Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:43 AM GMT

PDB ID	:	2E3D
Title	:	Crystal structure of E. coli glucose-1-phosphate uridylyltransferase
Authors	:	Thoden, J.B.; Holden, H.M.
Deposited on	:	2006-11-22
Resolution	:	1.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

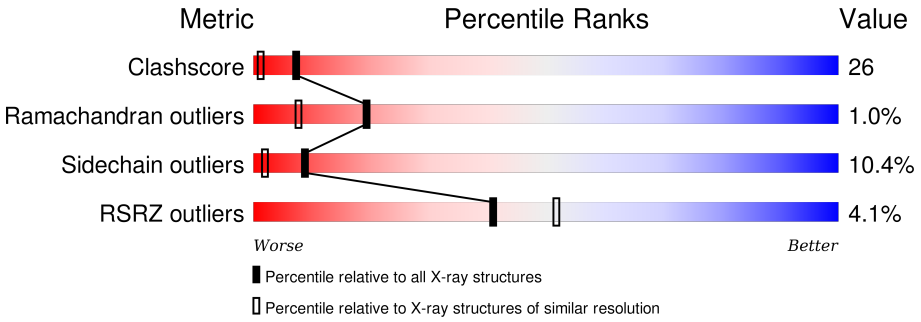
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 <=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	302	3% 55% 32% 7% 5%
1	B	302	5% 50% 36% 7% 7%
1	C	302	% 58% 29% 8% • 5%
1	D	302	6% 49% 34% 9% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9442 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 UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	2	0
			2199	1400	363	420	16			
1	B	281	Total	C	N	O	S	0	3	0
			2166	1376	361	413	16			
1	C	288	Total	C	N	O	S	0	0	0
			2195	1396	362	422	15			
1	D	278	Total	C	N	O	S	0	0	0
			2096	1331	346	404	15			

- Molecule 2 is water.

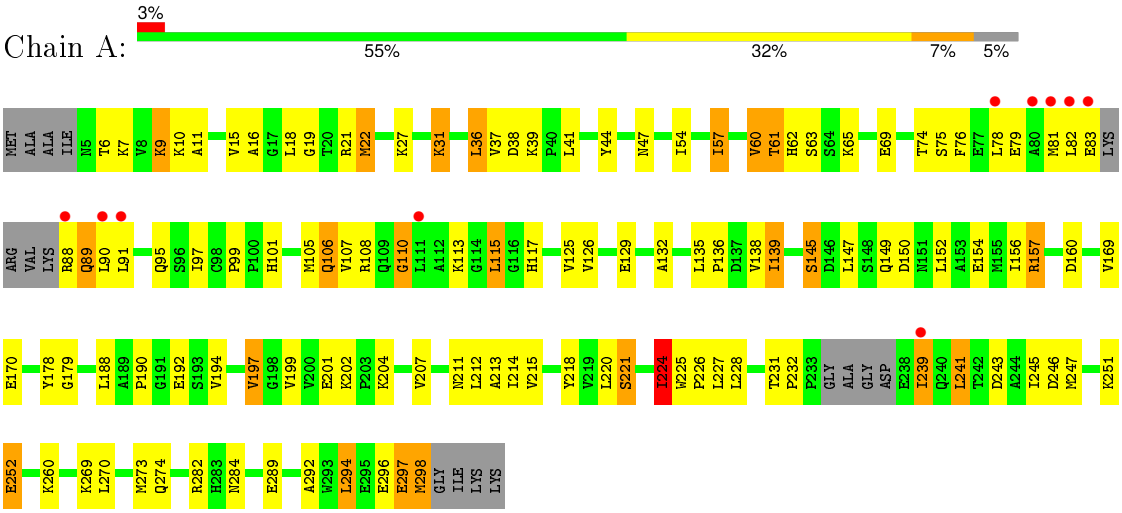
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	249	Total	O	0	0
			249	249		
2	B	194	Total	O	0	0
			194	194		
2	C	187	Total	O	0	0
			187	187		
2	D	156	Total	O	0	0
			156	156		

3 Residue-property plots

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

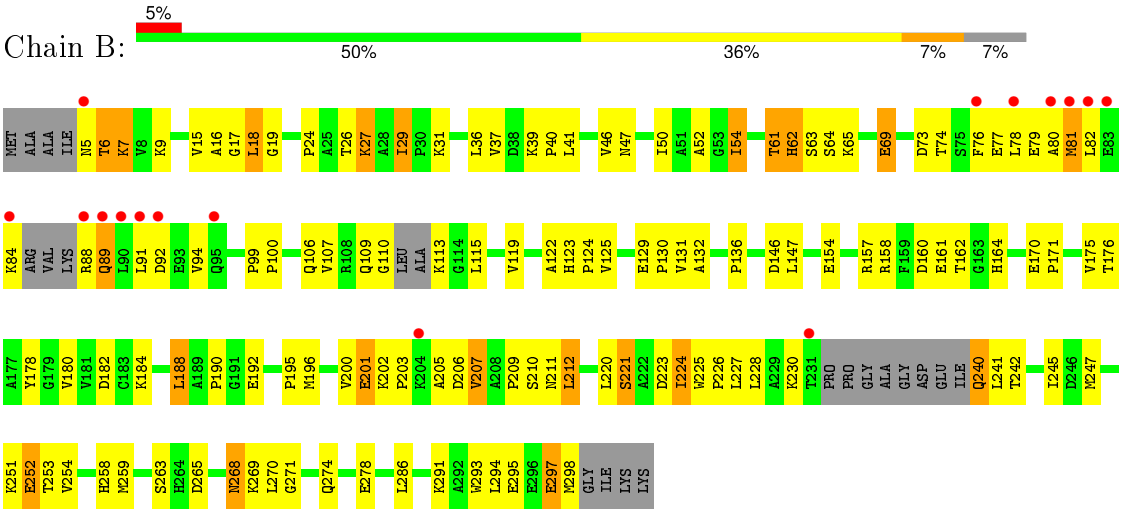
- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain A:



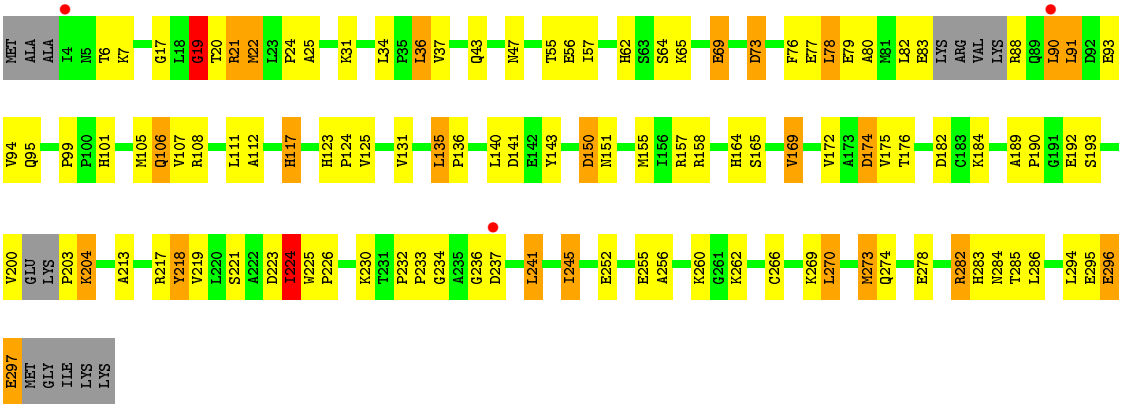
- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain B:



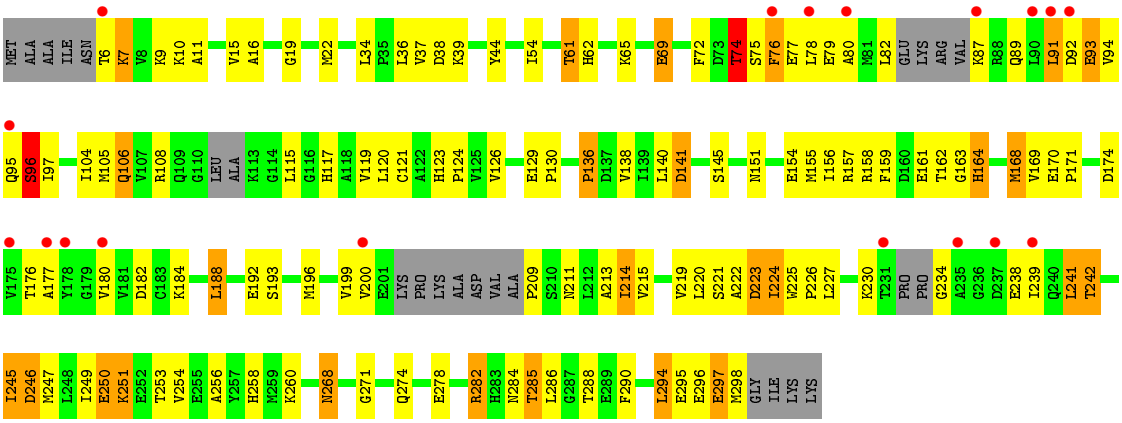
- Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain C:



• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.90Å 109.30Å 100.50Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-1.95) 98.6 (29.89-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 1.91Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.198 , 0.243 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 119.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 106814 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9442	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.83	1/2250 (0.0%)	1.47	24/3058 (0.8%)
1	B	0.77	0/2219	1.36	14/3011 (0.5%)
1	C	0.83	3/2235 (0.1%)	1.52	30/3038 (1.0%)
1	D	0.76	0/2131	1.42	18/2893 (0.6%)
All	All	0.80	4/8835 (0.0%)	1.44	86/12000 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	273	MET	SD-CE	-7.84	1.33	1.77
1	C	22	MET	SD-CE	5.26	2.07	1.77
1	C	165	SER	CB-OG	5.13	1.49	1.42
1	A	138	VAL	CB-CG1	5.04	1.63	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	282	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	D	108	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	C	217	ARG	NE-CZ-NH1	-9.06	115.77	120.30
1	C	73	ASP	CB-CG-OD1	8.74	126.17	118.30
1	C	22	MET	CG-SD-CE	8.48	113.77	100.20
1	C	273	MET	CG-SD-CE	-7.97	87.45	100.20
1	C	234	GLY	N-CA-C	-7.91	93.32	113.10
1	C	135	LEU	CB-CG-CD1	-7.73	97.86	111.00
1	C	282	ARG	NE-CZ-NH1	7.69	124.15	120.30
1	C	36	LEU	CB-CG-CD2	-7.24	98.69	111.00
1	A	228	LEU	CB-CG-CD2	-7.23	98.71	111.00
1	A	19	GLY	N-CA-C	7.22	131.14	113.10
1	A	252	GLU	N-CA-CB	-7.20	97.65	110.60
1	C	174	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	C	241	LEU	CB-CG-CD2	-6.91	99.25	111.00
1	D	223	ASP	CB-CG-OD1	6.86	124.47	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	286	LEU	CB-CG-CD2	-6.83	99.39	111.00
1	C	224	ILE	CB-CA-C	-6.65	98.31	111.60
1	C	108	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	158	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	D	22	MET	CG-SD-CE	6.39	110.42	100.20
1	A	241	LEU	CB-CG-CD2	-6.38	100.15	111.00
1	D	192	GLU	CB-CA-C	-6.36	97.69	110.40
1	B	27	LYS	CD-CE-NZ	-6.31	97.18	111.70
1	A	179	GLY	N-CA-C	-6.30	97.36	113.10
1	A	145	SER	CB-CA-C	-6.29	98.14	110.10
1	B	54	ILE	CG1-CB-CG2	-6.26	97.63	111.40
1	A	212	LEU	CB-CG-CD1	-6.21	100.44	111.00
1	A	150	ASP	CB-CG-OD1	-6.19	112.72	118.30
1	B	29	ILE	CG1-CB-CG2	6.17	124.98	111.40
1	B	147	LEU	CB-CG-CD1	6.15	121.46	111.00
1	D	34	LEU	CB-CG-CD1	-6.13	100.58	111.00
1	C	204	LYS	N-CA-C	-6.11	94.51	111.00
1	D	19	GLY	N-CA-C	6.07	128.29	113.10
1	A	246	ASP	CB-CA-C	6.04	122.49	110.40
1	A	150	ASP	CB-CA-C	-5.98	98.45	110.40
1	B	36	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	D	69	GLU	CA-CB-CG	-5.90	100.42	113.40
1	C	19	GLY	N-CA-C	5.88	127.80	113.10
1	B	212	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	A	145	SER	N-CA-CB	5.86	119.29	110.50
1	D	105	MET	CG-SD-CE	5.82	109.52	100.20
1	A	57	ILE	CG1-CB-CG2	-5.82	98.60	111.40
1	A	197	VAL	CG1-CB-CG2	5.81	120.20	110.90
1	A	135	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	A	115	LEU	CB-CG-CD2	5.75	120.77	111.00
1	A	60	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	A	61	THR	N-CA-C	5.69	126.37	111.00
1	A	224	ILE	CG1-CB-CG2	5.65	123.82	111.40
1	C	266	CYS	CA-CB-SG	-5.63	103.86	114.00
1	D	282	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	150	ASP	CB-CG-OD2	5.62	123.35	118.30
1	D	214	ILE	CG1-CB-CG2	-5.61	99.06	111.40
1	D	230	LYS	CB-CA-C	-5.60	99.20	110.40
1	C	57	ILE	CG1-CB-CG2	-5.59	99.11	111.40
1	A	36	LEU	N-CA-C	-5.57	95.96	111.00
1	C	270	LEU	CB-CG-CD1	5.53	120.40	111.00
1	C	218	TYR	CB-CA-C	-5.51	99.38	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	168	MET	CG-SD-CE	5.50	109.00	100.20
1	D	161	GLU	CB-CA-C	-5.49	99.41	110.40
1	C	151	ASN	N-CA-CB	-5.47	100.76	110.60
1	C	155	MET	CG-SD-CE	5.45	108.92	100.20
1	B	254	VAL	CB-CA-C	-5.44	101.06	111.40
1	C	36	LEU	N-CA-C	-5.43	96.33	111.00
1	D	138	VAL	CA-CB-CG2	-5.41	102.79	110.90
1	C	224	ILE	CG1-CB-CG2	5.41	123.29	111.40
1	B	113	LYS	N-CA-C	5.39	125.55	111.00
1	A	139	ILE	CG1-CB-CG2	-5.38	99.57	111.40
1	C	219	VAL	N-CA-C	-5.33	96.60	111.00
1	C	169	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	A	297	GLU	CB-CA-C	5.32	121.03	110.40
1	C	182	ASP	CB-CA-C	-5.28	99.85	110.40
1	A	147	LEU	CB-CG-CD1	-5.24	102.10	111.00
1	B	62[A]	HIS	N-CA-CB	-5.22	101.21	110.60
1	B	62[B]	HIS	N-CA-CB	-5.22	101.21	110.60
1	D	36	LEU	N-CA-C	-5.21	96.95	111.00
1	C	182	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	131	VAL	N-CA-CB	-5.16	100.15	111.50
1	B	36	LEU	CB-CG-CD2	5.15	119.75	111.00
1	B	52	ALA	C-N-CA	-5.14	111.50	122.30
1	A	41	LEU	CB-CA-C	-5.10	100.51	110.20
1	D	96	SER	N-CA-CB	-5.07	102.90	110.50
1	D	74	THR	CA-CB-CG2	-5.06	105.31	112.40
1	D	141	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	204	LYS	N-CA-C	-5.02	97.44	111.00
1	B	61	THR	N-CA-C	5.01	124.54	111.00

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	2199	0	2224	113	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2166	0	2187	140	0
1	C	2195	0	2215	98	0
1	D	2096	0	2076	128	0
2	A	249	0	0	20	0
2	B	194	0	0	12	0
2	C	187	0	0	7	0
2	D	156	0	0	6	0
All	All	9442	0	8702	449	0

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 (449) 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:22:MET:CE	1:C:22:MET:SD	2.07	1.42
1:D:117:HIS:HB2	1:D:239:ILE:HD13	1.17	1.11
1:C:21:ARG:HD3	1:C:21:ARG:H	1.24	1.01
1:D:117:HIS:HB2	1:D:239:ILE:CD1	1.90	1.00
1:B:298:MET:HE3	1:D:295:GLU:HG3	1.44	1.00
1:A:149:GLN:O	1:A:157:ARG:NH2	1.94	1.00
1:A:39:LYS:O	2:A:495:HOH:O	1.85	0.94
1:B:188:LEU:CD2	1:B:192:GLU:HB2	1.97	0.94
1:D:7:LYS:CD	1:D:130:PRO:HG3	1.98	0.93
1:D:285:THR:HG22	1:D:286:LEU:HG	1.51	0.92
1:B:295:GLU:HG2	1:D:298:MET:HE1	1.52	0.90
1:B:295:GLU:HG2	1:D:298:MET:CE	2.02	0.89
1:A:16:ALA:HB2	1:A:61:THR:HA	1.56	0.88
1:D:241:LEU:HG	1:D:245:ILE:HD12	1.55	0.87
1:A:269:LYS:HB3	1:A:273:MET:CE	2.04	0.87
1:C:21:ARG:N	1:C:21:ARG:HD3	1.90	0.85
1:A:239:ILE:HD12	1:A:239:ILE:H	1.39	0.85
1:B:62[B]:HIS:CE1	1:B:64:SER:H	1.94	0.85
1:B:298:MET:CE	1:D:295:GLU:HG3	2.07	0.83
1:A:79:GLU:HG2	1:A:91:LEU:HD11	1.60	0.83
1:B:80:ALA:HB1	1:B:84:LYS:HE3	1.59	0.82
1:B:16:ALA:CB	1:B:31:LYS:HD3	2.10	0.82
1:B:298:MET:HE2	1:D:294:LEU:HB3	1.60	0.81
1:B:176:THR:O	1:B:202:LYS:HB3	1.78	0.81
1:A:83:GLU:HG2	1:A:91:LEU:CD2	2.10	0.80
1:A:227:LEU:HD22	1:A:247:MET:HE2	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:HG11	1:B:209:PRO:CD	2.12	0.80
1:B:206:ASP:OD1	1:B:207:VAL:HG22	1.82	0.79
1:D:7:LYS:HD3	1:D:130:PRO:HG3	1.65	0.79
1:B:223:ASP:O	1:B:226:PRO:HD2	1.82	0.79
1:A:201:GLU:HG2	1:A:202:LYS:HG3	1.64	0.78
1:A:115:LEU:HD21	1:A:241:LEU:HD23	1.64	0.78
1:C:226:PRO:O	1:C:230:LYS:HG2	1.84	0.78
1:A:61:THR:HG21	1:A:106:GLN:OE1	1.84	0.78
1:D:247:MET:O	1:D:251:LYS:HD3	1.83	0.77
1:B:76:PHE:CD1	1:C:77:GLU:HG3	2.20	0.77
1:D:162:THR:HG23	1:D:164:HIS:H	1.50	0.77
1:A:78:LEU:HG	1:A:82:LEU:HD11	1.65	0.77
1:C:230:LYS:O	1:C:232:PRO:HD3	1.83	0.77
1:D:7:LYS:HD2	1:D:130:PRO:HG3	1.65	0.76
1:B:136:PRO:HG2	2:B:395:HOH:O	1.84	0.76
1:D:158:ARG:O	1:D:162:THR:HG22	1.84	0.76
1:D:159:PHE:O	1:D:163:GLY:N	2.19	0.76
1:C:31:LYS:HB2	2:C:419:HOH:O	1.85	0.75
1:D:115:LEU:O	1:D:119:VAL:HG23	1.87	0.75
1:C:123:HIS:HB3	1:C:124:PRO:HD3	1.68	0.74
1:B:200:VAL:HG11	1:B:209:PRO:HD3	1.68	0.74
1:B:39:LYS:HE3	2:B:316:HOH:O	1.85	0.74
1:C:79:GLU:O	1:C:83:GLU:HG3	1.88	0.74
1:B:298:MET:CE	1:D:294:LEU:HB3	2.16	0.73
1:A:296:GLU:HB2	1:A:297:GLU:OE1	1.90	0.72
1:B:80:ALA:HB1	1:B:84:LYS:CE	2.19	0.72
1:A:243:ASP:O	1:A:247:MET:HG3	1.89	0.71
1:A:115:LEU:HD21	1:A:241:LEU:CD2	2.21	0.71
1:B:295:GLU:CG	1:D:298:MET:HE1	2.21	0.70
1:C:112:ALA:HB1	1:C:117:HIS:CG	2.26	0.70
1:B:80:ALA:CA	1:B:84:LYS:HE3	2.21	0.70
1:C:200:VAL:HG12	1:C:203:PRO:HG3	1.71	0.70
1:D:117:HIS:CB	1:D:239:ILE:HD13	2.10	0.70
1:B:78:LEU:O	1:B:78:LEU:HD12	1.91	0.69
1:A:11:ALA:HB2	1:A:54:ILE:HD13	1.74	0.69
1:A:110:GLY:N	2:A:414:HOH:O	2.25	0.69
1:B:80:ALA:C	1:B:84:LYS:HE3	2.13	0.69
1:B:80:ALA:CB	1:B:84:LYS:HE3	2.21	0.69
1:B:19:GLY:HA3	1:B:31:LYS:HD2	1.75	0.68
1:A:107[B]:VAL:HG21	1:A:125:VAL:CG2	2.24	0.67
1:B:78:LEU:HD11	1:B:82:LEU:HD11	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:HB3	2:A:485:HOH:O	1.93	0.67
1:B:24:PRO:HD2	1:D:38:ASP:O	1.95	0.67
1:C:111:LEU:HG	1:D:74:THR:HG21	1.75	0.67
1:D:251:LYS:N	1:D:251:LYS:HD2	2.08	0.67
1:C:22:MET:HE3	1:C:269:LYS:HG2	1.76	0.67
1:D:241:LEU:HG	1:D:245:ILE:CD1	2.24	0.67
1:B:178:TYR:O	1:B:202:LYS:HA	1.94	0.67
1:A:6:THR:HB	1:A:160:ASP:OD2	1.95	0.67
1:A:284:ASN:OD1	2:A:476:HOH:O	2.12	0.66
1:B:79:GLU:HA	1:B:82:LEU:HD12	1.77	0.66
1:C:270:LEU:O	1:C:274:GLN:HG3	1.95	0.66
1:C:19:GLY:HA3	1:C:31:LYS:HD3	1.76	0.66
1:A:270:LEU:O	1:A:274:GLN:HG3	1.95	0.66
1:C:143:TYR:CE1	1:C:282:ARG:HD2	2.30	0.65
1:B:7:LYS:HB3	1:B:130:PRO:HG3	1.78	0.65
1:B:291:LYS:O	1:B:295:GLU:HG3	1.97	0.65
1:D:151:ASN:O	1:D:155:MET:HG3	1.96	0.65
1:B:129:GLU:HB3	1:B:130:PRO:HD2	1.79	0.65
1:B:15:VAL:O	1:B:62[A]:HIS:NE2	2.31	0.64
1:D:154:GLU:O	1:D:158:ARG:HG3	1.97	0.64
1:A:22:MET:HE3	1:A:269:LYS:HG3	1.80	0.64
1:B:268:ASN:HD21	1:B:271:GLY:HA3	1.61	0.64
1:A:188:LEU:CD2	1:A:194:VAL:HG23	2.27	0.64
1:A:61:THR:HG21	1:A:106:GLN:CD	2.18	0.64
1:C:189:ALA:HB3	1:C:192:GLU:OE2	1.98	0.64
1:D:61:THR:HG21	1:D:106:GLN:HG3	1.79	0.63
1:C:143:TYR:CD1	1:C:282:ARG:HD2	2.33	0.63
1:A:269:LYS:HB3	1:A:273:MET:HE3	1.78	0.63
1:A:83:GLU:HG2	1:A:91:LEU:HD22	1.78	0.63
1:C:22:MET:CE	1:C:269:LYS:HG2	2.28	0.63
1:B:295:GLU:HG2	1:D:298:MET:HE3	1.81	0.62
1:C:91:LEU:O	1:C:91:LEU:HD12	1.99	0.62
1:D:91:LEU:O	1:D:91:LEU:HD12	2.00	0.62
1:A:16:ALA:HB2	1:A:61:THR:CA	2.28	0.62
1:B:7:LYS:HE2	1:B:7:LYS:HA	1.81	0.62
1:B:188:LEU:HD22	1:B:192:GLU:HB2	1.78	0.62
1:B:73:ASP:OD1	1:B:74:THR:N	2.30	0.62
1:B:16:ALA:O	2:B:389:HOH:O	2.16	0.62
1:A:220:LEU:HB3	1:A:224:ILE:HG12	1.81	0.62
1:C:83:GLU:HG2	1:C:91:LEU:HD21	1.82	0.62
2:A:496:HOH:O	1:C:22:MET:HE2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:MET:HE3	1:C:269:LYS:CG	2.30	0.61
1:B:27:LYS:HE2	1:D:75:SER:OG	2.00	0.61
1:D:188:LEU:HD13	1:D:258:HIS:HB2	1.82	0.61
1:B:9:LYS:O	2:B:387:HOH:O	2.16	0.61
1:D:171:PRO:HA	1:D:211:ASN:O	2.00	0.61
1:D:296:GLU:O	1:D:297:GLU:C	2.38	0.61
1:A:211:ASN:OD1	2:A:483:HOH:O	2.16	0.61
1:B:293:TRP:O	1:B:297:GLU:HB2	2.01	0.60
1:C:78:LEU:HD23	1:C:82:LEU:HD12	1.84	0.60
1:B:80:ALA:HB1	1:B:84:LYS:NZ	2.15	0.60
1:A:169:VAL:HA	1:A:213:ALA:O	2.01	0.60
1:A:188:LEU:HD22	1:A:192:GLU:O	2.02	0.60
1:C:90:LEU:HD23	1:C:90:LEU:N	2.15	0.60
1:B:62[B]:HIS:ND1	1:B:64:SER:N	2.44	0.60
1:A:78:LEU:HG	1:A:82:LEU:CD1	2.32	0.60
1:A:292:ALA:O	1:A:296:GLU:HG3	2.02	0.60
1:C:157:ARG:NH1	2:C:470:HOH:O	2.35	0.60
1:A:91:LEU:O	1:A:95:GLN:HG3	2.01	0.59
1:D:180:VAL:CG2	1:D:209:PRO:HD2	2.32	0.59
1:D:115:LEU:HD21	1:D:241:LEU:HD22	1.84	0.59
1:D:75:SER:O	1:D:78:LEU:HB3	2.02	0.59
1:C:241:LEU:HG	1:C:245:ILE:HD12	1.85	0.59
1:D:180:VAL:HG23	1:D:209:PRO:HD2	1.83	0.59
1:A:113:LYS:HB2	1:A:117:HIS:CG	2.38	0.59
1:A:107[B]:VAL:HG21	1:A:125:VAL:HG21	1.84	0.59
1:D:268:ASN:ND2	1:D:271:GLY:H	2.01	0.59
1:C:143:TYR:CD1	1:C:282:ARG:CD	2.86	0.58
1:B:225:TRP:HB2	1:B:226:PRO:HD3	1.85	0.58
1:A:38:ASP:O	1:C:24:PRO:HD2	2.03	0.58
1:B:62[B]:HIS:ND1	1:B:63:SER:N	2.51	0.58
1:B:247:MET:HG3	2:B:490:HOH:O	2.03	0.58
1:A:47:ASN:ND2	2:A:316:HOH:O	2.28	0.58
1:B:6:THR:HB	1:B:160:ASP:OD2	2.03	0.58
1:B:265:ASP:HB2	2:B:427:HOH:O	2.04	0.58
1:C:224:ILE:N	1:C:224:ILE:HD12	2.18	0.58
1:D:224:ILE:HA	1:D:227:LEU:HD12	1.86	0.57
1:A:99:PRO:HB2	1:A:101[B]:HIS:CE1	2.39	0.57
1:B:298:MET:HE3	1:D:295:GLU:HA	1.86	0.57
1:B:123:HIS:HB3	1:B:124:PRO:HD3	1.86	0.57
1:C:203:PRO:C	1:C:204:LYS:O	2.35	0.57
1:B:223:ASP:HB3	2:B:374:HOH:O	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PRO:HB3	1:C:101:HIS:CE1	2.39	0.57
1:A:61:THR:HG23	1:A:62:HIS:N	2.19	0.57
1:A:136:PRO:HD2	2:A:395:HOH:O	2.03	0.57
1:A:36:LEU:O	2:A:495:HOH:O	2.18	0.57
1:A:91:LEU:O	1:A:91:LEU:HD12	2.05	0.56
1:D:174:ASP:OD1	1:D:177:ALA:HB2	2.06	0.56
1:A:221:SER:O	1:A:224:ILE:HG13	2.04	0.56
1:A:21:ARG:NH2	2:A:422:HOH:O	2.28	0.56
1:D:7:LYS:HD3	1:D:130:PRO:CG	2.35	0.56
1:B:188:LEU:HD13	1:B:258:HIS:HB2	1.87	0.56
1:D:115:LEU:CD2	1:D:241:LEU:HD22	2.36	0.56
1:B:82:LEU:CD1	1:B:94:VAL:HG21	2.36	0.56
1:A:61:THR:OG1	1:A:62:HIS:N	2.36	0.55
1:B:76:PHE:CE1	1:C:77:GLU:HG3	2.41	0.55
1:D:274:GLN:O	1:D:278:GLU:HG3	2.06	0.55
1:D:16:ALA:HB2	1:D:61:THR:HA	1.87	0.55
1:A:273:MET:HE3	1:C:286:LEU:CD1	2.36	0.55
1:B:78:LEU:C	1:B:78:LEU:HD12	2.26	0.55
1:A:298:MET:HE2	1:C:294:LEU:HB3	1.88	0.55
1:B:18:LEU:HD12	1:B:18:LEU:H	1.72	0.55
1:C:203:PRO:N	2:C:424:HOH:O	2.39	0.55
1:B:170:GLU:HB2	1:B:171:PRO:HD2	1.89	0.55
1:A:75:SER:O	1:A:76:PHE:C	2.44	0.55
1:A:224:ILE:HD12	1:A:225:TRP:N	2.21	0.55
1:C:99:PRO:CB	1:C:101:HIS:CE1	2.89	0.55
1:A:239:ILE:HD12	1:A:239:ILE:N	2.15	0.55
1:B:7:LYS:CA	1:B:7:LYS:HE2	2.36	0.55
1:D:7:LYS:HD2	1:D:159:PHE:HE2	1.72	0.54
1:A:273:MET:HE3	1:C:286:LEU:HD13	1.90	0.54
1:D:250:GLU:C	1:D:251:LYS:HD2	2.27	0.54
1:C:20:THR:HB	1:C:21:ARG:HH11	1.72	0.54
1:D:145:SER:OG	1:D:260:LYS:O	2.26	0.54
1:A:78:LEU:O	1:A:81:MET:HB3	2.08	0.54
1:C:82:LEU:HB3	1:C:91:LEU:HD22	1.90	0.54
1:D:234:GLY:HA3	1:D:238:GLU:O	2.08	0.54
1:A:273:MET:CE	1:C:286:LEU:CD1	2.87	0.53
1:C:236:GLY:O	1:C:237:ASP:HB2	2.07	0.53
1:A:188:LEU:HD21	1:A:194:VAL:HG23	1.89	0.53
1:D:182:ASP:OD1	1:D:184:LYS:N	2.37	0.53
1:A:44:TYR:HE2	2:A:495:HOH:O	1.91	0.53
1:D:92:ASP:HB2	1:D:93:GLU:OE2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107[B]:VAL:CG2	1:A:125:VAL:HG21	2.39	0.53
1:D:10:LYS:HE3	1:D:126:VAL:HA	1.91	0.53
1:A:15:VAL:O	1:A:15:VAL:HG23	2.07	0.53
1:D:247:MET:HA	1:D:250:GLU:OE2	2.08	0.53
1:A:273:MET:HE1	1:C:286:LEU:HD12	1.91	0.53
1:B:200:VAL:HG13	1:B:200:VAL:O	2.08	0.53
1:A:75:SER:O	1:A:78:LEU:N	2.42	0.53
1:D:156:ILE:HG13	1:D:219:VAL:HG21	1.90	0.52
1:D:91:LEU:CD1	1:D:95:GLN:NE2	2.72	0.52
1:B:80:ALA:O	1:B:84:LYS:HE3	2.08	0.52
1:B:223:ASP:OD2	1:B:252:GLU:OE2	2.28	0.52
1:A:22:MET:HE3	1:A:269:LYS:CG	2.39	0.52
1:B:164:HIS:CE1	1:B:253:THR:HB	2.45	0.52
1:B:46:VAL:O	1:B:50:ILE:HG13	2.10	0.52
1:B:178:TYR:O	1:B:202:LYS:N	2.42	0.52
1:A:76:PHE:N	2:A:505:HOH:O	2.31	0.52
1:C:174:ASP:OD1	1:C:176:THR:OG1	2.23	0.52
1:D:251:LYS:N	1:D:251:LYS:CD	2.73	0.51
1:B:76:PHE:CG	1:C:77:GLU:HG3	2.45	0.51
1:A:27:LYS:NZ	1:C:73:ASP:O	2.29	0.51
1:B:178:TYR:O	1:B:202:LYS:CA	2.58	0.51
1:C:150:ASP:CG	1:C:260:LYS:HE3	2.31	0.51
1:D:246:ASP:HA	1:D:249:ILE:HD12	1.93	0.51
1:D:61:THR:CG2	1:D:106:GLN:HG3	2.40	0.51
1:A:60:VAL:HG22	1:A:107[A]:VAL:CG1	2.40	0.51
1:D:75:SER:HB2	1:D:78:LEU:HB3	1.92	0.51
1:B:61:THR:HG22	1:B:106:GLN:CG	2.40	0.51
1:D:11:ALA:HB2	1:D:54:ILE:HD12	1.92	0.51
1:A:108:ARG:NH1	1:B:73:ASP:OD2	2.39	0.51
1:B:293:TRP:HA	2:B:455:HOH:O	2.10	0.51
1:C:77:GLU:O	1:C:80:ALA:HB3	2.10	0.51
1:D:225:TRP:N	1:D:226:PRO:CD	2.74	0.51
1:C:218:TYR:N	1:C:218:TYR:CD1	2.78	0.51
1:D:226:PRO:HD2	1:D:227:LEU:H	1.75	0.50
1:D:77:GLU:O	1:D:80:ALA:HB3	2.10	0.50
1:B:298:MET:CE	1:D:295:GLU:N	2.75	0.50
1:A:36:LEU:N	2:A:495:HOH:O	2.30	0.50
1:D:74:THR:OG1	1:D:74:THR:O	2.29	0.50
1:B:15:VAL:HG12	1:B:15:VAL:O	2.10	0.50
1:B:82:LEU:HD13	1:B:94:VAL:HG21	1.93	0.50
1:A:199:VAL:HG21	1:A:245:ILE:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:O	1:A:202:LYS:N	2.38	0.50
1:B:154:GLU:O	1:B:158[A]:ARG:HG3	2.11	0.50
1:A:76:PHE:CE2	1:D:77:GLU:HA	2.47	0.50
1:D:82:LEU:C	1:D:91:LEU:HD22	2.32	0.50
1:C:90:LEU:CD2	1:C:90:LEU:N	2.75	0.50
1:C:223:ASP:OD2	1:C:252:GLU:OE2	2.30	0.50
1:C:224:ILE:HD12	1:C:225:TRP:N	2.26	0.50
1:A:214:ILE:O	2:A:545:HOH:O	2.20	0.50
1:B:115:LEU:O	1:B:119:VAL:HG23	2.11	0.50
1:D:62:HIS:HB3	1:D:65:LYS:HG3	1.94	0.49
1:D:162:THR:CG2	1:D:164:HIS:HB2	2.43	0.49
1:B:182:ASP:HA	1:B:209:PRO:HB2	1.93	0.49
1:A:76:PHE:CD2	1:D:77:GLU:HB2	2.47	0.49
1:B:7:LYS:HB3	1:B:130:PRO:CG	2.42	0.49
1:C:296:GLU:O	1:C:297:GLU:C	2.50	0.49
1:D:199:VAL:HG21	1:D:214:ILE:HD11	1.95	0.49
1:B:61:THR:CG2	1:B:106:GLN:CG	2.91	0.49
1:C:21:ARG:N	1:C:21:ARG:CD	2.71	0.49
1:D:140:LEU:HD23	1:D:140:LEU:N	2.25	0.49
1:D:182:ASP:C	1:D:182:ASP:OD1	2.51	0.49
1:A:105:MET:HG2	1:B:125:VAL:HG22	1.94	0.49
1:D:242:THR:O	1:D:246:ASP:OD1	2.31	0.49
1:D:225:TRP:N	1:D:226:PRO:HD3	2.28	0.49
1:B:7:LYS:CB	1:B:130:PRO:HG3	2.43	0.49
1:B:77:GLU:HA	1:C:76:PHE:CE2	2.48	0.49
1:B:16:ALA:HB2	1:B:31:LYS:HD3	1.90	0.48
1:A:63:SER:HB3	1:A:108:ARG:NH1	2.28	0.48
1:D:169:VAL:HA	1:D:213:ALA:O	2.13	0.48
1:D:123:HIS:HB3	1:D:124:PRO:HD3	1.93	0.48
1:B:130:PRO:HA	1:B:220:LEU:O	2.13	0.48
1:D:180:VAL:C	1:D:199:VAL:HG13	2.33	0.48
1:D:76:PHE:O	1:D:80:ALA:N	2.42	0.48
1:D:253:THR:HB	2:D:388:HOH:O	2.12	0.48
1:C:175:VAL:O	1:C:203:PRO:HD2	2.14	0.48
1:A:74:THR:HG23	1:A:79:GLU:OE1	2.14	0.48
1:D:242:THR:HG23	2:D:372:HOH:O	2.13	0.48
1:D:16:ALA:HB2	1:D:61:THR:CA	2.44	0.48
1:C:76:PHE:HB3	2:C:462:HOH:O	2.14	0.48
1:B:62[B]:HIS:CE1	1:B:64:SER:N	2.75	0.47
1:D:15:VAL:O	1:D:15:VAL:HG23	2.12	0.47
1:B:78:LEU:HD11	1:B:82:LEU:CD1	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:THR:C	1:C:56:GLU:HG3	2.35	0.47
1:D:151:ASN:HB3	1:D:168:MET:CE	2.43	0.47
1:A:22:MET:CE	1:A:269:LYS:CG	2.92	0.47
1:A:83:GLU:HG2	1:A:91:LEU:HD21	1.94	0.47
1:C:78:LEU:O	1:C:82:LEU:HB2	2.14	0.47
1:C:169:VAL:HA	1:C:213:ALA:O	2.15	0.47
1:A:10:LYS:HD2	1:A:126:VAL:HA	1.97	0.47
1:C:17:GLY:O	1:C:65:LYS:NZ	2.35	0.47
1:A:273:MET:CE	1:C:286:LEU:HD12	2.44	0.47
1:A:239:ILE:H	1:A:239:ILE:CD1	2.18	0.47
1:B:223:ASP:O	1:B:227:LEU:HG	2.14	0.47
1:D:74:THR:HB	1:D:79:GLU:OE2	2.14	0.47
1:A:22:MET:CE	1:A:269:LYS:HG3	2.43	0.47
1:B:122:ALA:O	1:B:123:HIS:C	2.53	0.47
1:D:121:CYS:O	1:D:124:PRO:HD2	2.15	0.47
1:A:152:LEU:O	1:A:156:ILE:HG13	2.14	0.47
1:C:91:LEU:O	1:C:95:GLN:HG3	2.15	0.46
1:B:17:GLY:O	1:B:65:LYS:NZ	2.46	0.46
1:C:164:HIS:HD2	1:C:255:GLU:OE2	1.97	0.46
1:B:171:PRO:HA	1:B:211:ASN:O	2.15	0.46
1:B:274:GLN:O	1:B:278:GLU:HG3	2.15	0.46
1:A:113:LYS:HB2	1:A:117:HIS:ND1	2.30	0.46
1:D:124:PRO:HD3	2:D:352:HOH:O	2.14	0.46
1:B:40:PRO:O	1:B:41:LEU:C	2.53	0.46
1:B:62[B]:HIS:CE1	1:B:64:SER:OG	2.69	0.46
1:D:223:ASP:O	1:D:226:PRO:HD2	2.15	0.46
1:A:207:VAL:O	1:A:207:VAL:HG22	2.16	0.46
1:D:174:ASP:OD2	1:D:176:THR:CB	2.64	0.46
1:C:6:THR:OG1	1:C:7:LYS:N	2.49	0.46
1:C:99:PRO:HB3	1:C:101:HIS:HE1	1.81	0.46
1:C:221:SER:O	1:C:224:ILE:HG13	2.15	0.46
1:C:34:LEU:HD23	1:C:34:LEU:HA	1.69	0.46
1:C:203:PRO:CD	2:C:424:HOH:O	2.64	0.45
1:D:74:THR:HG22	2:D:436:HOH:O	2.15	0.45
1:A:188:LEU:HD23	1:A:194:VAL:HG23	1.96	0.45
1:C:224:ILE:HD12	1:C:225:TRP:H	1.81	0.45
1:C:99:PRO:HB2	1:C:101:HIS:CE1	2.50	0.45
1:A:16:ALA:HB2	1:A:61:THR:C	2.35	0.45
1:D:246:ASP:O	1:D:250:GLU:HG3	2.16	0.45
1:C:24:PRO:O	1:C:25:ALA:C	2.55	0.45
1:A:227:LEU:HD22	1:A:247:MET:CE	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LYS:O	1:C:273:MET:HG3	2.16	0.45
1:B:107[B]:VAL:HG21	1:B:125:VAL:HG21	1.98	0.45
1:D:162:THR:HG23	1:D:164:HIS:HB2	1.97	0.45
1:C:91:LEU:O	1:C:95:GLN:HB2	2.16	0.45
1:C:189:ALA:O	1:C:190:PRO:C	2.54	0.45
1:D:6:THR:O	1:D:6:THR:HG22	2.16	0.45
1:D:298:MET:HE2	1:D:298:MET:HB3	1.58	0.45
1:B:74:THR:C	2:B:464:HOH:O	2.54	0.45
1:B:107[B]:VAL:HG21	1:B:125:VAL:CG2	2.46	0.45
1:A:132:ALA:HA	1:A:218:TYR:O	2.17	0.45
1:B:69:GLU:OE1	2:B:402:HOH:O	2.20	0.45
1:A:79:GLU:O	1:A:83:GLU:HG3	2.16	0.45
1:B:201:GLU:O	1:B:202:LYS:C	2.56	0.45
1:B:7:LYS:CE	1:B:7:LYS:HA	2.40	0.45
1:D:39:LYS:HE3	2:D:323:HOH:O	2.17	0.45
1:B:80:ALA:O	1:B:84:LYS:CE	2.65	0.45
1:D:91:LEU:HD12	1:D:95:GLN:NE2	2.32	0.45
1:A:225:TRP:HB2	1:A:226:PRO:HD3	1.99	0.45
1:D:74:THR:HG23	1:D:74:THR:H	1.40	0.44
1:A:129:GLU:HG2	2:A:420:HOH:O	2.17	0.44
1:D:241:LEU:O	1:D:245:ILE:HD12	2.17	0.44
1:D:246:ASP:OD1	1:D:246:ASP:N	2.51	0.44
1:B:78:LEU:CD1	1:B:82:LEU:HD11	2.46	0.44
1:C:43:GLN:O	1:C:47:ASN:ND2	2.50	0.44
1:B:82:LEU:HB2	1:B:91:LEU:HD13	2.00	0.44
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.61	0.44
1:A:201:GLU:HG2	1:A:202:LYS:CG	2.40	0.44
1:A:115:LEU:CD2	1:A:241:LEU:CD2	2.95	0.44
1:B:61:THR:HG21	1:B:106:GLN:HG3	2.00	0.44
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.58	0.44
1:A:154:GLU:HA	1:A:157:ARG:CZ	2.48	0.44
1:D:75:SER:O	1:D:79:GLU:HG3	2.18	0.44
1:C:106:GLN:NE2	2:C:463:HOH:O	2.51	0.44
1:D:129:GLU:C	1:D:222:ALA:HB2	2.38	0.44
1:A:60:VAL:HG22	1:A:107[A]:VAL:HG12	1.99	0.44
1:C:69:GLU:H	1:C:69:GLU:HG2	1.65	0.44
1:A:36:LEU:CB	2:A:495:HOH:O	2.66	0.44
1:D:159:PHE:O	1:D:163:GLY:CA	2.65	0.44
1:C:285:THR:HG22	1:C:286:LEU:HG	2.00	0.44
1:B:79:GLU:OE2	2:B:341:HOH:O	2.20	0.44
1:D:92:ASP:O	1:D:96:SER:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:THR:CG2	1:D:106:GLN:CG	2.96	0.43
1:C:135:LEU:HA	1:C:136:PRO:HD3	1.87	0.43
1:C:200:VAL:HG12	1:C:203:PRO:CG	2.42	0.43
1:D:16:ALA:HB2	1:D:61:THR:C	2.39	0.43
1:B:158[B]:ARG:CZ	1:B:162:THR:HG21	2.48	0.43
1:B:270:LEU:O	1:B:274:GLN:HG3	2.17	0.43
1:C:62:HIS:CE1	1:C:64:SER:HG	2.36	0.43
1:C:22:MET:HE1	1:C:269:LYS:HA	2.00	0.43
1:B:200:VAL:HG11	1:B:209:PRO:HD2	1.98	0.43
1:C:83:GLU:CG	1:C:91:LEU:HD21	2.46	0.43
1:C:78:LEU:HD23	1:C:82:LEU:CD1	2.48	0.43
1:D:174:ASP:O	1:D:177:ALA:HB3	2.18	0.43
1:C:295:GLU:O	1:C:296:GLU:C	2.56	0.43
1:B:241:LEU:HD12	1:B:241:LEU:HA	1.69	0.43
1:A:115:LEU:CD2	1:A:241:LEU:HD23	2.41	0.43
1:D:223:ASP:O	1:D:227:LEU:HD12	2.18	0.43
1:B:61:THR:CG2	1:B:106:GLN:HG3	2.48	0.43
1:C:78:LEU:CD2	1:C:94:VAL:HG11	2.49	0.43
1:A:289:GLU:HB2	2:A:479:HOH:O	2.19	0.43
1:A:61:THR:CG2	1:A:106:GLN:CD	2.85	0.43
1:A:107[B]:VAL:CG2	1:A:125:VAL:CG2	2.96	0.43
1:A:22:MET:HE1	1:A:269:LYS:HA	2.01	0.43
1:B:78:LEU:CD1	1:B:82:LEU:CD1	2.97	0.43
1:C:262:LYS:HE3	1:C:278:GLU:OE1	2.18	0.43
1:B:99:PRO:HA	1:B:100:PRO:HD3	1.82	0.43
1:B:131:VAL:HG22	1:B:132:ALA:N	2.33	0.42
1:A:252:GLU:HG2	2:A:386:HOH:O	2.19	0.42
1:C:283:HIS:CE1	1:C:285:THR:HB	2.55	0.42
1:B:180:VAL:HG12	1:B:210:SER:OG	2.19	0.42
1:D:288:THR:HB	2:D:421:HOH:O	2.19	0.42
1:D:115:LEU:CD2	1:D:241:LEU:CD2	2.97	0.42
1:B:61:THR:HG21	1:B:106:GLN:NE2	2.34	0.42
1:B:18:LEU:HD12	1:B:18:LEU:N	2.33	0.42
1:B:200:VAL:CG1	1:B:209:PRO:CD	2.91	0.42
1:B:89:GLN:HG2	1:B:89:GLN:H	1.55	0.42
1:C:172:VAL:O	1:C:172:VAL:HG23	2.19	0.42
1:A:231:THR:HA	1:A:232:PRO:HD3	1.65	0.42
1:B:188:LEU:HD21	1:B:192:GLU:HB2	1.96	0.42
1:C:135:LEU:HD23	1:C:135:LEU:N	2.34	0.42
1:C:193:SER:HA	1:C:256:ALA:O	2.19	0.42
1:B:221:SER:O	1:B:224:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:MET:SD	1:B:263:SER:HB3	2.59	0.42
1:D:249:ILE:HG13	1:D:254:VAL:HG21	2.02	0.42
1:D:193:SER:HA	1:D:256:ALA:O	2.20	0.42
1:A:89:GLN:HB3	1:A:89:GLN:HE21	1.50	0.42
1:B:146:ASP:OD1	1:B:146:ASP:C	2.58	0.42
1:D:199:VAL:HG12	1:D:200:VAL:N	2.34	0.42
1:C:204:LYS:HG2	2:C:377:HOH:O	2.20	0.42
1:D:95:GLN:O	1:D:97:ILE:N	2.52	0.42
1:D:170:GLU:HG2	1:D:215:VAL:HG22	2.01	0.42
1:C:105:MET:SD	1:C:125:VAL:HG11	2.60	0.42
1:B:157:ARG:O	1:B:161:GLU:HG3	2.19	0.41
1:D:162:THR:HG23	1:D:164:HIS:N	2.28	0.41
1:C:224:ILE:CD1	1:C:225:TRP:N	2.83	0.41
1:B:188:LEU:HD23	1:B:192:GLU:HB2	1.92	0.41
1:D:115:LEU:HD21	1:D:241:LEU:CD2	2.48	0.41
1:D:87:LYS:O	1:D:91:LEU:N	2.31	0.41
1:D:72:PHE:CB	1:D:104:ILE:HD13	2.49	0.41
1:D:141:ASP:OD2	1:D:282:ARG:NH2	2.45	0.41
1:D:15:VAL:HG12	1:D:136:PRO:HG3	2.01	0.41
1:A:139:ILE:HD12	1:A:139:ILE:HG23	1.80	0.41
1:A:9:LYS:HZ2	1:A:9:LYS:HB3	1.86	0.41
1:B:65:LYS:HE2	2:B:389:HOH:O	2.21	0.41
1:A:76:PHE:HB3	2:A:505:HOH:O	2.21	0.41
1:C:141:ASP:OD2	1:C:282:ARG:NH2	2.53	0.41
1:D:180:VAL:O	1:D:199:VAL:HG13	2.20	0.41
1:A:294:LEU:O	1:A:298:MET:HB2	2.20	0.41
1:A:31:LYS:HE3	1:A:31:LYS:HB2	1.60	0.41
1:A:170:GLU:HG2	1:A:215:VAL:HG22	2.02	0.41
1:B:298:MET:CE	1:D:295:GLU:HA	2.49	0.41
1:B:15:VAL:O	1:B:62[A]:HIS:CD2	2.73	0.41
1:B:242:THR:HA	1:B:245:ILE:HB	2.03	0.41
1:D:290:PHE:O	1:D:294:LEU:HB2	2.21	0.41
1:A:154:GLU:HA	1:A:157:ARG:NH2	2.36	0.41
1:B:81:MET:HA	1:B:84:LYS:HB2	2.01	0.41
1:B:26:THR:HG21	1:B:31:LYS:HB3	2.03	0.41
1:D:140:LEU:HD22	1:D:140:LEU:HA	1.87	0.41
1:D:123:HIS:N	1:D:124:PRO:CD	2.83	0.41
1:B:240:GLN:HE21	1:B:240:GLN:HB2	1.71	0.41
1:A:154:GLU:HG3	1:A:157:ARG:HE	1.86	0.40
1:B:69:GLU:CD	1:B:106:GLN:HE21	2.25	0.40
1:B:78:LEU:C	1:B:78:LEU:CD1	2.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASN:HA	1:B:50:ILE:HD12	2.04	0.40
1:B:61:THR:HG22	1:B:106:GLN:HG2	2.02	0.40
1:D:39:LYS:HB2	1:D:44:TYR:CE2	2.56	0.40
1:B:109:GLN:O	1:B:110:GLY:C	2.60	0.40
1:C:22:MET:CE	1:C:269:LYS:CG	2.94	0.40
1:B:31:LYS:H	1:B:31:LYS:HG2	1.73	0.40
1:C:78:LEU:CD2	1:C:82:LEU:HD12	2.49	0.40
1:B:82:LEU:CB	1:B:91:LEU:HD13	2.51	0.40
1:D:182:ASP:HA	1:D:209:PRO:HB2	2.03	0.40
1:B:175:VAL:HG23	1:B:203:PRO:HG2	2.02	0.40
1:B:294:LEU:HD13	1:D:298:MET:HG3	2.02	0.40

There are no symmetry-related clashes.

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	282/302 (93%)	265 (94%)	14 (5%)	3 (1%)	17 6
1	B	276/302 (91%)	261 (95%)	13 (5%)	2 (1%)	26 14
1	C	282/302 (93%)	264 (94%)	15 (5%)	3 (1%)	17 6
1	D	268/302 (89%)	243 (91%)	22 (8%)	3 (1%)	17 6
All	All	1108/1208 (92%)	1033 (93%)	64 (6%)	11 (1%)	19 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	96	SER
1	A	37	VAL
1	B	37	VAL
1	D	37	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	37	VAL
1	C	19	GLY
1	B	205	ALA
1	C	296	GLU
1	D	76	PHE
1	A	110	GLY
1	A	97	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	246/254 (97%)	222 (90%)	24 (10%)	10 2
1	B	242/254 (95%)	215 (89%)	27 (11%)	7 1
1	C	243/254 (96%)	225 (93%)	18 (7%)	17 5
1	D	227/254 (89%)	197 (87%)	30 (13%)	5 1
All	All	958/1016 (94%)	859 (90%)	99 (10%)	9 2

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	9	LYS
1	A	18	LEU
1	A	22	MET
1	A	31	LYS
1	A	57	ILE
1	A	65	LYS
1	A	69	GLU
1	A	88	ARG
1	A	89	GLN
1	A	90	LEU
1	A	106	GLN
1	A	145	SER
1	A	157	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	190	PRO
1	A	197	VAL
1	A	221	SER
1	A	224	ILE
1	A	239	ILE
1	A	251	LYS
1	A	260	LYS
1	A	282	ARG
1	A	294	LEU
1	A	298	MET
1	B	5	ASN
1	B	6	THR
1	B	7	LYS
1	B	18	LEU
1	B	29	ILE
1	B	54	ILE
1	B	69	GLU
1	B	81	MET
1	B	88	ARG
1	B	89	GLN
1	B	92	ASP
1	B	184	LYS
1	B	188	LEU
1	B	190	PRO
1	B	195	PRO
1	B	196	MET
1	B	201	GLU
1	B	207	VAL
1	B	221	SER
1	B	224	ILE
1	B	230	LYS
1	B	240	GLN
1	B	251	LYS
1	B	252	GLU
1	B	268	ASN
1	B	269	LYS
1	B	297	GLU
1	C	21	ARG
1	C	36	LEU
1	C	69	GLU
1	C	78	LEU
1	C	88	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	90	LEU
1	C	91	LEU
1	C	93	GLU
1	C	106	GLN
1	C	107	VAL
1	C	117	HIS
1	C	140	LEU
1	C	184	LYS
1	C	224	ILE
1	C	233	PRO
1	C	245	ILE
1	C	284	ASN
1	C	297	GLU
1	D	7	LYS
1	D	9	LYS
1	D	61	THR
1	D	69	GLU
1	D	74	THR
1	D	89	GLN
1	D	91	LEU
1	D	93	GLU
1	D	94	VAL
1	D	106	GLN
1	D	120	LEU
1	D	136	PRO
1	D	157	ARG
1	D	164	HIS
1	D	188	LEU
1	D	196	MET
1	D	220	LEU
1	D	221	SER
1	D	224	ILE
1	D	241	LEU
1	D	242	THR
1	D	245	ILE
1	D	246	ASP
1	D	250	GLU
1	D	251	LYS
1	D	268	ASN
1	D	284	ASN
1	D	285	THR
1	D	294	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	297	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	109	GLN
1	A	211	ASN
1	B	89	GLN
1	B	106	GLN
1	B	109	GLN
1	B	164	HIS
1	B	240	GLN
1	B	268	ASN
1	B	274	GLN
1	C	47	ASN
1	C	89	GLN
1	C	109	GLN
1	C	149	GLN
1	C	274	GLN
1	C	284	ASN
1	D	89	GLN
1	D	95	GLN
1	D	109	GLN
1	D	117	HIS
1	D	149	GLN
1	D	240	GLN
1	D	268	ASN
1	D	274	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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

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, 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	286/302 (94%)	-0.07	10 (3%) 48 58	6, 21, 72, 98	0
1	B	281/302 (93%)	0.03	16 (5%) 27 37	5, 24, 74, 100	0
1	C	288/302 (95%)	-0.15	3 (1%) 84 89	5, 21, 72, 92	0
1	D	278/302 (92%)	0.15	18 (6%) 22 32	4, 29, 79, 100	0
All	All	1133/1208 (93%)	-0.01	47 (4%) 41 52	4, 23, 75, 100	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	235	ALA	7.1
1	A	111	LEU	6.6
1	B	84	LYS	6.0
1	B	88	ARG	5.4
1	D	237	ASP	4.7
1	C	237	ASP	4.5
1	A	82	LEU	4.3
1	B	81	MET	4.2
1	D	91	LEU	4.1
1	B	82	LEU	4.0
1	D	239	ILE	3.9
1	A	81	MET	3.8
1	D	78	LEU	3.7
1	D	90	LEU	3.5
1	D	231	THR	3.4
1	A	88	ARG	3.4
1	A	91	LEU	3.3
1	B	89	GLN	3.3
1	B	91	LEU	3.2
1	B	95	GLN	2.7
1	A	80	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	83	GLU	2.6
1	B	83	GLU	2.6
1	B	78	LEU	2.6
1	D	180	VAL	2.6
1	D	76	PHE	2.5
1	D	175	VAL	2.5
1	B	76	PHE	2.5
1	D	92	ASP	2.4
1	B	90	LEU	2.4
1	B	231	THR	2.4
1	D	80	ALA	2.3
1	D	95	GLN	2.3
1	A	78	LEU	2.3
1	D	177	ALA	2.3
1	D	178	TYR	2.3
1	D	200	VAL	2.2
1	C	90	LEU	2.2
1	B	92	ASP	2.2
1	D	6	THR	2.2
1	D	87	LYS	2.2
1	C	4	ILE	2.1
1	B	80	ALA	2.1
1	B	204	LYS	2.0
1	B	5	ASN	2.0
1	A	239	ILE	2.0
1	A	90	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.