Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 01:23 pm BST

PDB ID	:	1GXB
Title	:	ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE IN COMPLEX WITH PYROPHOSPHATE AND MAGNESIUM
Authors	:	Mayans, O.; Ivens, A.; Nissen, L.J.; Kirschner, K.; Wilmanns, M.
Deposited on	:	2002-04-02
Resolution	:	2.65 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

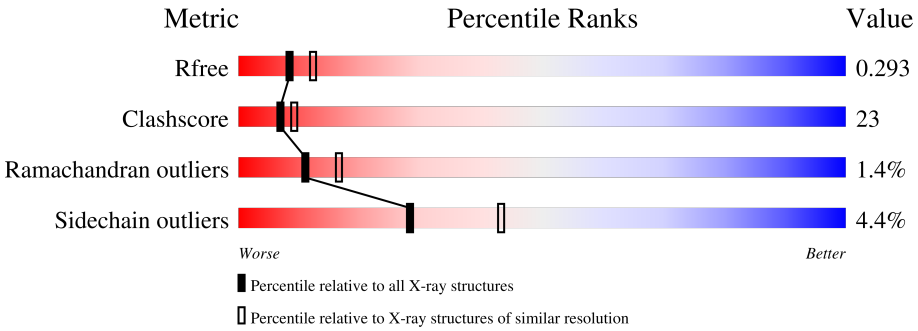
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	345	63% 32%
1	B	345	58% 35% 5%
1	C	345	55% 39%
1	D	345	60% 37%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	POP	D	1349	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10753 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.

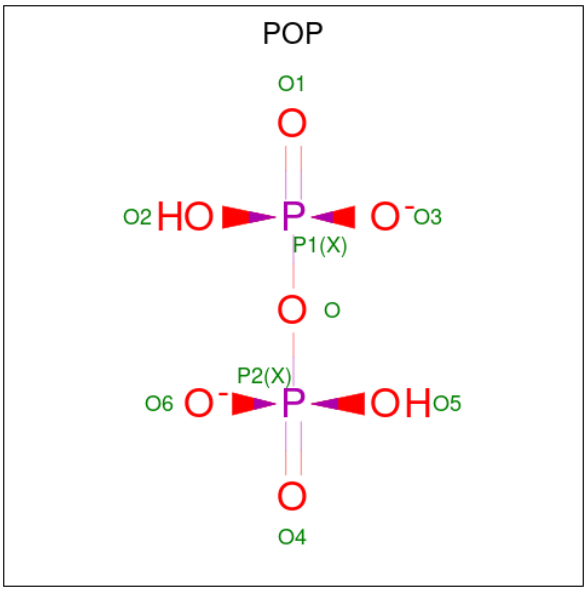
- Molecule 1 is a protein called ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	1
			2609	1674	440	488	7			
1	B	340	Total	C	N	O	S	0	0	1
			2611	1675	440	489	7			
1	C	341	Total	C	N	O	S	0	0	0
			2619	1679	441	492	7			
1	D	345	Total	C	N	O	S	0	0	0
			2642	1691	445	499	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 9 7 2	0	0
3	B	1	Total O P 9 7 2	0	0
3	C	1	Total O P 9 7 2	0	0
3	D	1	Total O P 9 7 2	0	0

- Molecule 4 is water.

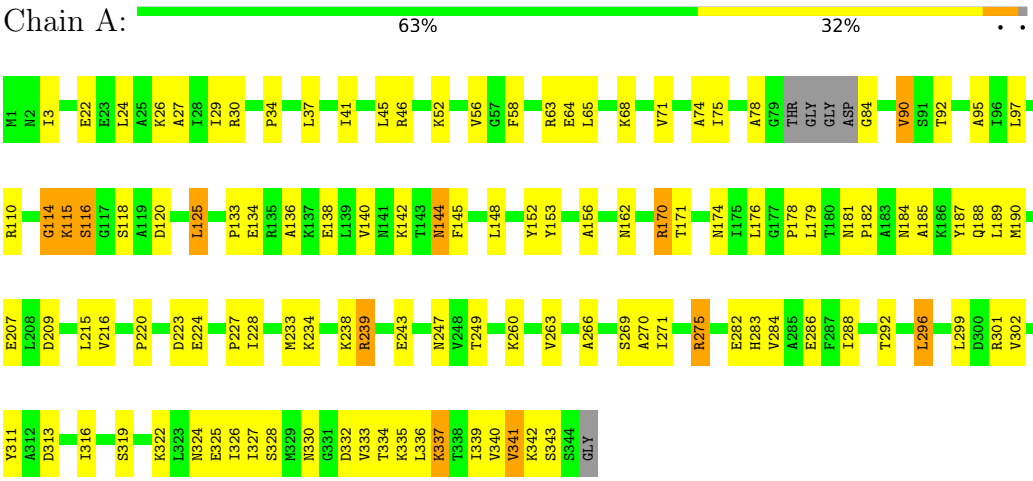
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	61	Total O 61 61	0	0
4	B	56	Total O 56 56	0	0
4	C	66	Total O 66 66	0	0
4	D	50	Total O 50 50	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

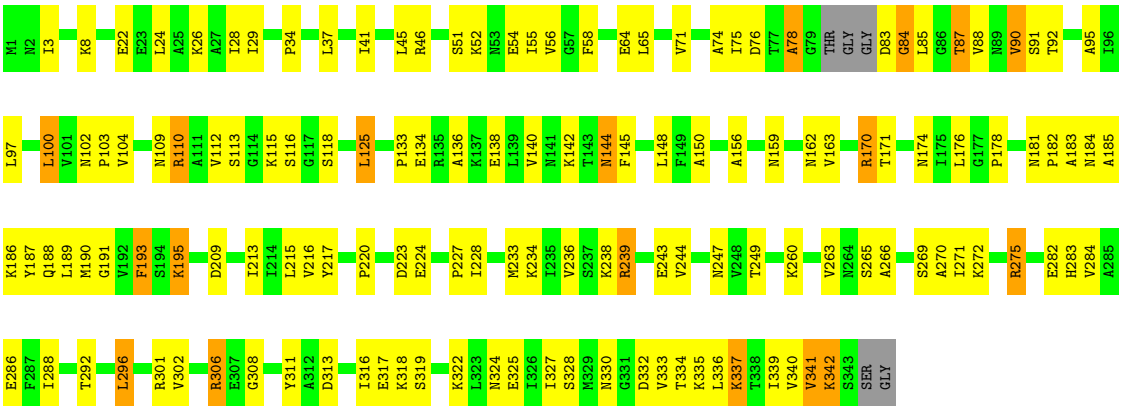
• Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE

Chain A:



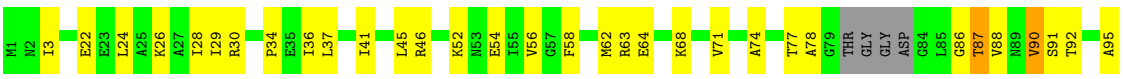
• Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE

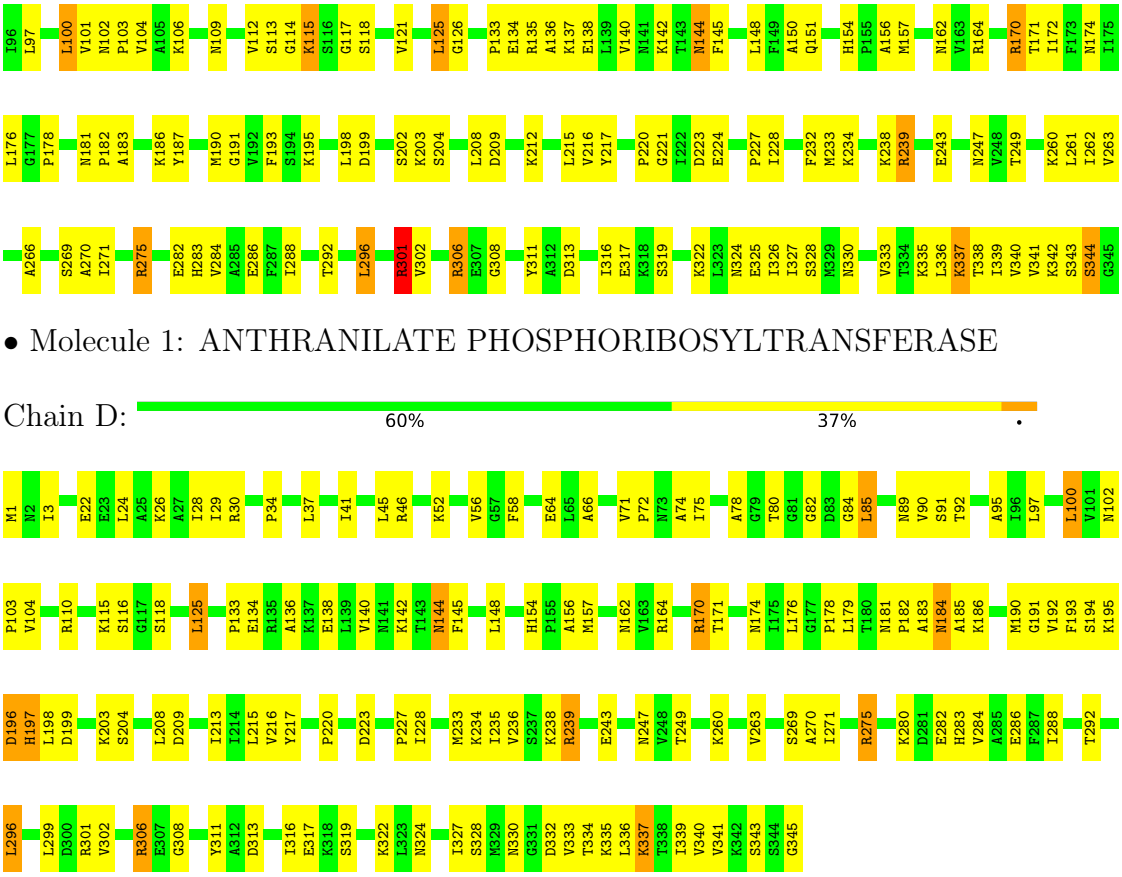
Chain B:



• Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE

Chain C:





• Molecule 1: ANTHRANILATE PHOSPHORIBOSYLTRANSFERASE

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.84Å 65.47Å 115.37Å 90.00° 107.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 19.69 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.65) 99.0 (19.69-2.63)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.63Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.223 , 0.297 0.282 , 0.293	Depositor DCC
R_{free} test set	1158 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	62.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10753	wwPDB-VP
Average B, all atoms (Å^2)	75.0	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 20.66 % 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 8.2807e-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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, POP

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	0.40	0/2645	0.97	11/3573 (0.3%)
1	B	0.38	0/2647	0.83	10/3576 (0.3%)
1	C	0.40	0/2655	0.99	11/3584 (0.3%)
1	D	0.36	0/2679	0.82	10/3618 (0.3%)
All	All	0.39	0/10626	0.91	42/14351 (0.3%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	301	ARG	NE-CZ-NH1	-23.00	108.80	120.30
1	C	301	ARG	NE-CZ-NH2	20.39	130.49	120.30
1	A	306	ARG	NE-CZ-NH2	19.56	130.08	120.30
1	A	306	ARG	NE-CZ-NH1	-19.42	110.59	120.30
1	A	275	ARG	NE-CZ-NH1	-15.11	112.75	120.30
1	D	275	ARG	NE-CZ-NH2	-15.10	112.75	120.30
1	C	275	ARG	NE-CZ-NH1	-14.95	112.83	120.30
1	B	275	ARG	NE-CZ-NH2	-14.85	112.88	120.30
1	A	275	ARG	NE-CZ-NH2	14.35	127.47	120.30
1	C	275	ARG	NE-CZ-NH2	14.23	127.42	120.30
1	D	275	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	B	275	ARG	NE-CZ-NH1	13.98	127.29	120.30
1	B	170	ARG	NE-CZ-NH2	-13.79	113.41	120.30
1	C	170	ARG	NE-CZ-NH1	-13.61	113.50	120.30
1	A	170	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	C	170	ARG	NE-CZ-NH2	13.34	126.97	120.30
1	D	170	ARG	NE-CZ-NH1	-13.01	113.80	120.30
1	B	170	ARG	NE-CZ-NH1	12.93	126.77	120.30
1	A	170	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	D	170	ARG	NE-CZ-NH2	12.38	126.49	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	301	ARG	CD-NE-CZ	10.54	138.36	123.60
1	A	306	ARG	CD-NE-CZ	9.51	136.92	123.60
1	D	301	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	B	275	ARG	CD-NE-CZ	7.63	134.28	123.60
1	D	275	ARG	CD-NE-CZ	7.61	134.26	123.60
1	C	275	ARG	CD-NE-CZ	7.59	134.22	123.60
1	A	301	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	275	ARG	CD-NE-CZ	7.51	134.11	123.60
1	A	301	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	D	301	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	C	170	ARG	CD-NE-CZ	6.76	133.06	123.60
1	C	306	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	D	306	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	B	306	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	D	170	ARG	CD-NE-CZ	6.54	132.76	123.60
1	B	306	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	301	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	170	ARG	CD-NE-CZ	6.38	132.54	123.60
1	B	301	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	170	ARG	CD-NE-CZ	6.37	132.51	123.60
1	D	306	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	306	ARG	NE-CZ-NH1	6.24	123.42	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2609	0	2725	109	0
1	B	2611	0	2725	128	0
1	C	2619	0	2734	127	0
1	D	2642	0	2752	130	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	9	0	0	0	0
3	B	9	0	0	2	0
3	C	9	0	0	1	0
3	D	9	0	0	4	0
4	A	61	0	0	11	0
4	B	56	0	0	14	0
4	C	66	0	0	19	0
4	D	50	0	0	23	0
All	All	10753	0	10936	496	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 23.

All (496) 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:109:ASN:HD22	1:C:150:ALA:HB3	1.10	1.12
1:A:78:ALA:HB2	1:A:188:GLN:OE1	1.62	0.98
1:D:280:LYS:HE3	1:D:345:GLY:H	1.32	0.93
1:A:178:PRO:HB2	1:A:190:MET:HE2	1.48	0.93
1:C:171:THR:H	1:C:174:ASN:ND2	1.67	0.92
1:D:171:THR:H	1:D:174:ASN:ND2	1.66	0.92
1:A:171:THR:H	1:A:174:ASN:ND2	1.70	0.90
1:B:171:THR:H	1:B:174:ASN:ND2	1.70	0.89
1:A:84:GLY:N	4:A:2016:HOH:O	2.06	0.89
1:B:83:ASP:HB3	4:B:2014:HOH:O	1.73	0.88
1:B:78:ALA:HB3	1:B:190:MET:HA	1.53	0.88
1:B:78:ALA:HB2	1:B:188:GLN:NE2	1.88	0.88
1:D:82:GLY:CA	1:D:170:ARG:HH22	1.87	0.86
1:C:342:LYS:HD2	4:C:2055:HOH:O	1.75	0.85
1:D:235:ILE:HD11	4:D:2036:HOH:O	1.76	0.85
1:A:29:ILE:CG2	1:A:65:LEU:HD12	2.08	0.83
1:A:78:ALA:HA	4:A:2018:HOH:O	1.78	0.82
1:D:171:THR:H	1:D:174:ASN:HD22	1.25	0.82
1:C:109:ASN:ND2	1:C:150:ALA:HB3	1.94	0.81
1:C:62:MET:HE1	4:C:2017:HOH:O	1.80	0.81
1:C:88:VAL:HG13	1:C:261:LEU:O	1.80	0.81
1:C:109:ASN:HD21	1:C:151:GLN:HG3	1.44	0.81
1:A:116:SER:HA	4:A:2044:HOH:O	1.81	0.80
1:D:208:LEU:HG	4:D:2013:HOH:O	1.81	0.80
1:B:171:THR:H	1:B:174:ASN:HD22	1.28	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:ALA:CB	1:D:178:PRO:HB3	2.11	0.80
1:C:171:THR:H	1:C:174:ASN:HD22	1.28	0.79
1:D:181:ASN:HD21	1:D:183:ALA:HB3	1.47	0.79
1:A:178:PRO:HB2	1:A:190:MET:CE	2.13	0.78
1:A:171:THR:H	1:A:174:ASN:HD22	1.29	0.78
1:A:266:ALA:HA	4:A:2044:HOH:O	1.84	0.78
1:D:170:ARG:HB3	4:D:2027:HOH:O	1.82	0.77
1:B:181:ASN:ND2	1:B:185:ALA:H	1.82	0.77
1:B:188:GLN:NE2	1:B:190:MET:HB2	1.99	0.77
1:C:97:LEU:HD22	1:C:319:SER:OG	1.85	0.77
1:B:97:LEU:HD22	1:B:319:SER:OG	1.85	0.76
1:D:82:GLY:HA2	1:D:170:ARG:HH22	1.47	0.76
1:D:190:MET:O	1:D:215:LEU:HA	1.85	0.76
1:A:97:LEU:HD22	1:A:319:SER:OG	1.86	0.75
1:D:97:LEU:HD22	1:D:319:SER:OG	1.85	0.75
1:B:78:ALA:CB	1:B:188:GLN:NE2	2.50	0.74
1:D:164:ARG:NH1	4:D:2025:HOH:O	2.19	0.74
1:B:87:THR:HG23	1:B:88:VAL:O	1.86	0.74
1:C:78:ALA:CB	1:C:178:PRO:HB3	2.17	0.74
1:B:234:LYS:HE2	1:B:243:GLU:HG3	1.70	0.74
1:D:216:VAL:HG12	1:D:233:MET:HB3	1.69	0.74
1:B:327:ILE:HD12	1:B:336:LEU:HD22	1.69	0.74
1:C:234:LYS:HE2	1:C:243:GLU:HG3	1.70	0.73
1:D:235:ILE:CG1	4:D:2036:HOH:O	2.36	0.73
1:D:234:LYS:HE2	1:D:243:GLU:HG3	1.71	0.73
1:C:216:VAL:HG12	1:C:233:MET:HB3	1.69	0.72
1:D:82:GLY:HA2	1:D:170:ARG:NH2	2.04	0.72
1:A:29:ILE:HG21	1:A:65:LEU:HD12	1.71	0.72
1:C:88:VAL:HG12	1:C:263:VAL:HG13	1.70	0.72
1:D:78:ALA:HB1	1:D:178:PRO:HB3	1.72	0.72
1:D:328:SER:HA	1:D:333:VAL:HG22	1.73	0.71
1:A:234:LYS:HE2	1:A:243:GLU:HG3	1.73	0.71
1:A:216:VAL:HG12	1:A:233:MET:HB3	1.70	0.71
1:B:148:LEU:HD13	1:B:182:PRO:HB2	1.71	0.71
1:A:336:LEU:O	1:A:340:VAL:HG23	1.90	0.71
1:D:327:ILE:HD12	1:D:336:LEU:HD22	1.71	0.70
1:C:327:ILE:HD12	1:C:336:LEU:HD22	1.72	0.70
1:A:327:ILE:HD12	1:A:336:LEU:HD22	1.74	0.70
1:A:75:ILE:HA	1:A:187:TYR:O	1.91	0.70
1:C:328:SER:HA	1:C:333:VAL:HG22	1.74	0.69
1:B:193:PHE:H	1:B:193:PHE:HD1	1.40	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:SER:HA	1:B:333:VAL:HG22	1.73	0.69
1:D:239:ARG:HD3	1:D:239:ARG:H	1.59	0.68
1:A:328:SER:HA	1:A:333:VAL:HG22	1.74	0.68
1:D:171:THR:N	1:D:174:ASN:HD22	1.91	0.68
1:C:28:ILE:HA	4:C:2008:HOH:O	1.93	0.68
1:B:324:ASN:ND2	4:B:2052:HOH:O	2.26	0.68
1:A:239:ARG:H	1:A:239:ARG:HD3	1.57	0.67
1:D:170:ARG:HG2	4:D:2010:HOH:O	1.95	0.67
1:A:29:ILE:HG22	1:A:65:LEU:HD12	1.76	0.67
1:B:216:VAL:HG12	1:B:233:MET:HB3	1.75	0.67
1:C:336:LEU:O	1:C:340:VAL:HG23	1.94	0.67
1:D:336:LEU:O	1:D:340:VAL:HG23	1.93	0.67
1:B:116:SER:OG	4:B:2021:HOH:O	2.13	0.67
1:C:137:LYS:HB2	4:C:2027:HOH:O	1.95	0.66
1:D:275:ARG:HG2	1:D:343:SER:HB2	1.77	0.66
1:C:171:THR:N	1:C:174:ASN:HD22	1.93	0.66
1:C:239:ARG:H	1:C:239:ARG:HD3	1.59	0.66
1:C:172:ILE:HA	4:C:2041:HOH:O	1.95	0.66
1:D:80:THR:HG21	1:D:193:PHE:H	1.61	0.66
1:B:336:LEU:O	1:B:340:VAL:HG23	1.96	0.65
1:A:156:ALA:HB2	4:A:2013:HOH:O	1.96	0.65
1:B:171:THR:N	1:B:174:ASN:HD22	1.95	0.65
1:D:116:SER:O	4:D:2019:HOH:O	2.15	0.65
1:D:233:MET:SD	4:D:2036:HOH:O	2.54	0.65
1:A:125:LEU:HB3	1:A:327:ILE:HD11	1.79	0.64
1:B:181:ASN:HD22	1:B:185:ALA:H	1.43	0.64
1:B:239:ARG:H	1:B:239:ARG:HD3	1.61	0.64
3:D:1349:POP:P1	4:D:2048:HOH:O	2.54	0.64
1:B:324:ASN:HD21	1:B:337:LYS:HE3	1.63	0.64
1:C:125:LEU:HB3	1:C:327:ILE:HD11	1.78	0.64
1:B:125:LEU:HB3	1:B:327:ILE:HD11	1.80	0.64
1:D:333:VAL:O	1:D:336:LEU:HB3	1.97	0.64
1:C:125:LEU:O	1:C:327:ILE:HD13	1.98	0.64
1:D:125:LEU:HB3	1:D:327:ILE:HD11	1.79	0.64
1:B:85:LEU:HD23	1:B:85:LEU:O	1.97	0.63
1:B:333:VAL:O	1:B:336:LEU:HB3	1.98	0.63
1:A:134:GLU:HG3	1:D:328:SER:O	1.98	0.63
1:A:171:THR:N	1:A:174:ASN:HD22	1.95	0.63
1:C:324:ASN:HD21	1:C:337:LYS:HE3	1.63	0.63
1:A:333:VAL:O	1:A:336:LEU:HB3	1.99	0.63
1:D:78:ALA:HB3	1:D:178:PRO:HB3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ASP:OD1	4:A:2034:HOH:O	2.15	0.63
1:C:115:LYS:HG2	1:C:266:ALA:HB2	1.80	0.63
1:B:340:VAL:C	1:B:342:LYS:H	2.02	0.62
1:D:125:LEU:O	1:D:327:ILE:HD13	2.00	0.62
1:A:148:LEU:HD13	1:A:182:PRO:HB2	1.81	0.62
1:B:271:ILE:O	1:B:275:ARG:HG3	1.99	0.62
1:D:46:ARG:HD2	1:D:170:ARG:O	2.00	0.61
1:B:76:ASP:HB3	1:B:188:GLN:HG3	1.81	0.61
1:C:46:ARG:HD2	1:C:170:ARG:O	2.01	0.61
1:C:333:VAL:O	1:C:336:LEU:HB3	2.01	0.61
3:D:1349:POP:O1	4:D:2048:HOH:O	2.15	0.61
1:A:125:LEU:O	1:A:327:ILE:HD13	2.01	0.61
1:A:333:VAL:HG23	4:A:2058:HOH:O	2.01	0.61
1:A:335:LYS:HG3	4:A:2059:HOH:O	2.00	0.61
1:D:324:ASN:HD21	1:D:337:LYS:HE3	1.63	0.60
1:D:24:LEU:HD11	1:D:41:ILE:HD13	1.82	0.60
1:A:271:ILE:O	1:A:275:ARG:HG3	2.02	0.60
1:D:181:ASN:ND2	1:D:183:ALA:H	2.00	0.60
1:A:34:PRO:HD2	1:A:37:LEU:HD12	1.84	0.60
1:D:82:GLY:C	1:D:170:ARG:HH22	2.04	0.60
1:B:78:ALA:HB1	1:B:178:PRO:HB3	1.84	0.60
1:D:271:ILE:O	1:D:275:ARG:HG3	2.01	0.59
1:A:324:ASN:HD21	1:A:337:LYS:HE3	1.67	0.59
1:B:34:PRO:HD2	1:B:37:LEU:HD12	1.85	0.59
1:C:24:LEU:HD11	1:C:41:ILE:HD13	1.84	0.59
1:B:188:GLN:HE22	1:B:190:MET:HB2	1.63	0.59
1:B:193:PHE:CD1	1:B:193:PHE:N	2.69	0.59
1:B:46:ARG:HD2	1:B:170:ARG:O	2.03	0.59
1:C:88:VAL:HG12	1:C:263:VAL:CG1	2.33	0.58
1:C:68:LYS:HE3	4:C:2016:HOH:O	2.03	0.58
1:C:109:ASN:ND2	1:C:151:GLN:HG3	2.16	0.58
1:B:29:ILE:CG2	1:B:65:LEU:HD12	2.33	0.58
1:C:199:ASP:OD2	1:C:203:LYS:HE3	2.04	0.58
1:A:46:ARG:HD2	1:A:170:ARG:O	2.03	0.58
1:A:195:LYS:O	1:A:198:LEU:HB2	2.04	0.58
1:D:34:PRO:HD2	1:D:37:LEU:HD12	1.85	0.58
1:A:340:VAL:O	1:A:342:LYS:N	2.37	0.58
1:B:125:LEU:O	1:B:327:ILE:HD13	2.04	0.57
1:B:75:ILE:HA	1:B:187:TYR:O	2.05	0.57
1:A:78:ALA:HB3	1:A:190:MET:HA	1.86	0.57
1:B:24:LEU:HD11	1:B:41:ILE:HD13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:VAL:CG2	4:C:2057:HOH:O	2.51	0.57
1:A:27:ALA:HB1	4:A:2005:HOH:O	2.05	0.57
1:C:34:PRO:HD2	1:C:37:LEU:HD12	1.87	0.57
1:B:178:PRO:HB2	1:B:190:MET:SD	2.45	0.56
1:B:184:ASN:ND2	1:B:186:LYS:HE2	2.20	0.56
1:B:341:VAL:HG12	1:B:341:VAL:O	2.04	0.56
1:D:28:ILE:HA	4:D:2006:HOH:O	2.05	0.56
1:D:235:ILE:CD1	4:D:2036:HOH:O	2.40	0.56
1:C:216:VAL:HG12	1:C:233:MET:CB	2.36	0.56
1:A:216:VAL:HG12	1:A:233:MET:CB	2.36	0.56
1:C:26:LYS:HE2	1:C:64:GLU:OE1	2.06	0.56
1:D:216:VAL:HG12	1:D:233:MET:CB	2.34	0.56
1:B:41:ILE:O	1:B:45:LEU:HB2	2.06	0.56
1:A:190:MET:O	1:A:215:LEU:HA	2.06	0.55
1:B:195:LYS:HG2	1:B:217:TYR:CD2	2.42	0.55
1:C:186:LYS:HD2	4:C:2046:HOH:O	2.06	0.55
1:D:26:LYS:HE2	1:D:64:GLU:OE1	2.05	0.55
1:C:36:ILE:HG13	4:C:2010:HOH:O	2.06	0.55
1:C:109:ASN:HD21	1:C:151:GLN:CG	2.18	0.55
1:A:24:LEU:HD11	1:A:41:ILE:HD13	1.88	0.55
1:C:121:VAL:HG21	4:C:2057:HOH:O	2.06	0.55
1:B:125:LEU:CD1	1:B:270:ALA:HB1	2.38	0.54
1:C:78:ALA:HB1	1:C:178:PRO:HB3	1.86	0.54
1:C:126:GLY:HA2	4:C:2024:HOH:O	2.07	0.54
1:A:92:THR:OG1	1:A:118:SER:HB2	2.08	0.54
1:B:26:LYS:HE2	1:B:64:GLU:OE1	2.07	0.54
1:A:78:ALA:CB	1:A:188:GLN:OE1	2.48	0.54
1:B:22:GLU:HG2	1:B:26:LYS:HE3	1.90	0.54
1:A:134:GLU:CD	1:A:134:GLU:H	2.12	0.53
1:A:26:LYS:HE2	1:A:64:GLU:OE1	2.07	0.53
1:C:271:ILE:O	1:C:275:ARG:HG3	2.07	0.53
1:D:220:PRO:HD3	1:D:228:ILE:HD13	1.91	0.53
1:D:92:THR:CB	4:D:2016:HOH:O	2.55	0.53
1:D:134:GLU:H	1:D:134:GLU:CD	2.12	0.53
1:D:148:LEU:HD13	1:D:182:PRO:HB2	1.90	0.53
1:D:170:ARG:HA	1:D:174:ASN:ND2	2.23	0.53
1:B:178:PRO:HB2	1:B:190:MET:HG3	1.91	0.53
1:B:216:VAL:HG12	1:B:233:MET:CB	2.39	0.53
1:B:92:THR:OG1	1:B:118:SER:HB2	2.09	0.53
1:D:191:GLY:O	1:D:223:ASP:HB2	2.09	0.53
1:A:292:THR:HG22	1:A:296:LEU:HD22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:GLU:HG2	1:C:26:LYS:HE3	1.92	0.52
1:C:125:LEU:CD1	1:C:270:ALA:HB1	2.39	0.52
1:C:171:THR:N	1:C:174:ASN:ND2	2.47	0.52
1:D:118:SER:HB3	4:D:2020:HOH:O	2.08	0.52
1:A:95:ALA:HB1	1:A:104:VAL:HG11	1.92	0.52
1:D:41:ILE:O	1:D:45:LEU:HB2	2.09	0.52
1:D:194:SER:HA	1:D:217:TYR:CE1	2.45	0.52
1:B:340:VAL:O	1:B:342:LYS:N	2.43	0.52
1:D:85:LEU:N	1:D:85:LEU:HD22	2.24	0.52
1:C:170:ARG:HA	1:C:174:ASN:ND2	2.23	0.52
1:C:343:SER:O	1:C:344:SER:CB	2.57	0.52
1:D:3:ILE:HG23	1:D:41:ILE:HD11	1.92	0.52
1:A:22:GLU:HG2	1:A:26:LYS:HE3	1.91	0.52
1:B:134:GLU:CD	1:B:134:GLU:H	2.13	0.52
1:B:292:THR:HG22	1:B:296:LEU:HD22	1.91	0.52
1:D:92:THR:OG1	1:D:118:SER:HB2	2.10	0.52
1:D:136:ALA:O	1:D:140:VAL:HG23	2.10	0.52
1:C:150:ALA:O	1:C:154:HIS:HB2	2.10	0.52
1:C:193:PHE:O	1:C:217:TYR:HE1	1.93	0.52
1:D:181:ASN:ND2	1:D:183:ALA:HB3	2.21	0.52
1:A:125:LEU:CD1	1:A:270:ALA:HB1	2.40	0.52
1:A:341:VAL:C	1:A:343:SER:H	2.12	0.52
1:B:75:ILE:HG13	1:B:187:TYR:O	2.10	0.52
1:B:318:LYS:NZ	4:B:2049:HOH:O	2.43	0.52
1:B:220:PRO:HD3	1:B:228:ILE:HD13	1.91	0.51
1:C:342:LYS:C	1:C:344:SER:H	2.13	0.51
1:D:22:GLU:HG2	1:D:26:LYS:HE3	1.91	0.51
1:A:170:ARG:HA	1:A:174:ASN:ND2	2.25	0.51
1:C:292:THR:HG22	1:C:296:LEU:HD22	1.91	0.51
1:C:3:ILE:HG23	1:C:41:ILE:HD11	1.92	0.51
1:C:187:TYR:CD1	1:C:187:TYR:N	2.78	0.51
1:C:134:GLU:CD	1:C:134:GLU:H	2.12	0.51
1:A:41:ILE:O	1:A:45:LEU:HB2	2.10	0.51
1:A:136:ALA:O	1:A:140:VAL:HG23	2.11	0.51
1:D:233:MET:HG3	4:D:2036:HOH:O	2.09	0.51
1:B:115:LYS:HE3	1:B:266:ALA:HB2	1.93	0.51
1:C:91:SER:HB2	3:C:1348:POP:P2	2.51	0.51
1:D:91:SER:HB2	3:D:1349:POP:O	2.11	0.50
1:A:114:GLY:O	1:A:115:LYS:C	2.50	0.50
1:D:80:THR:HG21	1:D:192:VAL:HA	1.93	0.50
1:D:292:THR:HG22	1:D:296:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:HA	1:B:174:ASN:ND2	2.26	0.50
1:D:140:VAL:O	1:D:144:ASN:HA	2.12	0.50
1:A:341:VAL:HG12	1:A:341:VAL:O	2.11	0.50
1:C:133:PRO:HG2	1:C:134:GLU:OE2	2.11	0.50
1:C:136:ALA:O	1:C:140:VAL:HG23	2.11	0.50
1:D:80:THR:CG2	1:D:192:VAL:HA	2.41	0.50
1:D:110:ARG:HG2	1:D:110:ARG:HH11	1.75	0.50
1:A:152:TYR:HD2	1:A:153:TYR:CE1	2.30	0.50
1:B:78:ALA:HB3	1:B:190:MET:CA	2.35	0.50
1:C:335:LYS:O	1:C:339:ILE:HG12	2.12	0.50
1:D:125:LEU:CD1	1:D:270:ALA:HB1	2.42	0.50
1:D:263:VAL:HG11	1:D:269:SER:HA	1.94	0.50
1:B:136:ALA:O	1:B:140:VAL:HG23	2.12	0.49
1:B:140:VAL:O	1:B:144:ASN:HA	2.11	0.49
1:B:159:ASN:HA	4:B:2026:HOH:O	2.10	0.49
1:C:112:VAL:O	1:C:114:GLY:N	2.45	0.49
1:C:190:MET:O	1:C:215:LEU:HA	2.11	0.49
1:D:80:THR:HG21	1:D:193:PHE:N	2.27	0.49
1:D:239:ARG:HG3	1:D:239:ARG:HH11	1.77	0.49
1:B:112:VAL:HG12	1:B:112:VAL:O	2.12	0.49
1:D:260:LYS:HG2	1:D:283:HIS:CD2	2.47	0.49
1:A:247:ASN:ND2	1:A:249:THR:HG23	2.27	0.49
1:A:260:LYS:HG2	1:A:283:HIS:CD2	2.47	0.49
1:A:335:LYS:O	1:A:339:ILE:HG12	2.12	0.49
1:B:95:ALA:HB1	1:B:104:VAL:HG11	1.94	0.49
1:B:247:ASN:ND2	1:B:249:THR:HG23	2.27	0.49
1:B:263:VAL:HG11	1:B:269:SER:HA	1.93	0.49
1:B:335:LYS:O	1:B:339:ILE:HG12	2.12	0.49
1:C:140:VAL:O	1:C:144:ASN:HA	2.12	0.49
1:B:3:ILE:HG23	1:B:41:ILE:HD11	1.94	0.49
1:C:112:VAL:HG11	4:C:2015:HOH:O	2.11	0.49
1:C:220:PRO:HD3	1:C:228:ILE:HD13	1.94	0.49
1:D:247:ASN:ND2	1:D:249:THR:HG23	2.28	0.49
1:B:272:LYS:NZ	4:B:2040:HOH:O	2.45	0.49
1:B:125:LEU:HD13	1:B:270:ALA:HB1	1.95	0.49
1:B:260:LYS:HG2	1:B:283:HIS:CD2	2.48	0.49
1:C:313:ASP:O	1:C:316:ILE:HG22	2.12	0.49
1:D:195:LYS:O	1:D:198:LEU:HB3	2.13	0.49
1:D:302:VAL:HG11	1:D:308:GLY:HA2	1.94	0.49
1:D:335:LYS:O	1:D:339:ILE:HG12	2.12	0.49
1:C:125:LEU:HD13	1:C:270:ALA:HB1	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:LYS:HG2	1:C:283:HIS:CD2	2.47	0.48
1:A:63:ARG:O	1:A:68:LYS:HE3	2.13	0.48
1:A:239:ARG:HG3	1:A:239:ARG:HH11	1.78	0.48
1:C:41:ILE:O	1:C:45:LEU:HB2	2.14	0.48
1:C:148:LEU:HD13	1:C:182:PRO:HB2	1.95	0.48
1:C:157:MET:HE1	4:C:2043:HOH:O	2.13	0.48
1:A:302:VAL:HG11	1:A:308:GLY:HA2	1.95	0.48
1:B:29:ILE:HG21	1:B:65:LEU:HD12	1.95	0.48
1:B:156:ALA:HB3	4:B:2025:HOH:O	2.12	0.48
1:C:239:ARG:HG3	1:C:239:ARG:HH11	1.77	0.48
1:D:66:ALA:HB2	1:D:154:HIS:CE1	2.48	0.48
1:D:195:LYS:HG3	1:D:217:TYR:CE2	2.48	0.48
1:D:271:ILE:HD12	4:D:2041:HOH:O	2.12	0.48
1:A:3:ILE:HG23	1:A:41:ILE:HD11	1.95	0.48
1:A:138:GLU:OE2	1:A:142:LYS:HE2	2.14	0.48
1:A:220:PRO:HD3	1:A:228:ILE:HD13	1.95	0.48
1:C:263:VAL:HG11	1:C:269:SER:HA	1.95	0.48
1:C:302:VAL:HG11	1:C:308:GLY:HA2	1.95	0.48
1:A:133:PRO:HG2	1:A:134:GLU:OE2	2.14	0.48
1:C:101:VAL:O	1:C:301:ARG:NH1	2.47	0.48
1:C:247:ASN:ND2	1:C:249:THR:HG23	2.29	0.48
1:C:342:LYS:C	1:C:344:SER:N	2.66	0.48
1:D:235:ILE:HG13	4:D:2036:HOH:O	2.09	0.48
1:B:138:GLU:OE2	1:B:142:LYS:HE2	2.14	0.47
1:D:100:LEU:HD13	1:D:322:LYS:HG2	1.97	0.47
1:C:227:PRO:HG2	1:C:228:ILE:HG23	1.97	0.47
1:D:78:ALA:O	1:D:190:MET:HA	2.14	0.47
1:C:164:ARG:HD2	4:C:2040:HOH:O	2.14	0.47
1:C:191:GLY:HA3	1:C:223:ASP:O	2.14	0.47
1:B:8:LYS:NZ	4:B:2002:HOH:O	2.47	0.47
1:B:109:ASN:ND2	1:B:150:ALA:HB3	2.29	0.47
1:C:181:ASN:HD21	1:C:183:ALA:HB3	1.79	0.47
1:A:140:VAL:O	1:A:144:ASN:HA	2.14	0.47
1:C:284:VAL:O	1:C:288:ILE:HG13	2.15	0.47
1:C:170:ARG:HG2	4:C:2011:HOH:O	2.14	0.47
1:C:78:ALA:HB3	1:C:178:PRO:HB3	1.97	0.47
1:B:302:VAL:HG11	1:B:308:GLY:HA2	1.97	0.47
1:A:263:VAL:HG11	1:A:269:SER:HA	1.96	0.47
1:C:92:THR:OG1	1:C:118:SER:HB2	2.14	0.46
1:C:204:SER:O	1:C:208:LEU:HD23	2.14	0.46
1:C:209:ASP:OD1	1:C:238:LYS:NZ	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ASP:OD1	1:D:203:LYS:HE3	2.16	0.46
1:B:239:ARG:HG3	1:B:239:ARG:HH11	1.80	0.46
1:B:328:SER:HA	1:B:333:VAL:CG2	2.43	0.46
1:C:198:LEU:HD11	1:C:232:PHE:O	2.15	0.46
1:B:341:VAL:C	1:B:342:LYS:HE3	2.36	0.46
1:D:24:LEU:HD11	1:D:41:ILE:CD1	2.45	0.46
1:D:284:VAL:O	1:D:288:ILE:HG13	2.15	0.46
3:B:1347:POP:O	4:B:2056:HOH:O	2.21	0.46
1:C:138:GLU:OE2	1:C:142:LYS:HE2	2.15	0.46
1:A:52:LYS:O	1:A:56:VAL:HG23	2.15	0.46
1:A:328:SER:HA	1:A:333:VAL:CG2	2.44	0.46
1:B:133:PRO:HG2	1:B:134:GLU:OE2	2.15	0.46
1:C:328:SER:HA	1:C:333:VAL:CG2	2.44	0.46
1:B:195:LYS:HG2	1:B:217:TYR:CE2	2.51	0.46
1:C:95:ALA:HB1	1:C:104:VAL:HG11	1.98	0.46
1:C:198:LEU:HD22	1:C:234:LYS:HG2	1.98	0.46
1:D:179:LEU:HD22	4:D:2013:HOH:O	2.14	0.46
1:A:22:GLU:O	1:A:26:LYS:HG3	2.16	0.46
1:B:184:ASN:HD21	1:B:186:LYS:HE2	1.80	0.46
1:D:71:VAL:HG12	1:D:74:ALA:HB2	1.97	0.46
1:A:110:ARG:NH1	1:A:120:ASP:OD1	2.46	0.46
1:B:342:LYS:N	1:B:342:LYS:HE3	2.31	0.46
1:C:90:VAL:HG21	1:C:224:GLU:HG2	1.98	0.46
1:A:187:TYR:CD2	1:A:299:LEU:HD23	2.51	0.45
1:A:313:ASP:O	1:A:316:ILE:HG22	2.15	0.45
1:C:30:ARG:NH2	4:C:2007:HOH:O	2.25	0.45
1:D:171:THR:N	1:D:174:ASN:ND2	2.47	0.45
1:A:115:LYS:HD3	1:A:266:ALA:CB	2.46	0.45
1:D:186:LYS:HA	1:D:186:LYS:HD3	1.69	0.45
1:A:125:LEU:HD13	1:A:270:ALA:HB1	1.97	0.45
1:A:138:GLU:O	1:A:142:LYS:HG2	2.16	0.45
1:B:91:SER:HB2	3:B:1347:POP:O2	2.17	0.45
1:B:340:VAL:C	1:B:342:LYS:N	2.69	0.45
1:D:145:PHE:C	1:D:145:PHE:CD2	2.89	0.45
1:D:220:PRO:HD3	1:D:228:ILE:CD1	2.46	0.45
1:C:86:GLY:O	1:C:262:ILE:HG23	2.17	0.45
1:A:52:LYS:NZ	1:A:207:GLU:OE2	2.45	0.45
1:A:171:THR:N	1:A:174:ASN:ND2	2.50	0.45
1:D:91:SER:HB2	3:D:1349:POP:P2	2.56	0.45
1:D:92:THR:HB	4:D:2016:HOH:O	2.16	0.45
1:D:138:GLU:OE2	1:D:142:LYS:HE2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ASP:O	1:D:198:LEU:N	2.49	0.45
1:D:328:SER:HA	1:D:333:VAL:CG2	2.43	0.45
1:B:113:SER:HA	4:B:2020:HOH:O	2.16	0.45
1:B:209:ASP:OD1	1:B:238:LYS:NZ	2.50	0.45
1:A:90:VAL:HG21	1:A:224:GLU:HG2	1.99	0.45
1:A:144:ASN:HA	1:A:144:ASN:HD22	1.61	0.45
1:A:209:ASP:OD1	1:A:238:LYS:NZ	2.50	0.45
1:A:341:VAL:C	4:A:2060:HOH:O	2.54	0.45
1:D:227:PRO:HG2	1:D:228:ILE:HG23	1.98	0.45
1:A:29:ILE:HG22	1:A:156:ALA:HB1	1.99	0.45
1:B:227:PRO:HG2	1:B:228:ILE:HG23	1.99	0.45
1:C:77:THR:O	1:C:106:LYS:HE2	2.17	0.45
1:D:102:ASN:CG	1:D:103:PRO:HD2	2.38	0.45
1:C:198:LEU:HD23	1:C:198:LEU:HA	1.84	0.44
1:D:209:ASP:OD1	1:D:238:LYS:NZ	2.50	0.44
1:D:133:PRO:HG2	1:D:134:GLU:OE2	2.15	0.44
1:B:52:LYS:O	1:B:56:VAL:HG23	2.17	0.44
1:C:338:THR:O	1:C:342:LYS:HG3	2.18	0.44
1:B:284:VAL:O	1:B:288:ILE:HG13	2.16	0.44
1:C:135:ARG:NE	4:C:2029:HOH:O	2.49	0.44
1:D:184:ASN:O	1:D:185:ALA:C	2.56	0.44
1:B:109:ASN:HD22	1:B:150:ALA:HB3	1.81	0.44
1:C:100:LEU:HD13	1:C:322:LYS:HG2	1.99	0.44
1:B:78:ALA:HB1	1:B:178:PRO:CB	2.45	0.44
1:B:102:ASN:CG	1:B:103:PRO:HD2	2.38	0.44
1:C:145:PHE:CD2	1:C:145:PHE:C	2.91	0.44
1:A:145:PHE:CD2	1:A:145:PHE:C	2.91	0.44
1:A:179:LEU:HG	1:A:190:MET:HE1	1.99	0.44
1:B:22:GLU:O	1:B:26:LYS:HG3	2.18	0.44
1:C:24:LEU:HD11	1:C:41:ILE:CD1	2.47	0.44
1:C:58:PHE:HB3	1:C:176:LEU:HD11	1.99	0.44
1:C:63:ARG:HH22	1:C:208:LEU:HB3	1.82	0.44
1:C:71:VAL:HG12	1:C:74:ALA:HB2	2.00	0.44
1:B:24:LEU:HD11	1:B:41:ILE:CD1	2.48	0.43
1:B:332:ASP:OD2	1:B:334:THR:OG1	2.33	0.43
1:C:239:ARG:HG3	1:C:239:ARG:NH1	2.34	0.43
1:D:313:ASP:O	1:D:316:ILE:HG22	2.18	0.43
1:D:110:ARG:HG2	1:D:110:ARG:NH1	2.33	0.43
1:D:95:ALA:HB1	1:D:104:VAL:HG11	2.01	0.43
1:B:163:VAL:HG23	4:B:2028:HOH:O	2.17	0.43
1:C:137:LYS:CB	4:C:2027:HOH:O	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:PRO:O	1:D:186:LYS:HB2	2.18	0.43
1:A:115:LYS:HD3	1:A:266:ALA:HB2	2.00	0.43
1:D:179:LEU:HD13	4:D:2013:HOH:O	2.18	0.43
1:A:71:VAL:HG12	1:A:74:ALA:HB2	2.01	0.43
1:A:343:SER:CB	4:A:2060:HOH:O	2.67	0.43
1:B:29:ILE:HG22	1:B:156:ALA:HB1	2.01	0.43
1:B:78:ALA:CB	1:B:188:GLN:HE22	2.31	0.43
1:B:220:PRO:HD3	1:B:228:ILE:CD1	2.49	0.43
1:D:82:GLY:HA2	1:D:170:ARG:CZ	2.48	0.43
1:A:227:PRO:HG2	1:A:228:ILE:HG23	2.01	0.43
1:A:332:ASP:OD2	1:A:334:THR:OG1	2.33	0.43
1:B:138:GLU:O	1:B:142:LYS:HG2	2.19	0.43
1:C:102:ASN:CG	1:C:103:PRO:HD2	2.39	0.43
1:C:195:LYS:HB2	1:C:217:TYR:CD2	2.54	0.43
1:D:328:SER:CA	1:D:333:VAL:HG22	2.46	0.43
1:A:322:LYS:HD2	1:A:325:GLU:HG2	2.01	0.43
1:C:337:LYS:O	1:C:341:VAL:HG23	2.19	0.42
1:D:125:LEU:HD13	1:D:270:ALA:HB1	2.00	0.42
1:D:332:ASP:OD2	1:D:334:THR:OG1	2.34	0.42
1:B:58:PHE:HB3	1:B:176:LEU:HD11	2.01	0.42
1:B:145:PHE:CD2	1:B:145:PHE:C	2.92	0.42
1:C:138:GLU:O	1:C:142:LYS:HG2	2.19	0.42
1:B:115:LYS:HB2	1:B:265:SER:HA	2.02	0.42
1:B:322:LYS:HD2	1:B:325:GLU:HG2	2.02	0.42
1:C:187:TYR:HA	1:C:212:LYS:O	2.17	0.42
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.84	0.42
1:B:90:VAL:HG21	1:B:224:GLU:HG2	2.01	0.42
1:A:282:GLU:O	1:A:286:GLU:HG3	2.19	0.42
1:D:282:GLU:HG3	1:D:283:HIS:N	2.35	0.42
1:C:217:TYR:CZ	1:C:221:GLY:HA2	2.55	0.42
1:D:1:MET:HG2	4:D:2001:HOH:O	2.19	0.42
1:D:58:PHE:HB3	1:D:176:LEU:HD11	2.02	0.42
1:A:52:LYS:HD2	1:A:207:GLU:OE2	2.19	0.42
1:B:313:ASP:O	1:B:316:ILE:HG22	2.18	0.42
1:C:87:THR:HG23	1:C:88:VAL:N	2.34	0.42
1:D:337:LYS:O	1:D:341:VAL:HG23	2.20	0.42
1:A:78:ALA:N	1:A:189:LEU:O	2.52	0.42
1:B:193:PHE:HD2	4:B:2014:HOH:O	2.00	0.42
1:C:220:PRO:HD3	1:C:228:ILE:CD1	2.50	0.42
1:A:26:LYS:HB3	1:A:30:ARG:NH1	2.34	0.42
1:A:325:GLU:HG3	1:A:326:ILE:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:O	1:B:58:PHE:HD1	2.03	0.42
1:B:83:ASP:O	1:B:84:GLY:C	2.58	0.42
1:B:110:ARG:NH1	4:B:2018:HOH:O	2.53	0.42
1:D:239:ARG:HG3	1:D:239:ARG:NH1	2.33	0.42
1:A:239:ARG:HG3	1:A:239:ARG:NH1	2.34	0.41
1:B:78:ALA:N	1:B:189:LEU:O	2.53	0.41
1:C:282:GLU:O	1:C:286:GLU:HG3	2.19	0.41
1:D:204:SER:O	1:D:208:LEU:HD23	2.19	0.41
1:A:58:PHE:HB3	1:A:176:LEU:HD11	2.02	0.41
1:B:100:LEU:HD13	1:B:322:LYS:HG2	2.02	0.41
1:B:144:ASN:HA	1:B:144:ASN:HD22	1.65	0.41
1:B:213:ILE:HG23	1:B:236:VAL:HB	2.02	0.41
1:C:97:LEU:O	1:C:100:LEU:HB2	2.18	0.41
1:D:280:LYS:HE3	1:D:345:GLY:N	2.15	0.41
1:A:24:LEU:HD11	1:A:41:ILE:CD1	2.50	0.41
1:B:190:MET:O	1:B:215:LEU:HA	2.20	0.41
1:D:29:ILE:HG22	1:D:156:ALA:HB1	2.02	0.41
1:B:282:GLU:HG3	1:B:283:HIS:N	2.36	0.41
1:B:282:GLU:O	1:B:286:GLU:HG3	2.20	0.41
1:D:26:LYS:HB3	1:D:30:ARG:NH1	2.35	0.41
1:D:97:LEU:O	1:D:100:LEU:HB2	2.20	0.41
1:A:97:LEU:O	1:A:100:LEU:HB2	2.21	0.41
1:A:178:PRO:HG2	1:A:190:MET:HE1	2.02	0.41
1:A:284:VAL:O	1:A:288:ILE:HG13	2.19	0.41
1:D:52:LYS:HE2	1:D:52:LYS:HB3	1.93	0.41
1:D:213:ILE:HG23	1:D:236:VAL:HB	2.01	0.41
1:D:313:ASP:O	1:D:317:GLU:HG3	2.21	0.41
1:A:100:LEU:HD13	1:A:322:LYS:HG2	2.02	0.41
1:C:90:VAL:CG2	1:C:224:GLU:HG2	2.51	0.41
1:C:313:ASP:O	1:C:317:GLU:HG3	2.20	0.41
1:D:52:LYS:O	1:D:56:VAL:HG23	2.20	0.41
1:B:118:SER:HB3	4:B:2056:HOH:O	2.20	0.41
1:D:154:HIS:HB3	1:D:157:MET:HG2	2.03	0.41
1:B:24:LEU:O	1:B:28:ILE:HG13	2.21	0.41
1:B:51:SER:O	1:B:55:ILE:HG12	2.21	0.41
1:C:26:LYS:HB3	1:C:30:ARG:NH1	2.35	0.41
1:C:282:GLU:HG3	1:C:283:HIS:N	2.36	0.41
1:D:75:ILE:HD12	1:D:299:LEU:HG	2.03	0.41
1:D:154:HIS:HA	4:D:2014:HOH:O	2.20	0.41
1:D:196:ASP:O	1:D:197:HIS:C	2.59	0.41
1:B:71:VAL:HG12	1:B:74:ALA:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:MET:CG	1:B:244:VAL:HB	2.52	0.41
1:B:313:ASP:O	1:B:317:GLU:HG3	2.20	0.41
1:C:52:LYS:O	1:C:56:VAL:HG23	2.20	0.41
1:D:89:ASN:CB	4:D:2019:HOH:O	2.69	0.41
1:A:181:ASN:ND2	1:A:185:ALA:H	2.19	0.40
1:B:191:GLY:HA3	1:B:223:ASP:O	2.20	0.40
1:C:198:LEU:O	1:C:202:SER:HB3	2.21	0.40
1:B:337:LYS:O	1:B:341:VAL:HG23	2.21	0.40
1:C:29:ILE:HG22	1:C:156:ALA:HB1	2.03	0.40
1:C:68:LYS:HG2	4:C:2016:HOH:O	2.21	0.40
1:C:325:GLU:HG3	1:C:326:ILE:N	2.36	0.40
1:D:138:GLU:O	1:D:142:LYS:HG2	2.21	0.40
1:A:90:VAL:CG2	1:A:224:GLU:HG2	2.51	0.40
1:A:282:GLU:HG3	1:A:283:HIS:N	2.36	0.40
1:B:328:SER:CA	1:B:333:VAL:HG22	2.46	0.40
1:C:22:GLU:O	1:C:26:LYS:HG3	2.21	0.40
1:A:337:LYS:O	1:A:341:VAL:HG23	2.21	0.40
1:C:54:GLU:O	1:C:58:PHE:HD1	2.04	0.40
1:B:183:ALA:O	1:B:184:ASN:HB3	2.21	0.40
1:D:282:GLU:O	1:D:286:GLU:HG3	2.20	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	336/345 (97%)	311 (93%)	20 (6%)	5 (2%)	10	15
1	B	336/345 (97%)	311 (93%)	21 (6%)	4 (1%)	13	19
1	C	337/345 (98%)	309 (92%)	23 (7%)	5 (2%)	10	15
1	D	343/345 (99%)	313 (91%)	25 (7%)	5 (2%)	10	15
All	All	1352/1380 (98%)	1244 (92%)	89 (7%)	19 (1%)	11	16

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	341	VAL
1	B	78	ALA
1	B	341	VAL
1	C	344	SER
1	A	114	GLY
1	A	115	LYS
1	B	84	GLY
1	C	117	GLY
1	D	84	GLY
1	C	113	SER
1	D	115	LYS
1	D	196	ASP
1	D	197	HIS
1	A	330	ASN
1	B	330	ASN
1	C	330	ASN
1	D	330	ASN
1	C	115	LYS

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	285/289 (99%)	274 (96%)	11 (4%)	32	48
1	B	285/289 (99%)	270 (95%)	15 (5%)	22	35
1	C	286/289 (99%)	274 (96%)	12 (4%)	30	45
1	D	288/289 (100%)	276 (96%)	12 (4%)	30	45
All	All	1144/1156 (99%)	1094 (96%)	50 (4%)	28	43

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	100	LEU
1	A	125	LEU
1	A	144	ASN
1	A	162	ASN
1	A	184	ASN
1	A	239	ARG
1	A	296	LEU
1	A	306	ARG
1	A	311	TYR
1	A	337	LYS
1	B	87	THR
1	B	90	VAL
1	B	100	LEU
1	B	110	ARG
1	B	125	LEU
1	B	144	ASN
1	B	162	ASN
1	B	193	PHE
1	B	195	LYS
1	B	239	ARG
1	B	296	LEU
1	B	306	ARG
1	B	311	TYR
1	B	337	LYS
1	B	342	LYS
1	C	87	THR
1	C	90	VAL
1	C	100	LEU
1	C	125	LEU
1	C	144	ASN
1	C	162	ASN
1	C	239	ARG
1	C	296	LEU
1	C	301	ARG
1	C	306	ARG
1	C	311	TYR
1	C	337	LYS
1	D	85	LEU
1	D	90	VAL
1	D	100	LEU
1	D	125	LEU
1	D	144	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	162	ASN
1	D	184	ASN
1	D	239	ARG
1	D	296	LEU
1	D	306	ARG
1	D	311	TYR
1	D	337	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	151	GLN
1	A	162	ASN
1	A	174	ASN
1	A	181	ASN
1	A	184	ASN
1	A	247	ASN
1	A	283	HIS
1	A	324	ASN
1	B	144	ASN
1	B	151	GLN
1	B	162	ASN
1	B	174	ASN
1	B	181	ASN
1	B	184	ASN
1	B	188	GLN
1	B	247	ASN
1	B	283	HIS
1	B	324	ASN
1	C	109	ASN
1	C	144	ASN
1	C	162	ASN
1	C	174	ASN
1	C	181	ASN
1	C	184	ASN
1	C	247	ASN
1	C	283	HIS
1	C	324	ASN
1	D	144	ASN
1	D	151	GLN
1	D	162	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	174	ASN
1	D	181	ASN
1	D	184	ASN
1	D	188	GLN
1	D	247	ASN
1	D	283	HIS
1	D	324	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	POP	D	1349	2	6,8,8	1.56	2 (33%)	13,13,13	1.04	1 (7%)
3	POP	C	1348	2	6,8,8	0.97	0	13,13,13	1.07	0
3	POP	A	1346	2	6,8,8	1.37	1 (16%)	13,13,13	1.20	1 (7%)
3	POP	B	1347	-	6,8,8	1.25	1 (16%)	13,13,13	1.01	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POP	D	1349	2	-	0/6/6/6	-
3	POP	C	1348	2	-	0/6/6/6	-
3	POP	A	1346	2	-	2/6/6/6	-
3	POP	B	1347	-	-	0/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1346	POP	P1-O1	3.06	1.60	1.50
3	D	1349	POP	P1-O1	2.78	1.59	1.50
3	B	1347	POP	P1-O3	2.13	1.63	1.54
3	D	1349	POP	P1-O3	2.01	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1349	POP	P2-O-P1	-2.27	125.03	132.83
3	B	1347	POP	P2-O-P1	-2.21	125.25	132.83
3	A	1346	POP	O2-P1-O	2.04	111.46	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1346	POP	P1-O-P2-O5
3	A	1346	POP	P1-O-P2-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1349	POP	4	0
3	C	1348	POP	1	0
3	B	1347	POP	2	0

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.