122:HIS:HD2	1:A:127:ARG:HH11	1.21	0.85
1:C:169:ASP:CB	2:C:1061:HOH:O	1.90	0.85
1:B:42:GLN:HG2	2:B:1494:HOH:O	1.75	0.85
1:C:8:ARG:HE	1:C:47:GLN:NE2	1.74	0.85
1:C:185:THR:HG22	1:C:188:GLU:H	1.42	0.84
1:F:239:ARG:HG2	2:F:1145:HOH:O	1.78	0.83
1:A:141:THR:HG21	1:A:198:ASP:OD2	1.79	0.83
1:E:185:THR:HG22	1:E:188:GLU:H	1.43	0.82
1:E:187:ASP:OD1	1:E:206:ARG:NH2	2.12	0.82
1:B:81:THR:HG21	1:B:133:ALA:N	1.93	0.81
1:A:185:THR:HG22	1:A:187:ASP:H	1.45	0.81
1:E:172:PRO:HA	1:E:175:HIS:HE2	1.44	0.81
2:B:1366:HOH:O	1:E:117:ARG:HD3	1.80	0.81
1:E:172:PRO:HA	1:E:175:HIS:CE1	2.17	0.80
1:A:141:THR:HG23	1:A:144:SER:H	1.46	0.80
1:F:55:GLY:O	1:F:59:ARG:CD	2.30	0.80
1:E:39:ILE:HD13	1:E:97:ALA:HB2	1.63	0.79
1:B:108:ASN:HB3	2:B:1124:HOH:O	1.81	0.79
1:D:185:THR:HG22	1:D:187:ASP:N	1.97	0.79
1:C:56:ASN:H	1:C:56:ASN:HD22	1.31	0.78
1:E:159:LEU:HD23	1:E:213:ARG:HB3	1.66	0.77
1:B:118:ARG:HD2	1:B:121:ARG:HH11	1.48	0.77
1:D:122:HIS:HD2	1:D:127:ARG:HH11	1.31	0.77
1:B:170:LYS:HD3	1:B:175:HIS:CD2	2.20	0.76
1:C:169:ASP:CG	2:C:1061:HOH:O	2.12	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASN:HD22	1:A:56:ASN:N	1.83	0.76
1:F:187:ASP:HB2	1:F:240:SER:HB2	1.67	0.76
1:D:180:ARG:NH1	1:D:180:ARG:HB3	2.01	0.76
1:F:176:SER:O	1:F:177:ASP:HB3	1.86	0.76
1:B:81:THR:CG2	1:B:133:ALA:N	2.49	0.75
1:E:156:ASP:O	1:E:211:PRO:HG2	1.87	0.75
1:E:165:ASP:O	1:E:180:ARG:HD3	1.87	0.75
2:A:1451:HOH:O	1:C:68:MET:SD	2.41	0.75
1:C:185:THR:CG2	1:C:188:GLU:H	1.99	0.74
1:E:196:VAL:CG1	1:E:214:ILE:HD11	2.09	0.74
1:A:68:MET:SD	2:A:1486:HOH:O	2.46	0.74
1:B:1:MET:CE	2:B:1438:HOH:O	2.05	0.74
1:B:75:HIS:HD2	2:D:1490:HOH:O	1.70	0.74
1:D:135:THR:HG22	1:D:137:ASN:H	1.53	0.74
1:E:141:THR:HG23	1:E:144:SER:H	1.52	0.73
1:D:11:LEU:HD11	1:D:217:MET:HE1	1.69	0.73
1:C:101:VAL:CG1	2:C:1471:HOH:O	2.26	0.73
1:F:21:ASP:HB3	2:F:1100:HOH:O	1.88	0.72
1:E:172:PRO:CA	1:E:175:HIS:NE2	2.53	0.72
1:D:90:ASP:OD2	1:D:94:LYS:CE	2.37	0.72
1:E:239:ARG:HD2	2:E:1130:HOH:O	1.89	0.72
1:D:192:GLN:HB2	1:D:194:LEU:HD22	1.72	0.72
1:B:235:LEU:HD11	1:B:237:GLN:HB2	1.72	0.72
1:F:108:ASN:HB3	2:F:1171:HOH:O	1.90	0.72
1:A:8:ARG:HH21	1:A:47:GLN:HE22	1.38	0.72
1:B:8:ARG:HH21	1:B:47:GLN:HE22	1.37	0.71
1:B:170:LYS:O	1:B:171:ASP:HB3	1.90	0.71
1:E:8:ARG:HE	1:E:47:GLN:NE2	1.88	0.71
1:D:180:ARG:HH11	1:D:180:ARG:HB3	1.54	0.70
1:A:33:ARG:HG3	2:A:1432:HOH:O	1.91	0.70
1:D:173:LYS:HE3	1:D:173:LYS:H	1.56	0.70
1:A:228:HIS:HE1	2:A:1337:HOH:O	1.75	0.70
1:E:122:HIS:HD2	1:E:127:ARG:HH11	1.39	0.70
1:F:141:THR:HG23	1:F:143:ASP:N	2.07	0.70
1:E:135:THR:HG22	1:E:137:ASN:H	1.57	0.69
1:F:176:SER:O	1:F:177:ASP:CB	2.40	0.69
1:F:141:THR:CG2	1:F:144:SER:H	2.04	0.69
1:E:168:TYR:CD1	1:E:172:PRO:HD2	2.28	0.68
1:C:135:THR:CG2	1:C:137:ASN:HD22	2.05	0.68
1:C:8:ARG:HH21	1:C:47:GLN:HE22	1.40	0.68
1:B:57:ILE:HD11	1:D:63:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:PRO:HB3	1:C:237:GLN:HE21	1.59	0.68
1:D:156:ASP:HB2	2:D:1208:HOH:O	1.93	0.67
1:A:122:HIS:CD2	1:A:127:ARG:HH11	2.07	0.67
1:A:141:THR:CG2	1:A:144:SER:H	2.07	0.67
1:B:122:HIS:HD2	1:B:127:ARG:HH11	1.40	0.67
1:F:164:VAL:HG22	1:F:168:TYR:CE1	2.30	0.66
1:B:118:ARG:HD2	1:B:121:ARG:NH1	2.10	0.66
1:E:12:LYS:O	1:E:12:LYS:HG3	1.95	0.66
1:C:197:MET:HE3	1:C:202:PHE:HA	1.77	0.66
1:F:90:ASP:O	1:F:94:LYS:HG3	1.94	0.66
1:C:8:ARG:HE	1:C:47:GLN:HE21	1.40	0.66
1:F:12:LYS:HE3	1:F:142:THR:HG22	1.77	0.66
1:A:8:ARG:HE	1:A:47:GLN:NE2	1.94	0.65
1:E:122:HIS:CD2	1:E:127:ARG:HH11	2.15	0.65
1:A:56:ASN:H	1:A:56:ASN:ND2	1.91	0.64
1:E:164:VAL:HG11	1:E:168:TYR:HE2	1.60	0.64
1:A:165:ASP:OD1	1:A:165:ASP:O	2.15	0.64
1:D:192:GLN:HB2	1:D:194:LEU:CD2	2.26	0.64
1:E:62:GLY:HA3	1:F:26:ILE:O	1.98	0.64
1:B:147:ALA:O	1:B:151:ILE:HG13	1.98	0.64
1:F:141:THR:HG21	1:F:198:ASP:OD2	1.97	0.64
1:A:165:ASP:HB3	2:A:1308:HOH:O	1.98	0.64
1:B:141:THR:HG22	1:B:144:SER:H	1.64	0.64
1:A:234:THR:N	2:A:1493:HOH:O	2.29	0.63
1:A:185:THR:HG22	1:A:187:ASP:N	2.12	0.63
1:C:18:LEU:HD22	1:C:31:ILE:HG13	1.80	0.63
1:A:78:MET:HE3	1:A:105:ILE:HD13	1.80	0.63
1:B:173:LYS:HG2	1:B:174:LYS:N	2.12	0.63
1:B:57:ILE:CD1	1:D:63:LEU:HD11	2.27	0.63
1:B:151:ILE:CD1	1:B:204:LEU:HD22	2.27	0.63
1:E:172:PRO:O	1:E:173:LYS:HB3	1.98	0.63
1:D:72:THR:HG22	1:D:76:MET:HE3	1.81	0.63
1:B:56:ASN:HD22	1:B:56:ASN:H	1.47	0.63
1:C:89:GLN:HG3	1:C:99:VAL:CG2	2.28	0.63
1:E:173:LYS:N	1:E:175:HIS:CE1	2.67	0.63
1:C:211:PRO:HB3	1:C:237:GLN:NE2	2.14	0.62
1:F:59:ARG:O	1:F:63:LEU:HB2	1.98	0.62
1:D:173:LYS:CE	1:D:173:LYS:H	2.12	0.62
1:A:34:LEU:HD12	1:A:88:MET:SD	2.39	0.62
1:C:108:ASN:H	1:C:108:ASN:HD22	0.70	0.62
1:D:3:GLU:HB2	2:D:1199:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HD12	1:B:204:LEU:HD22	1.82	0.62
1:C:102:MET:HE1	1:C:131:PHE:HE1	1.65	0.62
1:D:171:ASP:HB2	1:D:173:LYS:NZ	2.14	0.62
1:C:206:ARG:HE	1:C:239:ARG:HH22	1.45	0.62
1:B:170:LYS:O	1:B:171:ASP:CB	2.48	0.62
1:B:9:ILE:HD13	1:B:227:LEU:HD21	1.82	0.62
1:C:89:GLN:HG3	1:C:99:VAL:HG21	1.81	0.62
1:F:120:ILE:O	1:F:124:GLU:HG2	2.00	0.62
1:F:41:ALA:HB2	1:F:223:LEU:HD12	1.82	0.61
1:A:8:ARG:HE	1:A:47:GLN:HE21	1.48	0.61
1:C:116:ARG:HD2	1:C:152:GLU:O	2.00	0.61
1:F:92:LEU:HD13	1:F:128:ILE:HD11	1.81	0.61
1:D:59:ARG:NH1	2:D:1274:HOH:O	2.33	0.61
1:E:3:GLU:HA	1:E:3:GLU:OE2	2.00	0.61
1:A:175:HIS:O	1:A:177:ASP:N	2.34	0.61
1:B:235:LEU:CD1	1:B:237:GLN:HB2	2.31	0.61
1:C:3:GLU:HG3	1:C:4:LEU:H	1.66	0.61
1:C:56:ASN:HD22	1:C:56:ASN:N	1.98	0.61
1:C:127:ARG:NE	2:C:1348:HOH:O	2.14	0.60
1:A:23:ASP:HB2	2:A:1318:HOH:O	2.00	0.60
1:D:7:ARG:N	2:D:1208:HOH:O	2.30	0.60
1:B:62:GLY:HA3	1:D:26:ILE:O	2.01	0.60
1:E:13:LEU:HD11	1:E:34:LEU:HD11	1.82	0.60
1:A:175:HIS:C	1:A:177:ASP:H	2.04	0.60
1:E:75:HIS:HD2	2:F:1079:HOH:O	1.84	0.60
1:F:141:THR:HG23	1:F:143:ASP:H	1.65	0.60
1:E:70:ARG:NH1	1:E:74:ASP:OD1	2.35	0.60
1:C:89:GLN:HE21	1:C:99:VAL:HG23	1.67	0.59
1:F:18:LEU:HD12	2:F:1503:HOH:O	2.03	0.59
1:A:68:MET:HG2	1:A:69:ASP:N	2.17	0.59
1:C:109:ASP:OD2	2:C:1448:HOH:O	2.15	0.59
1:C:185:THR:HG23	1:C:187:ASP:H	1.67	0.59
1:A:175:HIS:C	1:A:177:ASP:N	2.55	0.59
1:E:237:GLN:HG2	1:E:238:GLY:N	2.18	0.59
1:E:172:PRO:CA	1:E:175:HIS:HE2	2.11	0.58
1:E:56:ASN:HD22	1:E:56:ASN:N	2.01	0.58
1:E:23:ASP:OD1	1:F:24:TYR:OH	2.16	0.58
1:A:239:ARG:HD3	2:A:1309:HOH:O	2.03	0.58
1:B:13:LEU:HD23	1:B:161:ALA:HB3	1.84	0.58
1:E:8:ARG:HE	1:E:47:GLN:HE21	1.52	0.58
1:D:121:ARG:HA	1:D:124:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:LYS:O	1:E:174:LYS:HB2	2.04	0.57
1:A:62:GLY:HA3	1:C:26:ILE:O	2.04	0.57
1:C:185:THR:HG23	1:C:187:ASP:N	2.20	0.57
1:C:3:GLU:HG2	2:C:1073:HOH:O	2.05	0.57
1:C:173:LYS:HD2	2:C:1282:HOH:O	2.03	0.57
1:F:143:ASP:OD1	1:F:160:LYS:HE3	2.05	0.57
1:A:120:ILE:HD11	1:A:153:ILE:HA	1.85	0.57
1:D:215:PHE:CZ	1:D:217:MET:HE2	2.39	0.57
1:D:235:LEU:CD2	1:D:237:GLN:HB2	2.35	0.57
1:E:185:THR:HG22	1:E:188:GLU:N	2.19	0.57
1:F:185:THR:OG1	1:F:240:SER:OG	2.12	0.56
1:A:9:ILE:HD13	1:A:227:LEU:HD21	1.87	0.56
1:B:174:LYS:O	1:B:175:HIS:ND1	2.38	0.56
1:B:141:THR:CG2	1:B:144:SER:H	2.17	0.56
1:E:33:ARG:HH11	1:E:33:ARG:HB3	1.68	0.56
1:A:93:GLU:OE1	1:F:117:ARG:NH2	2.38	0.56
1:C:137:ASN:HD21	1:F:135:THR:HG23	1.71	0.56
1:A:8:ARG:HH21	1:A:47:GLN:NE2	2.03	0.56
1:E:175:HIS:N	1:E:175:HIS:ND1	2.54	0.56
1:E:29:LYS:O	1:E:33:ARG:HG3	2.06	0.56
1:F:56:ASN:HD22	1:F:56:ASN:H	1.53	0.55
1:B:12:LYS:HD2	2:B:1468:HOH:O	2.07	0.55
1:E:82:VAL:O	1:E:86:LEU:HD22	2.06	0.55
1:A:8:ARG:NH2	1:A:47:GLN:HE22	2.04	0.55
1:B:70:ARG:HG2	1:B:139:PHE:CE1	2.41	0.55
1:D:56:ASN:N	1:D:56:ASN:HD22	1.96	0.55
1:E:55:GLY:O	1:E:59:ARG:HG3	2.07	0.55
1:F:171:ASP:HB3	1:F:175:HIS:CD2	2.42	0.55
1:E:26:ILE:HD11	1:E:84:ASN:HD22	1.71	0.55
1:F:92:LEU:HD22	1:F:128:ILE:CD1	2.37	0.55
1:C:213:ARG:HD2	1:C:232:ILE:O	2.07	0.55
1:E:76:MET:HE1	1:F:87:ALA:HB2	1.89	0.55
1:E:172:PRO:N	1:E:175:HIS:NE2	2.56	0.54
1:B:24:TYR:CD2	1:D:24:TYR:CD1	2.96	0.54
1:D:7:ARG:HD2	2:D:1424:HOH:O	2.08	0.54
1:B:169:ASP:HB2	1:B:181:TYR:CE1	2.43	0.54
1:E:158:LEU:HB2	1:E:210:LEU:HD21	1.90	0.54
1:A:165:ASP:OD1	1:A:233:GLY:HA2	2.07	0.54
1:B:68:MET:SD	1:B:76:MET:HE1	2.47	0.54
1:A:23:ASP:CB	2:A:1318:HOH:O	2.54	0.53
1:E:24:TYR:CE2	1:F:24:TYR:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:HIS:O	1:B:79:LEU:HD22	2.08	0.53
1:D:171:ASP:HB2	1:D:173:LYS:HZ1	1.72	0.53
1:D:68:MET:HB3	2:D:1168:HOH:O	2.08	0.53
1:D:169:ASP:HB3	1:D:179:VAL:H	1.74	0.53
1:E:84:ASN:N	2:E:1120:HOH:O	2.03	0.53
1:B:122:HIS:CD2	1:B:127:ARG:HH11	2.24	0.53
1:E:8:ARG:HH21	1:E:47:GLN:HE22	1.55	0.53
1:B:185:THR:HG22	1:B:188:GLU:N	2.10	0.52
1:C:112:GLU:OE2	1:C:118:ARG:NH1	2.42	0.52
1:C:127:ARG:NH2	2:C:1348:HOH:O	2.35	0.52
2:B:1366:HOH:O	1:E:117:ARG:CD	2.49	0.52
1:E:165:ASP:O	1:E:180:ARG:CD	2.57	0.52
1:D:173:LYS:HE3	1:D:173:LYS:N	2.21	0.52
1:A:68:MET:CG	1:A:69:ASP:N	2.72	0.52
1:C:211:PRO:CB	1:C:237:GLN:HE21	2.23	0.52
1:F:197:MET:CE	1:F:202:PHE:HA	2.40	0.52
1:E:33:ARG:HH11	1:E:33:ARG:CB	2.22	0.52
1:D:72:THR:HG22	1:D:76:MET:CE	2.40	0.52
1:E:185:THR:HG23	1:E:240:SER:N	2.25	0.52
1:E:81:THR:C	2:E:1120:HOH:O	2.49	0.52
1:C:185:THR:HG22	1:C:188:GLU:HG3	1.92	0.52
1:D:28:PRO:HA	1:D:31:ILE:HG22	1.92	0.52
1:B:72:THR:HG22	1:B:76:MET:CE	2.39	0.51
1:A:41:ALA:HB2	1:A:223:LEU:HD23	1.91	0.51
1:C:197:MET:CE	1:C:202:PHE:HA	2.39	0.51
1:A:185:THR:HG22	1:A:186:TYR:N	2.25	0.51
1:F:30:VAL:HG22	1:F:33:ARG:HH22	1.76	0.51
1:B:240:SER:HB2	2:B:1178:HOH:O	2.10	0.51
1:E:168:TYR:CD1	1:E:171:ASP:HA	2.45	0.51
1:E:135:THR:HG22	1:E:137:ASN:N	2.25	0.51
1:D:56:ASN:ND2	1:D:56:ASN:H	2.00	0.51
1:C:206:ARG:CZ	1:C:239:ARG:HH12	2.23	0.51
1:E:135:THR:CG2	1:E:137:ASN:HD22	2.24	0.51
1:C:137:ASN:ND2	1:F:135:THR:HG23	2.26	0.50
1:C:148:LEU:HG	2:C:1506:HOH:O	2.11	0.50
1:A:169:ASP:OD2	1:A:170:LYS:N	2.45	0.50
1:D:194:LEU:HD12	2:D:1110:HOH:O	2.10	0.50
1:E:41:ALA:HB1	1:E:227:LEU:HD11	1.94	0.50
1:C:135:THR:CG2	1:C:137:ASN:ND2	2.74	0.50
1:E:9:ILE:HD12	1:E:159:LEU:HD12	1.93	0.50
1:A:157:LEU:HD21	1:A:213:ARG:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:GLU:OE2	1:C:224:LEU:HB2	2.10	0.50
1:E:197:MET:HE3	1:E:202:PHE:HA	1.94	0.50
1:E:76:MET:CE	1:F:87:ALA:HB2	2.42	0.50
1:F:75:HIS:O	1:F:79:LEU:HD22	2.12	0.50
1:B:8:ARG:HE	1:B:47:GLN:NE2	2.09	0.50
1:A:214:ILE:HD12	1:A:214:ILE:N	2.27	0.49
1:A:24:TYR:CD1	1:C:24:TYR:CD2	3.00	0.49
1:B:8:ARG:HE	1:B:47:GLN:HE21	1.60	0.49
1:C:8:ARG:NE	1:C:47:GLN:NE2	2.54	0.49
1:F:12:LYS:HE3	1:F:142:THR:CG2	2.43	0.49
1:E:171:ASP:O	1:E:173:LYS:N	2.45	0.49
1:E:219:GLU:O	1:E:222:VAL:HG23	2.13	0.49
1:E:42:GLN:HG3	1:E:43:GLN:N	2.27	0.49
1:B:102:MET:HG2	1:B:112:GLU:HG3	1.94	0.49
1:E:56:ASN:H	1:E:56:ASN:HD22	1.59	0.49
1:E:239:ARG:HA	2:E:1130:HOH:O	2.12	0.49
1:C:26:ILE:HD11	1:C:84:ASN:HD22	1.78	0.49
1:F:122:HIS:HD2	1:F:127:ARG:HH11	1.61	0.49
1:C:65:ALA:O	1:C:67:GLY:N	2.45	0.48
1:F:92:LEU:HD22	1:F:128:ILE:HD11	1.94	0.48
1:F:89:GLN:HG3	1:F:99:VAL:CG2	2.35	0.48
1:B:38:VAL:HG13	1:B:48:VAL:HG21	1.95	0.48
1:B:107:ILE:HG22	1:B:110:VAL:HG13	1.94	0.48
1:B:184:LEU:O	1:B:236:VAL:HA	2.13	0.48
1:E:110:VAL:CG2	1:E:111:CYS:N	2.76	0.48
1:B:26:ILE:HD12	1:D:63:LEU:HD23	1.96	0.48
1:F:223:LEU:O	1:F:227:LEU:HG	2.13	0.48
1:F:197:MET:HE3	1:F:202:PHE:HA	1.96	0.48
1:D:16:GLU:H	1:D:16:GLU:CD	2.17	0.48
1:E:121:ARG:HA	1:E:124:GLU:HG3	1.95	0.48
1:C:102:MET:CE	1:C:131:PHE:HE1	2.27	0.48
1:E:172:PRO:CA	1:E:175:HIS:CE1	2.91	0.48
1:F:36:HIS:O	1:F:40:GLU:HG3	2.15	0.47
1:B:158:LEU:HD13	1:B:212:LEU:HD13	1.95	0.47
1:B:26:ILE:O	1:D:62:GLY:CA	2.51	0.47
1:B:72:THR:HG22	1:B:76:MET:HE3	1.95	0.47
1:B:185:THR:HG21	1:B:240:SER:C	2.34	0.47
1:D:148:LEU:CD1	1:D:149:ARG:NH1	2.77	0.47
1:F:39:ILE:O	1:F:43:GLN:HB2	2.15	0.47
1:A:-2:SER:O	1:A:-1:ASN:HB2	2.14	0.47
1:A:185:THR:CG2	1:A:186:TYR:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ASN:HD22	1:F:56:ASN:N	2.12	0.47
1:C:187:ASP:OD2	1:C:240:SER:N	2.42	0.47
1:B:187:ASP:OD1	1:B:206:ARG:NH1	2.46	0.47
1:E:107:ILE:HB	1:E:110:VAL:HG22	1.96	0.47
1:F:163:LYS:HE3	1:F:163:LYS:HA	1.97	0.47
1:F:223:LEU:HA	1:F:223:LEU:HD22	1.81	0.47
1:C:8:ARG:NH2	1:C:47:GLN:HE22	2.10	0.46
1:F:28:PRO:HA	1:F:31:ILE:HG22	1.97	0.46
1:A:26:ILE:O	1:C:62:GLY:HA3	2.15	0.46
1:D:185:THR:CG2	1:D:187:ASP:H	2.18	0.46
1:F:141:THR:HG22	1:F:144:SER:N	2.11	0.46
1:A:168:TYR:CE2	1:A:180:ARG:HB2	2.50	0.46
1:C:121:ARG:NH1	2:C:1280:HOH:O	2.47	0.46
1:C:197:MET:HE3	1:C:202:PHE:CA	2.46	0.46
1:C:6:TYR:HB3	2:C:1105:HOH:O	2.16	0.46
1:D:215:PHE:HZ	1:D:217:MET:HE2	1.80	0.46
1:D:135:THR:HG22	1:D:137:ASN:N	2.27	0.46
1:B:68:MET:HG2	1:B:69:ASP:N	2.31	0.46
1:A:122:HIS:HD2	1:A:127:ARG:NH1	2.00	0.46
1:C:190:ILE:HA	1:C:190:ILE:HD12	1.84	0.46
1:D:34:LEU:HD12	1:D:88:MET:SD	2.56	0.46
1:B:76:MET:HE3	1:D:86:LEU:HB3	1.98	0.46
1:C:206:ARG:NH2	1:C:239:ARG:HH12	2.14	0.46
1:E:164:VAL:CG1	1:E:168:TYR:HE2	2.28	0.46
1:B:138:PRO:O	1:B:139:PHE:HB2	2.16	0.46
1:C:185:THR:HG22	1:C:188:GLU:CG	2.46	0.46
1:E:185:THR:HA	1:E:237:GLN:O	2.16	0.46
1:D:150:ALA:HB3	1:D:210:LEU:HD11	1.97	0.45
1:E:222:VAL:O	1:E:226:ILE:HG13	2.16	0.45
1:F:89:GLN:CG	1:F:99:VAL:HG21	2.37	0.45
1:C:211:PRO:CG	1:C:237:GLN:HE21	2.30	0.45
1:D:161:ALA:CB	1:D:217:MET:HE3	2.47	0.45
1:A:116:ARG:O	1:A:120:ILE:HG12	2.16	0.45
1:C:32:ASN:HB3	2:C:1291:HOH:O	2.16	0.45
1:D:122:HIS:CD2	1:D:127:ARG:HH11	2.22	0.45
1:C:145:GLY:HA3	2:C:1474:HOH:O	2.17	0.45
1:D:161:ALA:HB2	1:D:217:MET:HE3	1.99	0.45
1:F:19:MET:HG2	1:F:56:ASN:HB2	1.98	0.45
1:A:183:SER:HA	1:A:235:LEU:O	2.17	0.44
1:B:39:ILE:CD1	1:B:95:LEU:HB3	2.47	0.44
1:A:185:THR:HB	2:A:1070:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LYS:HG3	1:D:113:ASP:OD1	2.17	0.44
1:B:235:LEU:CD1	1:B:237:GLN:CB	2.95	0.44
1:D:160:LYS:HE2	1:D:196:VAL:O	2.17	0.44
1:B:46:ALA:HB2	1:B:227:LEU:HD13	1.98	0.44
1:C:127:ARG:CZ	2:C:1348:HOH:O	2.59	0.44
1:A:14:SER:OG	1:A:16:GLU:HG2	2.18	0.44
1:A:175:HIS:O	1:A:178:ALA:N	2.45	0.44
1:D:61:ALA:O	1:D:65:ALA:HB2	2.17	0.44
1:E:185:THR:CG2	1:E:187:ASP:H	2.31	0.44
1:F:121:ARG:O	1:F:125:LYS:HG2	2.18	0.44
1:F:192:GLN:HB3	1:F:194:LEU:HG	2.00	0.44
1:A:39:ILE:CD1	1:A:95:LEU:HB2	2.47	0.44
1:F:164:VAL:CG2	1:F:168:TYR:CE1	3.01	0.44
1:F:187:ASP:HB2	1:F:240:SER:CB	2.43	0.44
1:D:156:ASP:CB	2:D:1208:HOH:O	2.61	0.44
1:A:41:ALA:HB1	1:A:227:LEU:HD11	2.00	0.43
1:B:141:THR:HG23	1:B:143:ASP:N	2.33	0.43
1:E:156:ASP:O	1:E:211:PRO:CG	2.62	0.43
1:E:163:LYS:HG2	2:E:1125:HOH:O	2.17	0.43
1:E:33:ARG:CB	1:E:33:ARG:NH1	2.80	0.43
1:B:185:THR:HG21	1:B:240:SER:OXT	2.18	0.43
1:F:87:ALA:O	1:F:90:ASP:OD2	2.36	0.43
1:A:-2:SER:HB3	1:A:-1:ASN:H	1.61	0.43
1:B:65:ALA:HB3	1:B:68:MET:HB2	2.01	0.43
1:D:11:LEU:HD11	1:D:217:MET:CE	2.43	0.43
1:A:185:THR:HB	1:A:188:GLU:HG3	2.00	0.43
1:B:134:GLY:HA2	2:B:1048:HOH:O	2.19	0.43
1:D:168:TYR:HA	1:D:180:ARG:HA	2.01	0.43
1:E:55:GLY:O	1:E:59:ARG:CG	2.65	0.43
1:F:186:TYR:OH	1:F:210:LEU:O	2.24	0.43
1:B:57:ILE:HB	1:B:80:ALA:HB1	2.01	0.43
1:C:101:VAL:HG22	1:C:111:CYS:HB2	2.01	0.43
1:B:75:HIS:CD2	2:D:1490:HOH:O	2.57	0.43
1:C:206:ARG:HE	1:C:239:ARG:NH2	2.15	0.43
1:D:168:TYR:CE2	1:D:180:ARG:HB2	2.54	0.43
1:E:158:LEU:HD23	1:E:159:LEU:N	2.34	0.43
1:A:107:ILE:HG23	1:C:105:ILE:HG21	2.01	0.43
1:D:147:ALA:O	1:D:151:ILE:HG13	2.19	0.43
1:D:187:ASP:OD2	1:D:239:ARG:HD2	2.19	0.43
1:E:185:THR:HG22	1:E:187:ASP:N	2.34	0.43
1:F:106:LYS:HA	1:F:113:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:LEU:HB3	1:D:236:VAL:HB	2.01	0.42
1:A:188:GLU:N	2:A:1070:HOH:O	2.51	0.42
1:C:186:TYR:CD2	1:C:206:ARG:HB2	2.54	0.42
1:E:175:HIS:HB3	2:E:1035:HOH:O	2.19	0.42
1:E:76:MET:CE	2:E:1511:HOH:O	2.59	0.42
2:E:1332:HOH:O	1:F:90:ASP:HB3	2.18	0.42
1:C:191:MET:HE3	2:C:1197:HOH:O	2.19	0.42
1:D:106:LYS:HG3	1:D:113:ASP:CG	2.40	0.42
1:E:26:ILE:HD11	1:E:84:ASN:ND2	2.34	0.42
1:A:-2:SER:O	1:A:-1:ASN:CB	2.68	0.42
1:A:186:TYR:CB	1:A:206:ARG:HG3	2.49	0.42
1:D:149:ARG:O	1:D:153:ILE:HG12	2.19	0.42
1:E:187:ASP:OD2	1:E:240:SER:N	2.52	0.42
1:D:214:ILE:HD12	1:D:214:ILE:N	2.35	0.42
1:A:186:TYR:HB3	1:A:206:ARG:HG3	2.02	0.42
1:A:34:LEU:C	1:A:34:LEU:HD13	2.39	0.42
1:B:151:ILE:HD13	1:B:208:SER:CB	2.50	0.42
1:B:95:LEU:HA	1:B:95:LEU:HD12	1.92	0.42
1:D:148:LEU:HD13	1:D:149:ARG:NH1	2.34	0.42
1:A:172:PRO:HA	1:A:178:ALA:HB3	2.01	0.42
1:D:122:HIS:HD2	1:D:127:ARG:NH1	2.09	0.42
1:F:77:GLY:O	1:F:81:THR:HG23	2.19	0.42
1:B:106:LYS:HB3	1:B:106:LYS:HE2	1.80	0.42
1:D:148:LEU:HD13	1:D:152:GLU:OE2	2.20	0.42
1:E:158:LEU:HB2	1:E:210:LEU:CD2	2.49	0.42
1:F:18:LEU:HA	2:F:1503:HOH:O	2.20	0.42
1:C:148:LEU:HD22	1:C:148:LEU:O	2.20	0.41
1:E:165:ASP:C	1:E:165:ASP:OD2	2.59	0.41
1:A:6:TYR:CE1	1:A:157:LEU:HG	2.55	0.41
1:F:141:THR:HG21	1:F:143:ASP:HB2	2.02	0.41
1:D:52:ILE:HB	2:D:1461:HOH:O	2.21	0.41
1:A:165:ASP:OD1	1:A:165:ASP:C	2.58	0.41
1:C:185:THR:HG21	1:C:240:SER:OXT	2.21	0.41
1:D:223:LEU:HD22	1:D:223:LEU:HA	1.81	0.41
1:E:172:PRO:O	1:E:173:LYS:CB	2.65	0.41
1:F:13:LEU:O	1:F:52:ILE:HA	2.20	0.41
1:D:106:LYS:H	1:D:106:LYS:HD2	1.86	0.41
1:D:158:LEU:HD12	1:D:210:LEU:CD1	2.51	0.41
1:F:90:ASP:OD2	1:F:91:ALA:N	2.53	0.41
1:C:8:ARG:HE	1:C:47:GLN:HE22	1.63	0.41
1:F:186:TYR:CD2	1:F:206:ARG:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:OE2	1:A:122:HIS:HE1	2.03	0.41
1:B:169:ASP:CG	1:B:181:TYR:HH	2.24	0.41
1:E:162:THR:HG22	1:E:163:LYS:N	2.36	0.41
1:E:15:GLY:O	1:E:18:LEU:HB2	2.21	0.41
1:B:158:LEU:HB2	1:B:210:LEU:HD22	2.03	0.41
1:C:148:LEU:HD12	2:C:1506:HOH:O	2.20	0.41
1:D:14:SER:HB3	1:D:16:GLU:HG2	2.02	0.41
1:D:171:ASP:HA	1:D:172:PRO:HD2	1.83	0.41
1:A:214:ILE:N	1:A:214:ILE:CD1	2.84	0.41
1:C:185:THR:HA	1:C:237:GLN:O	2.21	0.41
1:C:39:ILE:HD12	1:C:95:LEU:HB3	2.03	0.41
1:D:168:TYR:CZ	1:D:180:ARG:HB2	2.55	0.41
1:B:169:ASP:CG	1:B:181:TYR:OH	2.60	0.40
1:C:102:MET:O	1:C:131:PHE:HA	2.21	0.40
1:F:187:ASP:CB	1:F:240:SER:HB2	2.44	0.40
1:B:143:ASP:OD2	1:B:160:LYS:NZ	2.43	0.40
1:B:235:LEU:HD11	1:B:237:GLN:CB	2.48	0.40
1:E:120:ILE:O	1:E:124:GLU:HG3	2.20	0.40
1:D:186:TYR:CG	1:D:206:ARG:HG2	2.56	0.40
1:E:231:GLN:HA	1:E:231:GLN:NE2	2.36	0.40
1:E:12:LYS:HA	1:E:51:VAL:O	2.20	0.40
1:C:158:LEU:HD23	1:C:159:LEU:N	2.36	0.40
1:E:120:ILE:O	1:E:124:GLU:CG	2.69	0.40
1:A:35:ALA:HB2	1:A:88:MET:HE1	2.04	0.40
1:B:171:ASP:HB2	1:B:173:LYS:NZ	2.36	0.40
1:C:134:GLY:HA2	2:C:1474:HOH:O	2.20	0.40
1:D:106:LYS:HD2	1:D:106:LYS:N	2.37	0.40
1:D:171:ASP:OD1	1:D:175:HIS:HD2	2.05	0.40
1:F:16:GLU:HA	1:F:19:MET:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:SER:OG	1:D:228:HIS:O[2_565]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	241/243 (99%)	232 (96%)	7 (3%)	2 (1%)	22	23
1	B	238/243 (98%)	229 (96%)	7 (3%)	2 (1%)	22	23
1	C	236/243 (97%)	229 (97%)	6 (2%)	1 (0%)	38	42
1	D	238/243 (98%)	228 (96%)	8 (3%)	2 (1%)	22	23
1	E	236/243 (97%)	220 (93%)	10 (4%)	6 (2%)	6	4
1	F	236/243 (97%)	225 (95%)	9 (4%)	2 (1%)	22	23
All	All	1425/1458 (98%)	1363 (96%)	47 (3%)	15 (1%)	17	15

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	B	170	LYS
1	B	171	ASP
1	E	172	PRO
1	E	173	LYS
1	E	174	LYS
1	E	175	HIS
1	C	66	SER
1	E	239	ARG
1	D	170	LYS
1	F	65	ALA
1	A	176	SER
1	E	176	SER
1	D	171	ASP
1	F	177	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/186 (100%)	165 (89%)	21 (11%)	7	6
1	B	184/186 (99%)	158 (86%)	26 (14%)	4	3
1	C	182/186 (98%)	165 (91%)	17 (9%)	10	9
1	D	184/186 (99%)	158 (86%)	26 (14%)	4	3
1	E	181/186 (97%)	160 (88%)	21 (12%)	6	5
1	F	182/186 (98%)	159 (87%)	23 (13%)	5	4
All	All	1099/1116 (98%)	965 (88%)	134 (12%)	6	5

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	7	ARG
1	A	29	LYS
1	A	42	GLN
1	A	50	LEU
1	A	56	ASN
1	A	66	SER
1	A	70	ARG
1	A	86	LEU
1	A	88	MET
1	A	94	LYS
1	A	98	LYS
1	A	115	ILE
1	A	123	LEU
1	A	148	LEU
1	A	157	LEU
1	A	170	LYS
1	A	204	LEU
1	A	212	LEU
1	A	213	ARG
1	A	240	SER
1	B	23	ASP

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Mol	Chain	Res	Type
1	B	34	LEU
1	B	42	GLN
1	B	48	VAL
1	B	56	ASN
1	B	66	SER
1	B	70	ARG
1	B	79	LEU
1	B	81	THR
1	B	95	LEU
1	B	99	VAL
1	B	123	LEU
1	B	141	THR
1	B	148	LEU
1	B	157	LEU
1	B	158	LEU
1	B	173	LYS
1	B	175	HIS
1	B	176	SER
1	B	180	ARG
1	B	182	ASP
1	B	185	THR
1	B	204	LEU
1	B	210	LEU
1	B	213	ARG
1	B	224	LEU
1	C	16	GLU
1	C	56	ASN
1	C	86	LEU
1	C	95	LEU
1	C	106	LYS
1	C	108	ASN
1	C	113	ASP
1	C	123	LEU
1	C	148	LEU
1	C	157	LEU
1	C	183	SER
1	C	185	THR
1	C	190	ILE
1	C	210	LEU
1	C	224	LEU
1	C	235	LEU
1	C	239	ARG

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Mol	Chain	Res	Type
1	D	1	MET
1	D	32	ASN
1	D	40	GLU
1	D	42	GLN
1	D	56	ASN
1	D	70	ARG
1	D	79	LEU
1	D	86	LEU
1	D	95	LEU
1	D	101	VAL
1	D	108	ASN
1	D	110	VAL
1	D	113	ASP
1	D	123	LEU
1	D	135	THR
1	D	148	LEU
1	D	157	LEU
1	D	162	THR
1	D	170	LYS
1	D	173	LYS
1	D	180	ARG
1	D	210	LEU
1	D	213	ARG
1	D	218	SER
1	D	223	LEU
1	D	224	LEU
1	E	12	LYS
1	E	30	VAL
1	E	34	LEU
1	E	42	GLN
1	E	56	ASN
1	E	63	LEU
1	E	70	ARG
1	E	79	LEU
1	E	86	LEU
1	E	93	GLU
1	E	110	VAL
1	E	123	LEU
1	E	124	GLU
1	E	135	THR
1	E	148	LEU
1	E	169	ASP

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Mol	Chain	Res	Type
1	E	175	HIS
1	E	185	THR
1	E	206	ARG
1	E	223	LEU
1	E	235	LEU
1	F	7	ARG
1	F	16	GLU
1	F	50	LEU
1	F	56	ASN
1	F	79	LEU
1	F	86	LEU
1	F	110	VAL
1	F	123	LEU
1	F	128	ILE
1	F	141	THR
1	F	148	LEU
1	F	157	LEU
1	F	163	LYS
1	F	183	SER
1	F	188	GLU
1	F	191	MET
1	F	192	GLN
1	F	204	LEU
1	F	210	LEU
1	F	212	LEU
1	F	219	GLU
1	F	222	VAL
1	F	223	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	47	GLN
1	A	56	ASN
1	A	84	ASN
1	A	122	HIS
1	A	192	GLN
1	B	47	GLN
1	B	56	ASN
1	B	75	HIS
1	B	84	ASN

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Mol	Chain	Res	Type
1	B	122	HIS
1	B	192	GLN
1	C	32	ASN
1	C	47	GLN
1	C	56	ASN
1	C	84	ASN
1	C	89	GLN
1	C	108	ASN
1	C	137	ASN
1	C	192	GLN
1	C	237	GLN
1	D	56	ASN
1	D	84	ASN
1	D	122	HIS
1	D	175	HIS
1	D	192	GLN
1	E	43	GLN
1	E	47	GLN
1	E	56	ASN
1	E	84	ASN
1	E	108	ASN
1	E	122	HIS
1	E	137	ASN
1	E	192	GLN
1	E	228	HIS
1	E	231	GLN
1	F	56	ASN
1	F	84	ASN
1	F	122	HIS
1	F	137	ASN
1	F	175	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	243/243 (100%)	0.25	9 (3%) 42 53	24, 40, 58, 65	0
1	B	240/243 (98%)	0.45	15 (6%) 21 29	26, 41, 61, 71	0
1	C	238/243 (97%)	0.13	6 (2%) 58 67	25, 40, 56, 65	0
1	D	240/243 (98%)	0.64	31 (12%) 4 7	31, 49, 67, 73	0
1	E	238/243 (97%)	0.83	31 (13%) 4 6	36, 52, 68, 76	0
1	F	238/243 (97%)	0.46	22 (9%) 10 15	35, 51, 69, 75	0
All	All	1437/1458 (98%)	0.46	114 (7%) 13 20	24, 45, 65, 76	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	240	SER	9.9
1	E	168	TYR	9.3
1	E	176	SER	7.4
1	E	175	HIS	6.2
1	E	173	LYS	6.1
1	E	172	PRO	6.0
1	D	179	VAL	5.9
1	E	239	ARG	5.9
1	F	67	GLY	5.5
1	A	-2	SER	5.5
1	D	1	MET	4.9
1	D	171	ASP	4.6
1	E	174	LYS	4.4
1	D	178	ALA	4.2
1	B	173	LYS	4.2
1	F	178	ALA	4.2
1	E	66	SER	4.1
1	B	179	VAL	4.0
1	E	67	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	66	SER	3.9
1	D	176	SER	3.9
1	D	52	ILE	3.9
1	F	179	VAL	3.9
1	F	24	TYR	3.9
1	F	174	LYS	3.8
1	E	11	LEU	3.8
1	B	171	ASP	3.7
1	B	177	ASP	3.6
1	D	67	GLY	3.6
1	F	29	LYS	3.6
1	B	174	LYS	3.5
1	E	170	LYS	3.5
1	B	169	ASP	3.5
1	A	240	SER	3.5
1	F	239	ARG	3.4
1	D	51	VAL	3.4
1	E	178	ALA	3.3
1	E	225	ARG	3.3
1	C	240	SER	3.3
1	C	65	ALA	3.2
1	D	172	PRO	3.2
1	D	169	ASP	3.2
1	D	21	ASP	3.2
1	F	51	VAL	3.2
1	E	21	ASP	3.1
1	B	172	PRO	3.0
1	E	229	GLY	3.0
1	B	175	HIS	3.0
1	B	178	ALA	3.0
1	B	66	SER	3.0
1	E	179	VAL	3.0
1	C	7	ARG	3.0
1	D	240	SER	3.0
1	E	50	LEU	3.0
1	D	10	LEU	2.9
1	D	194	LEU	2.9
1	E	23	ASP	2.9
1	E	96	GLY	2.9
1	E	177	ASP	2.9
1	E	171	ASP	2.9
1	E	169	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	66	SER	2.9
1	E	10	LEU	2.9
1	D	177	ASP	2.8
1	E	51	VAL	2.8
1	D	2	SER	2.8
1	D	170	LYS	2.7
1	F	169	ASP	2.7
1	F	175	HIS	2.7
1	F	170	LYS	2.7
1	B	1	MET	2.6
1	D	88	MET	2.6
1	A	170	LYS	2.6
1	D	173	LYS	2.6
1	B	24	TYR	2.6
1	A	174	LYS	2.6
1	F	177	ASP	2.6
1	F	130	ILE	2.6
1	A	172	PRO	2.5
1	E	220	PRO	2.5
1	D	175	HIS	2.5
1	D	130	ILE	2.5
1	D	50	LEU	2.5
1	B	2	SER	2.5
1	A	21	ASP	2.5
1	D	13	LEU	2.5
1	F	10	LEU	2.4
1	F	229	GLY	2.4
1	B	158	LEU	2.4
1	E	161	ALA	2.4
1	D	181	TYR	2.3
1	F	168	TYR	2.3
1	F	68	MET	2.3
1	E	108	ASN	2.3
1	E	218	SER	2.3
1	D	86	LEU	2.2
1	F	218	SER	2.2
1	F	240	SER	2.2
1	C	52	ILE	2.2
1	D	49	ALA	2.2
1	A	179	VAL	2.2
1	D	66	SER	2.2
1	E	20	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	21	ASP	2.2
1	D	131	PHE	2.2
1	D	158	LEU	2.1
1	D	174	LYS	2.1
1	A	173	LYS	2.1
1	D	29	LYS	2.1
1	A	159	LEU	2.1
1	F	50	LEU	2.1
1	C	67	GLY	2.1
1	E	24	TYR	2.1
1	B	51	VAL	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.